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TWO-DIMENSIONAL MATHEMATICAL MODEL FOR FLUORIDE ION TRANSPORT IN SOIL UNDER STEADY FLOW CONDITIONS

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Abstract

Soil systems are a common receptor of anthropogenic and natural fluoride contamination. Soils play an important role in the containment or dispersion of pollution to surface water, groundwater or the atmosphere. The aim of this paper is to present a two-dimensional mathematical model for transport of fluoride ion in soil taking into consideration both longitudinal and transverse flow. The model has been developed for two-dimensional steady state case along with the appropriate initial and pulse type boundary conditions. The mathematical formulation encompasses various parameters such as: the mechanism for advection-convection transport, hydrodynamic dispersion, and retardation factor. These parameters are greatly involved in the contamination of water due to fluoride ion in soil and also in the increasing risk of fluorosis. The analytical solution of the partial differential equations, so obtained, has been obtained by using Laplace Transform method. The results for the concentration of fluoride ion with respect to spatial and temporal coordinates have been discussed in detail.

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1. Introduction

Fluoride occurring naturally in the earth's crust in the form of rocks, coal, clay, and soil is released into the environment via the natural process of weathering of minerals, in emissions from volcanic ash and in marine aerosols [30]. Other anthropogenic sources causing deposition of Fluoride into soil are both direct through phosphate fertilizers or indirect through atmospheric pollution from industrial activities and burning of fossil fuels [14]. In areas without natural phosphate or fluoride deposits, the total fluoride concentrations in soils range from 20 to $1{,}000\ \mu g/g$, whereas the concentration in organic soils are usually lower [13].

Fluoride is a micro nutrient required for dental and skeletal growth of mammals. At the same time, it is also one of the most important environmental micro pollutants responsible for soil and groundwater pollution causing dental and skeletal fluorosis [1, 3, 29]. The concentration of fluoride that occurs in groundwater and the rate by which fluoride migrates to groundwater are the key factors determining the risk for human health and the environment. Both these processes are strongly influenced by the interaction of dissolved fluoride with the soil solid phase via adsorption and desorption [12] and cation-anion exchange. Therefore, it is important to study the migration and transport of fluoride ion in soil.

The development of mathematical models is an integral component of any effort to understand and predict the transport phenomena of fluoride migration and its persistence in soil and groundwater. The attention to prevent, reduce and eliminate soil and groundwater pollution has been growing with the growing importance of groundwater resources and the models are helpful tools to design and implement soil and crop management practises which minimize soil and water contamination.

Over the years, various mathematical models for the process of transport of reactive contaminants through porous media have been developed [11, 19, 32] based on advection diffusion equation. The advection diffusion equation is parabolic second order partial differential equation built on the basis of conservation of mass and Fick's first law of diffusion.

Analytical solutions of one-dimensional solute transport problems with different initial and boundary conditions, in finite as well as semi-finite domain have been reported in the literature [17, 24]. Most of the works [5, 6, 25, 16] are based on assuming ideal conditions for porosity, seepage flow and dispersion.

Some works [28, 4, 27, 33] include the deviation in ideal conditions, due to adsorption, first order radio-active decay and/or chemical reactions. The study of uniform flow and unsteady flow against the dispersion in finite porous media were also undertaken [2, 20]. A numerical model for one dimensional fluoride transport in unsaturated stratified soil considering the retardation factor and source sink term has been also presented [36]. The development of solute transport problems in two dimensions involve both longitudinal as well as transverse dispersion along with porous media flow in addition to advection. The literature is replete with numerous works on solutions of two, three-dimensional advection-diffusion equations [7, 8, 21, 22, 23]. Convective-dispersive equation (CDE) and Convective-lognormal transport (CLT) models [1] were employed to study fluoride retardation factor in unsaturated and undisturbed soil column.

Mathematical model for two-dimensional solute transport in a semi-infinite heterogeneous porous medium with spatially and temporally dependent coefficients for pulse type input concentration of varying nature has been developed [34].

In the present paper a two-dimensional advection-dispersion model fluoride transport in soil is presented in which, the transverse component of velocity and dispersion coefficients are also considered along with the longitudinal components. The longitudinal and transverse seepage velocities are taken to be constant. The soil medium is assumed to be homogeneous, isotropic saturated and of semi-infinite in horizontal plane. Since fluoride is reactive in nature and has the tendency to get adsorbed in the medium, retardation factor and a first order decay term as a constant is also considered. A pulse type boundary condition is assumed which is in consonance with the realistic situation in the sense that generally industries or waste sites release pollution in a finite period or pesticides containing fluorides are applied for a certain duration of time with the awareness of the pollution or government regulation. Analytical solution is obtained for a fixed initial concentration with the help of Laplace transformation technique.

2. Mathematical Formulation of the Problem

The soil medium has been assumed to be a homogeneous and isotropic porous medium that is having same water content, bulk density and retention factor. The fluorides find their way into the soil subsurface predominantly by advection, that is by flow of groundwater, and by dispersion which is caused by mechanical mixing and molecular diffusion. Due to small seepage velocity molecular diffusion is neglected.

Assuming that the fluoride is introduced in to the soil system in the form of pulse i.e. for a time $t_0 = t$, the distance in downward direction i.e. longitudinal direction be represented by $x[L]$ and the distance in horizontal i.e. lateral direction be represented by $y[L]$. The two-dimensional advection-diffusion equation is given as

$$R\frac{\partial C}{\partial t} = D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} - u\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial y} - kC. \tag{1}$$

Here $C = C(x, y, t) =$ concentration of fluoride at any time t; $D_x[LT^{-2}] =$ Dispersion coefficient along longitudinal direction; $D_y[LT^{-2}] =$ Dispersion coefficient along transverse direction; $u[LT^{-1}] =$ uniform constant velocity along x or longitudinal direction and $v[LT^{-1}] =$ uniform constant velocity along y or transverse direction; $R =$ retardation factor (dimensionless); $k =$ degradation constant. The dispersion coefficient is proportional to a power of the seepage velocity which ranges between 1 and 2 [15]. In India, the experimental observation has shown that the dispersion is directly proportional to the seepage velocity with a power ranging from 1 to 1.2 [18] and is applicable to various porous media. In present study dispersion is assumed to be directly proportional to the seepage velocity. Therefore,

$$D_x = au \text{ and } D_y = bv, \tag{2}$$

where a and b are the coefficients having the dimensions [L] and depends upon pore geometry and average pore size diameter of the porous medium.

The source of fluoride contamination is taken to be uniform pulse-type point source that is, it is introduced into the porous medium continuously at a uniform rate up to a certain time period i.e. t_0 and for $t > t_0$ it becomes zero. The porous medium is considered to be having some inherent initial concentration of fluoride C_i. Flux type homogeneous conditions are assumed at far ends of the medium, along both the directions. So, writing initial and boundary conditions mathematically

$$C(x, y, t) = C_i; \; x \geq 0, \; y \geq 0, \; t = 0. \tag{3}$$

$$C(x, y, t) = \begin{cases} C_0; & 0 < t \leq t_0 \\ 0; & t > t_0 \end{cases}, \tag{4a}$$

$$\frac{\partial C}{\partial x} = 0; \; \frac{\partial C}{\partial y} = 0; \; x \to \infty, \; y \to \infty, \; t > t_0. \tag{4b}$$

3. Analytical Solution

The problem of fluoride transport modelling in homogeneous porous medium can be solved using numerical, analytical, statistical, finite element method etc. It has been observed that the analytical approach is more significant to estimate the pattern of solute concentration and various transport parameters from field data [18, 9].

Introducing a new space variable

$$z = x + y\sqrt{\frac{D_y}{D_x}}. \tag{5}$$

Using equation (5) in equation (1), the resultant equation obtained is

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial z^2} - U\frac{\partial C}{\partial z} - kC, \tag{6}$$

where,

$$D = D_x\left(1 + \frac{D_y^2}{D_x^2}\right), \tag{7}$$

and

$$U = u + v\sqrt{\frac{v}{u}}. \tag{8}$$

Using the new space variable z, the initial condition given by equation (3) and the boundary conditions given by (4a), (4b) are written as

$$C(z, t) = C_i;\ z \geq 0,\ t = 0. \tag{9}$$

$$C(z, t) = \begin{cases} C_0; & 0 < t \leq t_0 \\ 0; & t > t_0 \end{cases}, \tag{10a}$$

$$\frac{\partial C}{\partial z} = 0;\ z \to \infty,\ t > t_0. \tag{10b}$$

Now, in order to solve equation (6), the following transformation is introduced which removes the convective term $U \frac{\partial c}{\partial z}$:

$$C(z, t) = K(z, t) \exp\left\{\frac{Uz}{2D} - \frac{1}{R}\left(\frac{U^2}{4D} + k\right)t\right\}. \tag{11}$$

As a result, equation (6) on substitution and simplification gives the below equation

$$R \frac{\partial K}{\partial t} = D \frac{\partial^2 K}{\partial z^2}. \tag{12}$$

As a result of the transformation used, given by equation (11), the initial condition and the boundary conditions given by equation (9) and (10a), (10b) respectively get transformed to

$$K(z, t) = C_i \exp\left\{-\frac{Uz}{2D}\right\};\ z \geq 0,\ t = 0. \tag{13}$$

$$K(z, t) = \begin{cases} C_0 \exp\left\{-\frac{1}{R}\left(\frac{U^2}{4D} + k\right)t\right\}; & 0 < t \leq t_0 \\ 0; & t > t_0 \end{cases}, \tag{14a}$$

$$\frac{\partial K}{\partial z} + \frac{UK}{2D} = 0;\ z \to \infty,\ t > t_0. \tag{14b}$$

Applying the Laplace transform to equations (12), (14a) and (14b) the expression obtained is

$$\frac{d^2 \overline{K}}{dz^2} - \frac{Rs}{D}\overline{K} = -\frac{R}{D}\left[C_i \exp\left(-\frac{Uz}{2D}\right)\right]. \tag{15}$$

$$\overline{K}(z, s) = \frac{C_0}{\left\{s - \frac{1}{R}\left(\frac{U^2}{4D} + k\right)\right\}}\left[1 - \exp\left\{s - \frac{1}{R}\left(\frac{U^2}{4D} + k\right)\right\}t\right]; \; z = 0, \tag{16a}$$

$$\frac{\partial \overline{K}}{\partial z} + \frac{U\overline{K}}{2D} = 0; \; z \to \infty. \tag{16b}$$

Where

$$\overline{K} = \int_0^\infty K(z, t)\exp(-st)\,dt \tag{17}$$

s = parameter.

On solving equation (15) the general solution of the differential equation is given as

$$\overline{K}(z, s) = C_1 \exp\left(\sqrt{\frac{Rs}{D}}z\right) + C_2 \exp\left(-\sqrt{\frac{Rs}{D}}z\right) + C_i \frac{\exp\left(-\frac{Uz}{2D}\right)}{\left(s - \frac{U^2}{4RD}\right)}. \tag{18}$$

Where C_1 and C_2 are arbitrary constants, whose values are determined using equations (16a) and (16b). And the final expression obtained is

$$\overline{K}(z, s) = \frac{C_0}{\left\{s - \frac{1}{R}\left(\frac{U^2}{4D} + k\right)\right\}}\left[1 - \exp[\left\{s - \frac{1}{R}\left(\frac{U^2}{4D} + k\right)\right\}\right]t \exp\left(-\sqrt{\frac{Rs}{D}}z\right) \tag{19}$$

$$- C_i \frac{\exp\left(-\frac{Uz}{2D}\right)}{\left(s - \frac{U^2}{4RD}\right)} \exp\left(-\sqrt{\frac{Rs}{D}}z\right) + C_i \frac{\exp\left(-\frac{Uz}{2D}\right)}{\left(s - \frac{U^2}{4RD}\right)}.$$

Taking inverse Laplace transformation to equation (19) and resubstituting for $K(z, t)$. we get

$$C(z, t) = C_0 F(z, t) + C_i F_1(z, t); \; 0 < t \le t_0, \tag{20a}$$

$$C(z, t) = C_0 F(z, t) - C_0 F(z, t - t_0) + C_i F_1(z, t); \; t > t_0, \tag{20b}$$

Where

$$F(z, t) = \frac{1}{2} \exp\left[\frac{(U - \sqrt{U^2 + 4kD})z}{2D}\right] erfc\left[\frac{(Rz - \sqrt{U^2 + 4kD}\, t)}{2\sqrt{RDt}}\right] \quad (21a)$$

$$+ \frac{1}{2} \exp\left[\frac{(U + \sqrt{U^2 + 4kD})z}{2D}\right] erfc\left[\frac{(Rz + \sqrt{U^2 + 4kD}\, t)}{2\sqrt{RDt}}\right],$$

and

$$F_1(z, t) = \exp\left(-\frac{kt}{R}\right)\left[1 - \frac{1}{2} erfc\left\{\frac{Rz - Ut}{\sqrt{2DRT}}\right\} - \frac{1}{2} \exp\left(\frac{Uz}{D}\right) erfc\left\{\frac{Rz + Ut}{\sqrt{2DRT}}\right\}\right] \quad (21b)$$

4. Numerical Results and Discussion

In order to understand the concentration distribution of fluoride ion in soil the concentration values obtained from the analytical solution equation (20a) in the presence of initial fluoride concentration are discussed graphically for a chosen set of numerical values of the different variables.

Taking initial concentration of fluoride as $C_i = 0.05$ and $C_0 = 1.0$, where C_0 is the concentration of the pulse type source, where source is present for time $t_0 = 5$ days. The distances in longitudinal and transverse direction are taken to be $0 \leq x \leq 5$ and $0 \leq y \leq 5$, in meters respectively. In actual field like situations the dispersion or flow of fluoride in longitudinal direction will be faster than in transverse direction due to presence of gravitational force in the former direction. Taking this into account the lateral velocity and dispersion coefficients are considered one- tenth of that in longitudinal direction. The seepage velocity and the dispersion coefficients in longitudinal and transverse direction are as follows:

$u = 0.75\ m/day$; $v = 0.075\ m/day$; $D_x = 0.95\ m^2/day$; $D_y = 0.095\ m^2/day$; $k = 0.02/day$. Figure 1 and 2 show the concentration profiles for $t = 4$ days and $R = 1.5$ and $t = 2$ days and $R = 1.5$. The initial value of fluoride concentration profile is 1 for both the cases except that it is lower for smaller time and higher for larger time.

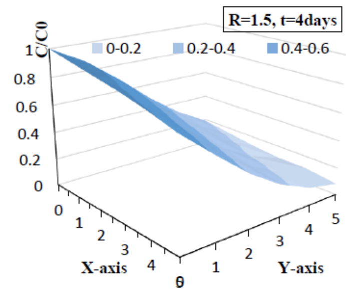

Figure 1. Concentration profiles of fluoride for steady for $t = 4$ days $(t < t_0)$ and $R = 1.5$.

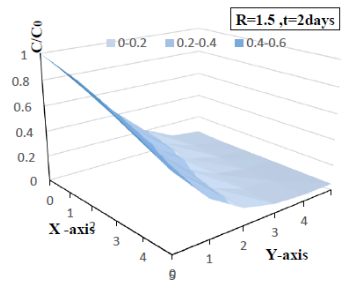

Figure 2. Concentration profiles of fluoride for steady flow for $t = 2$ days $(t < t_0)$ and $R = 1.5$.

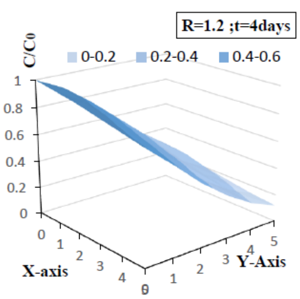

Figure 3. Concentration profiles of fluoride for steady flow for $t = 4$ days days $(t < t_0)$ and $R = 1.2$.

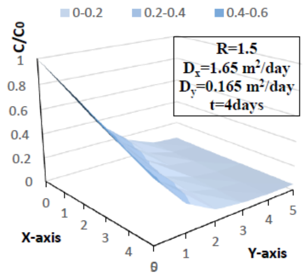

Figure 4. Concentration profiles of fluoride for steady flow for $t = 4$ days $(t < t_0)$ and $R = 1.5$ for higher Dispersion coefficient.

Figure 3 represents the concentration profile for $t = 4$ days and different value of retardation coefficient namely $R = 1.2$ and on comparing with figure 1 it is observed that the concentration profile is lower for higher and higher for lower retardation factor.

In Figure 4 the fluoride concentration profile has been presented for a higher longitudinal and transverse dispersion coefficient namely $D_x = 1.65\, m^2/day$ and $D_y = 0.165\, m^2/day$ and on comparison with figure 1 it is observed that the concentration levels are lower for lower and higher for higher dispersion coefficient.

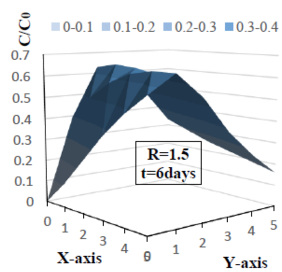

Figure 5. Concentration profiles of fluoride for steady flow for $t = 6$ days $(t > t_0)$ and $R = 1.5$.

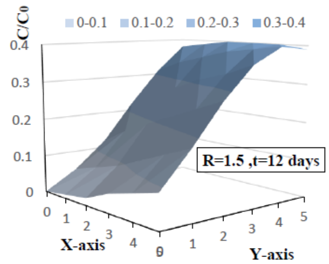

Figure 6. Concentration profiles of fluoride for flow for $t = 12$ days $(t > t_0)$ and $R = 1.5$.

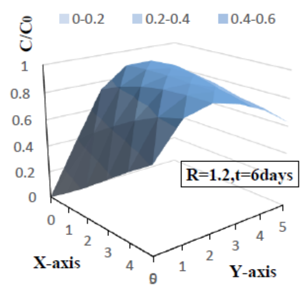

Figure 7. Concentration profiles of fluoride for steady flow for $t = 6$ days $(t > t_0)$ and $R = 1.2$.

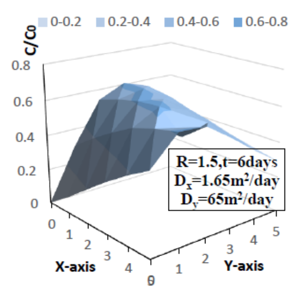

Figure 8. Concentration profiles of fluoride for steady flow for $t = 6$ days $(t > t_0)$ and $R = 1.5$ for higher Dispersion coefficients

Figure 5, 6, 7 and 8 represent fluoride concentration profile for the time $(t > t_0)$ when the source has been removed and is no longer present at the boundary.

The values of seepage velocity and dispersion coefficients in both longitudinal and transverse directions have been taken as stated earlier. Figure 5 and 6 are drawn at different time $t = 6$ days and $t = 12$ days and show that near the source boundary the concentration levels initially increases up to certain distance and then it deceases slowly with space. But for higher value of t the maxima of concentration profiles are lower than that for lower value of t.

On comparing the Figure 7 with Figure 5, it is observed that for high value of retardation factor, the concentration values are lower and vice-versa. Similarly, on comparing figure 8 with figure 5, it appears that near the source boundary the fluoride concentration levels initially increases for both and after some distance travelled it deceases but decreasing levels of concentration are lower for lower dispersion coefficient.

5. Conclusion

The present study presents a two-dimensional model for transport of fluoride ion in a homogeneous porous medium i.e., soil in steady state, considering both the longitudinal as well as transverse movement of the same. The equations so obtained have been solved analytically using Laplace transform technique. The numerical computation shows that the fluoride ion concentration decreases with respect to distance from origin along both longitudinal and transverse directions. There were often more influencing factors than initially anticipated, even in relatively simple systems. But on the whole, the transportation rules of fluorine ions are basically correct, which indicates that the established two-dimensional model can approximate the transportation rules of fluorine contaminants in homogeneous isotropic soils.

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