MATHEMATICAL STUDY OF VOLATILE ORGANIC COMPOUND (VOC) TYPE OF CONTAMINANTS TRANSPORT IN SOIL MEDIA

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Abstract

This study develops a mathematical model for one-dimensional solute transport of volatile organic compound type contaminates in a semi-infinite isotropic and homogeneous unsaturated soil medium. This phenomenon has been obtained in term of one-dimensional advection-dispersion equation. In this study the advection dispersion equation has been solved analytically by using Laplace transform, moving coordinates and Duhamel's theorem with appropriate initial and boundary condition. The final solution is obtained in terms of complementary error function and exponential form and it is concluded that the concentration profile decreases with time and depth.
Key words: *Advection, dispersion, Laplace transforms, Moving coordinates, Duhamel's theorem*

Introduction

The exhaustive size of natural resources and the large production of wastes in modern civilization often create a hazard to the groundwater quality and already have resultant in many incidents of groundwater pollution. Degradation of groundwater quality can take place over large areas from plane or diffuse sources like deep percolation from intensively farmed fields, or it can be caused by point sources such as septic tank, garbage disposal sites, cemeteries, mine spoils and oil spoils or other accidental entry of pollutants into the underground atmosphere. Another possibility is pollution by line sources of poor quality water, like seepage from polluted streams or intrusion of salt water, from oceans. These are main reason for volatile organic compound type contaminates enter to groundwater.

Analytical solutions in one-dimensional problems through semi-infinite or finite porous media have been studied by a number of researchers, like Bastian and Lapidus [1], Ebach and White [2] gives the longitudinal dispersion problem for an input concentration that varies periodically with time and Ogata and Banks [3] for a constant input concentration. Hoopes and Herteman [4] discussed the problem of dispersion in radial flow from a well fully penetrating, homogenous, isotropic non-adsorbing confined aquifers. Bruce and Street [5] considered both longitudinal and lateral dispersion in semi-infinite non adsorbing porous media in a steady unidirectional fluid flow for a constant input concentration. Marino [6] examined the input concentration varying exponentially with time. Al-Niami and Rushton [7] and Marino [6] studied the analysis of flow against dispersion in a porous media. Basak [8] consider an analytical solution the problem of evaporation from a horizontal soil column in which diffusivity increases linearly with moisture content and also to a problem of concentration dependent diffusion with decreasing concentration at the source. Hunt [9] applied perturbation method to longitudinal and lateral dispersion in non uniform seepage flow through heterogeneous aquifers. Sudheendra[10-12] Discussed the Mathematical Solutions of transport of pollutants through unsaturated porous media with adsorption in a finite domain and he gives the Mathematical Analysis of transport of pollutants through unsaturated porous media with adsorption and radioactive decay also gives the Mathematical Analysis of Solute Transport Exponentially Varies With Time In Unsaturated porous.

Mathematical Model

The advection-dispersion equation is playing a major role to understanding the mechanism of groundwater pollution problems. The advection-dispersion equation is a partial differential equation of parabolic type. The analytical solution of one dimensional advection-dispersion equation along with an initial condition and two boundary condition help to understand the contaminant

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concentration distribution behaviour through an unsaturated porous media. Soil is also a porous media, It can be written as.

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial z^2} - w\frac{\partial C}{\partial z} - \left(\frac{1-n}{n}\right) K_d C \qquad (1)$$

Initially, saturated flow of miscible type contaminant concentration, C = 0, takes place in the soil media. At t = 0, the concentration of the upper surface is immediately changed to $C = C_0$. Thus, the suitable boundary conditions for the given model are

$$\left.\begin{array}{ll} C(z,0) = 0 & z \geq 0 \\ C(0,t) = C_0 & t \geq 0 \\ C(\infty,t) = 0 & t \geq 0 \end{array}\right\} \qquad (2)$$

The problem then is to describe the concentration as a function of z and t.

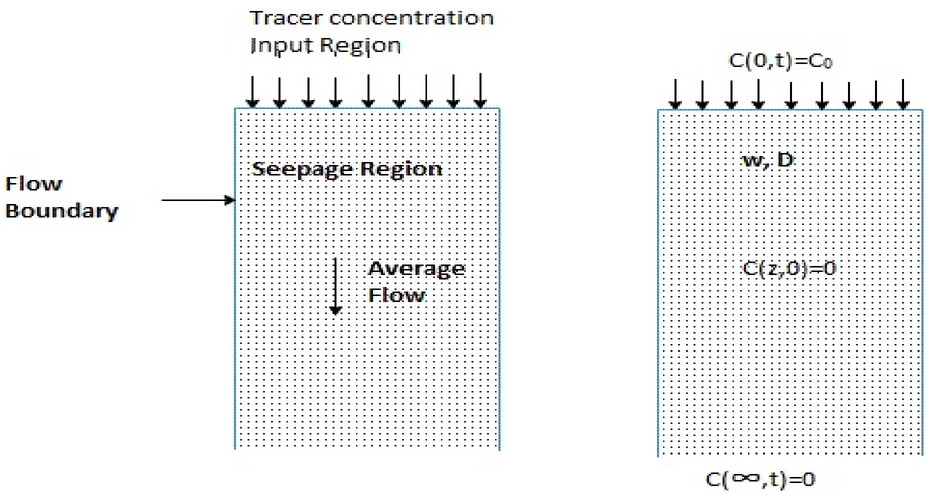

Figure 1: Physical Layout of the Model

Where the input condition is assumed at the origin and a second type or flux type homogeneous condition is assumed. C_0 is initial concentration. To reduce equation (3) to a more familiar form, we take

$$C(z,t) = \Gamma(z,t) Exp\left[\frac{wz}{2D} - \frac{w^2 t}{4D} - \frac{K_d(1-n)t}{n}\right] \qquad (3)$$

$$\frac{\partial \Gamma}{\partial t} = D\frac{\partial^2 \Gamma}{\partial z^2} \qquad (4)$$

Equation (1) can be transform to (4) and its initial and boundary conditions (2) transform to (5), when we substitute equation (3) to (1) and (2) respectively.

$$\left.\begin{array}{ll} \Gamma(0,t) = C_0\, Exp\left[\frac{w^2 t}{4D} + \frac{K_d(1-n)t}{n}\right] & t \geq 0 \\ \Gamma(z,0) = 0 & z \geq 0 \\ \Gamma(\infty,t) = 0 & t \geq 0 \end{array}\right\} \qquad (5)$$

Equation (4) may be solved for a time dependent influx of the fluid at z = 0. The solution of equation (4) may be obtained readily by use of Duhamel's theorem (Carslaw and Jaeger, 1947).

If $\boldsymbol{C = F(x,y,z,t)}$ is the solution of the diffusion equation for semi-infinite media in which the initial concentration is zero and its surface is maintained at concentration unity, then the solution of the problem in which the surface is maintained at temperature $\phi(t)$is

$$C = \int_0^t \phi(\tau)\frac{\partial}{\partial t}F(x,y,z,t-\tau)d\tau$$

This theorem is used principally for heat conduction problems, but the above has been specialized to fit this specific case of interest. Consider now the problem in which initial concentration is zero and the boundary is maintained at concentration unity. The boundary conditions are

$$\left.\begin{aligned} \Gamma(0,t) &= 0 \quad t \geq 0 \\ \Gamma(z,0) &= 1 \quad z \geq 0 \\ \Gamma(\infty,t) &= 0 \quad t \geq 0 \end{aligned}\right\}$$

When we Applying Laplace transform to equation (4) is reduced to an ordinary differential equation, that is,

$$\mathscr{L}\left[\frac{\partial \Gamma}{\partial t}\right] = \mathscr{L}\left[D\frac{\partial^2 \Gamma}{\partial z^2}\right]$$

$$\frac{\partial^2 \overline{\Gamma}}{\partial z^2} = \frac{p}{D}\overline{\Gamma} \qquad (6)$$

Where

$$\overline{\Gamma}(z,p) = \int_0^{\infty} e^{-pt}\,\Gamma(\mathrm{z},\mathrm{t})\mathrm{dt}$$ and p is the Laplace parameter

The solution of the equation is $\overline{\Gamma} = Ae^{-qz} + Be^{qz}$ where, $q = \pm\sqrt{\frac{p}{D}}$ boundary condition at z = 0 requires that $A = \frac{1}{p}$ and the boundary condition as $z \to \infty$ requires that B = 0 thus the particular solution of the Laplace transformed equation is

$$\overline{\Gamma} = \frac{1}{p}e^{-qz}$$

The inversion Laplace transforms of the above function is gives, the result

$$\Gamma = 1 - erf\left(\frac{z}{2\sqrt{Dt}}\right) = \frac{2}{\sqrt{\pi}}\int_{\frac{z}{2\sqrt{Dt}}}^{\infty} e^{-\eta^2}d\eta$$

Using Duhamel’s theorem, the solution of the problem with initial concentration zero and the time dependent surface condition at z = 0 is

$$\Gamma = \int_0^t \phi(\tau)\frac{\partial}{\partial t}\left[\frac{2}{\sqrt{\pi}}\int_{\frac{z}{2\sqrt{D(t-\tau)}}}^{\infty} e^{-\eta^2}d\eta\right]d\tau$$

Since $e^{-\eta^2}$ is a continuous function, it is possible to differentiate under the integral, which gives

$$\frac{2}{\sqrt{\pi}}\frac{\partial}{\partial t}\int_{\frac{z}{2\sqrt{D(t-\tau)}}}^{\infty} e^{-\eta^2}d\eta = \frac{z}{2\sqrt{Dt}(t-\tau)^{3/2}}Exp\left[\frac{-z^2}{4D(t-\tau)}\right]$$

The solution to the problem is

$$\Gamma = \frac{\mathrm{z}}{2\sqrt{\pi \mathrm{D}}}\int_0^t \phi(\tau)\,Exp\left[\frac{-z^2}{4D(t-\tau)}\right]\frac{d\tau}{(t-\tau)^{3/2}} \qquad (7)$$

Putting $\mu = \frac{z}{2\sqrt{D(t-\tau)}}$ then the equation (7) can be written as

$$\Gamma = \frac{2}{\sqrt{\pi}} \int_{\frac{z}{2\sqrt{Dt}}}^{\infty} \phi\left(t - \frac{z^2}{4D\,\mu^2}\right) e^{-\mu^2} \qquad (8)$$

Since $\phi(t) = C_0\, Exp\left(\frac{w^2 t}{4D} + \frac{K_d(1-n)t}{n}\right)$ the particular solution of the problem may be written as

$$\Gamma(z,t) = \frac{2C_0}{\sqrt{\pi}} \mathrm{Exp}\left(\frac{w^2 t}{4D} + \frac{K_d(1-n)t}{n}\right)\left\{\int_0^{\infty} \mathrm{Exp}\left(-\mu^2 - \frac{\varepsilon^2}{\mu^2}\right) d\mu - \int_0^{\alpha} \mathrm{Exp}\left(-\mu^2 - \frac{\varepsilon^2}{\mu^2}\right) d\mu\right\} \qquad (9)$$

Where, $\alpha = \frac{z}{2\sqrt{Dt}}$ and $\epsilon = \sqrt{\frac{w^2}{4D} + \frac{K_d(1-n)}{n}}\ \left(\frac{z}{2\sqrt{D}}\right)$

Integrating integral part of the equation (9) we get

$$\Gamma(z,t) = \frac{2C_0}{\sqrt{\pi}} \mathrm{Exp}\left(\frac{w^2 t}{4D} + \frac{K_d(1-n)t}{n}\right).\left[e^{2\varepsilon}\,\mathrm{erfc}\left(\alpha + \frac{\varepsilon}{\alpha}\right) + e^{-2\varepsilon}\,\mathrm{erfc}\left(\alpha - \frac{\varepsilon}{\alpha}\right)\right] \qquad (10)$$

From equations (3) and (10)

$$\frac{C}{C_0} = \frac{1}{2} Exp\left[\frac{wz}{2d}\right].\left[e^{2\varepsilon}\, erfc\left(\alpha + \frac{\varepsilon}{\alpha}\right) + e^{-2\varepsilon}\, erf\left(\alpha - \frac{\varepsilon}{\alpha}\right)\right]$$

Re-substituting for ε and α gives

$$\frac{c}{c_0} = \frac{1}{2}\left[Exp\left(\left(\frac{w}{2\sqrt{D}} + \sqrt{\frac{w^2}{4D} + \frac{(1-n)K_d}{n}}\right)\frac{z}{\sqrt{D}}\right) erfc\left(\frac{z}{2\sqrt{Dt}} + \sqrt{\frac{w^2 t}{4D} + \frac{(1-n)K_d t}{n}}\right)\right.$$
$$+ Exp\left(\left(\frac{w}{2\sqrt{D}} + \sqrt{\frac{w^2}{4D} + \frac{(1-n)K_d}{n}}\right)\frac{z}{\sqrt{D}}\right) erfc\left(\frac{z}{2\sqrt{Dt}}\right.$$
$$\left.\left. + \sqrt{\frac{w^2 t}{4D} + \frac{(1-n)K_d t}{n}}\right)\right] \qquad (11)$$

RESULTS & DISCUSSIONS

The Concentration profile C/C_0 of volatile organic compound type contaminant, decreases with time t and depth z. It means as the time increases dispersion process goes on dominating over the transport due to convection. In the case of unsteady flow similar but lesser effect would appear too. Though exponential form of seepage velocity is considered in the present analysis, there is no reason why other form of seepage velocity could not be used as long as the boundary conditions one dimensional transport model is selected because the groundwater flow is mixing of the groundwater contaminant is a good approximation in such deep aquifer. The time dependent behaviour of pollutants in subsurface is of interest for many practical problems where the concentration is observed or needs to be predicted at fixed positions. Problems of solute transport in one-dimension involving sequential first order decay reactions frequently occurs in soil, chemical engineering and groundwater systems.

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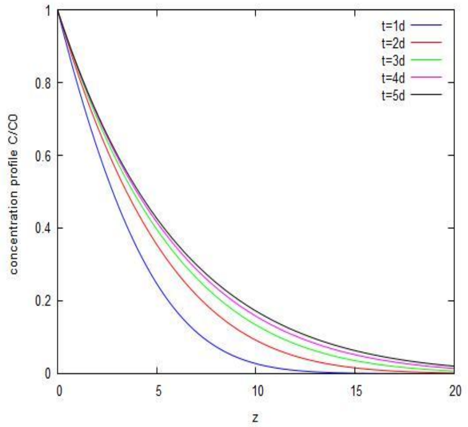


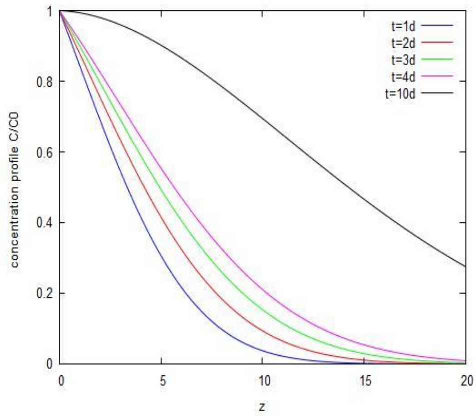
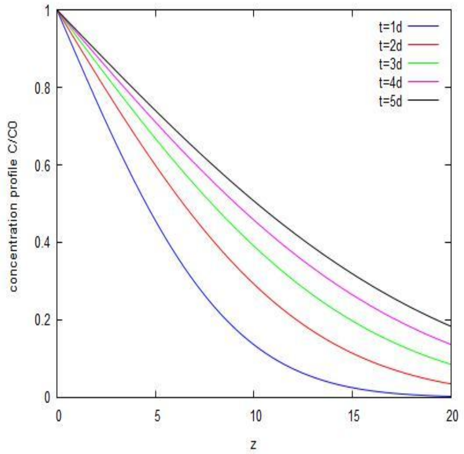


Fig. 1: Break-through-curve for C/C_0 v/s depth for n=0.5 & K_d=0.4

Fig. 2: Break-through-curve for C/C_0 v/s depth for n=0.5 & K_d=1



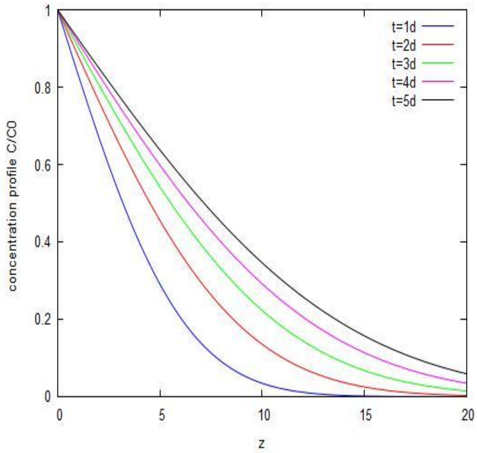


Fig. 3: Break-through-curve for C/C_0 v/s depth for n=1 & K_d=0.4

Fig. 4: Break-through-curve for C/C_0 v/s depth for n=1 & K_d=1

The above graphs 1 to 4 represents the concentration profile C/C_0 verses time t for different values of distribution coefficient and porosity n with fixed velocity w and dispersion coefficient D. it is observe that for a fixed K_d concentration increases slowly up to t=10 days because of less adsorption of pollutants on the solid surface and then reaches a constant value for longer time for small K_d. This study presents an analytical solution to solve the advection–dispersion equation for describing the one dimensional solute transport in a homogeneous porous media. In the derived solution, the components of velocity are assumed exponentially deceasing function of time, dispersion coefficient and first order decay are directly proportional to velocity. The hypothetical studies indicate that the effect of pollutant is not uniform but decrease as we move away from origin. The governing solute transport equation is solved analytically by employing Laplace Transformation Technique. The derived solution is an effective and useful for further application to verify the newly developed numerical transport model for predicting the one dimensional time-dependent transport of contaminants. The application results reveal that the solute transport process at the test site obeys the linearly time dependent dispersion model and that the linearly time-dependent assumption is valid in this real world example. The proposed solution can be applied to field problems where the hydrological properties of the medium and prevailing boundary and initial conditions are the same as, or can be approximated by, the ones considered in this study.

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