Mathematical Solutions of Transport of Pollutants through Unsaturated Porous Media with Adsorption in a finite domain

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Abstract: The objective of this paper is to demonstrate how mass transport, flow of pollutants and other technologies can be applied to define the behaviour of pollutants in the unsaturated and saturated soil zones. This paper is concerned with the development of analytical models for unsaturated and saturated flow behaviour in soils. Also, a comprehensive study on the effect of different soil parameters on the moisture movement and storage during different processes is carried out for homogeneous and isotropic soil media by considering adsorption term. The solution is obtained for the given mathematical model in a finite length initially solute free domain. The input condition is considered continuous of uniform and of increasing nature both. The solution has been obtained by using Duhamel's theorem and integral solution technique.

Introduction

In recent years numerous models have been developed based on finite differences, finite element and finite analytic methods for solving Richards equation. Rubin (1968) presented theoretical analysis of one-dimensional flow of water in an unsaturated soil by simulating transient transfer of water in a rectangular unsaturated soil slab using implicit finite difference method. Wang and Lakshminarayana (1968), Hanks et al., (1969) and Brutsaert (1971) solved the one and two-dimensional Richards equation using an implicit finite difference scheme with Newton iteration technique. Neuman et al., (1975) used the finite element method for analysis of one-dimensional flow in unsaturated soils considering water uptake (Adsorption) by roots.

Zyvoloski et al., (1976) and Cooley (1983) used the sub-domain finite element difference method in accomplishing a greater amount of nodal averaging of nonlinear quantities to improve stability. He also outlined new procedures for solving the nonlinear matrix equations and for locating positions of seepage faces. Kaluarachchi and Parker (1987) developed a two-dimensional Galerkin finite element model for flow through an unsaturated soil. They employed a fourth order Runge-Kutta time integration method that allows use of time steps at least two times greater than for a traditional finite difference approximation of time derivatives. This method has the advantage of requiring less computational effort while simulating problems having large time duration. Ross (1990a) developed two efficient finite difference methods namely fixed grid method and advancing front methods. He demonstrated that large time steps are possible when mass conserving mixed form of Richards equation is combined with an implicit scheme while a hyperbolic sine transform for the metric potential allows large spatial increments even in a dry inhomogeneous soil.

Celia et al., (1990) proposed a mixed form of Richards equation which combines the benefits inherent in both θ based and ψ based formulations for improving the poor mass balance and associated poor accuracy in ψ based formulation. Panoconi et al., (1991) evaluated the performance of iterative and non-iterative techniques while solving the Richards equation. The solutions of one, two and three-dimensional deterministic advection-dispersion equations have been investigated in numerous publications before and are still actively studied. For instance, Ogata and Banks (1961), Sauty (1980), and van Genuchten (1981) have provided analytical solutions of one-dimensional transport with the first-type (Dirichlet), second-type (Neumann), and third-type (Cauchy) boundary conditions, respectively. Yeh (1981) have given the generalised analytical one, two, and three-dimensional description and computer code for estimating the transport of waste in groundwater aquifers. Domenico and Robbins (1984) and Domenico (1987) have explored some multi-dimensional transport problems. Batu (1989, 1993) have studied the two-dimensional analytical solute transport model with the first and the second-type boundary conditions. Wexler (1992) and its cited references there have documented many previously derived analytical solutions with different initial and boundary conditions. Leij et al. (1993) have studied the non-equilibrium multi-dimensional transport using the Laplace and Fourier transforms and Leij et al. (2000) have used Green's functions to describe persistent solute source transport. Eungyu Park and Hongbin Zhan (2001) have developed an analytical solutions of contaminant transport from one, two, and three-dimensional finite sources in a finite-thickness aquifer using Green's function method. A graphically integrated MATLAB script is developed to calculate the temporal integrations in the analytical solutions and obtain the final solutions of concentration. He examined the analytical solutions by reproducing the solutions of some special cases discussed in previous studies. The objective of the problem is to develop the mathematical model to demonstrate how mass transport, flow of pollutants and other technologies can be applied to define the behaviour of pollutants in the unsaturated and saturated soil zones.

Mathematical Model

The Advection-Dispersion equation along with initial condition and boundary conditions can be written as

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

Initially, saturated flow of fluid of concentration, $C = 0$, takes place in the porous media. At $t = 0$, the concentration of the upper surface is instantaneously changed to $C=C_0$. Thus, the appropriate boundary conditions for the given model

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

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

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

Substituting equation (3) into equation (1) gives

$$\frac{\partial \Gamma}{\partial t} = D\frac{\partial^2 \Gamma}{\partial z^2} \tag{4}$$

The initial and boundary conditions (2) transform to

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

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 $C = F\,(x,\ y,\ z,\ t)$ 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

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

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

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

The Laplace transform of equation (4) is

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

Hence, it is reduced to an ordinary differential equation

$$\frac{\partial^2 \overline{\Gamma}}{\partial z^2} = \frac{p}{D}\overline{\Gamma} \tag{6}$$

The solution of the equation is $\overline{\Gamma} = Ae^{-qz} + Be^{qz}$ where, $q = \pm\sqrt{\dfrac{p}{D}}$.

The boundary condition as $z \to \infty$ requires that $B = 0$ and boundary condition at $z = 0$ requires that $A = \dfrac{1}{p}$ thus the particular solution of the Laplace transformed equation is

$$\overline{\Gamma} = \frac{1}{p}e^{-q\,z}$$

The inversion of the above function is given in any table of Laplace transforms. The result is

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

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

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

The solution to the problem is

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

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

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

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

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

where, $\alpha = \dfrac{z}{2\sqrt{D\,t}}$ and $\varepsilon = \sqrt{\left(\dfrac{w^2}{4D} + \dfrac{K_d(1-n)}{n}\right)}\left(\dfrac{z}{2\sqrt{D}}\right)$.

Evaluation of the integral solution

The integration of the first term of equation (9) gives

$$\int_0^{\infty} Exp\left(-\mu^2 - \frac{\varepsilon^2}{\mu^2}\right)d\mu = \frac{\sqrt{\pi}}{2} e^{-2\varepsilon}. \tag{10}$$

For convenience the second integral may be expressed on terms of error function (Horenstein, 1945), because this function is well tabulated.

Noting that

$$-\mu^2 - \frac{\varepsilon^2}{\mu^2} = -\left(\mu + \frac{\varepsilon}{\mu}\right)^2 + 2\varepsilon = -\left(\mu - \frac{\varepsilon}{\mu}\right)^2 - 2\varepsilon .$$

The second integral of equation (9) may be written as

$$I = \int_0^{\alpha} Exp\left(-\mu^2 - \frac{\varepsilon^2}{\mu^2}\right)d\mu = \frac{1}{2}\left\{e^{2\epsilon}\int_0^{\alpha} Exp\left[-\left(\mu + \frac{\varepsilon}{\mu}\right)^2\right]d\mu + e^{-2\epsilon}\int_0^{\alpha} Exp\left[-\left(\mu - \frac{\varepsilon}{\mu}\right)^2\right]d\mu\right\} \tag{11}$$

Since the method of reducing integral to a tabulated function is the same for both integrals in the right side of equation (11), only the first term is considered. Let $a = \varepsilon/\mu$ and the integral may be expressed as

$$\begin{aligned} I_1 &= e^{2\varepsilon}\int_0^{\alpha} Exp\left[-\left(\mu + \frac{\varepsilon}{\mu}\right)^2\right]d\mu \\ &= -e^{2\varepsilon}\int_{\varepsilon/\alpha}^{\infty}\left(1 - \frac{\varepsilon}{a^2}\right)Exp\left[-\left(\frac{\varepsilon}{a} + a\right)^2\right]da + e^{2\varepsilon}\int_{\varepsilon/\alpha}^{\infty} Exp\left[-\left(\frac{\varepsilon}{a} + a\right)^2\right]da . \end{aligned} \tag{12}$$

Further, let, $\beta = \left(\frac{\varepsilon}{a} + a\right)$

in the $\beta = \frac{\varepsilon}{a} + a$ first term of the above equation, then

$$I_1 = -e^{2\varepsilon} \int_{\alpha+\frac{\varepsilon}{\alpha}}^{\infty} e^{-\beta^2} d\beta + e^{2\varepsilon} \int_{\frac{\varepsilon}{\alpha}}^{\infty} Exp\left[-\left(\frac{\varepsilon}{a} + a\right)^2\right] da \, . \tag{13}$$

Similar evaluation of the second integral of equation (11) gives

$$I_2 = e^{-2\varepsilon} \int_{\varepsilon/\alpha}^{\infty} Exp\left[-\left(\frac{\varepsilon}{a} - a\right)^2\right] da - e^{-2\varepsilon} \int_{\varepsilon/\alpha}^{\infty} Exp\left[-\left(\frac{\varepsilon}{a} - a\right)^2\right] da \, .$$

Again substituting $-\beta = \frac{\varepsilon}{a} - a$ into the first term, the result is

$$I_2 = e^{-2\varepsilon} \int_{\frac{\varepsilon}{\alpha}-\alpha}^{\infty} e^{-\beta^2} d\beta - e^{-2\varepsilon} \int_{\varepsilon/\alpha}^{\infty} Exp\left[-\left(\frac{\varepsilon}{a} - a\right)^2\right] da \, .$$

Noting that

$$\int_{\varepsilon/\alpha}^{\infty} Exp\left[-\left(a + \frac{\varepsilon}{a}\right)^2 + 2\varepsilon\right] da = \int_{\varepsilon/\alpha}^{\infty} Exp\left[-\left(\frac{\varepsilon}{a} - a\right)^2 - 2\varepsilon\right] da$$

Substitution into equation (11) gives

$$I = \frac{1}{2}\left(e^{-2\varepsilon} \int_{\frac{\varepsilon}{\alpha}-\alpha}^{\infty} e^{-\beta^2} d\beta - e^{2\varepsilon} \int_{\alpha+\frac{\varepsilon}{\alpha}}^{\infty} e^{-\beta^2} d\beta\right). \tag{14}$$

Thus, equation (9) may be expressed as

$$\Gamma(z,t) = \frac{2C_0}{\sqrt{\pi}} Exp\left(\frac{w^2 t}{4D} + \frac{K_d(1-n)\,t}{n}\right)\left\{\frac{\sqrt{\pi}}{2} e^{-2\varepsilon} - \frac{1}{2}\left[e^{-2\varepsilon} \int_{\frac{\varepsilon}{\alpha}-\alpha}^{\infty} e^{-\beta^2} d\beta - e^{-2\varepsilon} \int_{\alpha+\frac{\varepsilon}{\alpha}}^{\infty} e^{-\beta^2} d\beta\right]\right\} \tag{15}$$

However, by definition,

$$e^{2\varepsilon} \int_{\alpha+\frac{\varepsilon}{\alpha}}^{\infty} e^{-\beta^2} d\beta = \frac{\sqrt{\pi}}{2} e^{2\varepsilon} \; erfc\left(\alpha + \frac{\varepsilon}{\alpha}\right)$$

also,
$$e^{-2\in} \int_{\frac{\varepsilon}{\alpha}-\alpha}^{\infty} e^{-\beta^2} d\beta = \frac{\sqrt{\pi}}{2} e^{-2\varepsilon}\left(1 + erf\left(\alpha - \frac{\varepsilon}{\alpha}\right)\right).$$

Writing equation (15) in terms of error functions, we get

$$\Gamma(z,t)=\frac{C_0}{2}Exp\left(\frac{w^2 t}{4D}+\frac{K_d(1-n)t}{n}\right)\left[e^{2\varepsilon}erfc\left(\alpha+\frac{\varepsilon}{\alpha}\right)+e^{-2\varepsilon}erfc\left(\alpha-\frac{\varepsilon}{\alpha}\right)\right] \qquad (16)$$

Thus, Substitution into equation (3) the solution is

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

Re-substituting for ε and α gives

$$\frac{C}{C_0}=\frac{1}{2}Exp\left[\frac{wz}{2D}\right]\left[Exp\left[\frac{\sqrt{w^2 n+4D(1-n)K_d}}{2D\sqrt{n}}z\right]\cdot erfc\left[\frac{z+\sqrt{w^2 n+4D(1-n)K_d}}{2\sqrt{Dnt}}t\right]+\right.$$

$$\left.\left[Exp\left[-\frac{\sqrt{w^2 n+4D(1-n)K_d}}{2D\sqrt{n}}z\right]\cdot erfc\left[\frac{z-\sqrt{w^2 n+4D(1-n)K_d}}{2\sqrt{Dnt}}t\right]\right] \qquad (17)$$

where boundaries are symmetrical the solution of the problem is given by the first term the equation (17). The second term is equation (17) is thus due to the asymmetric boundary imposed in the more general problem. However, it should be noted also that if a point a great distance away from the source is considered, then it is possible to approximate the boundary condition by $C(-\infty,t)=C_0$, which leads to a symmetrical solution.

Results and discussions

The present investigation describes theoretical considerations and presents tools for analyzing solute conditions during infiltration from a source. The partial differential equations describing solute transport are solved analytically by considering adsorption term. It is generally assumed that macroscopic transport by convection must take into account the average flow velocity as well as the mechanical or hydrodynamic dispersion. Taking into account the scope of the work, the investigation carried out in the field as well as in the laboratory, the observations made and the results obtained are presented under different sections.

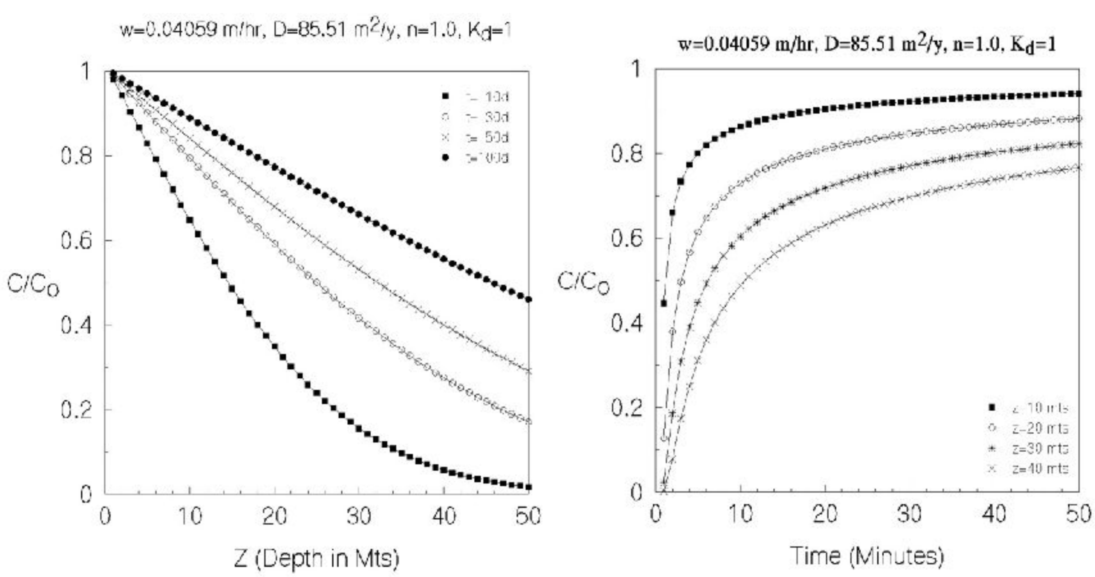
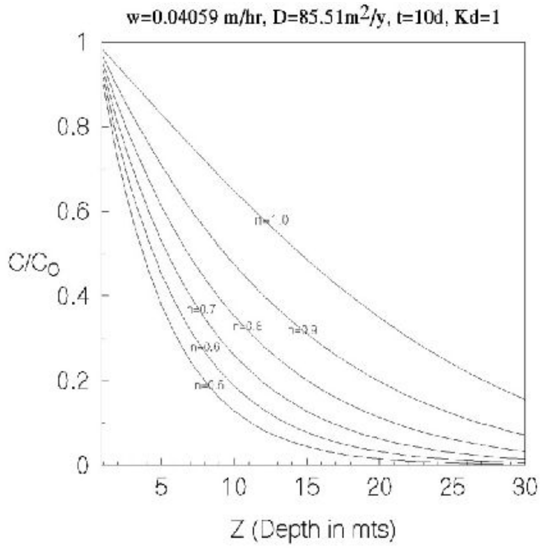


Figure 1: Break - through - curve for C/C_0 v/s Depth for different time interval

Figure 2: Break - through - curve for C/C_0 v/s Time for different depth



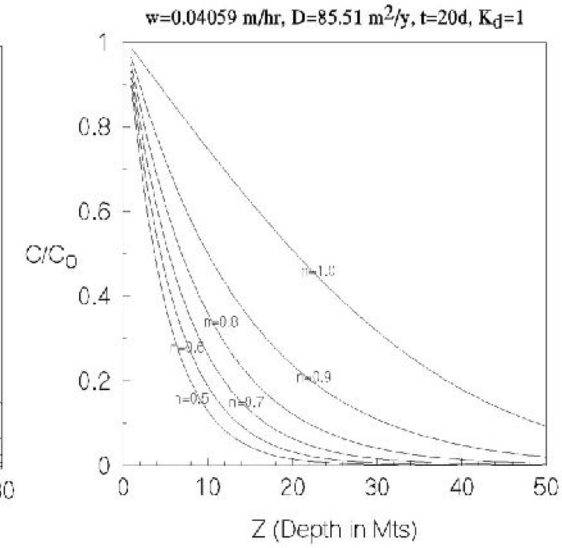
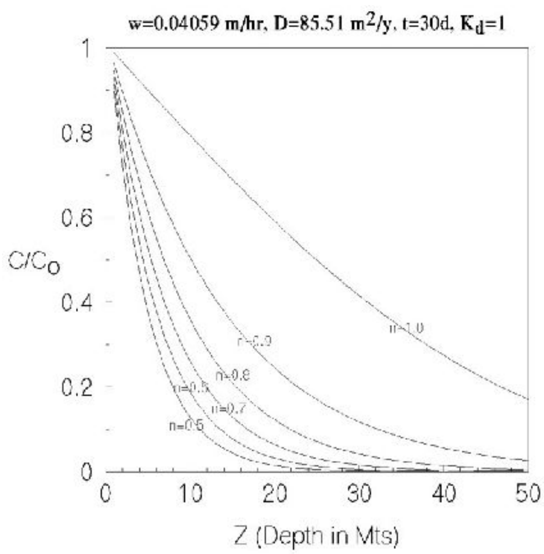


Figure 3: Break - through - curve for C/C_0 v/s Depth for different porosity at Time (t) = 10 days

Figure 4: Break - through - curve for C/C_0 v/s Depth for different porosity at Time (t) = 20 days



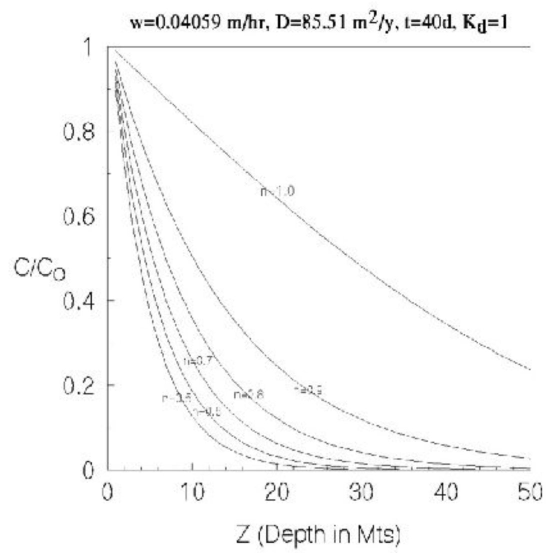


Figure 5: Break - through - curve for C/C_0 v/s Depth for different porosity at Time (t) = 30 days

Figure 6: Break - through - curve for C/C_0 v/s Depth for different porosity at Time (t) = 40 days

The Water containing pollutants such as sewage and radioactive wastes, infiltrate through the soil matrix from streams, ditches and lakes as well as direct flow from overland areas as result of runoff. This water eventually enters the aquifer - a source for potable water. During the passage of water through the soil, the pollutants are mixed, adsorbed, dispersed and diffused through the flowing flux and led to an intense effort to develop more accurate and economical models for predicting solute transport and fate, often from solute sources that exist in the unsaturated soil zone.

The solution presented in equation (17), the solute concentration C/C_0 was computed numerically with the help of 'Mathematica' and the results are presented graphically in figures (1) to (6). Figure (1) represent break through curve for C/C_0 v/s Depth for different time interval. Figure (2) represents break through curve for C/C_0 v/s time for different depth z. Figure (3) to (6) represents for break through curve for C/C_0 v/s Depth by taking porosity (0.5 to 1.0) for different time interval (10 days to 40 days). Figure (1) represents the solute concentration field decrease for different time intervals. In Figure (2), we have seen that the solute concentration field increases in the beginning and reaches a steady state value for a fixed z but decreases with an increase in the layer thickness. Most of the contaminants are attenuated in the unsaturated zone itself and thus the threat of groundwater being contaminated is minimized. Similar pattern is observed in the Figure (3) to (6) for different values of average velocity w and dispersion coefficient D. We conclude that solute concentration decreases with respect to the porosity and adsorption because of the surface tension and water uptake by the roots. The governing partial differential equation is solved in straight forward manner for general inlet and initial solute distributions by applying Laplace transform with respect to z & t.

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