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Mathematical Modelling Of Transport of Contaminants In Unsaturated Porous Media With Non-Uniform Flow

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Abstract

Over-pumping of groundwater for domestic, agricultural and industrial consumption will lower the water table and can accelerate the movement of pollutant-laden surface water into the groundwater. In unsaturated soil, the water content is less than the soil porosity, and the soil water pressure head (matric potential) is negative, being less than that of free water at the same location. The upper most region of the soil, the unsaturated zone, is the site of important process leading to pollutant attenuation.

In responding to the growing concern over deteriorating groundwater quality, groundwater flow models are rapidly coming to play a crucial role in the development of protection and rehabilitation strategies. These models provide forecasts of the future state of the groundwater aquifer systems.

The present study is concerned with the development of analytical models for transport of contaminants in unsaturated porous media with non-uniform flow

Introduction

The groundwater has been a major source of water supply throughout the ages. The groundwater is also an important source in the agriculture and industrial sector. In many parts of the world, groundwater resources are under increasing threat from growing demands, wasteful use and contamination. A good planning and management practices are needed to face this challenge. In order to understand the behaviour of contaminant transport through different types of media, several researchers are carrying out experimental investigations through laboratory and field studies. A porous medium is a material, which contains pores. Pores are filled with one or more different fluids, like air, water or oil. The porous medium is saturated if all the pores contain water and is unsaturated if some pores are filled with water and some with air. The saturation is defined as the fraction of the total volume of the fluid and pore volume. There exist many natural porous substances such as soil, rocks, wood, cork or bones.

The water flow and contaminant transport equations in the unsaturated zone are described by Bear [2], Pinder and Gray [6], and Freeze and Cherry [7]. Gray and Hassanizadeh [8] proposed a new set of equations to describe the unsaturated flow processes obtained from averaging theory coupled with an interface thermodynamic analysis. However, this set of equations contains many more unknowns than that of classical equations.

For simulating most field problems, exact analytical solutions are probably out weighted by errors introduced by simplifying approximations of the complex field environment that are required to apply the analytical approach (De Smedt and Wirenga, [5], Foussereau et al.,[9],Yates et al., [10]). Ebach and White [1] studied the longitudinal dispersion problem for an input concentration that varies periodically with time. Al-Niami and Rushton [3] studied the analysis of flow against dispersion in porous media. Hunt [4] applied the perturbation method to longitudinal and lateral dispersion in non-uniform seepage flow through heterogeneous aquifers. M Jalal Ahammad et al [11] studied dispersion and diffusion of solvent saturation with the help of a streamline-based Lagrangian methodology. Overall pressure drag on the diffusion and dispersion of solvent saturation was studied. Numerical results were in good agreement with the results obtained from asymptotic analysis.

In this paper, we have studied the mathematical modelling of transport of pollutants in unsaturated soil media with non-uniform flow. The basic approach is to reduce the advection-dispersion equation into a conduction equation by using moving coordinates which eliminates the convective term. We have used Laplace transform method to reduce the non-linear partial differential equation to ordinary differential equation. By introducing Duhamel's theorem, the general solution of ordinary differential equation is expressed in terms of error function.

Mathematical Formulation

The advection-dispersion equation of one-dimensional mathematical model for transport of pollutants through unsaturated porous media in non-uniform flow with initial and boundary conditions is of the form

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

where C is the constituent concentration in the soil solution, t is the time, D is the hydrodynamic dispersion coefficient, z is the depth, w is the average pore-water velocity, K_d is the dissipaton coefficient.

Let us consider a semi-infinte soil (porous) medium in an uni-directional flow field in which the input tracer concentration is $C_0 e^{-\gamma t}$, where C_0 is a reference concentration and γ is a constant. Initially, saturated flow of concentration, $C = 0$, in the porous media. At $t = 0$, the concentration of the upper surface is instantaneously changed to $C = C_0 e^{-\gamma t}$

Thus, the appropriate boundary conditions for the given model are

$$\left.\begin{aligned} &C(z,0)=0 && z\ge 0\\ &C(0,t)=C_o e^{-\gamma t} && t\ge 0\\ &C(\infty,t)=0 && t\ge 0\end{aligned}\right\} \tag{2}$$

The problem then is to characterize the concentration as $f(z,t)$, where the input condition is assumed at the origin and a second type boundary condition or flux type boundary condition is assumed. C_o is the initial concentration. Using

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

equation (1) reduces to

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

The initial and boundary conditions (2) transform to

$$\left.\begin{aligned} &\Gamma(0,t)=C_o\, exp\left[\frac{w^2t}{4D}+\frac{K_d(1-n)t}{n}-\gamma t\right] && :t\ge 0\\ &\Gamma(z,0)=0 && :z\ge 0\\ &\Gamma(\infty,t)=0 && :t\ge 0\end{aligned}\right\} \tag{5}$$

Equation (4) is solved for a time dependent influx of the fluid at $z = 0$ and is obtained by Duhamel's theorem stated as " If $C = F(x, y, z, \tau)$ is the solution of semi-infinite conduction equation in which, the initial concentration is zero and the solute concentration at the surface is unity. The solution of the given problem at temperature $\phi(t)$ will be $C=\int_0^t \phi(\tau)\frac{\partial}{\partial t}F(x,y,z,t-\tau)\,d\tau$". Consider the problem in which the initial concentration is zero. The boundary conditions are

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

The Laplace transform of equation (4) is given by $L\left[\frac{\partial\Gamma}{\partial t}\right]=L\left[D\frac{\partial^2\Gamma}{\partial z^2}\right]$ which reduces to

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

Its solution is $\bar{\Gamma}=Ae^{-qz}+Be^{qz}$ where $q=\pm\sqrt{\frac{p}{D}}$.

As $z\to\infty$, $B = 0$ and at $z = 0$, $A=\frac{1}{p}$, thus the general solution is of the form $\bar{\Gamma}=\frac{1}{p}e^{-qz}$. The inverse of the given function from the table of Laplace transforms is

$$\Gamma=1-erf\left(\frac{z}{2\sqrt{Dt}}\right)=\frac{2}{\sqrt{\pi}}\int_{\frac{z}{2\sqrt{Dt}}}^{\infty} e^{-\eta^2}d\eta \quad \text{with} \quad erf(z)=\frac{2}{\sqrt{\pi}}\int_0^z e^{-\eta^2}d\eta .$$

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

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

Since $e^{-\eta^2}$ is a continuous function, the differential under the integral reduces to

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

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

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

Since, $\varphi(t) = C_0 \exp\left(\frac{w^2 t}{4D} + \frac{K_d(1-n)t}{n} - \gamma t\right)$ the particular solution of the problem is

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

z

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

The integral 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 term is expressed in terms of error function.

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 term of the integral of equation (9) is

$$I = \int_0^{\alpha} \exp\left(-\mu^2 - \frac{\varepsilon^2}{\mu^2}\right) d\mu = \frac{1}{2}\left\{e^{2z} \int_0^{\alpha} \exp\left(-\left(\mu + \frac{\varepsilon}{\mu}\right)^2\right) d\mu + e^{-2z} \int_0^{\alpha} \exp\left(-\left(\mu - \frac{\varepsilon}{\mu}\right)^2\right) d\mu\right\}. \tag{11}$$

With $a = \varepsilon/\mu$, the first integral on R H S of equation (11) can be written as

$$I_1 = e^{2\varepsilon} \int_0^{\alpha} \exp\left[-\left(\mu + \frac{\varepsilon}{\mu}\right)^2\right] d\mu = -e^{2z} \int_{\frac{z}{\alpha}}^{\alpha} \left(1 - \frac{\varepsilon}{a^2}\right) \exp\left[-\left(\frac{\varepsilon}{a} + a\right)^2\right] da +$$

$$e^{2z} \int_{\frac{z}{\alpha}}^{\infty} \exp\left[-\left(\frac{\varepsilon}{a} + a\right)^2\right] da \tag{12}$$

Let $\beta = \left(\frac{\varepsilon}{a} + a\right)$, then the first integral term of the above equation becomes

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

Similarly, the second integral on R H S of equation (11) gives

$$I_2 = e^{2z}\int_{\frac{z}{\alpha}}^{\infty} exp\left[-\left(\frac{\varepsilon}{a}-a\right)^2\right]da - e^{-2z}\int_{\frac{z}{\alpha}}^{\infty} \exp\left[-\left(\frac{\varepsilon}{a}-a\right)^2\right]da \quad (14)$$

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

$$I_2 = e^{-2z}\int_{\frac{z}{\alpha}-\alpha}^{\infty} e^{-\beta^2}d\beta - e^{-2z}\int_{\frac{z}{\alpha}}^{\alpha} exp\left[-\left(\frac{\varepsilon}{a}-a\right)^2\right]da \quad (15)$$

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

Substitution into equation (11) gives

$$I = \frac{1}{2}\left(e^{-2z}\int_{\frac{Z}{\alpha}-\alpha}^{\infty} e^{-\beta^2}d\beta - e^{2z}\int_{\frac{Z}{\alpha}+\alpha}^{\infty} e^{-\beta^2}d\beta\right) \quad (16)$$

Thus, equation (9) may be expressed as

$$\Gamma(z,t) = \frac{2C_0}{\sqrt{\pi}}exp\left(\frac{w_L{}^2 t}{4D_L} + \frac{K_d(1-n)t}{n} - \gamma t\right).$$

$$\left\{\frac{\sqrt{\pi}}{2}e^{-2z} - \frac{1}{2}\left[e^{-2z}\int_{\frac{Z}{\alpha}-\alpha}^{\infty} e^{-\beta^2}d\beta - e^{2z}\int_{\frac{Z}{\alpha}+\alpha}^{\infty} e^{-\beta^2}d\beta\right]\right\} \quad (17)$$

But $e^{2z}\int_{\alpha+\frac{Z}{\alpha}}^{\infty} e^{-\beta^2}d\beta = \frac{\sqrt{\pi}}{2}e^{2z}erfc\left(\alpha+\frac{\varepsilon}{\alpha}\right)$, $e^{-2z}\int_{\frac{z}{\alpha}-\alpha}^{\infty} e^{-\beta^2}d\beta = \frac{\sqrt{\pi}}{2}e^{-2z}erfc\left(\alpha-\frac{\varepsilon}{\alpha}\right)$ Re-writing equation (17) in terms of error function, we get

$$\Gamma(z,t) = \frac{C_0}{2}exp\left(\frac{w^2 t}{4D} + \frac{K_d(1-n)t}{n} - \gamma t\right)\left[e^{2z}erfc\left(\alpha+\frac{\varepsilon}{\alpha}\right) + e^{-2z}erfc\left(\alpha-\frac{\varepsilon}{\alpha}\right)\right] \quad (18)$$

Thus, substitution into equation (3) gives the solution as

$$\frac{C}{C_0} = \frac{1}{2}exp\left(\frac{wz}{2D} - \gamma t\right)\left[e^{-2z}erfc\left(\alpha-\frac{\varepsilon}{\alpha}\right) + e^{2z}erfc\left(\alpha+\frac{\varepsilon}{\alpha}\right)\right] \quad (19)$$

Re-substituting for ε and α gives

$$\frac{C}{C_0} = \frac{1}{2}exp\left(\frac{wz}{2D} - \gamma t\right).$$

$$\left[exp\left(\frac{\sqrt{w^2 n + 4D(1-n)K_d - 4Dn\gamma}}{2D\sqrt{n}}z\right) erfc\left(\frac{z + \sqrt{w^2 n + 4D(1-n)K_d - 4Dn\gamma}\,t}{2\sqrt{Dnt}}\right)\right] +$$

$$\left[exp\left(-\frac{\sqrt{w^2 n + 4D(1-n)K_d - 4Dn\gamma}}{2D\sqrt{n}}z\right) erfc\left(\frac{z - \sqrt{w^2 n + 4D(1-n)K_d - 4Dn\gamma}\,t}{2\sqrt{Dnt}}\right)\right] \quad (20)$$

When the boundaries are symmetrical the solution of the problem is given by the first integral term of the equation (20). The second integral term of equation (20) is due to the asymmetric boundary condition imposed in the general problem. However, if a point at a large 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.

1. Results and Discussion

Equation (20) gives the value of the ratio $\frac{C}{C_0}$ for unsaturated non – uniform fluid flow at any distance z and time t. Fig. 1 and. Fig. 2 represents the concentration profiles verses time in the porous media for depth z for different velocity w = 0.0111 m/hr, D = 11.24 cm²/yr, K_d =1, n

= 0.5 and n = 1. Fig. 3 and. Fig. 4 represents the concentration profiles verses time in the porous media for depth z for different velocity w = 0.0111 m/hr, D = 11.24 cm²/yr, K_d =1, n = 0, $\gamma = 0$ and $\gamma = 1$.

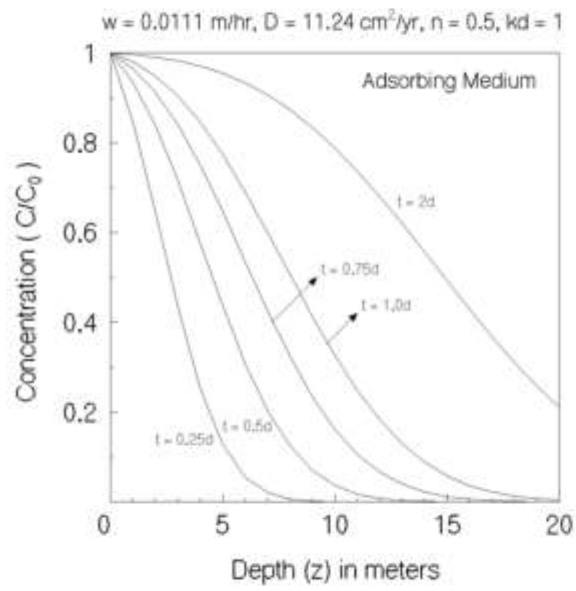

Fig.1 Break-through-curve for C/C_0 v/s depth Z for different time interval at porosity n = 0.5 and dissipation coefficient K_d = 1

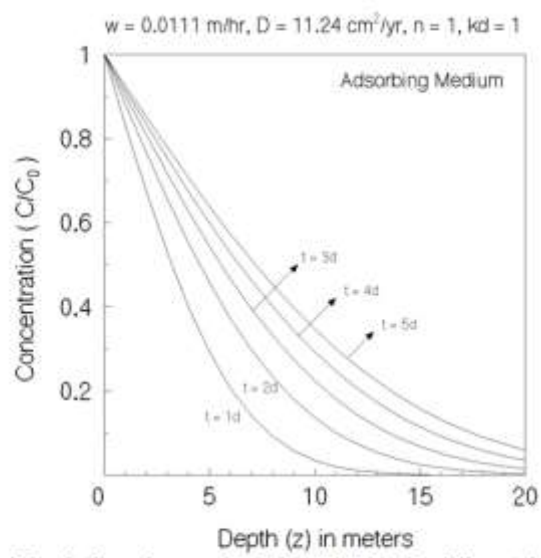

Fig.2 Break-through-curve for C/C_0 v/s depth Z for different time interval at porosity n = 1.0 and dissipation coefficient K_d = 1

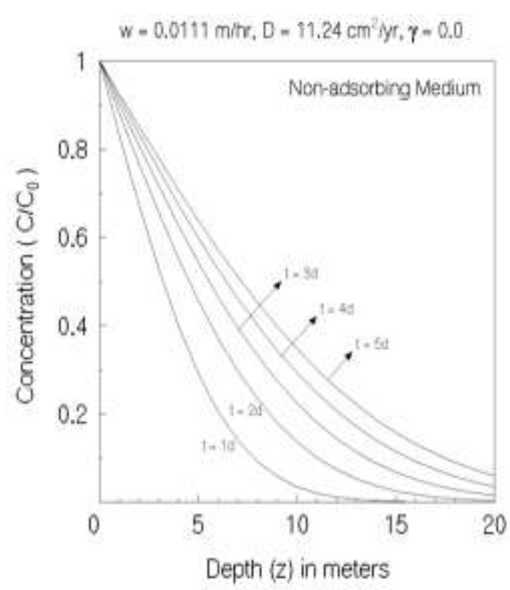

Fig.3 Break-through-curve for C/C_0 v/s Depth Z for different time interval at porosity n = 0.0, Dissipation Coefficient K_d = 1 and γ = 0.0

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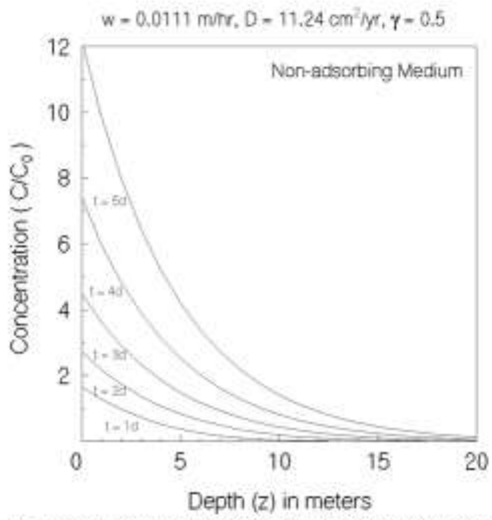

Fig.4 Break-through-curve for C/C_0 v/s depth Z for different time interval at porosity n = 0.0, dissipation coefficient K_d = 1 and γ = 0.5

From Fig. 1 and Fig.2, there is a decrease in $\frac{C}{C_0}$ with depth as porosity n decreases due to the distributive coefficient Kd . From Fig. 3 and Fig.4 there is a decrease in $\frac{C}{C_0}$ with depth as **γ** decreases and if time increases the concentration increases for different time.

Conclusions

The main limitations of the analytical methods are that the applicability is for relatively simple problems. The geometry of the problem should be regular. The properties of the soil in the region considered must be homogeneous in the sub region. The analytical method in somewhat more flexible than the standard form of the other methods for one-dimensional transport model. Accordingly, the analytical solutions derived for the finite domain will thus be particularly useful for analyzing the one-dimensional transport in unsaturated porous medium with a large dispersion coefficient whereas the analytical solution for semi-infinite domain is recommended to be applied for a medium system with a small dispersion coefficient. Moreover, the developed solution is especially useful for validating numerical model simulated solution because realistic problems generally have a finite domain.

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