Mathematical Modelling of Transport of Pollutants in Unsaturated Porous Media for One-Dimensional Flow

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Abstract—Contaminants containing different chemicals will pass through different hydro geologic zones as they migrate through the soil to the water table. The water table is the upper surface of the groundwater system. The pore space between soil particles above the water table are occupied by both air and water. Flow in this unsaturated zone is taken to be vertically downward, as liquid contaminants or solutions of contaminants and precipitation move under the force of gravity. 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 objective of the present work 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. The present study is concerned with the development of analytical models for unsaturated and saturated flow behaviour in soils.

Index Terms — Contaminants , water table, groundwater, flow, pollutants, aquifer, analytical models .

1 INTRODUCTION

The increasing demand for water for domestic, industrial and agricultural purposes is placing greater emphasis on the development of ground water resources. The exploitation of ground water resources at some parts of the country induces degradation of groundwater quality as well as the discharge of untreated effluents which add contaminants to the groundwater system. In recent years considerable interest and attention have been directed to dispersion phenomenon in flow through porous media.

The solutions of one, two and three-dimensional deterministic advection-dispersion equation have been investigated in numerous publications before and are still actively studied. [4] and its cited references there have documented many previously derived analytical solutions with different initial and boundary conditions. [2] have developed an analytical solutions of contaminant transport from one, two, three-dimensional finite sources in a finite-thickness aquifer using Green's function method. For simulating most field problems, the mathematical benefits of obtaining an exact analytical are probably out weighted by errors introduced by simplifying approximations of the complex field environment that are required to apply the analytical approach ([1] ,[3],[5]).

Not many analytical solutions are available for two and three-dimensional problems even through the numerical solutions exist. In spite of difficulties in obtaining solution for two and three-dimensional cases, in the present study, we have developed a mathematical model for one-dimensional flow assuming linear retardation, a zero order sink/source term, a first-order production/decay term, and using first and third type boundary conditions at the inlet. The governing partial differential equations are by applying Laplace transforms with respect to z and t; Fourier transforms with respect to x and y for a Cartesian coordinate system. The solute concentration in the real space and time domain is obtained by solving the ensuing algebraic equation and applying appropriate inverse integral transforms.

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2 MATHEMATICAL FORMULATION

We consider one-dimensional unsteady flow through the semi-infinite unsaturated porous media in the x-z plane in the presence of a toxic material. The uniform flow is in the z-direction. The medium is assumed to be isotropic and homogeneous so that all physical quantities are assumed to be constant. Initially the concentration of strength C_0 exists at the surface. The velocity of the groundwater is assumed to be constant. With these assumptions the basic equation governing the flow is

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial z}\left(D\frac{\partial C}{\partial z}\right)-\omega\frac{\partial C}{\partial z}-\frac{\rho}{\theta}\frac{\partial S}{\partial t} \quad (1)$$

where C is the constituent concentration in the soil solution, t is the time, S is the adsorbed constituent concentration, D is the hydrodynamic dispersion coefficient, z is the depth, ω is the average pore-water velocity, θ is the soil water content fraction and ρ is the bulk density of soil.

The first term on the right hand side of equation (1) represents the change in concentration due to hydrodynamic dispersion while the second term gives the effect of advective transport and the last term represents source/sink term i.e., chemical reaction or radioactive decay. The physical system assumes constant application of a Leachate constituent of concentration C_0 to the soil surface or large sources of wastes in a landfill that release a given constituent to the soil water system at a concentration.The third term on the right hand side of equation (1) represents adsorption.An equilibrium adsorption state will be assumed with a linear relationship between solution and adsorbed phases and this can be expressed as

$$S=K_d C \quad (2)$$

Where K_d is the partition or distribution coefficient. The distribution coefficient is expressed as the ratio of solute concentration on the adsorbent to solute aqueous concentration at equilibrium.

Differentiating equation (2) with respect to time and substituting it into (1) and rearranging, we get

$$R\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial z^2}-\omega\frac{\partial C}{\partial z} \quad (3)$$

Where $R=\left(1+\rho/\theta\ K_d\right)$ is called the coefficient of retardation. When no adsorption occurs (K_d = 0) the relation factor R reduces to unity. Then the advection-dispersion equation (3) can be written as

$$\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial z^2}-\omega\frac{\partial C}{\partial z} \quad (4)$$

Equation (4) with its auxiliary conditions is an appropriate mathematical model of the physical problem. The problem is solved when a unique C(z,t) is found that satisfies equation (4) and its auxiliary conditions. There are several well-known analytical and numerical methods for solving the mathematical model. However, an alternative formulation of the problem is possible with the aid of the calculus of variations. An extremum problem replaces the given differential equation. A functional is found such that the extremum function also satisfies the given differential equation and its auxiliary conditions. A necessary condition that an extremum function exists is that the function satisfies the Euler equation. In practice the natural boundary conditions of the problem are only approximately satisfied with no loss in the validity of the solution.

Initially saturated flow of fluid of concentration C = 0, takes place in the medium. At t = 0, the concentration of the plane source is instantaneously changed to C = C_0 Then the initial and boundary conditions for a semi-infinite column and for a step input are

$$C(z,0)=0: z\geq 0, C(0,t)=C_0: t\geq 0, C(\infty,t)=0: t\geq 0 \quad (5)$$

The physical meaning of the boundary conditions corresponds to a situation where a soluble constituent in leachate is continually supplied to the soil surfaces which do not contain the material initially. The chemical process represents irreversible adsorption precipitation and/or changes in the chemical state of the constituent being described.

Equation (5) is a concentration type initial and boundary condition. However, use of a different boundary condition, such as a flux-type boundary condition should have little effect on the final results. For uniform soils, value of value of hydrodynamic dispersion coefficient D and average velocity ω may be estimated by matching values of the relative concentration measured at specific depths as a function of time.

For layered soil, values for D and ω may be estimated by matching observed concentration vs time distributions at specific soil depths with those obtained for a numerical model which allow for depth dependent values of D, θ and ω .To reduce equation (4) to a more familiar form, we take

$$C(z,t) = \Gamma(z,t)\exp\left[\frac{\omega z}{2D} - \frac{\omega^2 t}{4D}\right] \quad (6)$$

Substitution of equation (6) reduced equation (4) to Fick's law of diffusion equation

$$\frac{\partial \Gamma}{\partial t} = D\frac{\partial^2 \Gamma}{\partial z^2} \quad (7)$$

The above initial and boundary conditions (5) transform to

$$\Gamma(0,t) = C_0 \exp\left(\frac{\omega^2 t}{4D}\right) : t \ge 0, \Gamma(z,0) = 0 : z \ge 0, \Gamma(\infty,t) = 0 : t \ge 0 \quad (8)$$

It is thus required that equation (7) can be solved for a time dependent influx of fluid at z=0. The solution of equation (7) can be obtained by using Duhamel's theorem.

If C=F(x,y,z,t) is the solution of differential 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 $\varphi(t)$ is

$$C = \int_0^t \varphi(\tau)\frac{\partial}{\partial t}F(x,y,z,t-\tau)\,d\tau \quad (9)$$

This theorem is used principally for heat conduction problem, but the above has been specified to fit this specific case of interest.

Let us consider the problem in which the initial concentration is zero and the boundary is maintained at concentration unity. the boundary conditions are

$$\Gamma(z,0) = 0 \ : z \ge 0, \Gamma(0,t) = 1 : t \ge 0, \Gamma(\infty,t) = 0 : t \ge 0 \quad (10)$$

This problem can be solved by the application of the Laplace transform. The concentration Γ which is a function of t and whatever space coordinates, say z, t, occur in the problem. We write

$$L\{\Gamma(z,t)\} = \overline{\Gamma}(z,p) = \int_0^\infty e^{-pt}\,\Gamma(z,t)\,dt \quad (11)$$

where p is a number whose real part is positive and large enough to make the integral (4) convergent.

By applying Laplace transformation (11) to equation (7), that is, multiplied by e^{-pt} and integrate with respect to t from 0 to ∞.Then the partial differential equation (7) is reduced to the ordinary differential equation below. The equation for $\overline{\Gamma}$ derived in this way we shall always refer to as the 'subsidiary equation'. When the subsidiary equation has been solved with the boundary conditions, the Laplace transform $\overline{\Gamma}$ of the solution of the problem is known. Before proceeding to the method of finding Γ from $\overline{\Gamma}$ it may be remarked that more general differential equation and more general boundary conditions lead in precisely the same way to an ordinary differential equation with boundary conditions at a and b, and hence to the value of $\overline{\Gamma}$.

If there is more one space variable, for example, if the general differential equation

$$\nabla^2\overline{\Gamma} - \frac{1}{D}\frac{\partial\overline{\Gamma}}{\partial t} = 0 \quad (12)$$

has to be solved in some region with initial and boundary conditions then the subsidiary equation will be

$$\frac{d^2\overline{\Gamma}}{dz^2} = \frac{p}{D}\overline{\Gamma} \quad (13)$$

The solution of equation can be written as $\overline{\Gamma} = Ae^{-qz} + Be^{+qz}$

where $q = \sqrt{\frac{p}{D}}$

The boundary condition as $z \to \infty$ requires that B=0 and boundary conditions at z=0 requires that A=1/p, thus the particular solution of the Laplace transform equation is

$$\overline{\Gamma} = \frac{1}{p}e^{-qz} \quad (14)$$

If the transformation $\overline{\Gamma}$ does not appear in the table, we determine Γ from $\overline{\Gamma}$ by the use of the Inversion theorem for the Laplace transformation. This states that

$$\Gamma(t) = \frac{1}{2\pi i}\int_{\gamma - i\infty}^{\gamma + i\infty} e^{kt}\Gamma(k)\,dk \quad (15)$$

Where γ is to be large that all the singularities of $\overline{\Gamma}$ (k) lie to the left of the line ($\gamma - i\infty$, $\gamma + i\infty$). k is written in place of p in equation (13) to emphasise the fact that in equation (15) we are considering the behaviour of $\overline{\Gamma}$ regarded as a function of a complex variable, while in the previous discussion p need not have been complex at all. Then the inversion of the above function is given by the table of Laplace transform .Equation (14) can be written in the form of Complementary Error Function (erfc). The error function to the probability integral is defined as

$$erf\left(z\right)=\frac{2}{\sqrt{\pi}}\int_{0}^{z}e^{-\eta^2}d\eta \qquad (16)$$

This integral arises in the solution of certain partial differential equations of applied mathematics and occupies an important position in the probability theory. The complementary error function erfc(z) is defined as

$$erfc\;(z)=1-erf\,(z)=\frac{2}{\sqrt{\pi}}\int_{z}^{\infty}e^{-\eta^2}d\eta \qquad (17)$$

then the equation (15) can be written in the form of complimentary error function,then the above result will be

$$\Gamma=1-erf\left(\frac{z}{2\sqrt{Dt}}\right)=\frac{2}{\sqrt{\pi}}\int_{z/2\sqrt{Dt}}^{\infty}e^{-\eta^2}d\eta \qquad (18)$$

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

$$\Gamma=\int_{0}^{t}\phi(\tau)\frac{\partial}{\partial t}F(z,t-\tau)d\tau \qquad (19)$$

Where

$$\Gamma(z,t-\tau)=\frac{2}{\sqrt{\pi}}\int_{z/2\sqrt{D(t-\tau)}}^{\infty}e^{-\eta^2}d\eta \qquad (20)$$

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

$$\frac{2}{\sqrt{\pi}}\frac{\partial}{\partial t}\int_{\frac{z}{2\sqrt{D(t-\tau)}}}^{\infty}e^{-\eta^2}d\eta=\frac{z}{2\sqrt{\pi D}(t-\tau)^{3/2}}\exp\left[\frac{-z^2}{4D(t-\tau)}\right] \qquad (21)$$

The solution to the problem is

$$\Gamma=\frac{z}{2\sqrt{\pi D}}\int_{0}^{t}\varphi(t)\exp\left[\frac{-z^2}{4D(t-\tau)}\right]\frac{d\tau}{(t-\tau)^{3/2}} \qquad (22)$$

putting

$$\mu=\frac{z}{2\sqrt{D(t-\tau)}} \qquad (23)$$

then the equation(21) can be written as

$$\Gamma=\frac{2}{\sqrt{\pi}}\int_{\frac{z}{2\sqrt{Dt}}}^{\infty}\varphi\left(t-\frac{z^2}{4D\mu^2}\right)e^{-\mu^2}d\mu \qquad (24)$$

By taking boundary condition as, $\phi(t)=C_0\exp\left(\frac{\omega^2 t}{4D}\right)$ the particular solution of the problem can be written as

$$\Gamma=\frac{2C_0}{\sqrt{\pi}}\exp\left[\frac{\omega^2 t}{4D}\right]\int_{z/2\sqrt{Dt}}^{\infty}\exp\left[-\mu^2-\frac{\varepsilon^2}{\mu^2}\right]d\mu \qquad (25)$$

Then the above equation can be written by changing the integral limits as

$$\Gamma(z,t)=\frac{2C_0}{\sqrt{\pi}}\exp\left[\frac{w^2 t}{4D}\right]\left\{\int_{0}^{\infty}\exp\left[-\mu^2-\frac{\varepsilon^2}{\mu^2}\right]d\mu-\int_{0}^{\alpha}\exp\left[-\mu^2-\frac{\varepsilon^2}{\mu^2}\right]d\mu\right\} \qquad (26)$$

Evaluation of the Integral Solution

The integration of the first term of the equation (25) gives

$$\int_{0}^{\infty}\exp\left[-\mu^2-\frac{\varepsilon^2}{\mu^2}\right]d\mu=\frac{\sqrt{\pi}}{2}e^{-2\varepsilon} \qquad (27)$$

For convenience the second integral can be expressed in terms of error function, because this function is well tabulated.

Noting that

$$-\mu^2-\frac{\varepsilon^2}{\mu^2}=-\left(\mu+\frac{\varepsilon}{\mu}\right)^2+2\varepsilon=-\left(\mu-\frac{\varepsilon}{\mu}\right)^2-2\varepsilon \qquad (28)$$

The second integral of equation can be written as

$$I=\int_{0}^{\alpha}\exp\left[-\mu^2-\frac{\varepsilon^2}{\mu^2}\right]d\mu$$
$$=\frac{1}{2}\left\{e^{2\varepsilon}\int_{0}^{\alpha}\exp\left[-\left(\mu+\frac{\varepsilon}{\mu}\right)^2\right]d\mu+e^{-2\varepsilon}\int_{0}^{\alpha}\exp\left[-\left(\mu-\frac{\varepsilon}{\mu}\right)^2\right]d\mu\right\} \qquad (29)$$

Since the method of reducing to a tabulated function is the same for both the integrals on the right side of equation (27) only first term is considered. Let $\alpha=\frac{\varepsilon}{\mu}$ adding and subtracting we get

$$e^{2\varepsilon}\int_{\varepsilon/\alpha}^{\infty}\exp\left[-\left(\frac{\varepsilon}{a}+a\right)^2\right]da \quad (30)$$

The integral can be expressed as

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

$$e^{2\varepsilon}\int_{\varepsilon/\alpha}^{\infty}\exp\left[-\left(\frac{\varepsilon}{a}+a\right)^2\right]da \quad (31)$$

Further, let $\beta=\left(\frac{\varepsilon}{a}+a\right)$ in the first term of the above equation, then

$$I_1=-e^{2\varepsilon}\int_{\alpha+\frac{\varepsilon}{\alpha}}^{\infty}e^{-\beta^2}d\beta+e^{2\varepsilon}\int_{\frac{\varepsilon}{2}}^{\infty}\exp\left[-\left(\frac{\varepsilon}{a}+a\right)^2\right]da \quad (32)$$

Similarly, the second integral of equation (27) reduces to

$$I_2=-e^{2\varepsilon}\int_{\frac{\varepsilon}{\alpha}}^{\alpha}\exp\left[-\left(\frac{\varepsilon}{a}-a\right)^2\right]da-e^{2\varepsilon}\int_{\frac{\varepsilon}{\alpha}}^{\alpha}\exp\left[-\left(\frac{\varepsilon}{a}-a\right)^2\right]da \quad (33)$$

Again substituting $-\beta=\left(\frac{\varepsilon}{a}-a\right)$ in to the first term, then the above equation reduces to

$$I_2=e^{2\varepsilon}\int_{\frac{\varepsilon}{\alpha}-\alpha}^{\infty}e^{-\beta^2}d\beta-e^{2\varepsilon}\int_{\frac{\varepsilon}{\alpha}}^{\alpha}\exp\left[-\left(\frac{\varepsilon}{a}-a\right)^2\right]da \quad (34)$$

Noting that

$$\int_{\frac{\varepsilon}{\alpha}}^{\alpha}\exp\left[-\left(\frac{\varepsilon}{a}+a\right)^2+2\varepsilon\right]da=\int_{\frac{\varepsilon}{\alpha}}^{\alpha}\exp\left[-\left(\frac{\varepsilon}{a}-a\right)^2-2\varepsilon\right]da \quad (35)$$

Substituting this in to equation (27) gives

$$I=e^{-2\varepsilon}\int_{\frac{\varepsilon}{\alpha}-\alpha}^{\infty}e^{-\beta^2}d\beta-e^{2\varepsilon}\int_{\frac{\varepsilon}{2}+\alpha}^{\infty}e^{-\beta^2}d\beta \quad (36)$$

Equation (26) can be expressed as

$$\Gamma(z,t)=\frac{2C_0}{\sqrt{\pi}}\exp\left[\frac{w^2t}{4D}\right]\left\{\frac{\sqrt{\pi}}{2}e^{-2\varepsilon}-\frac{1}{2}\left[e^{-2\varepsilon}\int_{\frac{\varepsilon}{\alpha}-\alpha}^{\infty}e^{-\beta^2}d\beta-e^{2\varepsilon}\int_{\frac{\varepsilon}{\alpha}+\alpha}^{\infty}e^{-\beta^2}d\beta\right]\right\} \quad (37)$$

However, by definition

$$e^{2\varepsilon}\int_{\alpha+\frac{\varepsilon}{\alpha}}^{\infty}e^{-\beta^2}d\beta=\frac{\sqrt{\pi}}{2}e^{2\varepsilon}\left[1+erf\left(\alpha+\frac{\varepsilon}{\alpha}\right)\right]=\frac{\sqrt{\pi}}{2}e^{2\varepsilon}erfc\left(\alpha+\frac{\varepsilon}{\alpha}\right) \quad (38)$$

$$e^{2\varepsilon}\int_{\frac{\varepsilon}{\alpha}-\alpha}^{\infty}e^{-\beta^2}d\beta=\frac{\sqrt{\pi}}{2}e^{-2\varepsilon}\left[1+erf\left(\alpha-\frac{\varepsilon}{\alpha}\right)\right]=\frac{\sqrt{\pi}}{2}e^{-2\varepsilon}erfc\left(\alpha-\frac{\varepsilon}{\alpha}\right) \quad (39)$$

Writing equation (37) in terms of error function, we get

$$\Gamma(z,t)=\frac{C_0}{2}\exp\left(\frac{\omega^2t}{4D}\right)\left[e^{2\varepsilon}erfc\left(\alpha+\frac{\varepsilon}{\alpha}\right)+e^{-2\varepsilon}erfc\left(\alpha-\frac{\varepsilon}{\alpha}\right)\right] \quad (40)$$

Substituting the value of $\Gamma(z,t)$ is equation then the solution reduces to

$$\frac{C}{C_0}=\frac{1}{2}\exp\left(\frac{\omega z}{2D}\right)\left[e^{2\varepsilon}erfc\left(\alpha+\frac{\varepsilon}{\alpha}\right)+e^{-2\varepsilon}erfc\left(\alpha-\frac{\varepsilon}{\alpha}\right)\right] \quad (41)$$

Resubstituting the value of ε and α gives

$$\frac{C}{C_0}=\frac{1}{2}\exp\left(\frac{\omega z}{2D}\right)\left\{\exp\left[\frac{\sqrt{\omega^2+4D}}{2D}z\right]erfc\left(\frac{z+\sqrt{\omega^2+4D}}{2\sqrt{Dt}}t\right)+\right.$$

$$\left.\exp\left[-\frac{\sqrt{\omega^2+4D}}{2D}z\right]erfc\left(\frac{z-\sqrt{\omega^2+4D}}{2\sqrt{Dt}}t\right)\right\} \quad (42)$$

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

Mathematical models have been developed for predicting the possible concentration of a given dissolved substance in steady unidirectional seepage flows through semi-infinite, homogeneous, and isotropic porous media subject to source concentrations that vary exponentially with time.

3 DISCUSSION OF RESULTS AND CONCLUSION

The water eventually enters the groundwater storage basin (aquifer)- a source for potable water. During the passage of water through the soil, the pollutants are mixed, 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 mixing takes place in the soil medium by two processes, viz., molecular diffusion and dispersion. Molecular diffusion is a physical process, which depends upon the kinetic properties of the fluid particles and cause mixing at the contact front between the two fluids. Dispersion, however, is defined as mechanical mixing process caused by the tortuous path followed by the fluid flowing in the geometrically complex interconnections of the flow channels and by the variations in equations solute transport are solved analytically and numerically. An analytical solution for one-dimensional model is obtained using Laplace transformation techniques.

To estimate the magnitude of the hazard posed by some of these chemicals, it is important to investigate the processes that control their movement from the soil surface through the root zone down to the groundwater table. At present, major thrust on the transport of contaminant and research is directed towards the definition and qualification of the process governing the behaviour of pollutants in sub surface environment, coupled with the development of mathematical models that integrate process descriptions with the pollutant properties and site characteristics.

The main limitations of the analytical method 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 or at least homogeneous in the sub region. The analytical method is somewhat more flexible than the standard form of other methods for one-dimensional transport model.

From the equation (42), C/C_0 was numerically computed using 'Mathematica' software. With an increase in most of the contaminants get absorbed by the solid surface and thereby retarding the movements of the contaminants as evident from the graphs. Most of the contaminants are attenuated in the unsaturated zone itself and thus the threat or groundwater being contaminated is minimized.

we conclude that the solute transport in semi-infinite homogeneous porous media is modelled analytically for one-dimensional flow assuming linear retardation, a zero order sink/source term, a first-order production/decay term, and using first and third-type boundary conditions at the inlet. The governing partial differential equation is solved in a straightforward manner for general inlet solute distributions by applying Laplace transform with respect to z and t.

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