

Mathematical Modelling of Transport of Pollutants of Longitudinal Dispersion in Unsaturated Porous Media

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Abstract- In order to understand the behavior of contaminant transport through different types of media, several researchers are carrying out experimental investigations through laboratory and field studies. Many of them are working on the analytical and numerical studies to simulate the movement of contaminants in soil and groundwater of the contaminant transport. A key to the management of groundwater is the ability to model the movement of fluids and contaminants in the subsurface environment. It is obvious that the contaminant source activities cannot be completely eliminated and perhaps our water bodies will continue to serve as receptors of vast quantities of waste. 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 using Laplace transform, moving coordinates and Duhamel's theorem is used to get the solution in terms of complementary error function.

Indexed Terms- Advection, dispersion, adsorption, Integral transforms, Fick's law, Moving coordinates, Duhamel's theorem

I. INTRODUCTION

The advection-dispersion equation is a partial differential equation and it is derived on the principle of conservation of mass using Fick's law, which is of parabolic in nature. For getting the analytical solutions the approach is to reduce the advection-dispersion equation into a diffusion equation by eliminating the convective term. This can be done by either introducing the moving coordinates of by including

another dependent variable. To get the desired result it can be made use of Laplace transforms technique.

II. MATHEMATICAL FORMULATION AND MODEL

The basic governing equation of the flow is

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial z^2} - u \frac{\partial C}{\partial z} \quad (1)$$

Basically, fluid concentration along the saturated flow, $C = 0$, carries in the medium. Later at $t = 0$, the concentration is changed to $C = C_0$. For a semi-infinite column the initial and boundary conditions (Fig.1) are

$$\left. \begin{aligned} C(z, 0) &= 0; & z &\geq 0 \\ C(0, t) &= C_0; & t &\geq 0 \\ C(\infty, t) &= 0; & t &\geq 0 \end{aligned} \right\} \quad (2)$$

Now, let

$$C(z, t) = \Gamma(z, t) \exp \left[\frac{uz}{2D} - \frac{u^2 t}{4D} - t \right] \quad (3)$$

Put equation (3) in equation (1), reduces to Fick's law of diffusion equation

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

The conditions (2) becomes

$$\left. \begin{aligned} \Gamma(0, t) &= C_0 \exp\left(\frac{u^2 t}{4D}\right); & t \geq 0 \\ C(z, 0) &= 0; & z \geq 0 \\ C(\infty, t) &= 0; & t \geq 0 \end{aligned} \right\} \quad (5)$$

For semi-infinite medium, the temperature $\phi(t)$ is

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

Now consider the model with the boundary conditions

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

We write

$$\bar{\Gamma}(z, p) = \int_0^\infty e^{-pt} \Gamma(z, t) dt$$

Now, if the equation (4) is multiplied by e^{-pt}

$$\frac{d^2 \bar{\Gamma}}{dz^2} = \frac{p}{D} \bar{\Gamma} \quad (6)$$

The solution is,

$$\bar{\Gamma} = A e^{-qz} + B e^{qz}$$

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

then,

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

Using the table of Laplace transforms to find the inverse of the above function (Carslaw and Jaeger, 1947). The result is

$$\Gamma = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = \frac{2}{\sqrt{\pi}} \int_{\frac{z}{2\sqrt{Dt}}}^\infty e^{-\eta^2} d\eta. \quad (7)$$

With the initial concentration 0 and time at $z = 0$ the solution of the problem using Duhamel's theorem is

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

using Leibnitz rule we have

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

Now the solution is

$$\Gamma(z, t) = \frac{2C_0}{\sqrt{\pi}} e^{\left(\frac{u^2}{4D}\right)t} \left\{ \int_0^\infty \exp\left(-\mu^2 - \frac{\varepsilon^2}{\mu^2}\right) d\mu - \int_0^\alpha \exp\left(-\mu^2 - \frac{\varepsilon^2}{\mu^2}\right) d\mu \right\} \quad (9)$$

Where

$$\varepsilon = \sqrt{\left(\frac{u^2}{4D}\right)} \frac{z}{2\sqrt{D}}$$

And

$$\alpha = \frac{z}{2\sqrt{Dt}}$$

III. EVALUATION OF INTEGRAL SOLUTION

In the equation (9) the integration of first term reduces to (Pierce, 1956)

$$\Gamma = \frac{z}{\pi\sqrt{D}} \int_0^t \phi(\tau) e^{-z^2/4D(t-\tau)} \frac{d\tau}{(t-\tau)^{3/2}}$$

Letting

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

the solution is

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

Since

$$\phi(t) = C_0 \exp\left(\frac{u^2 t}{4D} + t\right)$$

$$\int_0^{\infty} e^{-\mu^2 - \frac{\varepsilon^2}{\mu^2}} d\lambda = \frac{\sqrt{\pi}}{2} e^{-2\varepsilon}$$

Expressing second term as an error function (Horenstein, 1945),

$$\begin{aligned} -\mu^2 - \frac{\varepsilon^2}{\mu^2} &= -\left(\mu + \frac{\varepsilon}{\mu}\right)^2 + 2\varepsilon \\ &= -\left(\mu - \frac{\varepsilon}{\mu}\right)^2 - 2\varepsilon \end{aligned}$$

Now the integral of second term of equation (9) can be put as

$$I = \int_0^{\frac{\varepsilon}{\alpha}} \exp\left(-\mu^2 - \frac{\varepsilon^2}{\mu^2}\right) d\mu = \frac{1}{2} \left\{ e^{2\varepsilon} \int_0^{\frac{\varepsilon}{\alpha}} \exp\left[-\left(\mu + \frac{\varepsilon}{\mu}\right)^2\right] d\mu + e^{-2\varepsilon} \int_0^{\frac{\varepsilon}{\alpha}} \exp\left[-\left(\mu - \frac{\varepsilon}{\mu}\right)^2\right] d\mu \right\} \quad (10)$$

Let $a = \frac{\varepsilon}{\mu}$

Adding and subtracting the above term, we get

$$\begin{aligned} &e^{2\varepsilon} \int_{\frac{\varepsilon}{\alpha}}^{\infty} \exp\left[-\left(a + \frac{\varepsilon}{a}\right)^2\right] da \\ &= -e^{2\varepsilon} \int_{\frac{\varepsilon}{\alpha}}^{\infty} \left(1 - \frac{\varepsilon}{a^2}\right) \cdot \exp\left[-\left(\frac{\varepsilon}{a} + a\right)^2\right] da + e^{2\varepsilon} \int_{\frac{\varepsilon}{\alpha}}^{\infty} \exp\left[-\left(\frac{\varepsilon}{a} + a\right)^2\right] da \end{aligned}$$

further,

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

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

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

Making a note that

Now the integral can be expressed as

$$I = e^{2\varepsilon} \int_0^{\alpha} \exp\left[-\left(\mu + \frac{\varepsilon}{\mu}\right)^2\right] d\mu =$$

Substituting in the first term we have.

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

Substituting this into equation (10) which gives

$$I = e^{-2\varepsilon} \int_{\frac{\varepsilon}{\alpha} - \alpha}^{\infty} e^{-\beta^2} d\beta - e^{2\varepsilon} \int_{\frac{\varepsilon}{\alpha}}^{\infty} e^{-\beta^2} d\beta$$

Thus,

$$\Gamma(z, t) = \frac{2C_0}{\sqrt{\pi}} e^{\left(\frac{u^2}{4D}\right)t} \left\{ \frac{\sqrt{\pi}}{2} e^{-2\varepsilon} - \frac{1}{2} \left[e^{-2\varepsilon} \int_{\frac{\varepsilon}{\alpha} - \alpha}^{\infty} e^{-\beta^2} d\beta - e^{2\varepsilon} \int_{\frac{\varepsilon}{\alpha}}^{\infty} e^{-\beta^2} d\beta \right] \right\} \quad (11)$$

by definition

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

also,

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

Equation (11) reduces to,

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

Substituting the value of $\Gamma(z, t)$ in equation (3) the solution reduces to

$$\frac{C}{C_0} = \frac{1}{2} \exp \left[\frac{uz}{2D} \right] \left[e^{2\varepsilon} \operatorname{erfc} \left(\alpha + \frac{\varepsilon}{\alpha} \right) + e^{-2\varepsilon} \operatorname{erfc} \left(\alpha - \frac{\varepsilon}{\alpha} \right) \right] \quad (12)$$

Reconstituting the value of ε and α gives

$$\begin{aligned} \frac{C}{C_0} = & \frac{1}{2} \exp \left[\frac{uz}{2D} \right] \left[\exp \left[\frac{\sqrt{u^2 + 4D}}{2D} z \right] \cdot \operatorname{erfc} \left(\frac{z + \sqrt{u^2 + 4D}}{2\sqrt{Dt}} t \right) \right. \\ & \left. + \exp \left[-\frac{\sqrt{u^2 + 4D}}{2D} z \right] \cdot \operatorname{erfc} \left(\frac{z - \sqrt{u^2 + 4D}}{2\sqrt{Dt}} t \right) \right] \quad (13) \end{aligned}$$

The first and second terms are asymmetric in the above solution. It is possible to obtain the symmetrical solution by considering the boundary conditions $C(-\infty, t) = C_0$, with a long distance away from the source.

IV. RESULTS AND CONCLUSIONS

The important limitation for the analytical methods are that applications for a relatively simple problems. For one-dimensional transport model, analytical method is more convenient than the other standard methods. Figures 1 to 4 represents the concentration profiles against distance along the media for different values of porosity n . It is seen that for a fixed velocity w , dispersion coefficient D , $\frac{C}{C_0}$ decreases with depth as porosity n , whereas concentration profile versus time for different values of depth z . For a fixed z it is seen that because of lesser effect of dispersion coefficient D , the concentration increases at the

beginning and attains a steady-state value for greater time. Hence we conclude that by these solutions using integral transform we can find the steady-state concentration distributions and temporal moments. Likewise the transient concentration distribution is accessible through numerical inversions.

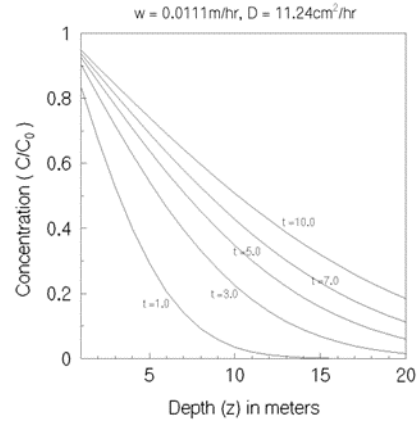


Fig. 1

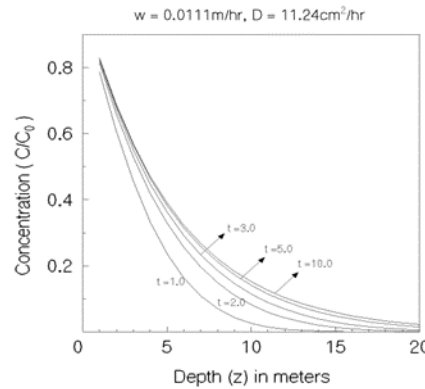


Fig. 2

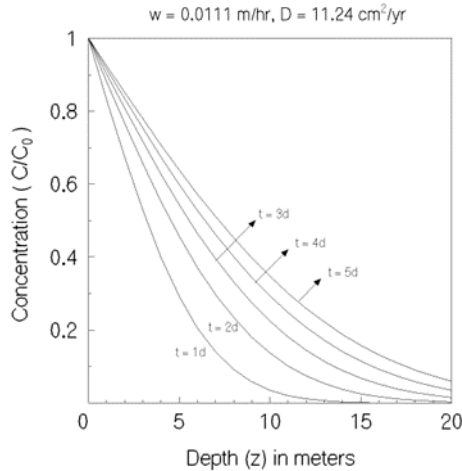


Fig. 3

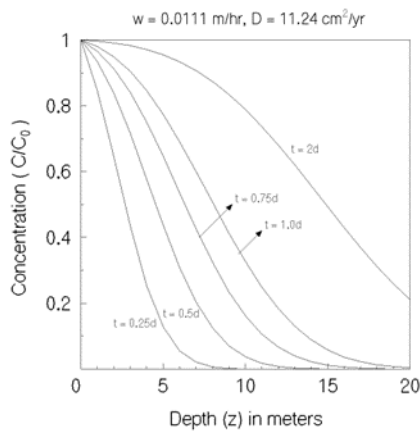


Fig. 4

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