MATHEMATICAL MODELLING OF CONCENTRATION DISTRIBUTION IN MISCIBLE FLUID FLOW THROUGH POROUS MEDIA

Vijayalakshmi A.R.
Department of Mathematics, Maharani's Science College for Women,
Palace Road, Bengaluru – 560 001. E-mail: drarv@rediffmail.com

Abstract

The present study is concerned with the development of analytical models for distribution in miscible fluid flow through porous media. The advection-dispersion equation is solved using Laplace-transform and Duhamel's theorem with appropriate initial and boundary condition. It is concluded that the concentration distribution of miscible fluids decreases with time.

Key words: Miscible fluid flow, porous media, advection-dispersion equation, Laplace transform, Duhamel's theorem

Introduction

Due to modern civilization, a large amount of waste is created which affects the ground water quality and results in ground water pollution. Among many flow problems in porous media, one involving fluid mixtures is called miscible fluids. A miscible fluid is a single phase fluid consisting of several completely dissolved homogenous fluid species, a distinct fluid-fluid interface doesn't exist in a miscible fluid. The study of miscible flow in porous media is important in oil recovery in petroleum engineering, contamination of ground water by waste product disposed , underground movement of mineral in the soil and recovery of spent liquors in pulping process. These problems of dispersion have been receiving considerable attention from chemical, environmental and petroleum engineers, hydrologists, mathematicians and soil scientists.

The solutions of one, two and three-dimensional deterministic advection-dispersion equation have been investigated in numerous publications before and are still actively studied. Wexler [6] and its cited references there have documented many previously derived analytical solutions with different initial and boundary conditions. Eungyu park and Hongbin Zhan [8] 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, 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, [4], Foussereau et al.,[5],Yates et al., [7]).

Most of the works have the assumption of homogenous porous media with constant porosity, steady seepage flow velocity and constant dispersion coefficient. Ebach and White [1] studied the longitudinal dispersion problem for an input concentration that varies periodically with time. Al-Niami and Rushton [2] studied the analysis of flow against dispersion in porous media. Hunt [3] applied the perturbation method to longitudinal and lateral dispersion in non uniform seepage flow through heterogeneous aquifers. Meher [10] and Mehta and Patel [9] studied the dispersion of miscible fluid in semi infinite porous media with unsteady velocity distribution. 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. This study is useful in examining how the flow regime may be optimized for enhanced oil recovery methods. Hendrata Wibisana et al. [12] studied the distribution value of total suspended solids and found that Landsat 8 satellite image can quite effectively and accurately be used to map the distribution of total suspended solid especially in the shallow water environment adjacent to ponds and estuary.

In this paper, the study is concerned with the development of analytical models for distribution in miscible fluid flow through confined and unconfined porous media.

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Mathematical Formulation

The one-dimensional advection-dispersion equation describing the concentration distribution of miscible fluids (contaminated or salt water with fresh water) flow in homogeneous porous media is given by

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

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

The above equation can be rewritten as

$$\frac{\partial C}{\partial t} = D_L\frac{\partial^2 C}{\partial z^2} - w_L\frac{\partial C}{\partial z} \qquad (2)$$

with $D_L = \frac{D}{R}$ and $w_L = \frac{w}{R}$, where $R = \left(1+\left(\frac{1-n}{n}\right)K_d\right)$ and K_d is the distribution coefficient.

Initially saturated flow of fluid of concentration $C = 0$ takes place in the porousmedia. At t = 0, the concentration of the plane source is instantaneously changed to C = C_0.

The boundary conditions for the given model are

$$\left.\begin{aligned} C(z,0) &= 0 \qquad && z \ge 0 \\ C(0,t) &= C_0 e^{-\gamma t} && t \ge 0 \\ C(\infty,t) &= 0 && t \ge 0 \end{aligned}\right\} \qquad (3)$$

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

$$C(z,t) = \Gamma(z,t)\exp\left[\frac{w_L z}{2D_L} - \frac{w_L^2 t}{4D_L}\right] \qquad (4)$$

Now equation (1) reduces to Fick's law of diffusion equation

$$\frac{\partial \Gamma}{\partial t} = D_L\frac{\partial^2 \Gamma}{\partial z^2} \qquad (5)$$

The above initial and boundary conditions (3) transform to

$$\left.\begin{aligned} \Gamma(0,t) &= C_0 \exp\left(\frac{w_L^2 t}{4D_L} - \gamma t\right) \qquad && t \ge 0 \\ \Gamma(z,0) &= 0 && z \ge 0 \\ \Gamma(\infty,t) &= 0 && t \ge 0 \end{aligned}\right\} \qquad (6)$$

The solution of equation (5) 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

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surface is maintained at unit concentration, then the solution of the problem in which the surface is maintained at temperature $\varphi(t)$ will be

$$C=\int_0^t \varphi(\tau)\frac{\partial}{\partial t}F(x,y,z,t-\tau)\,d\tau \tag{7}$$

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

$$\left.\begin{aligned}\Gamma(z,0)&=0 \quad z\geq 0\\ \Gamma(0,t)&=1 \quad t\geq 0\\ \Gamma(\infty,t)&=0 \quad t\geq 0\end{aligned}\right\} \tag{8}$$

This problem can be solved by using the Laplace transform defined by

$$L\{\Gamma(z,t)\}=\bar{\Gamma}(z,s)=\int_0^\infty e^{-st}\,\Gamma(z,t)\,dt \tag{9}$$

where s is a number whose real part is positive and large enough to make the above integral convergent.

By applying Laplace transformation equation (9), to equation (5) is reduced to the ordinary differential equation below. In this paper, the equation for $\bar{\Gamma}$ derived in this way is read as the 'subsidiary equation'. If there is one more space variable, for example, if the general differential equation

$$\nabla^2\bar{\Gamma}-\frac{1}{D_L}\frac{\partial\bar{\Gamma}}{\partial t}=0 \tag{10}$$

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

$$\frac{d^2\bar{\Gamma}}{dz^2}=\frac{s}{D_L}\bar{\Gamma} \tag{11}$$

whose solution can be written as $\bar{\Gamma}=Ae^{-qz}+Be^{+qz}$ where $q=\sqrt{\frac{s}{D_L}}$.

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

$$\bar{\Gamma}=\frac{1}{s}e^{-qz} \tag{12}$$

We determine Γ from $\bar{\Gamma}$ by the using the the Laplace inversion theorem which states that

$$\Gamma(t)=\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} e^{kt}\,\Gamma(k)\,dk \tag{13}$$

where γ is to be large so that all the singularities of $\bar{\Gamma}$ (k) lie to the left of the line ($\gamma-i\infty$, $\gamma+i\infty$). k is written in place of s in equation (13) to emphasise the fact that in equation (13) we are considering the behaviour of $\bar{\Gamma}$ regarded as a function of a complex variable, while in the previous discussion s need not have been complex at all. Equation (12) can be written in the form of complementary error function (erfc).

$$erfc(z)=1-erf(z)=\frac{2}{\sqrt{\pi}}\int_z^\infty e^{-\eta^2}\,d\eta \tag{14}$$

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Where, the error function to the probability integral is defined as

$$erf\,(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-\eta^2} d\eta \tag{15}$$

The equation (13) in terms of complimentary error function is

$$\Gamma = 1 - erf\left(\frac{z}{2\sqrt{D_L t}}\right) = \frac{2}{\sqrt{\pi}} \int_{z/2\sqrt{D_L t}}^{\infty} e^{-\eta^2} d\eta \tag{16}$$

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

$$\Gamma = \int_0^t \phi(\tau) \frac{\partial}{\partial t}\left[\frac{2}{\sqrt{\pi}} \int_{\frac{z}{2\sqrt{D_L t}}}^{\infty} e^{-\eta^2} d\eta\right] d\tau \tag{17}$$

Since $e^{-\eta^2}$ is a continuous function,

$$\frac{2}{\sqrt{\pi}} \frac{\partial}{\partial t} \int_{\frac{z}{2\sqrt{D_L(t-\tau)}}}^{\infty} e^{-\eta^2} d\eta = \frac{z}{2\sqrt{\pi D_L}\,(t-\tau)^{3/2}} \exp\left[\frac{-z^2}{4D_L(t-\tau)}\right] \tag{18}$$

The solution to the problem is

$$\Gamma = \frac{z}{2\sqrt{\pi D_L}} \int_0^t \varphi(t) \exp\left[\frac{-z^2}{4D_L(t-\tau)}\right] \frac{d\tau}{(t-\tau)^{3/2}} \tag{19}$$

By putting

$$\mu = \frac{z}{2\sqrt{D_L(t-\tau)}} \tag{20}$$

equation (18) can be written as

$$\Gamma = \frac{2}{\sqrt{\pi}} \int_{\frac{z}{2\sqrt{D_L t}}}^{\infty} \varphi\left(t - \frac{z^2}{4D_L \mu^2}\right) e^{-\mu^2} d\mu \tag{21}$$

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

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$$\Gamma = \frac{2C_0}{\sqrt{\pi}} \exp\left(\frac{w_L^2 t}{4D_L} - \gamma t\right) \int_{\frac{z}{2\sqrt{D_L t}}}^{\infty} \exp\left[-\mu^2 - \frac{\varepsilon^2}{\mu^2}\right] d\mu \qquad (22)$$

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

$$\Gamma(z,t) = \frac{2C_0}{\sqrt{\pi}} \exp\left(\frac{w_L^2 t}{4D_L} - \gamma t\right) \left\{ \int_0^{\infty} \exp\left[-\mu^2 - \frac{\varepsilon^2}{\mu^2}\right] d\mu - \int_0^{\alpha} \exp\left[-\mu^2 - \frac{\varepsilon^2}{\mu^2}\right] d\mu \right\} \qquad (23)$$

where $\varepsilon = \sqrt{\left(\frac{w_L^2}{4D_L} - \gamma\right) \frac{z}{2\sqrt{D_L}}}$ and $\alpha = \frac{z}{2\sqrt{D_L t}}$

The first integral of equation (23) can be written as

$$\int_0^{\infty} \exp\left(-\mu^2 - \frac{\varepsilon^2}{\mu^2}\right) d\mu = \frac{\sqrt{\pi}}{2} e^{-2\varepsilon} \qquad (24)$$

But

$$-\mu^2 - \frac{\varepsilon^2}{\mu^2} = -\left(\mu + \frac{\varepsilon}{\mu}\right)^2 + 2\varepsilon = -\left(\mu - \frac{\varepsilon}{\mu}\right)^2 - 2\varepsilon \qquad (25)$$

the second integral of equation (23) can be written as

$$I = \int_0^{\alpha} \exp\left[-\mu^2 - \frac{\varepsilon^2}{\mu^2}\right] d\mu = \frac{1}{2}\left\{ e^{2\varepsilon} \int_0^{\alpha} \exp\left[-\left(\mu + \frac{\varepsilon}{\mu}\right)^2\right] d\mu + e^{-2\varepsilon} \int_0^{\alpha} \exp\left[-\left(\mu - \frac{\varepsilon}{\mu}\right)^2\right] d\mu \right\} \qquad (26)$$

Since the method of reducing to a tabulated function is the same for both the integrals on the right side of equation (29) only first term is considered. Let $a = \frac{\varepsilon}{\mu}$.

The first integral of equation(26) can be written as

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

$$e^{2\varepsilon} \int_{\varepsilon/\alpha}^{\infty} \exp\left[-\left(\frac{\varepsilon}{a} + a\right)^2\right] da \qquad (27)$$

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

$$I_1 = -e^{2\varepsilon} \int_{\alpha+\frac{\varepsilon}{\alpha}}^{\infty} e^{-\beta^2} d\beta + e^{2\varepsilon} \int_{\frac{\varepsilon}{\alpha}}^{\infty} \exp\left[-\left(\frac{\varepsilon}{a} + a \right)^2 \right] da \tag{28}$$

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

$$I_2 = -e^{2\varepsilon} \int_{\frac{\varepsilon}{\alpha}}^{\alpha} \exp\left[-\left(\frac{\varepsilon}{a} - a \right)^2 \right] da - e^{2\varepsilon} \int_{\frac{\varepsilon}{\alpha}}^{\alpha} \exp\left[-\left(\frac{\varepsilon}{a} - a \right)^2 \right] da \tag{29}$$

Put $-\beta = \left(\frac{\varepsilon}{a} - a \right)$ in the first term in the above equation then equation (29) reduces to

$$I_2 = e^{2\varepsilon} \int_{\frac{\varepsilon}{\alpha}-\alpha}^{\infty} e^{-\beta^2} d\beta - e^{2\varepsilon} \int_{\frac{\varepsilon}{\alpha}}^{\alpha} \exp\left[-\left(\frac{\varepsilon}{a} - a \right)^2 \right] da \tag{30}$$

But

$$\int_{\frac{\varepsilon}{\alpha}}^{\alpha} \exp\left[-\left(\frac{\varepsilon}{a} + a \right)^2 + 2\varepsilon \right] da = \int_{\frac{\varepsilon}{\alpha}}^{\alpha} \exp\left[-\left(\frac{\varepsilon}{a} - a \right)^2 - 2\varepsilon \right] da \tag{31}$$

Equation (27) becomes

$$I = e^{-2\varepsilon} \int_{\frac{\varepsilon}{\alpha}-\alpha}^{\infty} e^{-\beta^2} d\beta - e^{2\varepsilon} \int_{\frac{\varepsilon}{2}+\alpha}^{\infty} e^{-\beta^2} d\beta \tag{32}$$

Equation (23) reduces to

$$\Gamma(z,t) = \frac{2C_0}{\sqrt{\pi}} \exp\left(\frac{\omega^2 t}{4D_L} - \gamma t \right) \left\{ \frac{\sqrt{\pi}}{2} e^{-2\varepsilon} - \frac{1}{2} \left[e^{-2\varepsilon} \int_{\frac{\varepsilon}{\alpha}-\alpha}^{\infty} e^{-\beta^2} d\beta - e^{2\varepsilon} \int_{\frac{\varepsilon}{\alpha}+\alpha}^{\infty} e^{-\beta^2} d\beta \right] \right\} \tag{33}$$

But, by definition

$$e^{2\varepsilon} \int_{\alpha+\frac{\varepsilon}{\alpha}}^{\infty} e^{-\beta^2} d\beta = \frac{\sqrt{\pi}}{2} e^{2\varepsilon} \left[1 + erf\left(\alpha + \frac{\varepsilon}{\alpha} \right) \right] = \frac{\sqrt{\pi}}{2} e^{2\varepsilon} erfc\left(\alpha + \frac{\varepsilon}{\alpha} \right) \tag{34}$$

$$e^{2\varepsilon} \int_{\frac{\varepsilon}{\alpha}-\alpha}^{\infty} e^{-\beta^2} d\beta = \frac{\sqrt{\pi}}{2} e^{-2\varepsilon} \left[1 + erf\left(\alpha - \frac{\varepsilon}{\alpha} \right) \right] = \frac{\sqrt{\pi}}{2} e^{-2\varepsilon} erfc\left(\alpha - \frac{\varepsilon}{\alpha} \right) \tag{35}$$

Writing equation (33) in terms of error function, we get

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$$\Gamma(z,t)=\frac{2C_0}{\sqrt{\pi}}\exp\left(\frac{\omega^2 t}{4D_L}-\gamma t\right)\left[e^{2\varepsilon}erfc\left(\alpha+\frac{\varepsilon}{\alpha}\right)+e^{-2\varepsilon}erfc\left(\alpha-\frac{\varepsilon}{\alpha}\right)\right] \qquad (36)$$

Substituting the value of $\Gamma(z,t)$ we get

$$\frac{C}{C_0}=\frac{1}{2}\exp\left(\frac{\omega^2 t}{4D_L}-\gamma t\right)\left[e^{2\varepsilon}erfc\left(\alpha+\frac{\varepsilon}{\alpha}\right)+e^{-2\varepsilon}erfc\left(\alpha-\frac{\varepsilon}{\alpha}\right)\right] \qquad (37)$$

Resubstituting the value of ε and α gives

$$\frac{C}{C_0}=\frac{1}{2}\left\{erfc\left(\frac{z+t\sqrt{w_L^2-4D_L\gamma}}{2\sqrt{D_L t}}\right)\exp\left[\frac{w_L t-2D_L\gamma t+z\sqrt{2w_L^2-4D_L\gamma}}{2D_L}z\right]+\right.$$
$$\left.erfc\left(\frac{z-t\sqrt{w_L^2-4D_L\gamma}}{2\sqrt{Dt}}\right)\exp\left[\frac{w_L t-2D_L\gamma t-z\sqrt{2w_L^2-4D_L\gamma}}{2D_L}z\right]\right\} \qquad (38)$$

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 due to the asymmetric boundary imposed in a general problem. If a point is far away from the source, then it is possible to approximate the boundary conditions by $C(-\infty,t)=C_0$, which leads to a symmetrical solution.

1. Results and discussion

Equation (38) gives the value of the ratio $\frac{C}{C_0}$ for the miscible fluid 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_L = 1.1 m/day, w_L = 1.60 m/day with respect to the dispersion coefficient D_L = 2.18 m²/day, D_L = 4.30 m²/day.

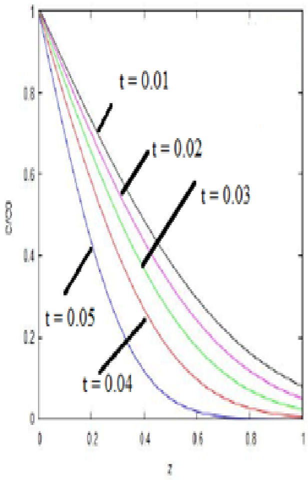

Fig 1. Break-through-curve for $\frac{C}{C_0}$ Vs depth for D_L = 2.18 m²/day and w_L =1.1 m/day

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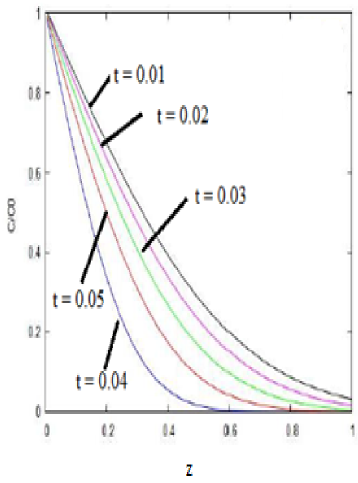

Fig 2. Break–through–curve for $\frac{C}{C_0}$ Vs depth for $D_L = 4.30$ m^2/day and w_L =1.60 m/day

There is a decrease in $\frac{C}{C_0}$ with depth as porosity n decreases due to the distributive coefficient Kd and if time increases the concentration decreases for different time.

Conclusion

This mathematical model depends on the physical phenomenon of the longitudinal dispersion of salt water or contaminated in porous medium. From the above graphs it can be seen that concentration of the miscible fluid decreases as the distance z and time t increases. Here we have used Laplace transform technique and Duhamel's principle to obtain analytical solution .The expressions obtained here are useful in making quantitative predictions on the possible contamination of groundwater supplies.

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