

Mathematical Modelling of Reactive Transport of Contaminants in Heterogeneous Flow of Saturated and Unsaturated Media

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Abstract— In this paper, an analytical first order solution to the one-dimensional advection-dispersion equation with adsorption term $C_0(1 - e^{-\gamma t})$ to study the transport of pollutant vary exponentially with time using a generalized integral transform method. In this chapter, we have investigated the transport of pollutant for adsorbing medium and non-adsorbing for reactive and non-reactive flow of saturated and unsaturated porous media. The solution is derived under conditions of steady-state flow and arbitrary initial and inlet boundary conditions using Duhamel's theorem and integral transform methods.

Keywords – Integral Transforms Method, Mathematical Modeling, Advection Dispersion Equation, Saturated porous media, unsaturated porous media, heterogeneous flow.

I. INTRODUCTION

In this study, the Advection Dispersion Equation has been resolved by using analytical methods to measure the solute transport of contaminants by considering the porosity and dissipation coefficient using input concentrations.

The Advection Dispersion Equation has been extensively used in simulation and modelling of reactive transference in groundwater. The convection-dispersion [Bear (1979), Gelhar (1973), Domenico (1998), Fetter (1999), Sudheendra (2010, 2011)] included hydrodynamic dispersion, advection, adsorption, first-order decay reaction, and possibly zeroth-order production.

Analytical solutions are generally derived from the basic physical principles and different from numerical dispersion. The other truncation errors usually occur in numerical simulations [Zheng and Bennett (1995)].

The solutions of one-dimensional Advection Dispersion Equation have been examined in many previously and are still actively studied. For example, Sauty (1980) and van Genuchten (1981), Sudheendra (2014) have been providing analytical solutions of the solute transference equation with the first, second and third type Boundary conditions. Yeh (1981) has given by analytical method and computer code for assessing the waste transportation in groundwater aquifers.

II MATHEMATICAL MODEL

The Advection Dispersion Equation along with Initial conditions and Boundary conditions can be written as

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

Consider a semi-infinite porous medium in a unidirectional flow field in which the input tracer concentration is $C_0(1 - e^{-\gamma t})$, where C_0 is a reference concentration and γ is a constant as show in the following figure (1).

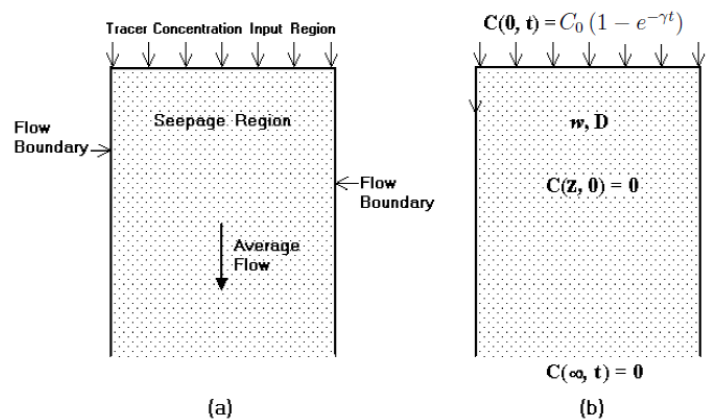


Figure 1: Schematic representation of semi-infinite porous medium in unidirectional flow field. Source concentrations is $C_0(1 - e^{-\gamma t})$

Hence, the suitable Boundary conditions for the given model

$$\left. \begin{aligned} C(z, 0) &= 0 & z \geq 0 \\ C(0, t) &= C_0(1 - e^{-\gamma t}) & t \geq 0 \\ C(\infty, t) &= 0 & t \geq 0 \end{aligned} \right\} \quad (2)$$

Then the problem is describe the concentration as a function of z and t , where the input condition is supposed at the source and a 2nd type condition is supposed. C_0 is initial

concentration. To reduce equation (3) in a more conversant form, we take

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

By substituting equation (3) in (1), we get

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

The Initial Conditions and Boundary conditions transform equation (2) to

$$\left. \begin{aligned} \Gamma(0, t) &= C_0 \text{Exp} \left[\frac{w^2t}{4D} + \frac{K_d(1-n)t}{n} - \gamma \right] & t \geq 0 \\ \Gamma(z, 0) &= 0 & z \geq 0 \\ \Gamma(\infty, t) &= 0 & t \geq 0 \end{aligned} \right\} \quad (5)$$

Equation (4) can be resolved for a time dependent arrival of the fluid at $z = 0$. The solution of equation (4) can be attained quickly by use of Duhamel's theorem, the same method already been used in the previous chapters.

The boundary conditions are

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

The Laplace Transform of equation (4) is

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

Later, it is reduced to an Ordinary Differential Equation

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

The resulting equation is $\bar{\Gamma} = A e^{-qz} + B e^{qz}$ where,

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

The Boundary conditions as $z \rightarrow \infty$ requires that $B = 0$ and

B C at $z = 0$ requires that $A = \frac{1}{p}$ thus the solution of the problem using Laplace transform method is

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

The inverse Laplace transform of the given function using the table. The result is

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

By Duhamel's theorem, the result of the problem with C_0 zero and the time dependent surface condition at $z = 0$ is

Since $e^{-\eta^2}$ is a constant function, , it becomes

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

The solution to the problem is

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

Putting $\mu = \frac{z}{2\sqrt{D(t-\tau)}}$ then the Equation (7)

becomes

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

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

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

Where, $\alpha = \frac{z}{2\sqrt{Dt}}$ and

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

III EVALUATION OF THE INTEGRAL SOLUTION

By integrating the 1st term of equation (9) we get

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

For convenience the 2nd integral can state in terms of the error function, thus the function was perfectly tabulated.

Observing that

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

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

The 2nd integral of equation (9) may be written as

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

Only by considering the 1st term of Equation. (11). Let

$a = \varepsilon/\mu$ and the integral can be stated as

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

Added, let, $\beta = \left(\frac{\varepsilon}{a} + a\right)$ in the $\beta = \frac{\varepsilon}{a} + a$ 1st term of the above Equation, then

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

Similar evaluation of the 2nd integral of Equation (11) gives

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

Again substituting $-\beta = \frac{\varepsilon}{a} - a$ into the 1st term, the solution is

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

Observing that

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

Substitute in equation (11) gives

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

Hence, equation (9) can be expressed as

$$\Gamma(z, t) = \frac{2C_0}{\sqrt{\pi}} \text{Exp}\left(\frac{w^2 t}{4D} + \frac{K_d(1-n)t}{n} - \gamma\right)$$

$$\left\{ \frac{\sqrt{\pi}}{2} e^{-2\varepsilon} - \frac{1}{2} \left[e^{-2\varepsilon} \int_{\alpha - \frac{\varepsilon}{\alpha}}^{\infty} e^{-\beta^2} d\beta - e^{2\varepsilon} \int_{\alpha + \frac{\varepsilon}{\alpha}}^{\infty} e^{-\beta^2} d\beta \right] \right\} \quad \dots\dots\dots(15)$$

But, by definition

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

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

Consider equation.(15) in terms of error functions, we have

$$\begin{aligned} \Gamma(z, t) &= \frac{C_0}{2} \text{Exp}\left(\frac{w^2 t}{4D} + \frac{K_d(1-n)t}{n} + \gamma\right) \\ &\left[e^{2\varepsilon} \text{erfc}\left(\alpha + \frac{\varepsilon}{\alpha}\right) + e^{-2\varepsilon} \text{erfc}\left(\alpha - \frac{\varepsilon}{\alpha}\right) \right] \quad \dots\dots\dots(16) \end{aligned}$$

By substituting this in equation (3) which gives

$$\frac{C}{C_0} = \frac{1}{2} \text{Exp}\left[\frac{wz}{2D} - \gamma\right] \left[\begin{aligned} &e^{-2\varepsilon} \text{erfc}\left(\alpha - \frac{\varepsilon}{\alpha}\right) \\ &+ e^{2\varepsilon} \text{erfc}\left(\alpha + \frac{\varepsilon}{\alpha}\right) \end{aligned} \right] \quad \dots\dots\dots(17)$$

Re-substituting for ε and α gives

IV ADSORBING MEDIUM:

$$\begin{aligned} C(z, t) &= \frac{C_0}{2} \left\{ \exp\left[\frac{z(w-\mu)}{2D}\right] \cdot \text{erfc}\left(\frac{z-\mu t}{2\sqrt{Dt}}\right) \right. \\ &+ \exp\left[\frac{z(w+\mu)}{2D}\right] \cdot \text{erfc}\left(\frac{z-\mu t}{2\sqrt{Dt}}\right) - \exp(-\gamma) \\ &\left. \left[\exp\left[\frac{z(w-\eta)}{2D}\right] \cdot \text{erfc}\left(\frac{z-\eta t}{2\sqrt{Dt}}\right) + \exp\left[\frac{z(w+\eta)}{2D}\right] \cdot \text{erfc}\left(\frac{z-\eta t}{2\sqrt{Dt}}\right) \right] \right\} \quad (18) \end{aligned}$$

in which

$$\mu = \left[\frac{w^2 n + 4D K_d(1-n)}{n} \right]^{\frac{1}{2}} \quad (19)$$

And

$$\eta = \left[\frac{w^2 n + 4D [K_d (1-n) - \gamma]}{n} \right]^{1/2} \quad (20)$$

$$C(z,t) = \frac{C_0}{2} \left\{ \operatorname{erfc} \left(\frac{z-wt}{2\sqrt{Dt}} \right) + \exp \left[\frac{wz}{D} \right] \cdot \operatorname{erfc} \left(\frac{z-wt}{2\sqrt{Dt}} \right) - \exp(-\gamma) \left[\exp \left[\frac{z(w-\xi)}{2D} \right] \cdot \operatorname{erfc} \left(\frac{z-\xi t}{2\sqrt{Dt}} \right) + \exp \left[\frac{z(w+\xi)}{2D} \right] \cdot \operatorname{erfc} \left(\frac{z-\xi t}{2\sqrt{Dt}} \right) \right] \right\} \quad (21)$$

in which in which

$$\xi = (w^2 - 4D\gamma)^{1/2} \quad (22)$$

where boundaries are symmetrical then the solution of problem is specified by the 1st term in Equation (18) and (21), and the 2nd term in equation (18) and (22) is thus due to the asymmetric boundary imposed in the more general problem. Though, it should also be noted that if a point an immense distance away from the basis is measured, then it is probable to estimate the boundary condition by $C(-\infty, t) = C_0$, which tends to a symmetrical solution.

VI RESULTS AND DISCUSSIONS

This water finally enters the groundwater storage basin - a basis for drinking water. Throughout the passageway of water through the soil, the pollution is combined, and then 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 causes mixing at the contact front between the two fluids.

Dispersion, however, is defined as a mechanical mixing process caused by the twisting path followed by the fluid owing in the geometrically complex interconnections of the flow channels and by the variations in equations relating to solute transport are resolved analytically and numerically. Analytical solutions for the one-dimensional model are obtained using Laplace transformation techniques.

To estimate the magnitude of the danger 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 ground water table. At present, foremost drive on the transportation of pollutants and research is directed towards the definition and quantification of the process governing the behaviour of pollutants in subsurface environment, combined with the development of mathematical models that integrate process descriptions with the pollutant properties and site characteristics.

From the equation (18) and (22), C/C_0 was numerically computed using 'Mathematica' and the outcomes are presented

realistically in figures 5 to 9. Figures 5 to 9 represent the Break through Curves for C/C_0 vs time for different depth z . It is seen that the concentration field increases in the initial and reaches a constant state value for a static z but decreases with an increase in the layer width. Similar pattern is observed in figures 5 to 9 for distinct values of w and D .

Figures 5 to 9 represent the Break-Through-Curves for C/C_0 , and is maximum at the surface $z=0$ and decreases to reaches zero at the depth of 100 meters. With an increase in most of the contaminants get absorbed by the solid surface and thus suspending the movements of the contaminants as evident from the graphs. The majority of the pollutants are reduced in unsaturated area itself, hence the risk of ground water being polluted is diminished.

Distance (cm)	ADE				sFADE				
	v (cm/min)	D (cm ² /min)	r^2	RMSE	v (cm/min)	D_f (cm ² /min)	α	r^2	RMSE
30	0.762	0.985	0.981	0.056	0.779	0.557	1.260	0.993	0.034
60	0.728	0.809	0.991	0.041	0.736	0.369	1.339	0.994	0.034
90	0.721	1.859	0.994	0.031	0.727	0.576	1.302	0.996	0.027
120	0.599	1.179	0.997	0.023	0.602	0.367	1.253	0.994	0.030
150	0.844	4.210	0.994	0.029	0.856	0.909	1.201	0.986	0.045
180	1.098	4.802	0.984	0.053	1.119	1.241	1.374	0.989	0.045
210	1.242	13.933	0.977	0.060	1.286	1.664	1.166	0.983	0.051
Minimum	0.599	0.809	0.977	0.023	0.602	0.367	1.166	0.983	0.027
Maximum	1.242	13.933	0.998	0.06	1.286	1.664	1.374	0.996	0.051
Max-to-Min ratio ^a	2.073	17.222	-	-	2.136	4.534	-	-	-
Mean	0.856	3.968	0.991	0.042	0.872	0.812	1.271	0.991	0.038
Standard deviation	0.213	4.328	0.007	0.013	0.225	0.453	0.068	0.004	0.008

^aMax-to-Min ratio denotes the ratio of the maximum value of a parameter to its minimum value; v - average pore-water velocity; D - dispersion coefficient; r^2 - determination coefficient; RMSE - root mean square error; α - fractional differentiation order

Table 1: Estimated parameters and statistical criteria for advection dispersion equation and spatial fractional advection dispersion equation at various distances in heterogeneous soil

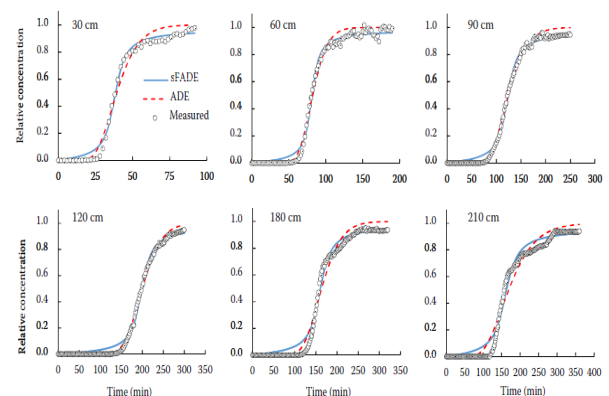


Figure 2: Comparison of the observed breakthrough curves with those fitted by advection dispersion equation and spatial fractional advection dispersion equation for heterogeneous soil at different distances

Distance (cm)	Homogeneous soil				Heterogeneous soil			
	ADE		sFADE		ADE		sFADE	
	r^2	RMSE	r^2	RMSE	r^2	RMSE	r^2	RMSE
60	0.989	0.044	0.994	0.032	0.985	0.052	0.982	0.059
90	0.963	0.088	0.969	0.080	0.974	0.067	0.978	0.061
120	0.970	0.076	0.977	0.066	0.608	0.239	0.626	0.234
150	0.966	0.084	0.973	0.074	0.879	0.133	0.935	0.097
180	0.961	0.089	0.969	0.079	0.353	0.336	0.510	0.292
210	0.964	0.085	0.973	0.073	0.020	0.395	0.241	0.348
Minimum	0.961	0.044	0.969	0.032	0.020	0.052	0.241	0.059
Maximum	0.989	0.089	0.994	0.080	0.985	0.395	0.982	0.348
Mean	0.969	0.078	0.976	0.067	0.636	0.204	0.712	0.182
SD	0.009	0.016	0.008	0.016	0.355	0.130	0.278	0.115

r^2 – determination coefficient; RMSE – root mean square error; SD – standard deviation

Table 2: Values of statistical criteria as the indicators of performance for advection dispersion equation and spatial fractional advection dispersion equation at subsequent distances using the best estimated parameters at 30 cm

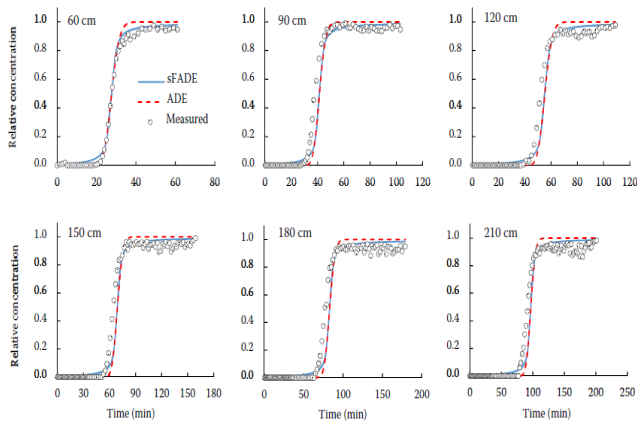


Figure 3: Predicted breakthrough curves in the homogeneous soil at different distances by advection dispersion equation and spatial fractional advection dispersion equation using parameters determined at 30 cm

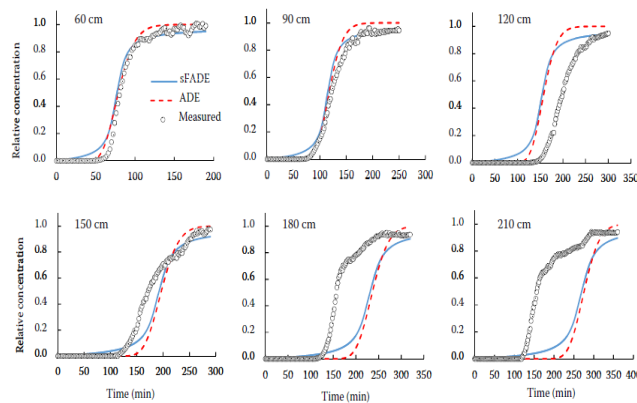


Figure 4: Predicted breakthrough curves in the heterogeneous soil at different distances by advection dispersion equation and spatial fractional advection dispersion equation using parameters determined at 30 cm

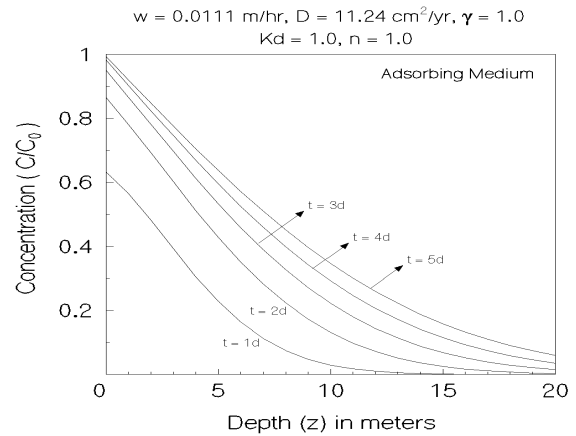


Figure 5: BTC for C/C_0 v/s depth for $n = 1.0, k_d = 1.0$ & $\gamma = 1.0$

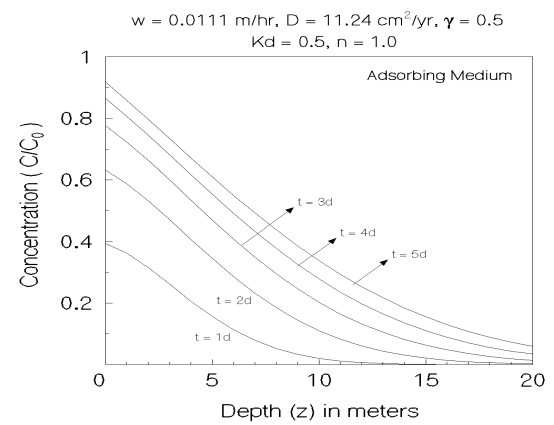


Figure 6: BTC for C/C_0 v/s depth for $n = 1.0, k_d = 0.5$ & $\gamma = 0.5$

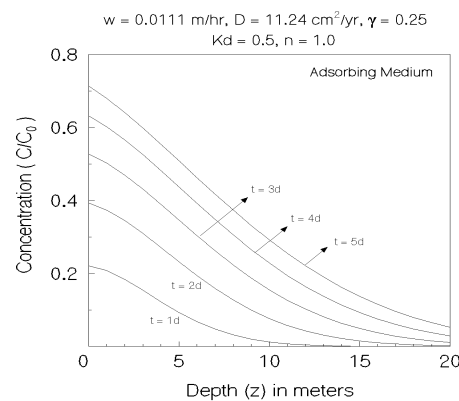


Figure 7: BTC for C/C_0 v/s depth for $n = 1.0, k_d = 0.5$ & $\gamma = 0.25$

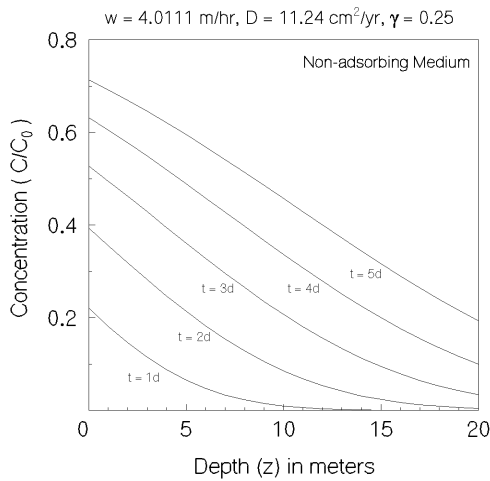


Figure 8: BTC for C/C_0
 v/s depth for $n = 1.0$, $k_d = 1.0$ & $\gamma = 0.25$

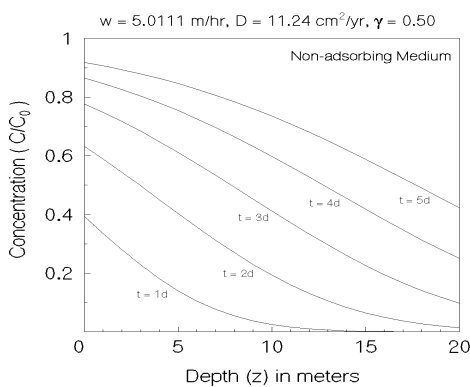


Figure 9: BTC for C/C_0
 v/s depth for $n = 0.5$, $k_d = 1.0$ & $\gamma = 0.25$

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