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Mathematical Study of Time - Exponentially Dependent Pollutant Transport in Unsaturated Porous Media

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Abstract

There are many factors that make it hard to assess the quality of groundwater. As water moves downward from the surface to the water table, different chemicals with various properties pass through different layers. These equations describe the movement of a substance that is both carried by water and slowed down by the medium, in a steady, one-directional flow through a material that is the same in all directions. These systems also remove the substance at a rate that depends on its concentration, while the concentration from sources decreases in an exponential way over time. We have developed a new analytical method to solve the advection-diffusion-reaction equation, which is commonly used to model how pollutants spread and move when influenced by the porosity of the material and a constant Weibull distribution of the substance coming from sources. A solution is found using the Laplace transform, and an error function is introduced using a method that moves coordinates and applies Duhamel's theorem to present the solution. Once certain values for the medium and fluid are known, mathematical models can be created to predict the concentration of pollutants in materials that can absorb them. It is safe to say that the variety of contamination sources is one of several factors that make it hard to assess the quality of groundwater. Different chemicals with various characteristics will travel through different parts of the water system.

Key words: Advection, dispersion, adsorption, Integral transforms, Fick's law, Moving coordinates, Duhamel's theorem

Mathematical Model

In recent times, there has been considerable attention on the study of substance movement through porous substances. Scientists have devised statistical techniques to assess concentration patterns and dispersion indices. The advection-diffusion equation elucidates how solutes traverse a medium due to both diffusion and convection. This equation is a type of partial differential equation grounded in the principle of mass conservation and Fick's law. With growing concerns about environmental degradation and air pollution, hydrologists, civil engineers, and mathematicians are focusing more on this equation.

Analytical and numerical methods that incorporate initial and boundary conditions facilitate understanding of contaminant dispersion across various mediums, including air, rivers, lakes, and underground water sources. These findings are vital for crafting tactics to minimize harm. This equation finds applications in various disciplines, such as soil physics, petroleum engineering, chemical engineering, and biological sciences.

In early experiments, investigators aimed to simplify the advection-diffusion equation in theoretical scenarios by transforming it into a diffusion equation by eliminating the convection terms by introducing an additional dependent variable. They accomplished this through the use of dynamic coordinates or by incorporating an additional dependent factor. The Laplace transformation method was subsequently employed to obtain the required solutions.

Tracy (1995) devised one-dimensional solutions by transforming the nonlinear advection-diffusion equation into a linear form, thereby enabling the derivation of two-dimensional and three-dimensional solutions. Numerous approaches have been suggested for addressing transport equations concerning solutes within porous substances, taking into account velocity fluctuations and dispersion rates (Van Kooten 1996, Sudheendra et al.). 2014.

Additional research revealed that certain extensive underground structures exhibit varying dispersivity over time or spatial distances. The method of analyzing one-dimensional solute transport using a temporal moment solution was employed to interpret the results from soil column experiments (Pang et al.). In 2003, Sudheendra and colleagues published their study. The year 2014. A technique was devised to study the movement of reactive substances in water as it infiltrates and redistributes under non-equilibrium conditions.

Molecules of solute travel via advection and adhere to linear kinetics. Methods were provided to study the movement of substances in rivers, taking into account phenomena such as temporary storage and degradation (Smedt 2006, Sudheendra 2011, 2012). In studies examining groundwater contamination in complex geological formations (Sirin 2006), the flow velocity through pores was modeled as a stochastic function that varies both spatially and temporally.

This explanation of the solution to the dispersion process equation is presented in a clearer manner here. It is assumed that there is no movement of matter between the solid and liquid phases, and that the porous medium is evenly distributed and uniform. Another assumption is that a planar region is multiplied by a diffusion constant, and the concentration difference is taken into account. The medium is viewed as having a one-dimensional structure, with uniform velocity throughout the flow area. This document outlines strategies to address two issues related to solute movement within a confined space. The initial challenge examines how solute distribution evolves with time in fully turbulent flow through a smooth enclosure. The condition of the output remains unchanged while a differential condition is present.

The Advection-Dispersion Equation along with initial and boundary conditions can be written as follows: initially, fluid flows through the porous material with a concentration of zero.

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

At time t = 0, the upper surface of the material instantly changes to a concentration of C0. This gives the correct boundary conditions for the model.

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

The problem then is to characterize the concentration as a function of z and *t*.

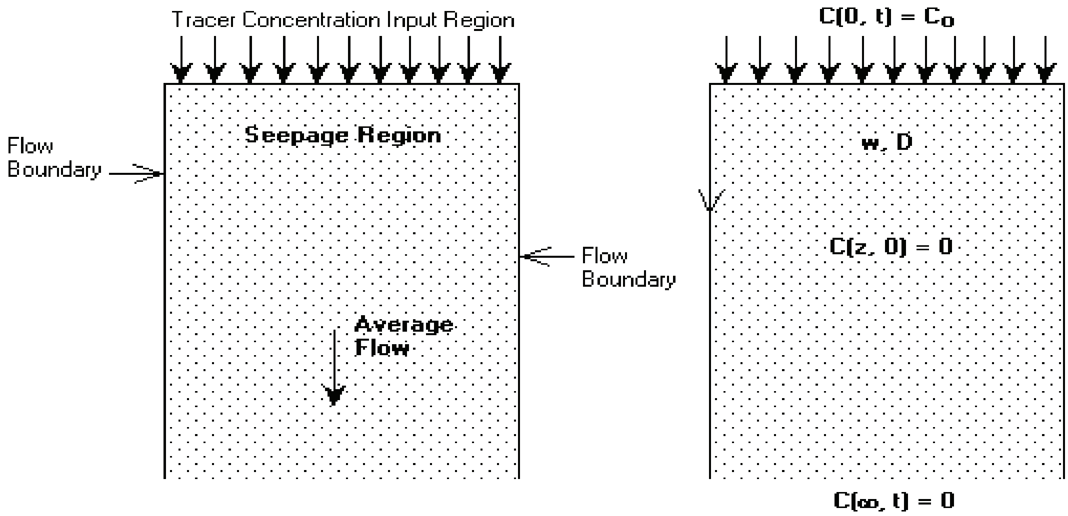

Figure 1 : Physical Layout of the Model

The input condition starts at the origin, and a second type of condition, which is about movement, is assumed. C0 is the original concentration. To make equations (3) look more familiar, we use the following approach.

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

Substituting equation (3) into equation (1) gives

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

The initial and boundary conditions (2) transform to

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

Equation (4) can be used to solve an influx of the fluid at z = 0. Using Duhamel's theorem (Carslaw and Jaeger, 1947), the solution to equation (4) can be found easily.

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

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

This theorem is often used in heat transfer problems, but we have adapted it for our specific case. Now we focus on the case where the initial concentration is zero and the boundary is fixed at a concentration of one. 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

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

Hence, it is reduced to an ordinary differential equation

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

The solution of the equation is $\overline{\Gamma} = Ae^{-qz} + Be^{qz}$ where, $q = \pm\sqrt{\frac{p}{D}}$.

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

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

The inversion of the above function is given in any table of Laplace transforms. The result is

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

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

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

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

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

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

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

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

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

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

Evaluation of the integral solution

The integration 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 may be expressed on terms of error function (Horenstein, 1945), because this function is well tabulated.

Noting that

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

The second integral of equation (9) may be written as

$$I=\int_0^\alpha Exp\left(-\mu^2-\frac{\varepsilon^2}{\mu^2}\right)d\mu$$

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

Since the method for reducing the integral to a known function is the same for both integrals on the right side of equation (11), we only need to consider the first term. Let $a=\varepsilon/\mu$, and the integral can be rewritten as:

Since the method of reducing integral to a tabulated function is the same for both integrals in the right side of equation (11), only the first term is considered. Let $a=\varepsilon/\mu$ and the integral may be expressed as

$$I_1=e^{2\varepsilon}\int_0^\alpha Exp\left[-\left(\mu+\frac{\varepsilon}{\mu}\right)^2\right]d\mu$$

$$=-e^{2\varepsilon}\int_{\varepsilon/\alpha}^{\infty}\left(1-\frac{\varepsilon}{a^2}\right)Exp\left[-\left(\frac{\varepsilon}{a}+a\right)^2\right]da+e^{2\varepsilon}\int_{\varepsilon/\alpha}^{\infty}Exp\left[-\left(\frac{\varepsilon}{a}+a\right)^2\right]da \quad (12)$$

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

in the $\beta=\frac{\varepsilon}{a}+a$ first term of the above equation, then

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

Similar evaluation of the second integral of equation (11) gives

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

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

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

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

Noting that

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

Substitution into equation (11) gives

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

Thus, equation (9) may be expressed as

$$\Gamma(z,\ t) = \frac{2C_0}{\sqrt{\pi}} Exp\ \left(\frac{w^2 t}{4D} + \frac{K_d(1-n)t}{n} - \gamma t\right) .\left\{\frac{\sqrt{\pi}}{2} e^{-2\varepsilon}\ \ \frac{1}{2}\left[e^{-2\varepsilon} \int_{\frac{\varepsilon}{\alpha}-\alpha}^{\infty} e^{-\beta^2} d\beta - e^{2\varepsilon} \int_{\alpha+\frac{\varepsilon}{\alpha}}^{\infty} e^{-\beta^2} d\beta\right]\right\} \tag{15}$$

However, by definition,

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

also,

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

Writing equation (15) in terms of error functions, we get

$$\Gamma(z,\ t) = \frac{C_0}{2} Exp\ \left(\frac{w^2 t}{4D} + \frac{K_d(1-n)\ t}{n} - \gamma t\right).\left[e^{2\varepsilon} erfc\ \left(\alpha+\frac{\varepsilon}{\alpha}\right) + e^{-2\varepsilon} erfc\ \left(\alpha-\frac{\varepsilon}{\alpha}\right)\right] \tag{16}$$

Thus, Substitution into equation (3) the solution is

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

Re-substituting for ε and α gives

$$\frac{C}{C_0} = \frac{1}{2}\ Exp\left[\frac{wz}{2D} - \gamma t\right]\left[Exp\left[\frac{\sqrt{w^2 n + 4D(1-n)K_d - 4Dn\gamma}}{2D\sqrt{n}} z\right] \cdot erfc\left[\frac{z + \sqrt{w^2 n + 4D(1-n)K_d - 4Dn\gamma}}{2\sqrt{Dnt}} t\right] + \left[Exp\left[-\frac{\sqrt{u^2 n + 4D(1-n)K_d - 4Dn\gamma}}{2D\sqrt{n}} z\right] \cdot erfc\left[\frac{z - \sqrt{u^2 n + 4D(1-n)K_d - 4Dn\gamma}}{2\sqrt{Dnt}} t\right] \quad (17)$$

where the boundaries are symmetrical, the solution of the problem is given by the first term of equation (17). The second term in equation (17) is due to the asymmetry introduced in the more general problem. However, it's also important to note that if you look at a point far away from the source, you can approximate the boundary condition as $C(-\infty, t) = C_0$, which gives a symmetrical solution.

4. Results & Discussions:

The analytical methods have some important limits. They work best when the problems are not too complicated and when the shape of the area being studied is regular. The soil must be the same in all parts of the area being studied. Compared to other methods for solving one-dimensional transport models, the analytical approach is a bit more flexible. Figures 1 to 4 show how the concentration of a substance changes as it moves through different parts of the media, depending on the amount of empty space (porosity). When the speed of fluid flow, the spread of the substance (dispersion), and the way it sticks to the soil (distribution coefficient) are constant, the ratio of current concentration to original concentration (C/C0) decreases as the depth increases, especially when porosity is lower. When you look at how concentration changes over time at different depths, it starts to increase because the spread effect (dispersion coefficient) has less impact. Eventually, it reaches a steady level after a longer period of time.

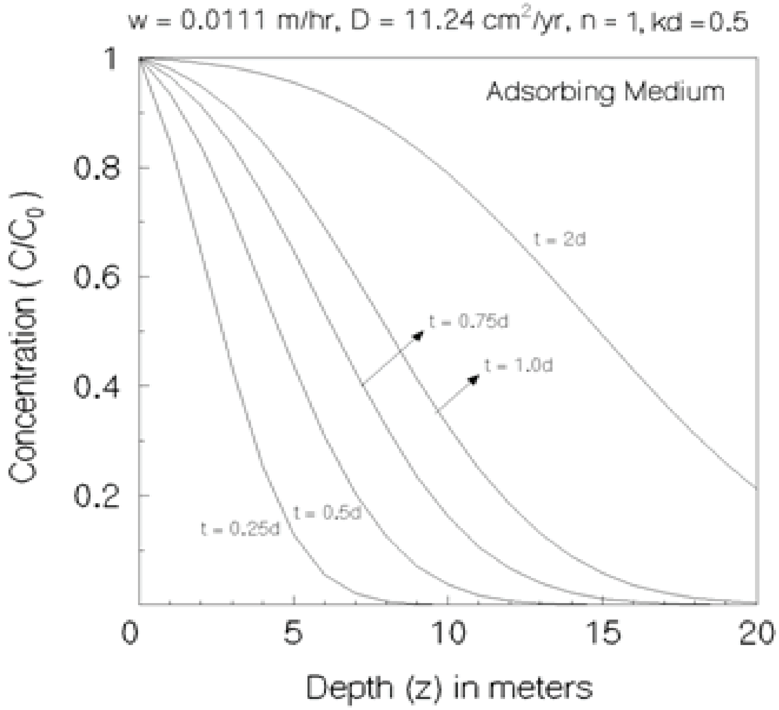

Fig. 1: Break-through-curve for C/C_0 v/s depth for n=1.0, K_d=0.5 & γ = 0

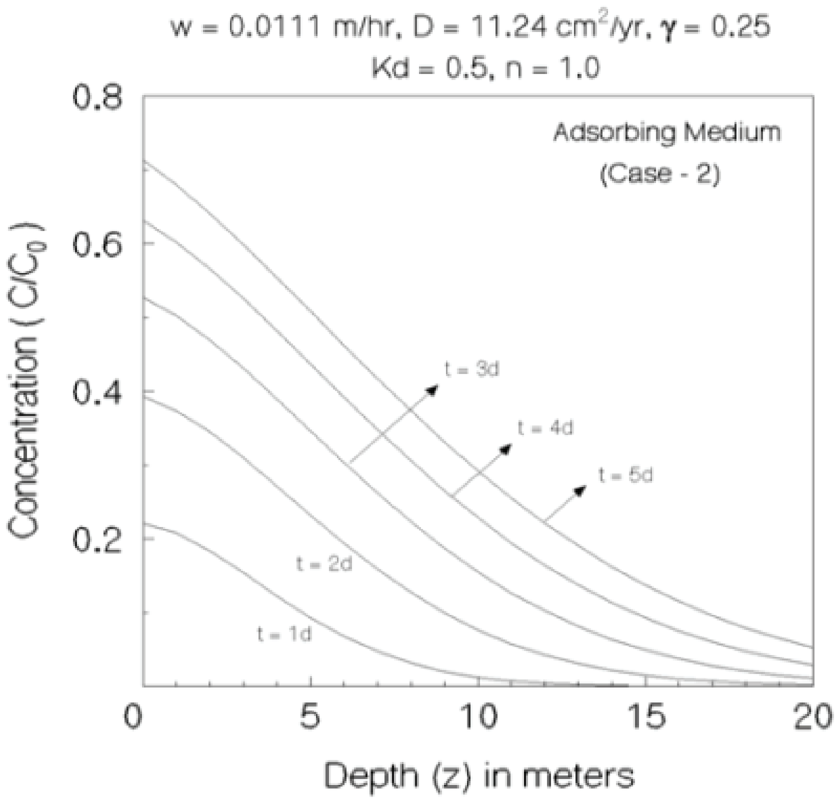

Fig. 2: Break-through-curve for C/C_0 v/s depth for n=1.0, K_d=0.5 & γ = 0.25

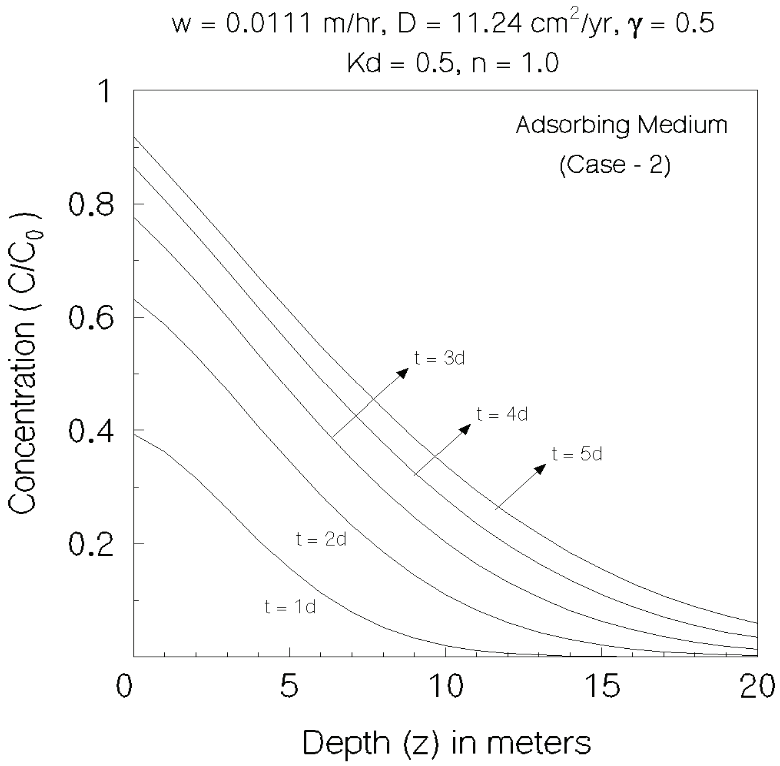

Fig. 3: Break-through-curve for C/C_0 v/s depth for n=1.0, K_d=0.5 & γ = 0.5

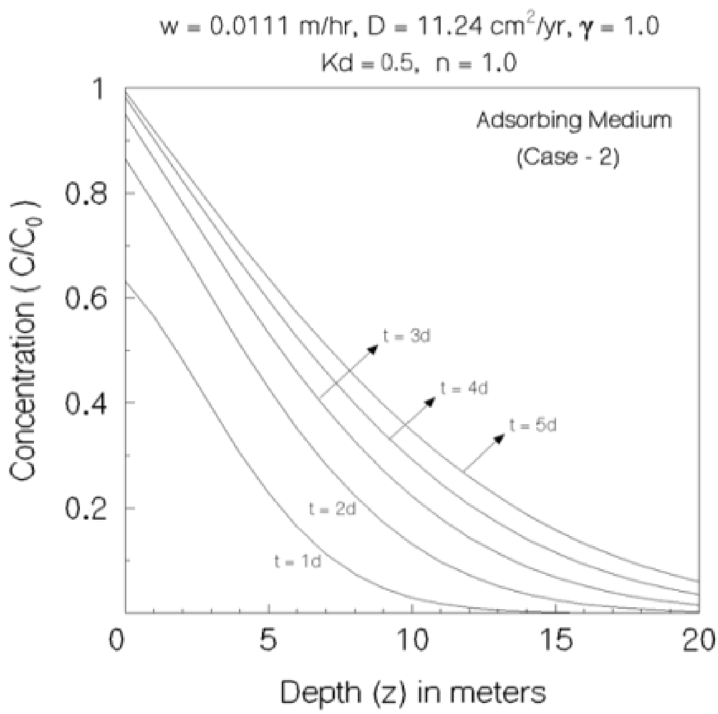

Fig. 4: Break-through-curve for C/C_0 v/s depth for n=1.0, K_d=0.5 & γ = 1.0

For a range of distribution coefficient K_d values, the figures show C/C0 versus time. Because there is less adsorption of pollutants on the solid surface, concentration rises gradually for a fixed K_d up to t=10 days. After that, it achieves a constant value for a longer period of time where the distribution coefficient K_d has no influence. We come to the conclusion that the integral transform approach is an effective way to provide analytical answers for the solute transport of an adsorption under various flow conditions and homogenous porous media. These solutions can be used to directly generate steady-state concentration distributions and temporal moments, and numerical inversion can be used to access transient concentration distributions. The derived solutions are of great value for bench-marking numerical reactive transport codes.

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