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An Analytical Solution of One-dimensional Advection-Diffusion Equation in a Porous Media in Presence of Radioactive Decay

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Abstract

We present a solution of the Transport of Pollutants with Radioactive Decay in Porous Media considering boundary conditions. The solutions are obtained by using Duhamel's theorem and integral solution technique. The effects of the concentration with time and depth on the solute transport are studied separately with the help of graphs.

Keywords: Advection-diffusion equation; Analytical solution; Fick's law; Mathematical Modelling.

Introduction
In recent years considerable interest and attention have been directed to dispersion phenomena in flow through porous media. Numerous analytical solutions have been developed to qualitatively describe one-dimensional convective-dispersive solute transport. In this paper, a more direct method is presented for solving the differential equation governing the process of dispersion. It is assumed that the porous medium is homogeneous and isotropic and that no mass transfer occurs between the solid and liquid phases. It is assumed also that the solute transport, across any fixed plane, due to microscopic velocity variations in the flow tubes, may be quantitatively expressed

as the product of dispersion co-efficient and the concentration gradient. The flow in the medium is assumed to be unidirectional and the average velocity is taken to be constant throughout the length of the flow field.

Reactive transport in porous media is of growing interest because of frequent contamination of aquifers with reactive substances like petroleum hydrocarbons and chlorinated solvents [Vogel et al. (1987), Hinchee et al. (1994), Wiedemeier et al. (1999), and Peter et al. (2001)].

Convective-dispersive system is common in many scientific and technologic domains such as: hydrogeology, soil science, biology, medicine and chemical engineering. To learn about the dynamic behaviour of the major components of such a system, mathematical and laboratory models are constructed and tracers are often utilized.

The analysis has been restricted here to one-dimensional cases. While this is an obvious limitation, many useful applications can be treated as one-dimensional. The various solutions of the one-dimensional convective-dispersive system are presented here in a systematic fashion. Several cases still remain, especially for nonequilibrium reactions, where analytic solutions are not available. To facilitate the discussion of the initial and boundary conditions and the effect of decay and chemical reaction on the distribution of tracers, these solutions have been presented in a unified form whenever possible as functions of non-dimensional variable.

The solutions for transport of decay in porous media, derived in this paper are useful for several reasons: First, they are widely applicable. Although only radioactive decay is a true first-order process, also chemical and biological transformations can be often described approximately in terms of first-order decay.

Mathematical Formulation and Model

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 the contaminant in the media is assumed to be zero and a constant source of 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

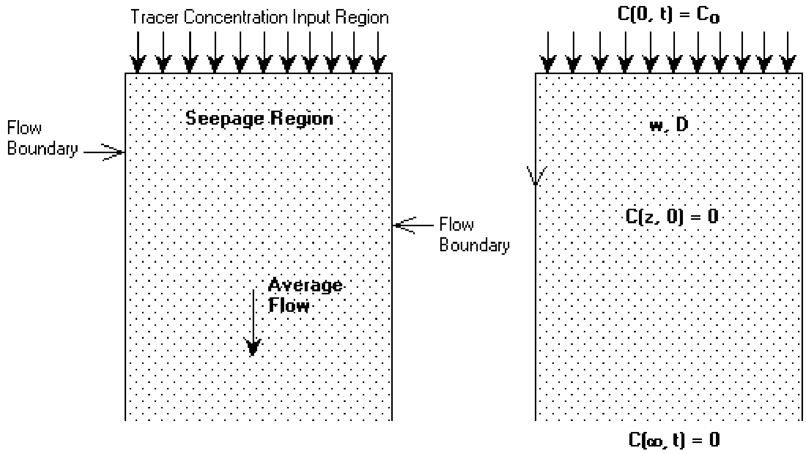
$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial z^2} - u\frac{\partial C}{\partial z} - \lambda C \tag{1}$$

where C is the constituent concentration in the soil solution, t is the time in minutes, D is the hydrodynamic dispersion coefficient, z is the depth, u is the average pore-water velocity and λ is the radioactive decay (Chemical reaction term).

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

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

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



Physical Layout of the Model

To reduce equation (1) to a more familiar form, let

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

Substitution of equation (3) reduces equation (1) to Fick's law of diffusion equation

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

The above initial and boundary conditions (2) transform to

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

It is thus required that equation (4) be solved for a time dependent influx of fluid at z = 0. The solution of equation (4) can be obtained by using Duhamel's theorem [Carslaw and Jeager, 1947].

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

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

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

Consider now the problem in which initial concentration is zero and the boundary is maintained at concentration unity. The boundary conditions are

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

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

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

Hence, if equation (4) is multiplied by e^{-pt} and integrated term by term it is reduced to an ordinary differential equation

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

The solution of the equation (6) can be written as

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

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

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

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

The inversion of the above function is given in a table of Laplace transforms (Carslaw and Jaeger, 1947). The result is

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

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

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

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

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

The solution of the problems is

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

Letting

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

the solution can be written as

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

Since $\phi(t) = C_0 \exp\left(\frac{u^2 t}{4D} + \lambda t\right)$ the particular solution of the problem can be written as

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

where $\varepsilon = \sqrt{\left(\frac{u^2}{4D} + \lambda\right)} \frac{z}{2\sqrt{D}}$ and $\alpha = \frac{z}{2\sqrt{Dt}}$.

Evaluation of the Integral Solution

The integration of the first term of equation (9) gives (Pierce, 1956)

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

For convenience the second integral can be expressed in 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) can be written as

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

Since the method of reducing integral to a tabulated function is the same for both integrals in the right side of equation (10), only the first term is considered. Let $a=\frac{\varepsilon}{\mu}$ and adding and subtracting, we get

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

The integral can be expressed as

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

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

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

in the first term of the above equation, then

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

Similar evaluation of the second integral of equation (10) 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

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

substitute this into equation (10) gives

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

Thus, equation (9) can be expressed as

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

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 (11) in terms of the error functions, we get

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

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

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

Resubstituting the value of ε and α gives

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

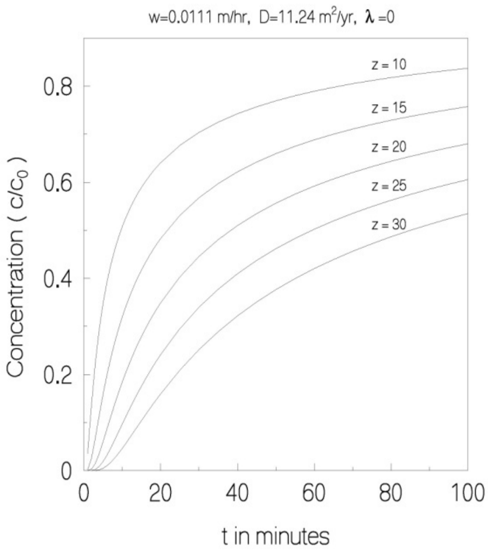
Results and Discussion

The main limitations of the analytical method are the applicability 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 (13) C/C_0 was numerically computed using `Mathematica' and the results are presented graphically in figures 1 to 12. Figures 1 to 6 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 beginning and reaches a steady state value for a fixed z but decreases with an increase in the radioactive decay coefficient λ. An increase in λ will make the solute concentration decreasing as evident from the physical grounds. Similar pattern is observed in figures 4 to 6 for different values of average velocity w and dispersion coefficient D.

Figures 7 to 12 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 λ 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 of groundwater being contaminated is minimized. Similar pattern is observed in the graphs 10 to 12 for different values of average velocity w and dispersion coefficient D.

We conclude that the integral transform method is a powerful method to derive analytical solutions for solute transport of a decay chain and adsorption in homogeneous porous media and under different flow conditions. Steady-state concentration distributions and temporal moments can be directly derived from these solutions and transient concentration distribution is accessible via numerical inversion. The derived solutions are of great value for bench-marking numerical reactive transport codes.



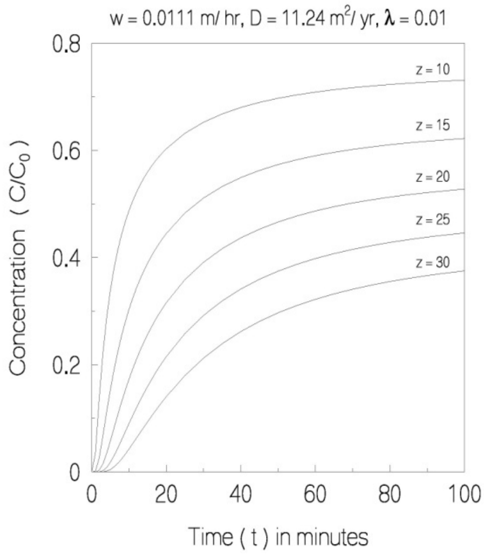
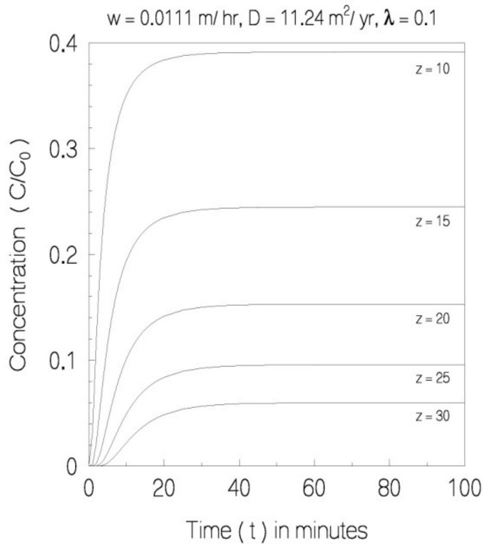


Figure 1 Figure 2



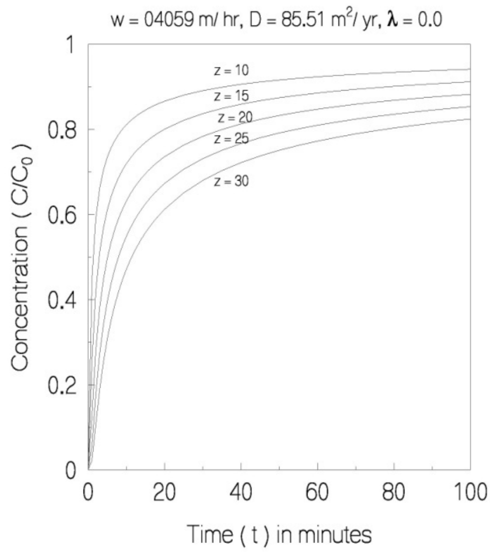
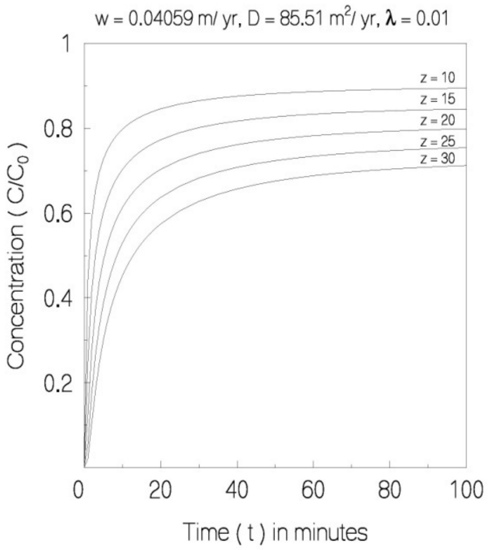


Figure 3 Figure 4



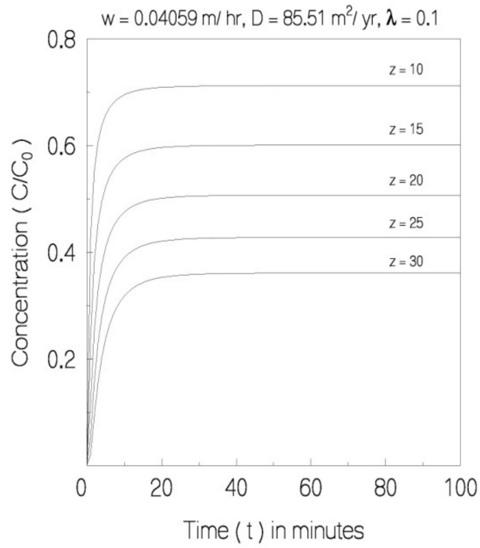
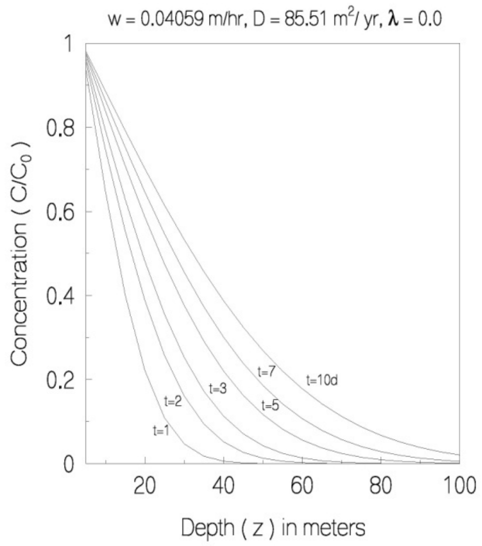


Figure 5 Figure 6



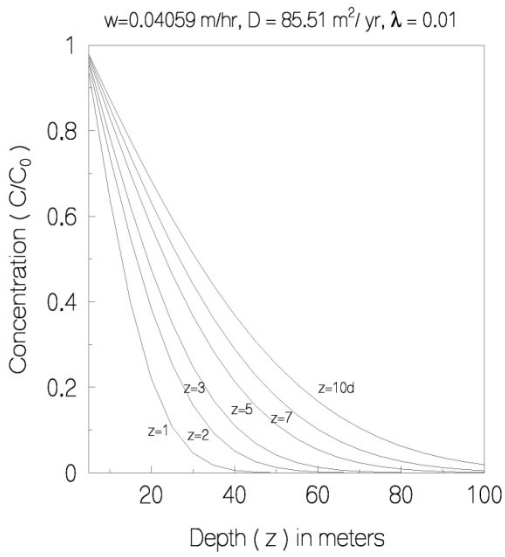
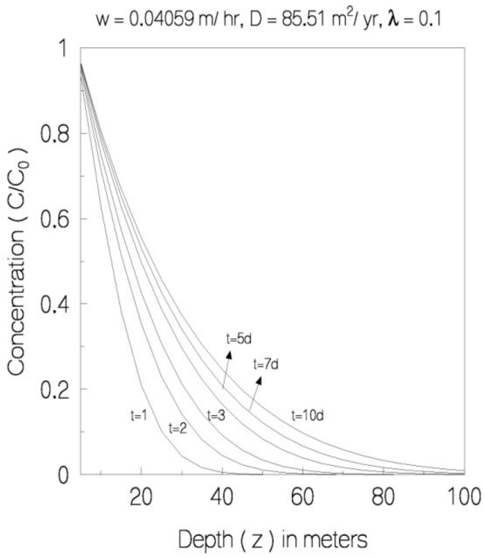


Figure 7 Figure 8



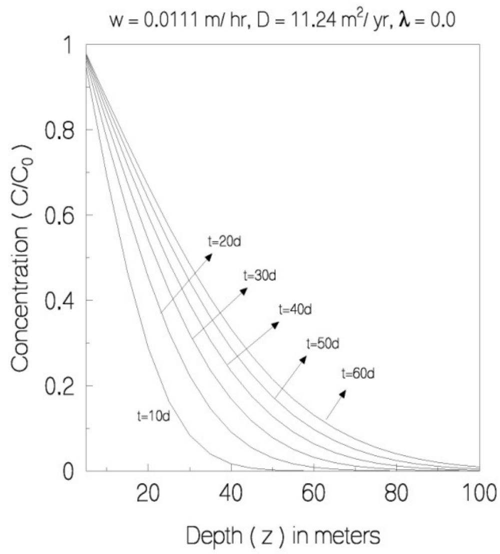
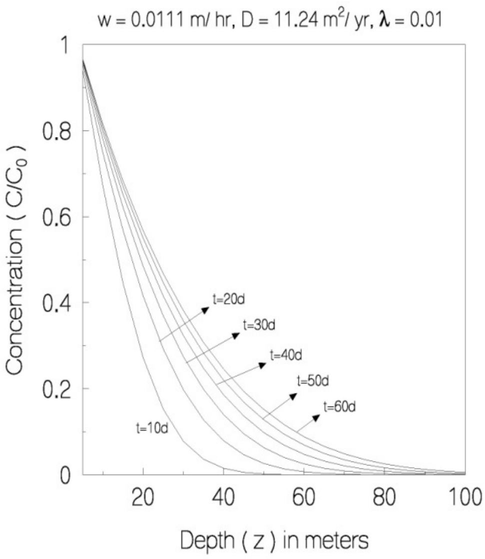


Figure 9 Figure 10



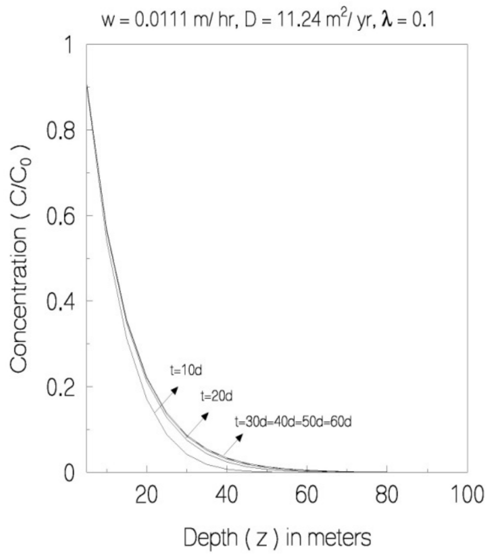


Figure 11 Figure 12

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