Mathematical Analysis of Transport of Pollutants through Unsaturated Porous Media with Adsorption and Radioactive Decay

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Abstract: A mathematical analysis is presented for simultaneous dispersion and adsorption of a solute within homogeneous and isotropic porous media in steady unidirectional flow fields. The dispersion systems are adsorbing the solute at rates proportional to their concentration and are subject to input concentrations that vary with time as well as depth. The solution is obtained with Laplace transform, Duhamel's theorem and moving coordinates to convert nonlinear partial differential equation to ordinary differential equation. Mathematical solutions are developed for predicting the concentration of contaminants in adsorbing and radioactive decay for prescribed media and fluid parameters.

Introduction

The main objective of the study is to provide mathematical model for better understanding of transport of pollutant through unsaturated porous media. A mathematical model is an important tool and can play a crucial role in understanding the mechanism of groundwater pollution problems. It is a simplified description of physical reality expressed in mathematical terms. Mathematical models that attempt to simulate atmospheric processes involved in groundwater pollution are based, in general, on the equation of mass conservation for individual pollutant species. Such models relate in one equation the effects of all the physical aspects and dynamic processes that influence the mass balance on groundwater which include transport, diffusion, removal of pollutants and loss or transformation through chemical reactions.

In this Paper, we have developed a mathematical model, which enables prediction of spatial and temporal concentration distribution of pollutants in groundwater. We study the solute transport and groundwater pollution problems by formulating different mathematical models incorporating all the important features which influence the dispersion of groundwater pollution problems. These models are developed analytically, because of exact values and easy to understand the concepts of the problems. These solutions possess a greater exhibility and do not suffer from some of the errors associated with numerical solutions. These analytical solutions can provide an acceptable indication of distribution of pollutants more quickly and cheaply than by monitoring network. An application of mathematical modelling on groundwater pollution is for determination of optimum depth so that people living around it will be less affected by the pollutants. The analytical solutions also pave the way to predict the influence of new sources of pollution on the water quality and decide as to which standards must set for these new sources in order to maintain the desired level of groundwater quality.

The solutions of one, two and three-dimensional deterministic advection-dispersion equations have been investigated in numerous publications before and are still actively studied. For instance, Ogata and Banks (1961), Sauty (1979), and van Genuchten (1981) have provided analytical solutions of one-dimensional transport with the first-type (Dirichlet), second-type (Neumann), and third-type (Cauchy) boundary conditions, respectively. Yeh (1981) have given the generalized analytical one, two, and three-dimensional description and computer code for estimating the transport of waste in groundwater aquifers. Domenico and Robbins (1984) and Domenico (1987) have explored some multi-dimensional transport problems. Batu (1989, 1993) have studied the two-dimensional analytical solute transport model with the first and the second-type boundary conditions. Wexler (1992) and its cited references there have documented many previously derived analytical solutions with different initial and boundary conditions. Leij et al. (1993) have studied the non-equilibrium multi-dimensional transport using the Laplace and Fourier transforms and Leij et al. (2000) have used Green's functions to describe persistent solute source transport. Narasimhan and Witherspoon (1976) have developed an integrated finite difference method for simulating fluid flow in porous media. This method uses an integral form of the governing equations whereas the standard finite difference method uses a differential form of the equation. An explicit finite difference mixing cell model was proposed by Van Ommen (1985). In this model the time and spatial derivative are approximated by a forward difference and backward difference respectively.

Mathematical Model

The Advection-Dispersion equation along with initial condition and boundary conditions can be written as

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

Initially, saturated flow of fluid of concentration, $C = 0$, takes place in the porous media. At $t = 0$, the concentration of the upper surface is instantaneously changed to $C=C_0$. Thus, the appropriate boundary conditions for the given model

$$\left.\begin{array}{ll} C(z,0) = 0 & z \geq 0 \\ C(0,t) = C_0 & t \geq 0 \\ C(\infty,t) = 0 & t \geq 0 \end{array}\right\}. \tag{2}$$

The problem then is to characterize the concentration as a function of z and t. where the input condition is assumed at the origin and a second type or flux type homogeneous condition is assumed. C_0 is initial concentration. To reduce equation (3) to a more familiar form, we take

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

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

$$\left.\begin{array}{ll} \Gamma(0,t) = C_0\ Exp\left[\dfrac{w^2 t}{4D} + \dfrac{K_d(1-n)\,t}{n} + \lambda t\right] & t \geq 0 \\ \Gamma(z,0) = 0 & z \geq 0 \\ \Gamma(\infty,t) = 0 & t \geq 0 \end{array}\right\} \tag{5}$$

Equation (4) may be solved for a time dependent influx of the fluid at $z = 0$. The solution of equation (4) may be obtained readily by use of Duhamel's theorem (Carslaw and Jaeger, 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

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

This theorem is used principally for heat conduction problems, but the 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

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

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

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

where, $\alpha = \frac{z}{2\sqrt{D t}}$ and $\varepsilon = \sqrt{\left(\frac{w^2}{4D} + \frac{K_d(1-n)}{n} + \lambda\right)} \cdot \left(\frac{z}{2\sqrt{D}}\right)$

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

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

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

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

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

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

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

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

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

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

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,

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

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

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

Thus, Substitution into equation (3) the solution is

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

Re-substituting for ε and α gives

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

$$\left. \left[Exp\left[-\frac{\sqrt{w^2 n + 4D(1-n)K_d + \lambda}}{2D\sqrt{n}} z\right] \cdot erfc\left[\frac{z - \sqrt{w^2 n + 4D(1-n)K_d + \lambda}}{2\sqrt{Dnt}} t\right]\right] \tag{17}$$

where boundaries are symmetrical the solution of the problem is given by the first term the equation (17). The second term is equation (17) is thus due to the asymmetric boundary imposed in the more general problem. However, it should be noted also that if a point a great distance away from the source is considered, then it is possible to approximate the boundary condition by $C(-\infty, t) = C_0$, which leads to a symmetrical solution.

Results and discussions

The main limitations of the analytical methods are, that the applicability is for relatively simple problems. The geometry of the problem should be regular. The properties of the soil in the region considered must be homogenous 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. The partial differential equations describing solute transport are solved analytically by considering adsorption and isotopes. It is generally assumed that macroscopic transport by convection must take into account the average flow velocity as well as the mechanical or hydrodynamic dispersion.

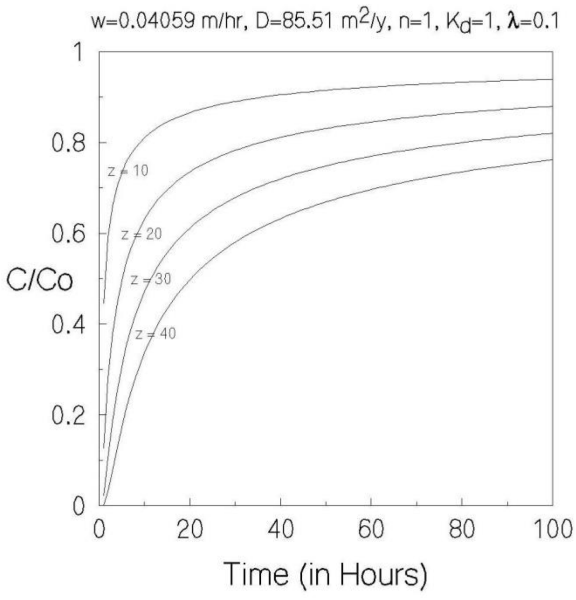

Figure 1: Break - through - curve for C/C_0 v/s Time for different Depth

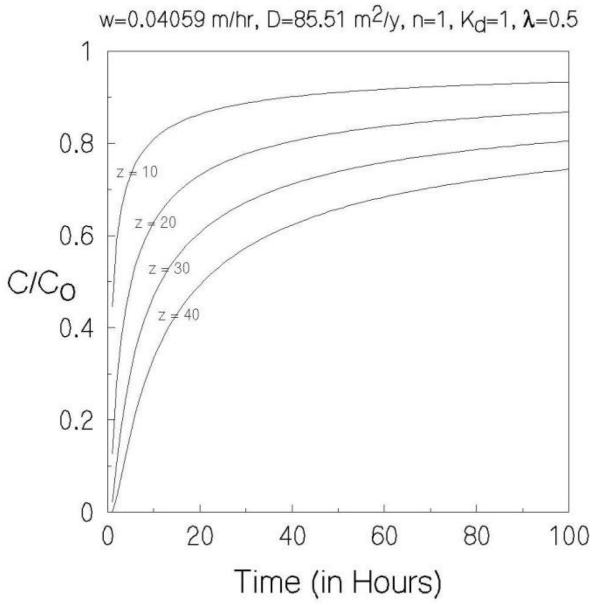

Figure 2: Break - through - curve for C/C_0 v/s Time for different depth

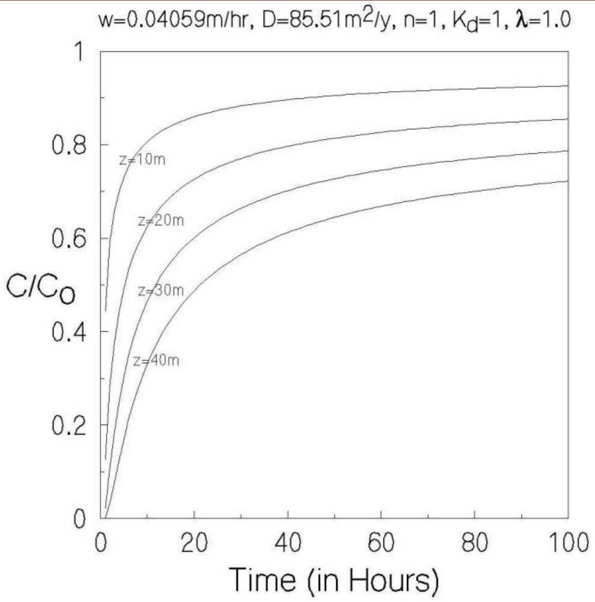

Figure 3: Break - through - curve for C/C_0 v/s Time for different Depth

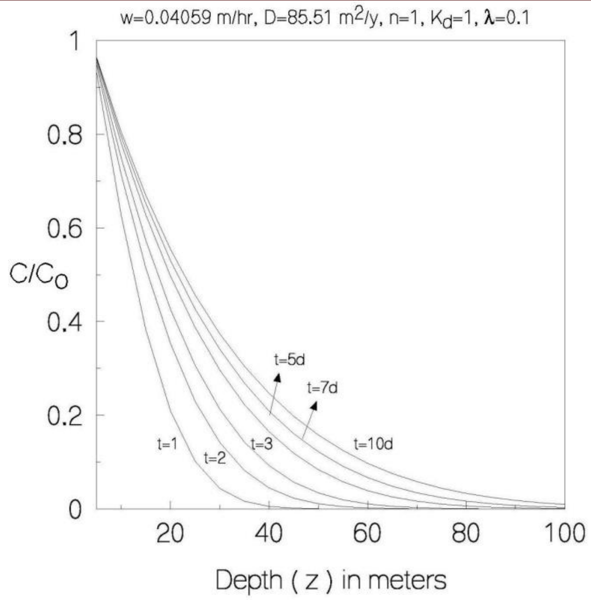

Figure 4: Break - through - curve for C/C_0 v/s Depth for different time interval

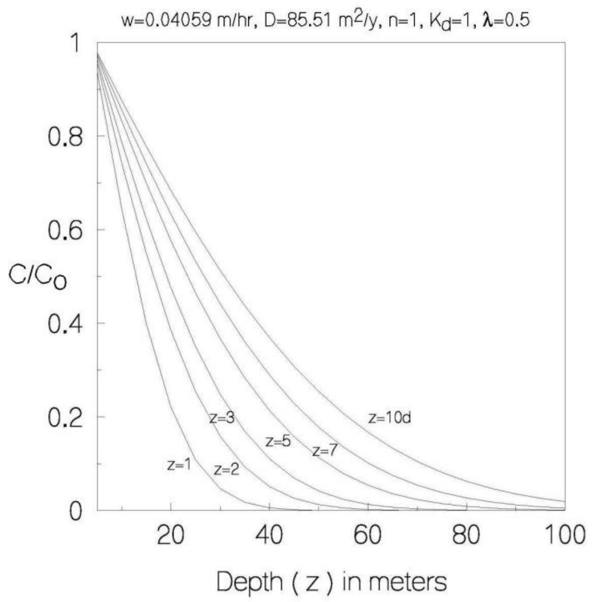

Figure 5: Break - through - curve for C/C_0 v/s Depth for different time interval

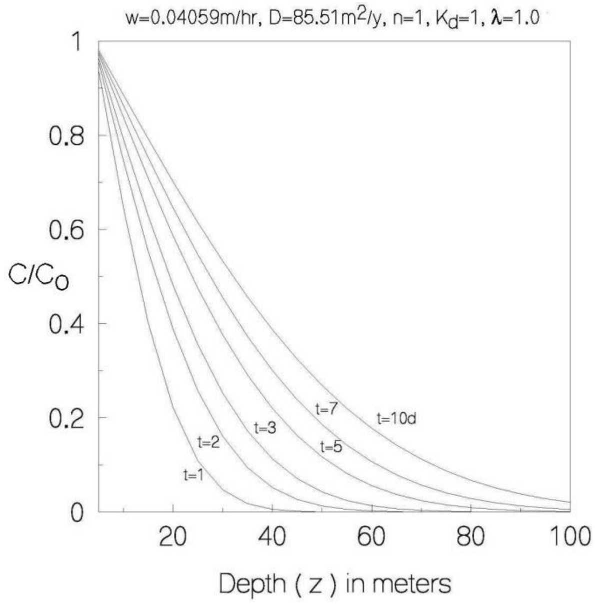

Figure 6: Break - through - curve for C/C_0 v/s Depth for different time interval

Figure (1), (2) and (3) represents the concentration profiles v/s time in the adsorbing media for different values of depth z, porosity n, and radioactive decay λ. It is seen that for a fixed velocity w, dispersion coefficient D and distribution coefficient K_d, C/C_0 increases with time as porosity n increases due to the distributive coefficient K_d and if time decreases the concentration increases for different time and decay chain. Figures (4), (5) and (6) represent the solute concentration v/s depth in the porous adsorbing media for different values of time, porosity n, and radioactive decay l. It is been observed that for a fixed velocity w, dispersion coefficient D and distribution coefficient K_d, the solute concentration decreases with depth as porosity n decreases due to dissipation coefficient K_d and if depth increases the solute concentration decreases for different depth and radioactive decay.

We conclude that the mathematical solutions have been developed for predicting the possible concentration of a given dissolved substance in steady unidirectional seepage flows through semi-infinite, homogeneous, and isotropic porous media subject to source concentrations that vary with time and isotopes. The expressions take into account the decay of a radioactive contaminants as well as mass transfer from the liquid to the solid phase due to adsorption. For simultaneous dispersion and adsorption of a solute, the dispersion system is considered to be adsorbing at a rate proportional to its concentrations. Mass due to adsorption plays an important role in mass transport within natural flow systems. In general the outcome of any contaminant introduced into the groundwater system is largely dependent on the capacity of the solid matrix material to adsorb the dissolved substance. Approximation to the adsorption rate is used in the mathematical analysis for lack of better data that take into account the macroscopic aspects of adsorption in groundwater system.

The analytical expressions developed herein should prove helpful in making quantitative predictions on the possible contaminant of groundwater supplies resulting from seepage of high salt concentrations in drainage ditches, canals, stream and from groundwater movement through buried wastes. In addition, they should prove useful for other processes such as ion exchange in soil and decay of organic substances.

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