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Study of Specially and Temporally Dependent Adsorption Coefficient in Heterogeneous Porous Medium

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Abstract

One-dimensional advection-dispersion equation **(**ADE) is studied along unsteady longitudinal flow through a semi-infinite heterogeneous medium. Adsorption coefficient is considered temporally and spatially–dependent function i.e., expressed in degenerate form. The dispersion parameter is considered as inversely proportional to adsorption coefficient. The input source is of pulse type. The Laplace Transformation Technique (LTT) is used to obtain the analytical solution by introducing certain new independent variables through separate transformations. The effects of adsorption, heterogeneity and unsteadiness are investigated and discussed with the help of various graphs.

Keywords: Adsorption; Advection; Dispersion; Heterogeneous; Porous Medium

AMS 2010 Classification: 34B05, 35G15, 44A10, 35Q35, 60J60

1. Introduction

One fundamental assumption of the theory which refers to the homogeneity of the adsorbent surface is not justified in many cases. In case of inhomogeneous/heterogeneous, the adsorption points are distributed over different levels. Such studies are of great importance in the remedial processes of groundwater, soil, industrial and blood where substances are in mixture form as well as in the environmental protection processes Dabrowski (2001). Most of natural environments are heterogeneous. On the basis of field evidence, experiment studies and statistical approach, many authors have suggested that the porosity of a porous medium varies with position and time due to the heterogeneity. Hence velocity of the flow through the medium also depends upon position and time variable. An adsorption is a process in which solute concentration in the liquid phase is attracted by the solid boundaries of the pores and is deposited on them (a process in which molecules accumulate in the interfacial layer). A theory of the monomolecular adsorption on energetically homogeneous surfaces is first given by Langmuir and latter tried to extend theoretical approach to account for heterogeneity of solid adsorbent and the multilayer character of adsorption. The fundamental practical applications of adsorption and related areas are separation and purification of liquid and gas mixtures, recovery of chemicals from industrial and vent gases.

The longitudinal dispersion coefficient is linearly and squarely proportional to the fluid velocity have been considered in previous decades and obtained analytical solutions for dispersion problems in a porous medium Ogata and Banks (1961), Al-Niami and Rushton (1977). Most of such type of works has been compiled by van Genuchten, and Alves (1982). We have studied some important hydro-dynamic dispersion problems based on theories of Scheidegger (1957), Ebach and White (1958), Matheron and de Marsily (1980) and solved some problems analytically Jaiswal et al. (2009), Kumar et al. (2010) Jaiswal et al. (2011).

In the works of Yates (1990), Zoppou and Knight (1997), the dispersion coefficient was also considered as spatially dependent. But to go on increasing as x increases along the semi-infinite domain, hence its limiting value was assumed. The solution may be used more effectively than previous ones to construct the mass transport function for a new type of transient infinite element Zhao and Valliappan (1994), Zhao (2009) and other numerical solutions in a semi-infinite domain van Genuchten et al. (2013a,b). Analytical solution for a physical aspect is of fundamental importance to understanding the role of all the parameters in the physical phenomenon. Jaiswal et al. (2012, 2013, 2014) and Yadav et al. (2010, 2012) obtained an analytical solutions with the help of Laplace transform technique (LTT) in finite and semi-infinite domain for dispersion problems with different boundary conditions related to physical and real scenario.

Singh and Das (2016) presented a paper with mathematical modeling of solute transport in porous media to predict the contaminant distribution pattern in groundwater by using Laplace transform technique. They used the concept of dispersion related seepage velocity, together with the concept of Reynolds number. Wang and Shao (2016) proposed a novel solution to the convection–dispersion equation (CDE) for predicting profiles of solute concentrations and estimating transport parameters. They adapted solution from polynomial and exponential boundary-layer (BL) solutions based on BL theory. The accuracy of the new BL solution was dependent on the number of polynomial terms and the properties of the soil. Alam and Tunc (2016), have been used the $\exp\{-\phi(\xi)\}$- expansion method to transformed into nonlinear ordinary differential equations and construct to many families of exact solutions of nonlinear evolution equations (NLEEs) via the nonlinear diffusive predator–prey system and the Bogoyavlenskii equations.

In the present paper, the adsorption coefficient is considered directly proportional to the dispersion parameter. To introduction of new independent space and time variables the ADE with variable coefficients is reduced into constant coefficients. The two coefficients dispersion and adsorption of the ADE are considered in degenerate form i.e., as functions of independent (space and time) variables while the flow velocity is considered temporally dependent. An analytical solution is obtained for a one-dimensional advection-dispersion equation (ADE) by using LTT.

2. Mathematical Formulations

A one dimensional ADE derived on the principle of conservation of mass and Fick's law of diffusion in general form may be written as,

$$\frac{\partial C}{\partial t}+\frac{1-n_p}{n_p}\frac{\partial F}{\partial t}=\frac{\partial}{\partial x}\left(D(x,t)\frac{\partial C}{\partial x}-u(x,t)C\right), \tag{1}$$

where C is the solute concentration at position x at time t in liquid phase and F is the concentration in the solid phase at time t, n_p is porosity. $D(x,t)$ and $u(x,t)$ are dispersion coefficient and velocity of the flow, respectively. In equation (1), D and u may be constants or functions of independent variables. This equation is solved in which one or both the coefficients either functions of independent variables or both constant. Lapidus and Amundson (1952) considered two cases, namely

$$F=k_1C^n+k_2, \tag{2}$$

and

$$\frac{\partial F}{\partial t}=k_1C^n-k_2, \tag{3}$$

Equilibrium and non-equilibrium relation between the concentrations in the two phases, where k_1 and k_2 are constants of the medium. The relations is linear if $n=1$ and is non-linear if $n>1$. The former relationship is adopted in the present paper. This assumption is generally valid when the adsorption process is fast in relation to the ground-water velocity Cherry et al. (1984). Using equation (2) in equation (1) for $n=1$ we may get,

$$\frac{\partial C}{\partial t}+\frac{1-n_p}{n_p}\frac{\partial\left(k_1C+k_2\right)}{\partial t}=\frac{\partial}{\partial x}\left(D(x,t)\frac{\partial C}{\partial x}-u(x,t)C\right), \tag{4}$$

or

$$R(x,t)\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left(D(x,t)\frac{\partial C}{\partial x}-u(x,t)C\right), \tag{5}$$

where

$R(x,t)=1+\frac{1-n_p}{n_p}k_1$ is the adsorption coefficient.

The dispersion and adsorption parameter is considered inversely proportional to each other. It means when adsorption will be higher then dispersion processes will be slow and vice-versa. It is shown in real and physical situations. Thus we may write,

$$D(x,t) \propto \frac{1}{R(x,t)} \quad \text{or} \quad R(x,t) \propto \frac{1}{D(x,t)}\ , \tag{6}$$

As a consequence of the heterogeneity of the medium, the dispersion coefficient transporting the solute particles spread out is considered spatially dependent. The dispersion is also considered temporally dependent. The expression for dispersion is written in degenerate form as,

$$D(x,t) = D_0 f(mt)(1+ax), \tag{7}$$

where m may be termed as an unsteady parameter of dimension inverse of the dimension of t. While choosing an expression for $f(mt)$, it is ensured that $f(mt)=1$ for $m=0$ and $t=0$.

The former case represents the steady flow. The latter case represents the velocity at the initial stage. Therefore the adsorption parameter and velocity may be written as,

$$R(x,t) = \frac{R_0}{f(mt)(1+ax)} \quad \text{and} \quad u(x,t) = u_0 f(mt), \tag{8}$$

then the equation (1) becomes,

$$\frac{R_0}{f(mt)(1+ax)}\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_0 f(mt)(1+ax)\frac{\partial C}{\partial x} - u_0 f(mt)C \right)\ , \tag{9}$$

Introduce a new independent variable X Jaiswal et al. (2009), using a transformation which is

$$X = -\int \frac{1}{(1+ax)^2}dx, \tag{10}$$

As ax and mt are non-dimensional terms, so the constants u_0 and D_0 in equation (9) may be referred to as uniform velocity of dimension LT^{-1} and the initial dispersion coefficient of dimension L^2T^{-1}, respectively. Using equation (10), equation (9) may be written as

$$\frac{R_0}{f^2(mt)}\frac{\partial C}{\partial t} = a^2 D_0 X^2 \frac{\partial^2 C}{\partial X^2} + \left(a^2 D_0 + au_0\right) X \frac{\partial C}{\partial X}\ , \tag{11}$$

where

$$X = \frac{1}{a(1+ax)}\ .$$

Again using a transformation Crank (1975),

$$T = \int_0^t \frac{f^2(mt)}{R_0} dt \,. \tag{12}$$

An expression of $f(mt)$ is chosen such that for $t = 0$, we get $T = 0$, so that the nature of initial condition does not change. The advection-diffusion equation (11) becomes,

$$\frac{\partial C}{\partial T} = a^2 D_0 X^2 \frac{\partial^2 C}{\partial X^2} + \left(a^2 D_0 + a u_0\right) X \frac{\partial C}{\partial X} \,, \tag{13}$$

Now with the help of other independent variables introduced through the transformation,

$$Z = -\ln aX \,, \tag{14}$$

the variable coefficients of the advection-diffusion equation are reduced to constant coefficients,

$$\frac{\partial C}{\partial T} = a^2 D_0 \frac{\partial^2 C}{\partial Z^2} - a u_0 \frac{\partial C}{\partial Z} \,, \, (0 \le Z < \infty \,,\ T > 0) \,, \tag{15}$$

3. Analytical Solutions

The medium is considered to be of semi-infinite and heterogeneous. For this instance, seepage velocity depends upon time. In a non-porous medium, such as air or a surface water body, velocity is rarely uniform. Since in porous domain like as soil, blood, aquifers and groundwater, the velocity is changed with time and position.

3.1. Continuous pulse type point source condition

It is assumed that initially the medium is solute free. The input point source which is of pulse type be introduced at the origin of the medium. It is assumed C_0 till $t = t_0$ i.e., t_0 is the time when the point source is eliminated and beyond that it is assumed zero. A flux type homogeneous condition is assumed at end of the medium. Thus initial and boundary conditions are as follows,

$$C(x,t) = 0 \;\; (t = 0 \,, x \ge 0) \,, \tag{16}$$

$$C(x,t) = \begin{cases} C_0, & 0 < t \le t_0 \\ 0, & t > t_0, \end{cases} ; \; x = 0, \;\; t > 0, \tag{17}$$

$$\frac{\partial C}{\partial x} = 0 \,, \, (\, x \to \infty \,,\ t \ge 0 \,) \,. \tag{18}$$

The initial and boundary conditions equations (16-18) may be written in the (Z,T) domain as,

$$C(Z,T)=0, \quad (T=0\,,\ Z\geq 0\,), \tag{19}$$

$$C(Z,T)=\begin{cases} C_0,\ 0<T\leq T_0, \\ 0,\ T>T_0, \end{cases};\ Z=0, \tag{20}$$

$$\frac{\partial C}{\partial Z}=0\,,\ (Z\to\infty\,,\ T\geq 0\,). \tag{21}$$

Applying Laplace transformation on equation and using back transformations equations (14), (12) and (10), the analytical solution may be written as using table of van Genutchen and Alves (1982),

$$C(x,T)=\frac{C_0}{2}\left[G_1(x,T)+G_2(x,T)\right],\ 0<T\leq T_0\,, \tag{22a}$$

$$C(x,T)=\frac{C_0}{2}\left[G_1(x,T)-G_1(x,T-T_0)+G_2(x,T)-G_2(x,T-T_0)\right],T>T_0\,, \tag{22b}$$

where

$$G_1(x,T)=erfc\left\{\frac{\ln(1+ax)}{2\sqrt{a^2D_0T}}-\beta\sqrt{T}\right\},$$

$$G_1(x,T)=\exp\left\{\left(\frac{u_0}{aD_0}\right)\ln(1+ax)\right\}erfc\left\{\frac{\ln(1+ax)}{2\sqrt{a^2D_0T}}+\beta\sqrt{T}\right\},$$

$$T=\int_0^t\frac{f^2(mt)}{R_0}dt \text{ and } \beta^2=\frac{u_0^2}{4D_0}\,.$$

3.2. Varying pulse type input point source condition

The input point source condition defined by equation (17) is of uniform nature. But in real cases, due to increasing human and other responsible activities such as in garbage disposal site, pesticides in the agriculture field, the infiltration of pollutants from the earth surface into an aquifer may increase. Since all human activity is closely connected with the natural environment. This more realistic scenario may be defined by a condition of mixed type of non-homogeneous nature which is

$$-D(x,t)\frac{\partial C(x,t)}{\partial x}+u(x,t)C(x,t)=\begin{cases} u_0C_0,\ \ 0<t\leq t_0, \\ 0,\ \ t>t_0, \end{cases};(x=0). \tag{23}$$

Now to proceed further, here expression for $f\left(mt\right)$ will be chosen. Let the expression be of exponentially decreasing nature. Let $f\left(mt\right)=\exp(-mt)$. From equation (12), we get the expression for new time variable as,

$$T=\frac{1}{2mR_0}\left[1-\exp(-2mt)\right]. \tag{24}$$

From the above expression of T, we may write $f\left(mt\right)$ in terms of T as follows,

$$f\left(mt\right)=\exp(-mt)=\left(1-2mR_0T\right)^{1/2}. \tag{25}$$

So condition (23) becomes in terms of (Z,T) by using previous transformations equations (12) and (14),

$$-\frac{\partial C(Z,T)}{\partial Z}+\frac{u_0}{aD_0}C(Z,T)=\begin{cases}-\dfrac{u_0C_0}{aD_0}\left(1+mR_0T\right), & 0<T\le T_0,\\ 0, & T>T_0,\end{cases} \tag{26}$$

where the series $o(m^2)$ from the binomial expansion of right side of equation (25) is neglected as m is chosen much smaller, i.e. less than 1.0. Applying Laplace transformation on equation and using back transformations equations (14), (12) and (10), the analytical solution may be written as using table of van Genutchen and Alves (1982):

$$C(x,T)=\frac{C_0}{2}\left[G_{11}(x,T)+G_{22}(x,T)\right],\ \ 0<T\le T_0\ , \tag{27a}$$

$$C(x,T)=\frac{C_0}{2}\left[G_{11}(x,T)-G_{11}(x,T-T_0)+G_{22}(x,T)-G_{22}(x,T-T_0)\right],T>T_0\ , \tag{27b}$$

where

$$G_{11}(x,T)=\left[2u_0\sqrt{\frac{T}{\pi D_0}}\exp\left(\frac{u_0\ln(1+ax)}{2aD_0}-\frac{u_0{}^2T}{4D_0}-\frac{\ln(1+ax)^2}{4a^2D_0T}\right)+\text{erfc}\left(\frac{\ln(1+ax)-au_0T}{2a\sqrt{D_0T}}\right)\right.$$
$$\left.-\left(1+\frac{u_0\ln(1+ax)}{aD_0}+\frac{u_0{}^2T}{D_0}\right)\exp\left(\frac{u_0\ln(1+ax)}{aD_0}\right)\text{erfc}\left(\frac{\ln(1+ax)+au_0T}{2a\sqrt{D_0T}}\right)\right],$$

$$G_{22}(x,T)=\frac{mD_0R_0}{u_0{}^2}\left\{2u_0\sqrt{\frac{T}{\pi D_0}}\left(1+\frac{u_0\ln(1+ax)}{2aD_0}+\frac{u_0{}^2T}{2D_0}\right)\right.$$

$$\times\exp\left(\frac{u_0\ln(1+ax)}{2aD_0}-\frac{u_0{}^2T}{4D_0}-\frac{\ln(1+ax)^2}{4a^2D_0T}\right)$$

$$-\left(1+\frac{u_0\ln(1+ax)}{aD_0}-\frac{u_0{}^2T}{D_0}\right)\mathrm{erfc}\left(\frac{\ln(1+ax)-au_0T}{2a\sqrt{D_0T}}\right)$$

$$+\left(1-\frac{u_0{}^2T}{D_0}-\frac{u_0{}^2}{2a^2D_0{}^2}\left\{\ln(1+ax)+au_0T\right\}^2\right)$$

$$\left.\left.\times\exp\left(\frac{u_0\ln(1+ax)}{aD_0}\right)\mathrm{erfc}\left(\frac{\ln(1+ax)+au_0T}{2a\sqrt{D_0T}}\right)\right\}\right],$$

where

$$T=\frac{1}{2mR_0}\left[1-\exp(-2mt)\right].$$

4. Results and Discussion

A new position variable X equation (10) introduced through a transformation which is like the transformation $Z=x-ut$ Bear (1972) i.e., as a moving coordinate which eliminates the advection term from the ADE with constant coefficient. The effects of heterogeneity and unsteadiness are studied and illustrated. More expressions for $f(mt)$ may be chosen. Thus an analytical solution of ADE with variable coefficients describing solute transport from the perspective Schiedegger's (1957) theory has been obtained by using the Laplace Integral Transform Technique (LITT).

The solute concentration distribution are evaluated from the analytical solutions (22a,b) for continuous pulse type input point source and (27a,b) for varying pulse type input point source in the context of contaminants dispersion along the flow in a finite domain $0\le x(\mathrm{km})\le 10$ of semi-infinite medium. The input data are considered as $C_0=1.0$, $u_0=0.58$ (km / month), $D_0=0.93$ (km^2 / month) in the presence of the source $t(\mathrm{month})=1$, 3 and 5 and in the absence of the source $t(\mathrm{month})=7$, 9 and 11. In addition to these, the heterogeneous parameter $a=0.1$ (km)$^{-1}$, unsteady parameter $m=0.1(\mathrm{month})^{-1}$ and adsorption coefficient $R_0=1.25$ have been taken for both cases (3.1 and 3.2). In all figures, horizontal axis shows position while vertical axis represents the concentration (C/C_0).

Figures 1 and 2 are drawn for continuous pulse type input point source. The three bold solid curves in Figures 1 and 2, represents the distribution of solute concentration values in the presence of the source and absence of the source at different time $t(\mathrm{month})$ respectively, where the elimination of the source of the pollution is $t_0(\mathrm{month})=6.0$. It is observed that, in the presence of the source, solute concentration values are increase with increasing time at particular position and after elimination of the source of the pollution the solute concentration values are decreases with increasing time at particular position.

Figures 3 and 4 illustrate the concentration profile for varying pulse type input point source. The three bold solid curves in Figures 3 and 4 represents the concentration values at various time $t(\text{month})$. The concentration levels at the source boundary are higher for higher time in Figure 3. The concentration decreases with position for all time in Figure 4. On other hand in the absence of the source of pollution $(t > t_0)$ the concentration levels is lower for the higher adsorption.

The parameters a, m and R play an important role on concentration profile in the domain. In all figures, comparisons of three parameters i.e., heterogeneous parameter a is shown by bold dashed line, adsorption parameter R_0 is shown by thin dashed line and unsteady parameter m is shown by thin solid line. Distribution of concentration for $a = 0.2\ (\text{meter})^{-1}$, $m = 0.25(\text{day})^{-1}$ and $R_0 = 1.45$ at a particular time $t(\text{month}) = 3$ are shown in the Figures 1 and 3, i.e., in the presence of source at $t(\text{month}) = 3.0$ and in Figures 2 and 4, i.e., in the absence of source concentration at time $t(\text{month}) = 9$. It is observed that from all figures, the distribution of concentration at particular time with heterogeneous parameter a increases and decreases with adsorption and unsteady parameters. These show that the physical phenomena of present problem and it are found in real scenario. Distribution of solute concentration with heterogeneity, unsteadiness and adsorption parameters are discussed in this section with suitable figures. This study different from other literatures since in several papers discussed only dispersion and advection coefficients where as in this paper all parameters are discussed i.e., unsteadiness, heterogeneity including adsorption coefficient which reflect the most physical problems.

5. Conclusion

An analytical solution of one-dimensional advection-dispersion equation is obtained along unsteady longitudinal flow through a semi-infinite heterogeneous medium. Adsorption coefficient is considered temporally and spatially–dependent function and inversely proportional to the dispersion parameter. The Laplace Transformation Technique (LTT) is used to obtain the analytical solution by introducing certain new independent variables through separate transformations for input source which is of pulse type. The changes in distribution of concentration due to adsorption, dispersion and unsteadiness by choosing appropriate values of their respective parameters are studied in present paper. From this study, it is found that when adsorption coefficient is higher the dispersion coefficient is lower and vise-versa. The analytical solutions of ADE validate the numerical solutions and have many applications in surface water, groundwater, environment, industries etc., pollution along with heterogeneity and unsteadiness with effective adsorption coefficient.

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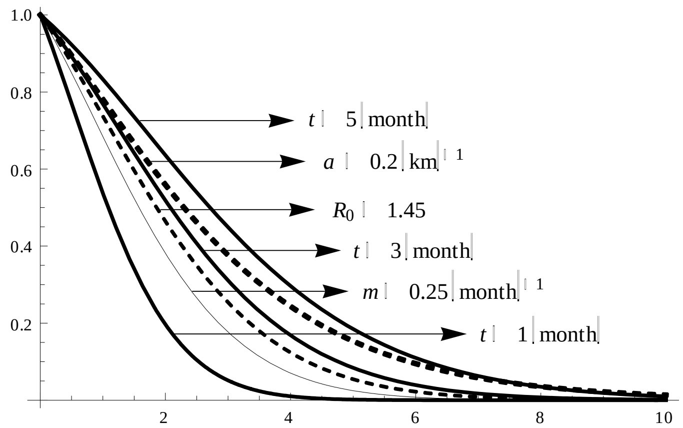

Figure 1. Distribution of solute in the presence of source ($t < t_0$) at different time for equation (22a)

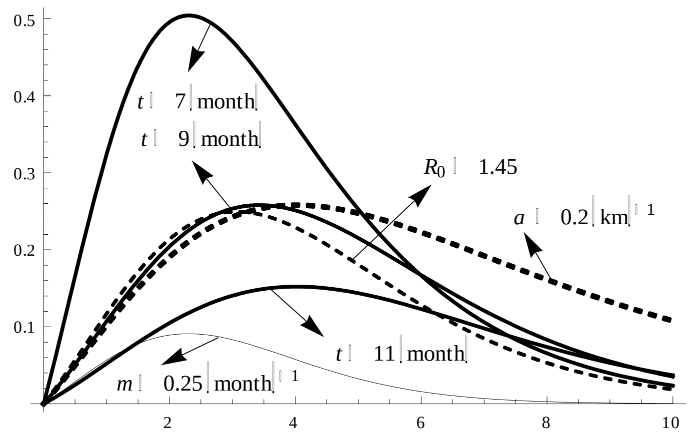

Figure 2. Distribution of solute in the absence of source ($t > t_0$) at different time for equation (22b)

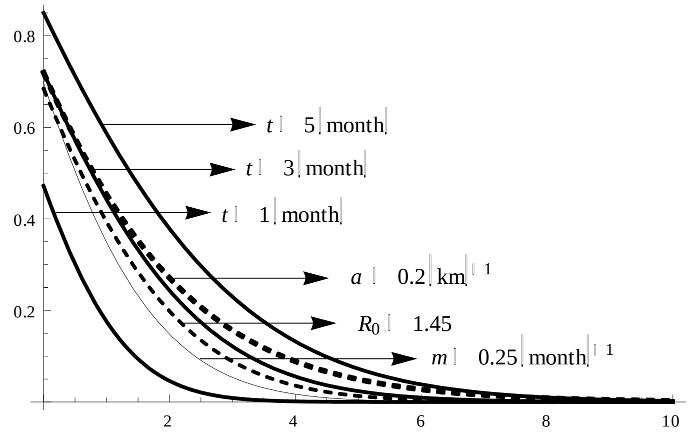

Figure 3. Distribution of solute in the presence of source ($t < t_0$) at different time for equation (27a)

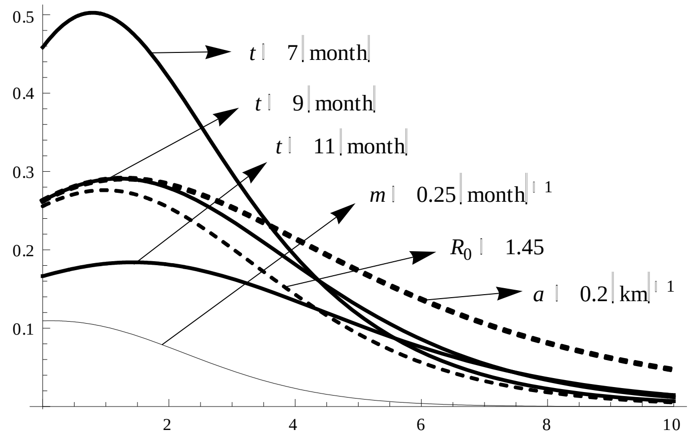

Figure 4. Distribution of solute in the absence of source ($t > t_0$) at different time for equation (27b)