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One-Dimensional Advection-Dispersion Equation of Pollutant Concentration

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Abstract
The purpose of this study is to obtain analytical solutions for the unsteady one-dimensional advection-dispersion equations that are used to describe the pollutant concentration in a river. The unsteady flow in a river is considered as a one-dimensional characterized by a single spatial distance whereas the concentration of pollutant is assumed to be variedwith time along the length of the river. With the application of Laplace Transform technique and addition of transform variable, the model equations can be solved and analyzed. Results obtained have shown that the concentration of pollutant increases from upstream to downstream. In zero dispersion case, the pollutant concentration is caused only by pure convection and rate of pollutant addition along the river. These mathematical models and their analytical solutions can predict water quality and provide reliable tools for water management in affected river areas.

Keywords One-Dimensional Advection-Dispersion Equation; Pollutant Concentration; Laplace Transform.

1. Introduction

The advection-diffusion equation (ADE) explains the flow of heat, particles, oil reservoir simulations, transport of mass and energy, global weather production or other physical quantities in conditions where there are both diffusion and convection or advection. Advection is understood as the motion of particles along the bulk flow while diffusion is the net movement of particles from high concentration to a lower concentration.

During the initial works while obtaining the analytical solutions of dispersion problems in ideal conditions, the basic approach was to reduce the advection–diffusion equation into a diffusionequation by eliminating the convective term(s). It was done either by introducing moving co- ordinates (Ogata and Banks 1961; Harleman and Rumer 1963; Bear 1972; Guvanasen and Volker 1983; Aral and Liao 1996; Marshal *et al* 1996) or by introducing another dependent variable (Banksand Ali 1964; Ogata 1970; Lai and Jurinak 1971; Marino 1974 and Al-Niami and Rushton 1977). Then, Laplace transformation technique has been used to get desired solutions. In addition to thismethod, Hankel transform method, Aris moment method, perturbation approach, method using Green's function, superposition method has also been used to get the analytical solutions of the advection–diffusion equations in one, two and three dimensions. Yet, Laplace transformation technique has been commonly used because of being simpler than other methods and the analytical solutions using this method being more reliable in verifying the numerical solutions in terms of accuracy and the stability.

Analytical solutions for one-dimensional transport in composite media are often derived with Laplace transforms (Carslaw and Jaeger 1959) and sometimes with Green's functions. Adjoin solution arbitrary initial and boundary conditions, as well as with different variations of dispersion and velocity, for which analytical solutions are not available (Djordjevich and Savovic 2013; Savovic and Djordjevich 2012, 2013; Savovic and Caldwell 2003, 2009).

Mathematical models have been used extensively to predict water quality and to provide reliable tools for water quality management in affected areas. According to research by Martinus Th. et al (2013) on the exact analytical solutions for contaminant transport in rivers, mathematical models have long proved useful for analyzing and predicting the transport of contaminants in streams. Due to the many complexes and often nonlinear physical, chemical and biological processes affecting contaminant transport in streams and rivers, numerical models are now increasingly used for prediction purposes (e.g., Anderson and Phanikumar, 2011; O'Connor et al., 2009; Runkel, 1998; Runkel and Chapra, 1993). Still, analytical and quasi-analytical approaches are useful for simplified analyses of a variety of contaminant transport scenarios, especially for relatively long spatial and time scales, when insufficient data are available to warrant the use of a comprehensive numerical model, and for testing numerical models.

The paper released by Zanke, Patzold and von Rohden (2016) explored analytical solutions for reactive transport in rivers and their application in testing numerical models. The development and validation of analytical solutions for reactive transport in rivers used the idealized Homogeneous Reactor-in-Series (HRS) model. Analytical solutions for the ADE in rivers are represented by the HRS model to demonstrate the pollutant transport and reaction processes inriver systems. In addition to that, sensitivity analysis is also used to investigate the influence of different parameters on reactive transport processes. The analysis can deduce the effects of flow velocity, reaction rate coefficients, and initial concentrations on pollutant transport and transformation in rivers. On the other hand, Ristic and Papic (2019) explored another possible method to present an approximate analytical solution based on a perturbation method. The perturbation method is used to obtain a solution that captures the time- dependent behavior of the dispersion coefficient.

Singh et al. (2018) studied analytical solutions for solute transport in rivers with time-varying velocity and dispersion coefficient. It focused on the solute transport processes in rivers, specifically considering the time-varying natureof velocity and dispersion coefficients. The paper emphasized that the velocity and dispersion coefficients in rivers can exhibit temporal variations due to factors such as diurnal variations, tidal effects, and flow regime changes. These variations significantly influence solute transport processes and need to be accounted for in accurate modelling. The method used is the method of characteristics, a mathematical technique used for solving partial differential equations, to derive analytical solutions for solute transport in rivers with time-varying velocity and dispersion coefficients.

In more recent years, Keshav Paudel (2021) further researching advection-dispersion equation of pollutant concentration using Laplace Transformation. The main assumptions in the research are similar such as one-dimensional steady state flow with constant dispersion coefficient and negligible chemical reactions. In addition to that, it also shared similar conditions such as homogeneous and isotropic medium where the pollutant is transported in uniform properties in all directions. It is later determined via numerical studies that the pollutant concentration along with time is caused only by pure convection and rate of pollutant addition along the river. If the added pollutant rate along the river is in a very small amount, the variation of pollutant concentration along the river at different times coincides with each other.

This present study will formulate the mathematical model of one-dimensional equation of pollutant concentration which includes a source term and is treated as two different regions of upstream and downstream.

2. Mathematical Model

This study will focus on obtaining an analytical solution for one-dimensional advection-diffusion equation using Laplace transform. In the river, the unsteady flow is considered one-dimensional characterized by a single spatial distance x (m).

It is established that the river is divided into two regions x ≥ 0 and x ≤ 0 and the origin is at $x = 0$. The variation of $C(x, t)$ with the time t from t = 0 up to $t \rightarrow \infty$ is also taken into account in this problem. The specialcase for which the dispersion coefficient D = 0 is studied in detail.

The governing equations of one-dimensional ADE representing pollutant concentration along a river can be written as (Pimpunchat et al, 2009; Ali S Wadi et al, 2014):

$$\frac{\partial\,(\mathrm{AC}_1)}{\partial \mathrm{t}} = D\frac{\partial^2(\mathrm{AC}_1)}{\partial x^2} - \frac{\partial(\mathrm{vA}C_1)}{\partial \mathrm{x}} - k_1\frac{X}{X+k}AC_1, \qquad x \le 0, \qquad t > 0$$

$$\frac{\partial\,(\mathrm{AC}_2)}{\partial \mathrm{t}} = D\frac{\partial^2(\mathrm{AC}_2)}{\partial x^2} - \frac{\partial(\mathrm{vA}C_2)}{\partial \mathrm{x}} - k_1\frac{X}{X+k}AC_2 + q\,, \qquad 0 \le x < L \le \infty, \qquad t > 0$$

C_1 and C_2 are the concentrations of the pollutant in the two regions respectively (kgm^{-3})
A is the cross-section area of the river (m^2)
D is the dispersion coefficient of pollutant in x direction $(m^2.day^{-1})$
v is the water velocity in the x direction $(m.day^{-1})$
$k_1$is the degradation rate coefficient for pollutant (day^{-1})
k is the half-saturated oxygen demand concentration for pollutant decay (kgm^{-3})
$X(x,t)$ is the concentration of the dissolved oxygen within the river (kgm^{-3})

The initial and boundary conditions associated are as follows;

$$C_1(x,0) = C_2(x,0) = 0$$

$$C_1(0,t) = C_2(0,t), \qquad t > 0$$

$$\frac{dC_1(0,t)}{dx} = \frac{dC_2(0,t)}{dx}, \qquad t > 0$$

3. Analytical Solution

Laplace transformation technique is used to get the analytical solution. It is estimated that the concentration of pollutant increases as x increases from the upstream to downstream. It is also predicted that the pollutant concentration is caused only by pure convection and rate of pollutant addition along the river.

By implementing the laplace transform method, the following solutions can be obtained.

$$\tilde{C}_1(x,p) = \frac{D}{k_1+p}.\alpha_1 exp\left[x\left(\delta + \sqrt{\frac{\alpha+p}{D}}\right)\right] + \frac{D}{k_1+p}.\alpha_2 exp\left[x\left(\delta - \sqrt{\frac{\alpha+p}{D}}\right)\right]$$

$$\tilde{C}_2(x,p) = \frac{q}{Ap(k_1+p)} + \frac{D}{k_1+p}.\alpha_3 exp\left[x\left(\delta + \sqrt{\frac{\alpha+p}{D}}\right)\right] + \frac{D}{k_1+p}.\alpha_4 exp\left[x\left(\delta - \sqrt{\frac{\alpha+p}{D}}\right)\right]$$

$\alpha_1, \alpha_2, \alpha_3$ and α_4 are constants that can be determined using the boundary condition, $\tilde{C}_1(0,p) = \tilde{C}_2(0,p)$ and $\frac{d\tilde{C}_1(0,p)}{dx} = \frac{d\tilde{C}_2(0,p)}{dx}$.

The inverse of the equations have been obtained by taking the inverse Laplace transformation and applying the convolution theorem and shift theorem. Thus, $C_1(x,t)$and $C_2(x,t)$ are given by:

$$C_1(x,t) = \frac{q}{4k_1A}\{\exp[(\delta-\beta)x]\}erfc\left(-\frac{x}{2\sqrt{Dt}}+\sqrt{\alpha t}\right)+\frac{q}{4k_1A}\{\exp[(\delta+\beta)x]\}erfc\left(-\frac{x}{2\sqrt{Dt}}-\sqrt{\alpha t}\right)$$
$$-\frac{q}{2k_1A}\{\exp[-k_1t]\}erfc\left(-\frac{x}{2\sqrt{Dt}}+\sqrt{(\alpha-k_1)t}\right)$$
$$-\frac{q}{4k_1A}\frac{\delta}{\beta}\{\exp[(\delta+\beta)x]\}erfc\left(-\frac{x}{2\sqrt{Dt}}-\sqrt{\alpha t}\right)$$
$$+\frac{q}{4k_1A}\frac{\delta}{\beta}\{\exp[(\delta-\beta)x]\}erfc\left(-\frac{x}{2\sqrt{Dt}}+\sqrt{\alpha t}\right)$$

where $x \le 0$.

$$C_2(x,t) = \frac{q}{k_1A}-\frac{q}{k_1A}\{\exp[-k_1t]\}-\frac{q}{4k_1A}\{\exp[(\delta-\beta)x]\}erfc\left(\frac{x}{2\sqrt{Dt}}-\sqrt{\alpha t}\right)$$
$$+\frac{q}{4k_1A}\frac{\delta}{\beta}\{\exp[(\delta+\beta)x]\}erfc\left(\frac{x}{2\sqrt{Dt}}+\sqrt{\alpha t}\right)+\frac{q}{2k_1A}\{\exp[-k_1t]\}erfc\left(\frac{x}{2\sqrt{Dt}}+\sqrt{(\alpha-k_1)t}\right)$$
$$-\frac{q}{4k_1A}\{\exp[(\delta+\beta)x]\}erfc\left(\frac{x}{2\sqrt{Dt}}+\sqrt{\alpha t}\right)-\frac{q}{4k_1A}\{\exp[(\delta-\beta)x]\}erfc\left(\frac{x}{2\sqrt{Dt}}-\sqrt{\alpha t}\right)$$

where $x \ge 0$.

By substituting the dimensionless variables into the equation,

$$C_1^*(x^*,t^*) = \frac{1}{4}\{\exp[(\delta^*-\beta^*)x^*]\}erfc\left(\frac{-x^*+2D^*\beta^*t^*}{2\sqrt{D^*t^*}}\right)+\frac{1}{4}\{\exp[(\delta^*+\beta^*)x^*]\}erfc\left(\frac{-x^*+2D^*\beta^*t^*}{2\sqrt{D^*t^*}}\right)$$
$$-\frac{1}{2}\{\exp[-t^*]\}erfc\left(\frac{-x^*+2D^*\beta^*t^*}{2\sqrt{D^*t^*}}\right)-\frac{\delta^*}{4\beta^*}\{\exp[(\delta^*+\beta^*)x^*]\}erfc\left(\frac{-x^*-2D^*\beta^*t^*}{2\sqrt{D^*t^*}}\right)$$
$$+\frac{\delta^*}{4\beta^*}\{\exp[(\delta^*-\beta^*)x^*]\}erfc\left(\frac{-x^*+2D^*\beta^*t^*}{2\sqrt{D^*t^*}}\right)$$

$$C_2^*(x^*,t^*) = 1-\exp[-t^*]-\frac{\delta^*}{4\beta^*}\{\exp[(\delta^*+\beta^*)x^*]\}erfc\left(\frac{x^*-2D^*\beta^*t^*}{2\sqrt{D^*t^*}}\right)$$
$$+\frac{\delta^*}{4\beta^*}\{\exp[(\delta^*+\beta^*)x^*]\}erfc\left(\frac{x^*+2D^*\beta^*t^*}{2\sqrt{D^*t^*}}\right)+\frac{1}{2}\{\exp[t^*]\}erfc\left(\frac{x^*-2D^*\beta^*t^*}{2\sqrt{D^*t^*}}\right)$$
$$-\frac{1}{4}\{\exp[(\delta^*+\beta^*)x^*]\}erfc\left(\frac{x^*+2D^*\beta^*t^*}{2\sqrt{D^*t^*}}\right)-\frac{1}{4}\{\exp[(\delta^*-\beta^*)x^*]\}erfc\left(\frac{x^*-2D^*\beta^*t^*}{2\sqrt{D^*t^*}}\right)$$

<u>Special Case of Zero Dispersion</u>

Another case is the model including time and zero dispersion, where $r \gg 0$ and is approximately zero. Hence, the case equation is reduced to:

$$\frac{\partial(AC_3)}{\partial t} = \frac{\partial(vAC_3)}{\partial x} - k_1AC_3 + q$$

It is later solved by applying Laplace transformation and subsequently summarized to this form:

$$C_3(x,t) = \frac{q}{k_1A}-\frac{q}{k_1A}\{\exp[-(k_1t)]\}+p_1\{exp-(k_1t)]\}-\frac{q}{k_1A}\left\{\exp\left[-\left(\frac{k_1}{v}\right)x\right]\right\}+\frac{q}{k_1A}\left\{\exp\left[-\left(\frac{k_1}{v}x+k_1t\right)\right]\right\}$$
$$-p_1\left\{\exp\left[-\left(\frac{k_1}{v}x+k_1t\right)\right]\right\}+p_2\left\{\exp\left[-\left(\frac{k_1}{v}\right)x\right]\right\}$$

Its dimensionless form is as follows:

$C_3^*(x^*,t^*) = 1-\exp[-t^*]+p_1^*\exp[-t^*]-\exp[-x^*]+\exp[-(x^*+t^*)]-p_1^*\{\exp[-(x^*+t^*)]\}+$
$p_2^*\{\exp[-x^*]\}$

<u>Special Case of Steady State Solution</u>

The steady state solution is obtained by taking the limit of $t \to \infty$. Hence, in the case of $C_1(x)$, $C_2(x)$

and $C_3(x)$ take the form of;

$$C_1(x) = \frac{q}{k_1 A}\left(\frac{\beta-\delta}{2\beta}\right)\{\exp[(\delta+\beta)x]\} \quad , x \le 0$$

$$C_2(x) = \frac{q}{k_1 A}\left(1-\left(\frac{\beta+\delta}{2\beta}\right)\right)\{\exp[(\delta-\beta)x]\} \quad , x \ge 0$$

$$C_3(x) = \frac{q}{k_1 A}\left(1-\left\{\exp\left[-\left(\frac{k_1}{v}\right)x\right]\right\}\right)$$

For $x \le 0$, the time t has very small effect on C_1. For $x \ge 0$, as t increases C_2 increases and reaches its maximum value as $t \to \infty$.

<u>Special Case of Time and Zero Dispersion</u>

Another case to be explored is the model including time and zero dispersion, $D = 0$. The equation is as follows:

$$\frac{\partial \tilde{C}_3(x,p)}{\partial x} + (k_1+p)\frac{\tilde{C}_3(x,p)}{v} = \frac{1}{v}\left(p_1 + \frac{q}{Ap}\right)$$

Where $p > 0$. This p represents the Laplace transform variable. Therefore, the general solution of the equation is

$$\tilde{C}_3(x,p) = \left(\frac{q}{Ap}+p_1\right)\frac{1}{(k_1+p)} + \alpha_5\{\exp\,[-\left(\frac{k_1+p}{v}\right)x]\}$$

α_5 is an arbitrary constant. When $\tilde{C}_3(0,p)=\frac{p_2}{p}$ is applied,

$$\frac{p_2}{p} = \left(\frac{q}{Ap}+p_1\right)\frac{1}{(k_1+p)} + \alpha_5\{\exp\,[-\left(\frac{k_1+p}{v}\right)0]\}$$

$$\tilde{C}_3(x,p) = \frac{q}{Ap(k_1+p)} + \frac{p_1}{k_1+p} - \frac{q}{Ap(k_1+p)}\left\{\exp\left[-\left(\frac{k_1+p}{v}\right)x\right]\right\} - \frac{p_1}{k_1+p}\left\{\exp\left[-\left(\frac{k_1+p}{v}\right)x\right]\right\} + \frac{p_2}{p}\left\{\exp\left[-\left(\frac{k_1+p}{v}\right)x\right]\right\}$$

The inverse of Laplace transform of equation is;

$$\tilde{C}_3(x,t) = \frac{q}{A}(\frac{1}{k_1} - \frac{1}{k_1}\{\exp[-(k_1t)]\}) + p_1\{exp-(k_1t)]\} - \frac{q}{A}(\frac{1}{k_1} - \frac{1}{k_1}\{\exp[-(k_1t)]\})$$
$$\otimes\left(\exp\left[-\left(\frac{k_1}{v}\right)x\right]H\left(t-\frac{x}{v}\right)\right) - p_1\left\{\exp\left[-\left(\left(\frac{k_1}{v}\right)x+k_1t\right)\right]H\left(t-\frac{x}{v}\right)\right\}$$
$$+ p_2\left\{\exp\left[-\left(\left(\frac{k_1}{v}\right)x\right)\right]H\left(t-\frac{x}{v}\right)\right\}$$

Where $H\left(t-\frac{x}{v}\right)$ is a Heaviside function defined by:

$H\left(t-\frac{x}{v}\right) = 1$ if $t > \frac{x}{v}$

and

$H\left(t-\frac{x}{v}\right) = 0$ if $t < \frac{x}{v}$

Additionally, $\otimes$ also denotes the multiplication operation in the Convolution Theorem. By using the Convolution Theorem equation,

$$C_3(x,t) = \frac{q}{k_1A} - \frac{q}{k_1A}\{\exp[-(k_1t)]\} + p_1\{exp - (k_1t)]\} - \frac{q}{k_1A}\left\{\exp\left[-\left(\frac{k_1}{v}\right)x\right]\right\} + \frac{q}{k_1A}\left\{\exp\left[-\left(\frac{k_1}{v}x + k_1t\right)\right]\right\} - p_1\left\{\exp\left[-\left(\frac{k_1}{v}x + k_1t\right)\right]\right\} + p_2\left\{\exp\left[-\left(\frac{k_1}{v}\right)x\right]\right\}$$

Where $t > \frac{x}{v}$. To write the equation in dimensionless form, the following dimensionless variables are used:

$$x^* = \frac{k_1}{v}x, \qquad t^* = k_1t, \qquad C_3^*(x^*,t^*) = \frac{C_3(x,t)}{\frac{q}{k_1A}}, \qquad p_1^* = \frac{p_1}{\frac{q}{k_1A}}, \qquad p_2^* = \frac{p_2}{\frac{q}{k_1A}}$$

Where $\frac{v}{k_1}$ scale for length and $\frac{q}{k_1A}$ scale for concentration. Hence,

$$C_3^*(x^*,t^*) = 1 - \exp[-t^*] + p_1^*\exp[-t^*] - \exp[-x^*] + \exp[-(x^* + t^*)] - p_1^*\{\exp[-(x^* + t^*)]\} + p_2^*\{\exp[-x^*]\}$$

In the steady state case where $t \to \infty$,

$$C_3(x) = \frac{q}{k_1A} - \frac{q}{k_1A}\left\{\exp\left[-\left(\frac{k_1}{v}\right)x\right]\right\} + p_2\left\{\exp\left[-\left(\frac{k_1}{v}\right)x\right]\right\}$$

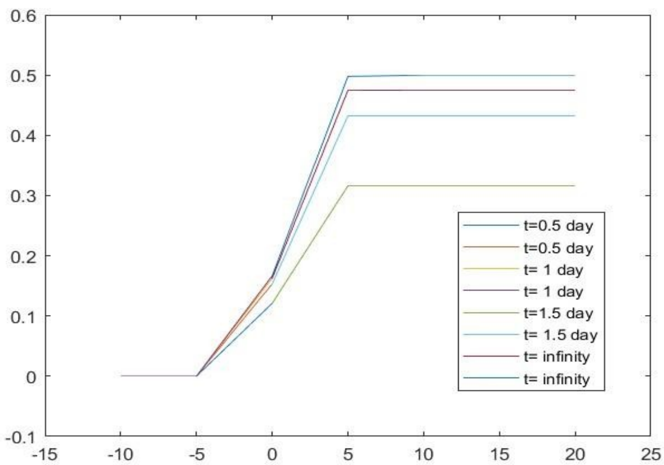
For the special case when $p_2 = 0$, the equation becomes as follows;

$$C_3(x) = \frac{q}{k_1A}\left(1 - \left\{\exp\left[-\left(\frac{k_1}{v}\right)x\right]\right\}\right)$$

4. Result and Discussion

Analytical solutions obtained from previous research have ignored the solution in the important interval of the time t, where $0 \le t \le \infty$. However, this solution in this particular period is important due to the fact that the remediation by aeration occurs in this period of time t, before the pollutant concentration reaches its maximum values as $t \to \infty$. Hence, this paper has been able to overcome this drawback and the pollutant concentration at any time t in the period $0 \le t \le \infty$ can beobtained.

In order to showcase the findings, MATLAB, a programming and numeric computing platform is used to analyze the data obtained.



zFigure 1 Analytical Unsteady State Solution with Dispersion for $C_1(x,t)$and $C_2(x,t)$at different time, t

Figure 1 shows the variation of (C_1, C_2) in the range of $-10 \le x \le 20$ (m) with the time t for the case when $D \ne 0$, for t = 0.5, t = 1.0 and t = 1.5 (in days) and as t approaches infinity. In orderto test the model, the parameters, A, v, q and D are taken to be equal to 1 and k_1 = 2. Based on the figure, it can be deduced that the time, t, has very small or minor effect on the pollutant concentration (C_1) for when the single spatial distance $x \leq 0$.

Generally, it can be analyzed that the concentration of pollutant increases as x increases from upstream to downstream.

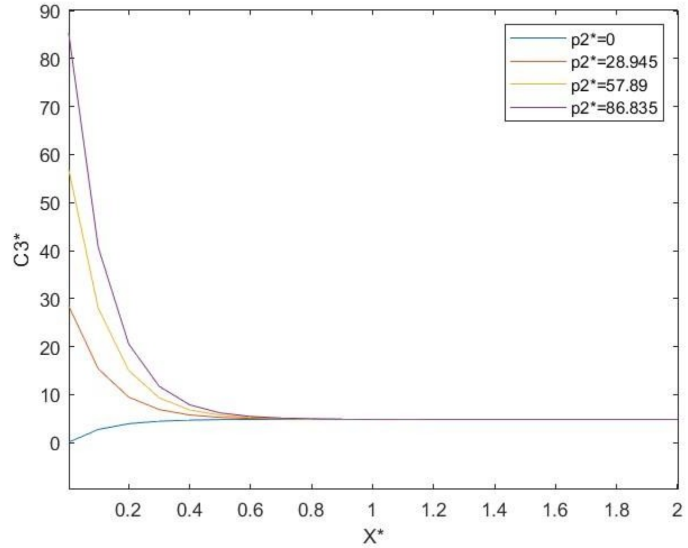


Figure 2 $C_3^*(x^*, t^*)$ as a function of space and time along the river with different values of p_2^* where p_1^* and t^* are constant

Next, Figure 2 shows the variation of C_3^* along the river with different values of p_2^*. The other values are as follows; $q = 0.06kgm^{-1}day^{-1}, k_1 = 8.27\ day^{-1}, A = 2100m^2$, $p_1 = 0, 0.0001, 0.0002, 0.0003kgm^{-3}$, $p_1^* = 2894.5, t^* = 6.616$. Based on the figure, for $p_2^* = 0$ (water without pollution) from the upstream of the river $x^* = 0,$ as x^* increases, C_3^* also increases due to the presence of p_1^*. For the other values of p_2^*, x^*increases causes C_3^* to decrease. Last but not least, at any cross-section where x^* = constant, C_3^* increases as p_2^* increases.

Special Case of Steady State Solution

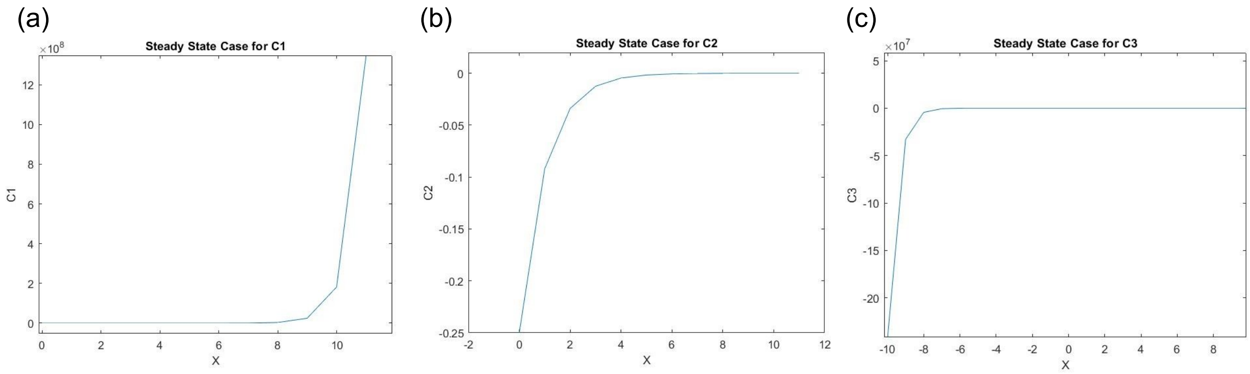


Figure 3 Steady State Case for C_1, C_2 and C_3

In the context of the advection-dispersion equation (ADE), the steady state case refers to a scenario where the concentration distribution of a substance being transported remains constant overtime. In other words, there is no change in the concentration of pollutant in the medium as time progresses. These are the equations for $C1(x)$, $C2(x)$ and $C3(x)$ as $t \rightarrow \infty$.

Conclusion

Using Laplace transformational method, the study derived analytical solutions for the unsteady pollutant concentration $C(x,t)$ in a one -dimensional advection-dispersion equation. This research is built upon the previous work by Pimpunchat et al. (2007), which focused on the steady-state case. The obtained solutions predicted the pollutant concentration as a function of space and time, considering various flow parameters. To simplify the analysis, the solution for pollutant concentration is expressed in dimensionless form as $C_1^*(x^*,t^*)$ and $C_2^*(x^*,t^*)$, both of which depend on only two dimensionless parameters $\frac{q}{k_1 A}$, representing the ratio of advection to dispersion and δ^*, representing the distance over which pollutant is transported. Through numerical studies, it is revealed that the variation of $C_3^*(x^*,t^*)$ increased as one of the dimensionless parameters (time, initial pollution at source) increased while holding the other two parameters constant. Furthermore, it is also found that the variation of C_3^* with time t^* is negligible for the special case when $p_1^* = p_2^* = 0$. In closing, it is generally acknowledged that as the distance from the pollution source (x) increases, the concentration of pollutant (C) approaches a constant value.

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