Proceedings of Science and Mathematics
Faculty of Science, Universiti Teknologi Malaysia
Vol. 18, 2023, page 207 – 212

Analytical Solution for Steady and Coupled Advection-Dispersion Equation of Pollutant Concentration in River

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Abstract
The advection-dispersion equation (ADE) is a commonly used mathematical model for studying pollutant transport and dispersion in rivers. It describes the movement and spreading of a pollutant as a result of advection (flow) and dispersion processes. This research project studies the mathematical model of coupled ADE describing the pollutant and dissolved oxygen concentrations. Specifically, to obtain the analytical solution of steady and coupled ADE with source term and with dispersion. The model is used to observe the concentrations by taking the dimension along the river together with the support of graphs obtained using MATLAB. The result indicates that the concentration of pollutant will increase along the river and hence, the concentration of dissolved oxygen will decrease along the river due to reaction with pollutants.

Keywords: Pollutant; dissolved oxygen; concentration; dispersion; analytical solution

1. Introduction

Fluid movement involves both advection and diffusion. During advection, properties are moved by the fluid's bulk motion as the fluid's velocity field is not zero. Advection, in accordance to Phillips and Castro (2014), is the mechanical movement of solutes in conjunction to the bulk flux of fluid. Advection is driven by the gradient in the total mechanical energy, often referring to the gravitational potential energy gradient. On the other hand, diffusion is the movement of molecules under a concentration gradient. The molecules move from higher to lower concentration until equilibrium is reached. It occurs in gases and liquids because random molecular movement is possible. Different solutes may have distinct diffusive fluxes, as their concentration distributions may vary within a single system. Plus, dispersion is another conveyance method that can be used in flowing water. It involves mixing processes driven by differential advection.

In real-world instances show that different types of pollutants from commercial and domestic sources end up in rivers. The bacteria that break down wastes may be consumed by an excess of oxygen in contaminated water. When this happens, the oxygen level may drop to dangerously low levels. This might also occur if polluted water contains nutrients that encourage the growth of algae. Dissolved oxygen is used up during the decomposition and death of the algae. This will have a negative impact on aquatic life, including plants and fish, considerably (Peterson & Risberg, 2009). Environmental engineers, hydrologists, chemical engineers, geologists, soil physicists, and mathematicians are all concerned about the pollution of rivers today. In order to analyse a model of river pollution, we assumed that the ADE may be a good approximation (Bhadane & Ghadle, 2016).

In a previous study conducted by Parsaie and Haghiabi (2017), they proposed a method that combines the finite volume method as a numerical technique with artificial neural networks as a soft computing technique for simulation. The ANN was utilized to predict the longitudinal dispersion coefficient, which was then incorporated as an input parameter in the numerical solution of the ADE. The researchers validated the model's performance by simulating the transmission of pollutants in the river and comparing the results with measured data. The comparison demonstrated that the model exhibited good performance improved the accuracy of the computer simulation in predicting pollution transmission in the river. Besides, Carr (2020) developed a semi-analytical Laplace-transform based solution for the one-dimensional linear advection-dispersion reaction problem in a layered medium. He developed a semi-analytical solution that extends and corrects previous Laplace transform based methods that merely take diffusion or reaction diffusion into consideration. The presented results are in great agreement with a standard numerical solution and other analytical results that are accessible in the literature. In addition, Abeye et al. (2022) focused on obtaining the numerical solution for an unsteady state fractional order ADE. They employed the Laguerre spectral collocation method in combination with the finite difference method to approximate the solution for the given problem. They validated the effectiveness of their method by providing examples and comparing the obtained solutions with the exact solution.

On the other hand, in a recent study conducted by Permanoon, Mazaheri, and Amiri (2022), they focused on addressing the issue of reconstructing pollutant source intensity functions for the pollutant transport equation in rivers, known as the inverse problem. They proposed a unique analytical method that combines the quasi-reversibility method with the Fourier transform tool. This method allows for solving the inverse problem of the ADE in rivers, considering a one-dimensional domain and different pollutant loading patterns. The analytical solution obtained through this method demonstrates its computational efficiency, high level of accuracy, and potential practical applicability, particularly when dealing with concentration data that may have errors. Also, Shilsar, Mazaheri, and Samani (2023) proposed semi-analytical solution aims to predict and describe pollutant transport in different river networks. The method focuses on one branch of the river network, considering advection and dispersion phenomena. Through the Laplace transform and considering diffusion and mass conservation equations, mass balance and diffusion matrices are obtained in terms of the Laplace variable. The results demonstrate that the proposed semi-analytical solution effectively models pollutant transport and captures critical features in complex river network configurations.

This research project will focus on the analytical solution for the one-dimensional ADE describing the pollutant and dissolved oxygen concentration in river. To be specific, the aim is to obtain the analytical solution of steady and coupled ADE of pollutant and dissolved oxygen concentration with source term and with dispersion.

2. Mathematical Model

In this case, a coupled equation for the concentration of pollutant, $C(x,t)(kgm^{-3})$ and dissolved oxygen, $X(x,t)(kgm^{-3})$ is considered. Dissolved oxygen refers to the amount of oxygen gas that is dissolved in the water of river ecosystem. It is a crucial factor in determining the environment of the river's quality. When oxygen and pollutant interact, a coupling scenario arises. In order to observe the concentration, a one-dimensional model is used along the length of river. According to Paudel, Kaffle and Bhandari (2022), the coupled equations in one dimension can be expressed as,

$$\frac{\partial(AC)}{\partial t} = D\frac{\partial^2(AC)}{\partial x^2} - \frac{\partial(uAC)}{\partial x} - k_1\frac{X}{X+k}AC + qH(x)\,; \quad 0 \le x < L\,, t > 0 \tag{1}$$

$$\frac{\partial(AX)}{\partial t} = D_x\frac{\partial^2(AX)}{\partial x^2} - \frac{\partial(uAX)}{\partial x} - k_2\frac{X}{X+k}AC + \alpha(S-X); 0 \le x < L, t > 0 \tag{2}$$

The Heaviside function $H(x)$ is represented in equation (1) by

$$H(x) = \begin{cases} 1 \text{ if } \ 0 < x < L \\ 0 \quad \text{otherwise} \end{cases} \tag{3}$$

Based on equations (1) and (2), $u(mday^{-1})$ denotes water velocity in the direction of x, $D(m^2day^{-1})$ denotes pollutant's dispersion coefficient in the same direction, $D_x(m^2day^{-1})$ is the dissolved oxygen's dispersion coefficient in the same direction, $S(kgm^{-3})$ is the saturation oxygen concentration, $k_1(day^{-1})$ is the pollutant's degradation rate coefficient, $k_2(day^{-1})$ is the dissolved oxygen's degradation rate coefficient, $\alpha(m^2day^{-1})$ is the mass transfer of oxygen from air to water, $q(kgm^{-1}day^{-1})$ is the additional pollutant rate along the river, $k(kgm^{-3})$ is the half-saturated oxygen demand concentration for pollutant decay and $A(m^2)$ is the cross-section of the river.

It is assumed that the parameters A, u, q, α and S are constants (Li, 2006). In the case of a river where pollutants and contaminants are discharged, the rate of growth of dissolved oxygen concentration is determined by the difference between the saturation concentration, S and the actual concentration of dissolved oxygen, X, represented as $\alpha(S - X)$. This difference influences the movement of oxygen from the air into the river. There is interaction between pollutant concentration, C, and the dissolved oxygen concentration, X. This equation is solved under the boundary conditions which are,

$$C(0) = 0 \tag{4}$$

$$X(0) = S \tag{5}$$

where C is the pollutant concentration and X is the dissolved oxygen concentration for the case when dispersion coefficient $D \neq 0$ and $D_x \neq 0$, and S is the saturated oxygen concentration.

3. Analytical Solution

A steady state model that involves dispersion terms, $D \neq 0, D_x \neq 0$ and k is negligible, $k = 0$ is utilized in this model. The equations can be expressed as,

$$D\frac{d^2(AC)}{dx^2} - \frac{d(uAC)}{dx} - k_1\frac{X}{X+k}AC + qH(x) = 0\,;\; x > L\,, t > 0 \tag{6}$$

$$D_x\frac{d^2(AX)}{dx^2} - \frac{d(uAX)}{dx} - k_2\frac{X}{X+k}AC + \alpha(S - X) = 0\,;\; x > L\,, t > 0 \tag{7}$$

The Heaviside function, $H(x) = 1$ is considered as mentioned in (3). Since $k = 0$, the equations (6) and (7) become,

$$D\frac{d^2(AC)}{dx^2} - \frac{d(uAC)}{dx} - k_1AC + q = 0 \tag{8}$$

$$D_x\frac{d^2(AX)}{dx^2} - \frac{d(uAX)}{dx} - k_2AC + \alpha(S - X) = 0 \tag{9}$$

From equation (8), it can be simplified to,

$$DA\frac{d^2(C)}{dx^2} - uA\frac{d(C)}{dx} - k_1AC + q = 0$$

or

$$\frac{d^2(C)}{dx^2} - \frac{u}{D}\frac{d(C)}{dx} - \frac{k_1}{D}C = -\frac{q}{DA} \tag{10}$$

This is the second order ordinary differential equations, where it can be shown that the general solution is

$$C(x) = c_1e^{(\delta-\beta)x} + c_2e^{(\delta+\beta)x} + \frac{q}{-k_1A}.$$

where

$$\delta = \frac{u}{2D}$$

and

$$\beta = \frac{\sqrt{u^2 + 4Dk_1}}{2D}$$

After applying the boundary condition (4), the pollutant concentration, $C(x)$ can be obtained as

$$C(x) = \begin{cases} \frac{q}{k_1 A}\left[1 - \left(\frac{\delta+\beta}{2\beta}\right)e^{(\delta-\beta)x}\right], & if\ x \geq 0 \\ \frac{q}{k_1 A}\left(\frac{\beta-\delta}{2\beta}\right)e^{(\delta+\beta)x}, & if\ x < 0 \end{cases} \tag{11}$$

On the other hand, equation (9) can be simplified as

$$AD_x \frac{d^2(X)}{dx^2} - uA\frac{d(X)}{dx} - k_2 AC + (\alpha S - \alpha X) = 0$$

or

$$\frac{d^2X}{dx^2} - \frac{u}{D_x}\frac{dX}{dx} - \frac{\alpha}{AD_x}X = \frac{k_2}{D_x}C - \frac{\alpha S}{AD_x}. \tag{12}$$

This is the second order ordinary differential equations, where it can be shown that the general solution is

$$X(x) = c_3 e^{(\gamma-\eta)x} + c_4 e^{(\gamma+\eta)x} - \left(\frac{k_2 AC + \alpha S}{\alpha}\right)$$

where

$$\gamma = \frac{u}{2D_x}$$

and

$$\eta = \frac{\sqrt{u^2 + \frac{4\alpha D_x}{2}}}{2D_x}$$

Hence, after applying the boundary condition (5), the general solution of dissolve oxygen concentration, $X(x)$ is obtained as

$$X(x) = \begin{cases} S - \frac{k_2 q}{k_1 \alpha} + \frac{k_2 q}{k_1}\left[\left(\frac{\delta+\eta}{2\eta\alpha} - \frac{\delta+\beta}{4\beta\eta A^*} + \frac{\delta-\beta}{4\beta\eta B^*}\right)e^{(\gamma-\eta)x} - \frac{\delta+\beta}{2\beta A^*}xe^{(\delta-\beta)x}\right], if\ x \geq 0 \\ S + \frac{k_2 q}{k_1}\left[\left(\frac{\delta-\eta}{2\eta\alpha} - \frac{\delta+\beta}{4\beta\eta A^*} + \frac{\delta-\beta}{4\beta\eta B^*}\right)e^{(\gamma+\eta)x} - \frac{\delta-\beta}{2\beta B^*}xe^{(\delta+\beta)x}\right], \ if\ x < 0 \end{cases} \tag{13}$$

where

$$A^* = 2AD_x(\delta - \beta) - uA$$

$$B^* = 2AD_x(\delta + \beta) - uA$$

4. Result and Discussion

Equation (11) is acquired by first utilising a steady state model that involves dispersion terms, $\boldsymbol{D \neq 0}$, $\boldsymbol{D_x \neq 0}$, and the concentration of half-saturated oxygen demand for pollutant degradation is negligible, $\boldsymbol{k = 0}$ to the coupled equations (1) and (2). The complementary function and particular integral of equation (10) are then used to solve the second order differential equation. Boundary condition (4) is then used to produce the final solution for pollutant concentration, $\boldsymbol{C}$ as shown in (11).

The same approach is used for equation (13) where the complementary function and particular integral of equation (12) are then used to solve the second order differential equation. The final solution of dissolved oxygen concentration, X, is obtained after applying boundary condition (5), producing (13). Equation (11) and (13) then can be used for plotting graphs in MATLAB in order to observe the behaviour of pollutant and dissolved oxygen concentration for $x \geq 0$.

Figure 1 illustrates the result of equation (11) formed by the process of second order differential equation. It shows the variation of pollutant concentration, C in the range $0 \leq x \leq 10$. In order to test the model, we consider parameters A, u, q, k_1 and D to be 1 (Wadi et al., 2014). From Figure 1, we can see that C increases as x increases. It reaches to maximum as $x \to \infty$. In general, concentration of pollutant increases as x increases.

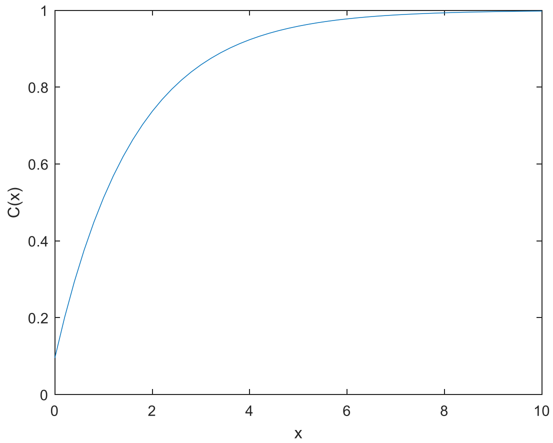

Figure 1 Steady and coupled ADE with source term and with dispersion described by equation (11) for $A, u, q, k_1, D = 1$.

Aside from that, Figure 2 illustrates the result of equation (13) using the same method as equation (11). It shows the variation of dissolved oxygen concentration, X in the range $0 \leq x \leq 10$. In order to test the model, we consider parameters A, S, u, q, D, D_x, k_1 and k_2 to be 1 and $\alpha = 0.99$ which is close to 1 (Wadi et al., 2014). Based on Figure 2, we can see that X decreases as x increases. It shows that oxygen level decreases due to reaction with pollutants. It reaches to minimum as $x \to \infty$.

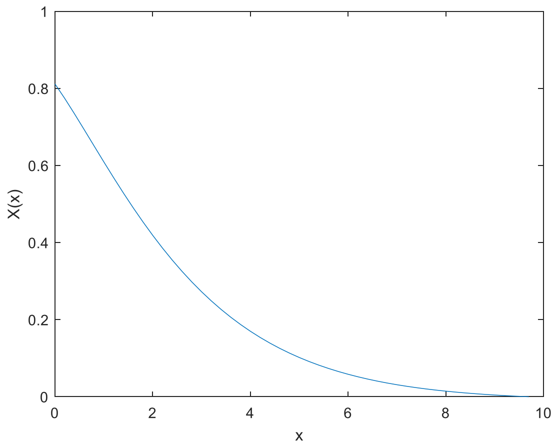

Figure 2 Steady and coupled ADE with source term and with dispersion described by equation (13) $A, S, u, q, D, D_x, k_1, k_2 = 1$ and $\alpha = 0.99$.

Conclusion

In general, the objectives of obtaining the analytical solution for the steady and coupled ADE with source term and with dispersion have been successfully accomplished. The mathematical model is solved using complementary function and particular integral describing the pollutant and dissolved oxygen concentration under the specified boundary conditions. Once the final analytical solution has been obtained, the outcomes are examined using MATLAB. The same sets of parameter values are applied but different values are used for the mass transfer of oxygen from the air to the water, α, in the dissolved oxygen concentration model. The outcome is then graphically analyzed on the behavior of pollutant and dissolved oxygen concentration. The result demonstrates that the concentration of pollutant will increases along the river and hence, the concentration of dissolved oxygen will decrease along the river due to reaction with pollutants.

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