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Advection-Diffusion Equation with Spatially Dependent Coefficients for Instantaneous Pollutant Injection in a River

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ARTICLE INFO	ABSTRACT
Article history: Received 25 October 2024 Received in revised form 15 November 2024 Accepted 15 December 2024 Available online 31 December 2024	River pollution is a major environmental concern globally, affecting ecosystems and water quality. Numerous strategies have been implemented to monitor and mitigate pollution, including mathematical modeling techniques. Among these, the advection-diffusion equation (ADE) has been widely applied to model the transport and dispersion of pollutants in rivers. Previous studies on the ADE have primarily examined pollutant concentration in rivers under scenarios where pollution enters the river continuously from the boundary or, if not continuous, is modelled with exponential decay in concentration. However, pollution in real situations can often be introduced to the river instantaneously. Furthermore, it has been demonstrated that the dispersion of the pollutant and the river velocity are not constant but varies with position (space). This research focuses on finding the analytical solution to the one-dimensional ADE with spatially dependent diffusion and velocity for the case where the pollutant is instantaneously introduced to the river. New space variables are introduced in the solution procedures to reduce the ADE to a simpler form with a single coefficient which is then solved using Laplace transform method. The findings demonstrate that velocity, diffusion coefficient, and medium inhomogeneity significantly influenced the pollutant concentration distribution in rivers. Since the pollutant is instantaneously injected, the peak concentration occurs not at the source of injection but at nearby location. While the spatially dependent effect with larger
solution	inhomogeneity demonstrates a much faster and broader pollutant distribution.

1. Introduction

River pollution occurs when harmful substances, such as chemical waste from industrial processes, enter rivers and contaminate the water. This is a major environmental concern with serious effects on aquatic ecosystems, human health, and water [1]. Contaminated water causes more deaths each year than war and all other forms of violence combined [2].

To address river pollution, various effective methods has been used. For instance, advanced treatment technologies, such as physical, chemical, and biological methods, can remove a wide range

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of contaminants [3]. Sustainable agricultural practices, such as reducing the use of chemical fertilizers and pesticides, can also help. Mathematically, the modelling based on ADE is commonly used to predict the concentration of pollutants in a river over time and space. By solving this equation, scientists and engineers can understand how pollutants spread, where they accumulate, and their impact on the river's ecosystem and water quality [1].

In the literature, various approaches have been used to model pollutant transport in different environmental settings. For example, De Smedt [4] have conducted a study on analytical solutions incorporating an ADE for solute transport in rivers with transient storage. Also, Parsaie and Haghiabi [1] developed a computational model for simulating pollution transmission in rivers. Their method integrates numerical solutions, particularly finite difference methods, to simulate the movement and dispersion of contaminants in river flow. While Chaudhary, Thakur, and Singh [5] study focused on one-dimensional pollutant transport in a semi-infinite groundwater reservoir. They applied Laplace transform method to solve the advection-diffusion equation (ADE), providing an analytical framework for understanding how contaminants move through groundwater. Their work is particularly relevant for cases where pollutants are introduced into a large or effectively infinite groundwater domain, making it a useful model for groundwater contamination studies. In another related study by Atshan et al., [6], they employed a pair of coupled reaction ADE that account for the pollutant and dissolved oxygen concentrations and solved it numerically. Also, Paudel et al., [7] conducted a study on simple analytical solution for the unsteady one-dimensional ADE describing the concentration of pollutant in one-dimension. Saleh et al., [8] developed a mathematical model to study the dispersion of pollutants in a river. They used Laplace transformation and an explicit finite difference scheme to solve the one-dimensional ADE with constant coefficients. Besides, Rahaman et al., [9] presented a mathematical model that was employed to study the movement of flowing pollution, specifically focusing on the one-dimensional ADE. The research investigated the utilization of the finite difference method to obtain numerical solutions for the ADE.

Overall, ADE can be used to model the movement of pollutants in rivers in several ways. The equation can be used to predict how pollutants will move downstream, how they will be distributed across the river, and how they will be affected by changes in the river's flow rate. However, in all the above works, the diffusion and velocity coefficients were assumed to be constant. While it has been demonstrated that these coefficients in the ADE can vary with position or space [5]. For example, the work by Zoppou and Knight [11], derived an analytical solution to the advection-diffusion equation with spatially variable coefficients using a coordinate transformation that reduces variable coefficients to constants, allowing for closed-form solutions. The paper by Yadav et al., [12] presented an analytical solution to the advection-dispersion equation (ADE) while incorporating spatially dependent parameters, such as variable dispersion and advection coefficients. The study enhances the understanding of how spatial heterogeneity impacts the transport processes. It was also shown that during the solute transport, the inhomogeneity of a medium causes' variation in the velocity of the flow through it [13]. Furthermore, Scheidegger [14] found that the solute dispersion parameter or diffusion was proportional to the square of the velocity. Also, in the study by Bruna and Chapman [15], diffusion has been proven to vary spatially. Even though the coefficient in the ADE has been proven to depend on space, many authors considered the diffusion and velocity as constant for simplicity.

Previous research on the ADE has largely focused on scenarios in which pollutants enter rivers either continuously from the boundaries or with an exponential decay in concentration. However, in real-world situations, pollutants can often be introduced instantaneously into the river. This study aims to derive an analytical solution for the one-dimensional ADE within a finite domain without a source term. A key contribution of this research is the incorporation of spatially dependent diffusion and velocity coefficients, which accounts for the inhomogeneity of the domain and the instantaneous introduction of pollutants. The solution will be obtained using Laplace transformation techniques.

2. Mathematical formulation

The one dimensional pollutant transport problem is govern by the advection diffusion equation (ADE)

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D_c \frac{\partial c}{\partial x} - u \frac{\partial c}{\partial x} \right) \tag{1}$$

where c [ML⁻³] is the concentration, while D_c [L²T⁻¹] and u [LT⁻¹] are the diffusion and velocity coefficients respectively. As mentioned in the introduction, it has been demonstrated that these coefficients can vary with position or space. In fact, the velocity varies due to inhomogeneity of the medium [13,16]. Therefore, in this study, the coefficients are defined to be spatially dependent, meaning they vary with position across the domain. This spatial variation reflects the inhomogeneity of the environment, allowing the model to more accurately represent real-world conditions where diffusion and velocity are not uniform. The coefficients are [12,13,16]:

$$D_c = D(x) = D_0(1 + ax)^2$$

and

$$u = u(x) = u_0(1 + ax)$$

where D_0 is initial diffusion coefficient, u_0 is initial velocity, and a [L⁻¹] is constant parameter due to inhomogeneity of the medium. The inhomogeneity of a river may be due to sediment characteristics or river morphology such as narrow, shallow or rivers with obstructions. The Eq. (1) can now be written as

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \Big(D_0 (1 + ax)^2 \frac{\partial c}{\partial x} - u_0 (1 + ax) c \Big),$$

Or

$$\frac{\partial c}{\partial t} = D_0 (1+ax)^2 \frac{\partial^2 c}{\partial x^2} + 2aD_0 (1+ax) \frac{\partial c}{\partial x} - u_0 (1+ax) \frac{\partial c}{\partial x} - u_0 ac.$$
(2)

Initially, there is c_i concentration in the domain. Meanwhile at x = 0 a source of pollution that releases a mass m [M] of a pollutant is introduced instantaneously. This situation accounts for scenarios such as sudden spills or burst of pollution. In addition, a flux type homogeneous condition is assumed at the other end of the domain. Hence, the initial and boundary conditions are

$$c(x,0) = c_i \tag{3}$$

$$c(0,t) = \frac{m}{\varrho}\delta(t),\tag{4}$$

$$\frac{\partial c}{\partial x}(L,t) = 0.$$
(5)

where Q [L³T⁻¹] is the volumetric flow rate, such that $\frac{m}{Q}\delta(t)$ essentially gives the instantaneous sharp injection of pollutant concentration localized at the boundary x = 0. The $\delta(t)$ term signifies that the release occurs at a single instant in time and does not persist beyond that moment ensuring an instantaneous effect.

3. Analytical Solution

To solve the model Eq. (2) along with the conditions Eq. (3 - 5), a new variable X is introduced, defined as

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

This substitution yields

$$\frac{\partial X}{\partial x} = -\frac{1}{(1+ax)^2},$$

$$\frac{\partial c}{\partial x} = -\frac{1}{(1+ax)^2} \frac{\partial c}{\partial x'},\tag{6}$$

and

$$\frac{\partial^2 c}{\partial x^2} = \frac{1}{(1+ax)^4} \frac{\partial^2 c}{\partial x^2}.$$
(7)

By substituting Eq. (6) and Eq. (7) into Eq. (2) will end up with

$$\frac{\partial c}{\partial t} = a^2 D_0 X^2 \frac{\partial^2 c}{\partial x^2} + (au_0 - 2a^2 D_0) X \frac{\partial c}{\partial x} - au_0 c.$$
(8)

Eq. (8) is further transformed into a partial differential equation with constant coefficients through the transformation

$$Z = -\log (aX) = \log (1 + ax).$$

This leads to

$$\frac{\partial c}{\partial t} = a^2 D_0 \frac{\partial^2 c}{\partial Z^2} - (au_0 - a^2 D_0) \frac{\partial c}{\partial} - au_0 c.$$
(9)

Consequently, the initial and boundary conditions from Eq. (3) - Eq. (5) are modified to

$$c(z,0) = c_i, \quad 0 \le Z \le Z_{0_i}, \quad Z_0 = \log(1+aL)$$
(10)

$$c(0,t) = \frac{m}{\rho}\delta(t),\tag{11}$$

$$\frac{\partial c}{\partial Z}(Z_0, t) = 0. \tag{12}$$

For simplification, Eq. (9) can be written as

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial z^2} - \nu \frac{\partial c}{\partial z} - \mu c, \tag{13}$$

where $D = a^2 D_0$, $v = (au_0 - a^2 D_0)$ and $\mu = au_0$.

To solve this ADE in Eq. (13), assume the solution of the form

$$c(Z,t) = K(Z,t) \exp\left[\frac{\nu Z}{2D} - \left(\frac{\nu^2}{4D} + \mu\right)t\right].$$
(14)

Differentiating with respect to t and z, and substituting into Eq. (13) will reduce Eq. (13) into diffusion equation

$$\frac{\partial K}{\partial t} = D \frac{\partial^2 K}{\partial Z^2}.$$
(15)

Following the assumption used in Eq. (14), the initial and boundary conditions Eq. (10) - (12) become

$$K(Z,0) = \frac{c_i}{exp\left[\frac{vZ}{2D}\right]},\tag{16}$$

$$K(0,t) = \frac{\frac{m}{Q}\delta(t)}{exp\left[-\left(\frac{v^2}{4D}+\mu\right)t\right]},\tag{17}$$

$$\frac{\partial K}{\partial Z} + \frac{v}{2D} K(Z_0, t) = 0.$$
(18)

By applying Laplace Transform method into Eq. (15) along with initial condition Eq. (16) produces

$$\frac{\partial^2 \widehat{K}}{\partial Z^2} - \frac{s}{D} \widehat{K} = -\frac{c_i}{D \exp\left[\frac{vZ}{2D}\right]}.$$

This is second order ordinary differential equation that can be solved using the method of undetermined coefficient, resulting in

$$\widehat{K}(Z,s) = C_1 \exp\left[-\sqrt{\frac{s}{D}}Z\right] + C_2 \exp\left[\sqrt{\frac{s}{D}}Z\right] - \frac{4c_i D}{(v^2 - 4sD) \exp\left[\frac{vZ}{2D}\right]}.$$

To determine C_1 and C_2 , make use of the boundary conditions Eq. (17) and Eq. (18) which in Laplace domain are

$$\widehat{K}(0,s) = \frac{m}{Q},$$

and

$$\frac{\partial \widehat{K}}{\partial Z} + \frac{v}{2D} \widehat{K} = 0 \quad ; Z \to Z_0.$$

After some necessary working, it is obtained that

$$C_1 = \frac{m}{Q} + \frac{4c_i D}{(v^2 - 4sD)} - \frac{\left(\sqrt{\frac{s}{D}} - \frac{v}{2D}\right) \left(\frac{m}{Q} + \frac{4c_i D}{(v^2 - 4sD)}\right)}{\left(\sqrt{\frac{s}{D}} - \frac{v}{2D}\right) + \left(\sqrt{\frac{s}{D}} + \frac{v}{D}\right) exp\left[2\sqrt{\frac{s}{D}}Z_0\right]}$$

and

$$C_2 = \frac{\left(\sqrt{\frac{s}{D}} - \frac{v}{2D}\right) \left(\frac{m}{Q} + \frac{4c_i D}{(v^2 - 4sD)}\right)}{\left(\sqrt{\frac{s}{D}} - \frac{v}{2D}\right) + \left(\sqrt{\frac{s}{D}} + \frac{v}{2D}\right) exp\left[2\sqrt{\frac{s}{D}}Z_0\right]}.$$

finally,

$$\widehat{K}(Z,s) = \begin{bmatrix} \frac{m}{Q} + \frac{4c_i D}{(v^2 - 4sD)} \\ - \left[\frac{\left(\sqrt{\frac{s}{D}} - \frac{v}{2D}\right) \left(\frac{m}{Q} + \frac{4c_i D}{(v^2 - 4sD)}\right)}{\left(\sqrt{\frac{s}{D}} - \frac{v}{2D}\right) + \left(\sqrt{\frac{s}{D}} + \frac{v}{D}\right) exp\left[2\sqrt{\frac{s}{D}}Z_0\right]} \end{bmatrix} exp\left[-\sqrt{\frac{s}{D}}Z \right] + \left[\frac{\left(\sqrt{\frac{s}{D}} - \frac{v}{2D}\right) \left(\frac{m}{Q} + \frac{4c_i D}{(v^2 - 4sD)}\right)}{\left(\sqrt{\frac{s}{D}} - \frac{v}{2D}\right) + \left(\sqrt{\frac{s}{D}} + \frac{v}{D}\right) exp\left[2\sqrt{\frac{s}{D}}Z_0\right]} \right] exp\left[\sqrt{\frac{s}{D}}Z \right] \\ - \frac{4c_i D}{(v^2 - 4sD) exp\left[\frac{vZ}{2D}\right]}.$$

$$(19)$$

The inverse Laplace transform of $\widehat{K}(Z,s)$ is computed using MATLAB, specifically utilizing the Stehfest algorithm. The Stehfest algorithm is a numerical technique for computing the inverse Laplace transform, widely used due to its efficiency and ability to handle Laplace-domain solutions without requiring closed-form inversions. This algorithm approximates the time-domain function by evaluating a weighted sum of the Laplace-domain function at specific points along the real axis. By applying the inverse Laplace transform to $\widehat{K}(Z,s)$, the time domain function K(Z,t) is obtained. Substituting K(Z,t) in Eq. (14) allows the intended solution to be determined.

4. Result and Discussion

Concentration profiles are analysed using the parameter values listed in Table 1, which are based on references relevant to river environments. Generally, the diffusion coefficient and velocity in rivers are influenced by various environmental and hydrodynamic factors. As shown in Table 1, diffusion coefficients range from 0.13 m²/day to 1.28×10^8 m²/day, while velocities range from 0.05 m/day to 5.96×10^4 m/day. For this study, parameter values from [22], which pertains to Malaysian rivers is utilized. Other parameters chosen are a = 0.01 m⁻¹ [17], $c_i = 1, m = 100, Q = 5$.

Diffusion and velocity parameter values of river based on some references			
References	Diffusion, D_0	Velocity, u_o	
Pimpunchat et al., [18]	$3.456 \times 10^6 \text{ m}^2/\text{day}$	$4.32 \times 10^4 \text{ m/day}$	
	(2400 m²/min)	(30 m/min)	
Deng et al., [19]	1.9 – 1486.45 m²/s	0.13 – 0.553 m/s	
	(1.6416 × 10 ⁵ – 1.28 × 10 ⁸ m ² /day)	$(1.123 \times 10^4 - 4.7 \times 10^4 \text{ m/day})$	
Ukpaka and Agunwamba [20]	72 – 104.4 m²/s	0.69 m/s	
	(6.22 × 10 ⁶ – 9.017 × 10 ⁶ m ² /day)	(5.96 × 104 m/day)	
Obi [21]	2.41 – 288.456 m²/s		
Fazli [22]	0.13 m ² /day	0.05 m/day	

Table 1

Diffusion and velocity parameter values of river based on some references

The results presented in Figure 1 demonstrate the concentration distributions based on parameters obtained from two studies, Fazli [22] and Pimpunchat *et al.*, [18] highlighting the influence of advection-diffusion parameters on pollutant transport. Take note that the time scale differs between the two, with the graph of Fazli expressing time in days while Pimpunchat *et al.* [18] expressing time in minutes. Both studies show a concentration peak near the source, with a decrease as time progresses. The highest concentration does not occur at the point it is injected because the pollutant is released as a single instant in time only, not continuously injected. Over time, the pollutant will travel to the neighbourhood space, causing the peak concentration to shift to a nearby location.

Furthermore, the diffusion coefficient, D_0 and velocity u_o are shown to significantly influence the dispersion patterns, with higher values in Pimpunchat *et al.*, [18] resulting in broader and faster pollutant spread compared to the localized dispersion in Fazli [22]. As can be seen, the pollutant concentration in Pimpunchat *et al.*, [18] demonstrates that the pollutant can travel significant distance, reaching up to 600 – 800 m from the source point within just a few minutes. In contrast, when the diffusion and velocity coefficient is very low as in Fazli [22], the pollutant's mobility is drastically reduced. Even after five days, the pollutant only disperses a short distance of 1 - 2 m only from where it is injected. This finding suggests that understanding the unique characteristics of pollutants in any situation is crucial, as seen by the notable difference in pollutant behaviour between high and low diffusion and velocity conditions.

Figure 2 illustrates the concentration distribution for different a which is the constant parameter due to inhomogeneity of the medium at two different times, Day 1 and Day 5. The findings reveal the significant impact of the inhomogeneity of the medium. At both Day 1 and Day 5, the concentration profiles demonstrate similar behaviour, with smaller a values (a = 0.001 and 0.1) result in a higher concentration peak near the source. This can be attributed to the fact that a smaller a corresponds to a lower diffusion and velocity, which allows more of the pollutant to remain concentrated near the source. Also, with less intense diffusion and advection effects, the pollutant travels a shorter distance resulting in a narrower dispersion. As a value becomes larger (a = 1,), the diffusion and velocity also become higher with x since the coefficients are spatially dependent. Therefore, the pollutant is more evenly distributed over a wider spatial range. However, this broader spread results in lower concentration values at any specific location. In addition, comparing the results between Day 1 and Day 5, it is evident that the pollutant disperses over a broader area as time progresses.



Fig. 1. Concentration distribution based on parameters obtained from two studies (a) Fazli [22] and (b) Pimpunchat *et al.*, [18]



Fig. 2. Concentration distribution for different *a*

5. Conclusion

This study focuses on deriving analytical solutions for a one-dimensional ADE with spatially varying coefficients under instantaneous boundary conditions. The spatial dependence of the diffusion and velocity coefficients illustrates how these parameters increase with distance (x) from the source due to the properties of the river environment. The Laplace transformation is used to derive the analytical solutions, introducing new space and dependent variables. The Stehfest algorithm in MATLAB is employed to perform the inverse Laplace transformation.

The findings highlight the critical role of the diffusion and velocity coefficient in pollutant dispersion. Smaller coefficients lead to sharper concentration peaks, indicating less spreading, while higher coefficients result in broader peaks, indicating greater spreading. Larger inhomogeneity shows steeper peaks arriving sooner and broader peaks arriving later, emphasizing the importance of accounting for spatial variations in riverbed properties when modelling pollutant transport. Given the important role of diffusion, velocity and inhomogeneity, this study proves the significance of carefully selecting accurate parameter values in in predicting real pollutant dispersion. Accurate

predictions are essential for designing effective mitigation strategies to manage pollution in river systems.

Future work should focus on validating the analytical solutions against experimental or field data to ensure the model's reliability. Additionally, extending the study to include other boundary conditions, time-dependent coefficients, or two-dimensional models would provide a more comprehensive understanding of pollutant dynamics in complex river systems.

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