Water Quality Analysis for the Depletion of Dissolved Oxygen due to Exponentially Increasing Form of Pollution Sources

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Analyzing and improving mathematical models for water quality investigation are imperative for water quality issues around the world. This study is aimed at presenting the 1D unsteady state regarding analytical and numerical solutions of dissolved oxygen (DO) concentration in a river, in which the increase of pollution from a source is considered as an exponential term. Laplace transformation was utilized to obtain analytical solutions, while the finite difference technique was selected for numerical solutions. The results show that the rate of pollutant addition along the river (q) and the arbitrary constants of an exponentially increasing pollution source term (λ) affected inversely, while the initial concentration $X_i$ affected directly, DO in the river. These solutions and simulations can be enabled for testing in various scenarios in terms of the behavior of oxygen depletion in polluted rivers.

1. Introduction

The quality of surface water is one of the crucial factors that influence the lives of humans and other creatures in the world. The measurement of water quality parameters consists of physicochemical parameters (pH, turbidity, conductivity, total suspended solids, total phosphorus, total solids, biochemical oxygen demand (BOD), dissolved oxygen (DO), nitrate-nitrogen, and heavy metals) and biological parameters (fecal and total coliform bacteria) [1]. In this paper, DO is taken as a principal indicator of water quality, as it is an essential element for aerobic communities living in aquatic systems. Other unwanted or waste matters, so-called pollutants, are chosen to be incorporated as from a hydrodynamic model of water pollution in a river. It is assumed that this waste is largely biochemical and undergoes various biochemical and biodegradation processes using dissolved oxygen. In Thailand, water contamination from land-based activities is largely associated with urbanization, industrialization, and agricultural activities. For the major rivers in Thailand, the observed water quality issues were dissolved oxygen depletion, decreased fish population, high amounts of ammonia and nitrogen, high coliform bacteria, and eutrophication phenomena [2]. If dissolved oxygen concentrations drop below a certain level, fish mortality rates will rise. Low oxygen or hypoxia (less than 2 mg/L) affects the biological system. For fish to survive, DO concentrations throughout a water system are required to remain at least 30% of the saturated value [3, 4]. Figure 1 shows a graph of raw data of DO concentrations which were obtained from a mobile application developed by the Regional Environmental Office 5, National Pollution Control Department (PCD) [5]. It shows the monitoring of DO during the second quarter of the year (April-June) between 2011 and 2018 and indicates that DO concentrations repeatedly exceeded the National Surface Water Quality Standards and Classification limits (red line 2-6 mg/L) throughout the river.

Mathematical modeling has been extensively utilized to forecast water quality and to provide reliable tools for water quality management in affected areas. One of the primary and most well-known environmental models was derived by Streeter and Phelps in 1925. It described how the balance of DO in rivers was affected by two processes; the first one was that oxygen is removed from water by the degradation of organic materials, and the second process
was “reaeration,” which is where oxygen is transferred into the water from the atmosphere [6]. Chapra stated the standard equations of water pollution by using advection-diffusion equations for the pollutant and DO concentrations [7]. Kumar et al. obtained analytical solutions for temporally and spatially dependent solute dispersion in a one-dimensional semi-infinite porous medium using the Laplace transform technique [8]. Pimpunchat et al. composed two coupled equations for the pollutant and DO concentrations and provided some analytical solutions at steady-state flows [9, 10], and Manitcharoen and Pimpunchat evaluated the unsteady-state analytical and numerical solutions for 1D advection-dispersion equations (ADE) of pollution concentration by considering the increasing terms of sources in two cases, uniformly and exponentially, respectively [11]. This study involved the relationship between oxygen concentrations from pollution degradation, in which oxygen depletion in a river is contrasted with increasing biochemical oxygen demand of organic waste. In [11], solutions with exponentially increasing pollution sources were found to be a suitable model for illustrating the behavior of increased pollution along a studied river (the Tha Chin river). The objective of this study is to evaluate unsteady-state solutions for 1D of the DO concentration by considering the rate of pollutant addition along a river in the case of an exponentially increasing form. It is thought that pollutant increment results from the pollution of the Tha Chin river. The contaminant in the lower portion of the river is higher than the upper portion, caused by geography, including various contributions from the branch river and main river, while the increasing wastewater is caused by swine and rice farming from the basin area. Analytical and numerical solutions are constructed for the model; analytical solutions are obtained utilizing the Laplace transform technique, and for numerical solutions, the explicit finite difference technique is used. Both solutions are compared to the values of the relative error. The parameter values that influence the concentration, such as the rate of pollutant addition along the river \( q \), the initial concentration of DO \( X_0 \), and arbitrary constants of exponentially increasing pollution source terms \( \lambda \), are presented to explain the behavior of dissolved oxygen in the river.

2. Materials and Methods

2.1. Governing Equation. The unsteady-state flow in the river is modeled by two coupled advection-dispersion equations, as 1D with spatial \( x \) and time \( t \) can be written as (2.1) and (2.2) in [10]:

\[
\frac{\partial (AP)}{\partial t} = D_p \frac{\partial^2 (AP)}{\partial x^2} - \frac{\partial (vAP)}{\partial x} - K_1 \frac{X}{X + k} AP + q \ (0 \leq x < L_{\infty}, t \geq 0),
\]

\[
\frac{\partial (AX)}{\partial t} = D_A \frac{\partial^2 (AX)}{\partial x^2} - \frac{\partial (vAX)}{\partial x} - K_2 \frac{X}{X + k} AP + \alpha (S - X) \ (0 \leq x < L_{\infty}, t \geq 0).
\]

The first equation includes both the rate of pollutant addition along the river \( q \) and its removal by aeration. The second equation is a mass balance for oxygen, in which oxygen is added at the river surface and it being consumed to remove pollutants. This equation is standard and was developed by Chapra [7]. We consider a river where pollutants are discharged in the form of waste. It is assumed that these pollutants \( P(x, t) \) use dissolved oxygen \( X(x, t) \) for various biochemical and biodegradation processes. The discharge of pollutants into the river is at the constant rate \( q \), \( A \) is the cross-section area of the river, \( D_p \) is the dispersion coefficient of pollutants, and \( D_A \) is the dispersion coefficient of DO in the \( x \)-direction, \( v \) is the water velocity in the \( x \)-direction, \( K_1 \) is the degradation rate coefficient for pollutants, \( K_2 \) is the reaeration rate coefficient for DO, \( \alpha \) is the mass transfer of oxygen from the air to water, and \( S \) is
saturated oxygen concentration. For convenience, all parameters are set to be constant values over time and space. The analysis is considered by the case of negligible $k$ ($k = 0$); then (1) and (2) can be written as follows:

$$\frac{\partial (AP)}{\partial t} = D_p \frac{\partial^2 (AP)}{\partial x^2} - \frac{\partial (vAP)}{\partial x} - K_1 AP + q,$$

(3)

$$\frac{\partial (AX)}{\partial t} = D_s \frac{\partial^2 (AX)}{\partial x^2} - \frac{\partial (vAX)}{\partial x} - K_2 AP + \alpha (S - X).$$

(4)

In this study, the result of DO concentration in (4) is determined by the case of an exponentially increasing form of pollution source, which is the same as (4) demonstrated as in [11], and can be written as

$$\frac{\partial (AP)}{\partial t} = D_p \frac{\partial^2 (AP)}{\partial x^2} - \frac{\partial (vAP)}{\partial x} - K_1 AP + q (1 - \exp (-\lambda x)), $$

(5)

where $\lambda$ is an arbitrary constant of an exponential term of pollution source. The initial and boundary conditions associated with the DO concentration (5) are

$$X(x, t) = X_i, \quad x \geq 0, \quad t = 0, \quad (6)$$

$$X(x, t) = X_0, \quad x = 0, \quad t > 0, \quad (7)$$

$$\frac{\partial X}{\partial x} (x, t) = 0, \quad x \to \infty, \quad t > 0,$$

(8)

where $X_i$ is the initial concentration and $X_0$ is the source concentration of DO at the origin.

2.2. Analytical Technique. The steady-state solution ($t \to \infty$) of pollutant concentration for an exponentially increasing form of source, as in (5), is given in [11] and can be written as

$$P(x) = q \frac{\exp (-\lambda x)}{AK_1} + \left( P_0 - q \frac{\exp (-\lambda x)}{AK_1} + q \frac{\exp (-\lambda x)}{AK_3} \right) \left( \frac{y - \beta}{\sqrt{D_p}} \right) x,$$

(9)

where $\gamma = \nu/2D_p$, $\beta = \sqrt{\nu^2/4D_p + K_1}$, and $K_3 = K_1 - \nu \lambda - D_p \lambda^2$. Applying the Laplace transformation to (4), we get

$$\hat{D}_A \frac{d^2 \hat{X}(x, s)}{d x^2} - \nu A \frac{d \hat{X}(x, s)}{d x} - \frac{K_2 A}{s} P(x, s) + \alpha \left( \frac{s}{s} - \hat{X}(x, s) \right)$$

$$- A (s \hat{X}(x, s) - X(x, 0)) = 0, \quad x \geq 0, \quad s > 0,$$

(10)

where $s$ is the transform variable. After this, transforming the initial and boundary conditions to (6), (7), and (8) in the Laplace domain gives

$$\hat{X}(x, 0) = X_i,$$

$$\hat{X}(0, s) = \frac{X_0}{s},$$

$$\frac{d \hat{X}}{d x} (x, s) = 0 \text{ as } x \to \infty.$$ 

(13)

Assessing (10), which uses the initial and boundary conditions (11), (12), and (13) and, finally, (9), obtains its solution in the Laplace domain as

$$\hat{X}(x, s) = \left( S - \frac{K_2 q}{K_1 \alpha} \right) \frac{1}{s} + \left( \frac{K_2 q}{K_1 \alpha} - S + X_i \right) \left( \frac{A}{A s + \alpha} \right)$$

$$+ \frac{K_2 q}{A K_3 s (s + C)} \exp (-\lambda x)$$

$$+ \frac{X_0}{s} - \frac{P_3 - \frac{K_2}{s + B^2}}{\frac{K_2}{s + B^2}} \exp \left( \frac{\delta - \frac{\beta^2}{D_p}}{D_p} x \right) - \frac{K_2 q}{A K_3 s (s + C^*)}$$

$$\cdot \exp \left( \frac{\delta - \frac{\beta^2}{D_p}}{D_p} x \right),$$

(14)

2.3. Numerical Technique. The numerical technique was displayed to utilize the explicit finite difference technique by using the forward differences scheme for time and the central derivatives for space. Thus, (4) in the finite difference form can be composed as

$$\frac{X_{m+1}^n - X_m^n}{\Delta t} = \frac{D_X}{\Delta x^2} (X_{m+1}^n - 2X_m^n + X_{m-1}^n) - \frac{\nu}{2 \Delta x} (X_{m+1}^n - X_{m-1}^n)$$

$$- K_2 P_m^n + \frac{\alpha}{A} (S - X_m^n) + 0 (\Delta x^2, \Delta t),$$

(15)

where indexes $m$ and $n$ refer to the discrete step size $\Delta x$ and the time step size $\Delta t$, respectively. $P_m^n$ is the pollutant concentration with an exponentially increasing pollution source, which is the same as (26) in [11]. The initial and boundary conditions of (6), (7), and (8) for (4) can be expressed in the finite difference form as

$$X_{m,0} = X_i, \quad x \geq 0,$$

$$X_{m,T} = X_0, \quad t > 0,$$

$$X_{M,n} = X_{m-1,n}, \quad x \to \infty, \quad t > 0.$$ 

(16)

3. Results and Discussion

3.1. Analytical Solution. Applying the invert Laplace transformation with the shift theorem and the convolution theorem [12, 13] to (14), the analytical solution of DO
concentration with an exponentially increasing pollution source of (4) is

\[ X(x,t) = S \frac{K_xq}{K_\alpha} + \left( X_0 - S + \frac{K_xq}{K_\alpha} \right) \exp \left( -\frac{x}{A} \right) \\
\times \left( 1 + \frac{1}{2} \left( \text{erf} \left( \frac{x - vt}{\sqrt{2}D_x} \right) + \exp (2\delta x) \text{erf} \left( \frac{x + vt}{\sqrt{2}D_x} \right) \right) \right) \\
+ \frac{1}{2} \left( X_0 - S + \frac{K_xq}{K_\alpha} + A_0 \right) \left( \exp (A_0x) \text{erf} \left( \frac{x}{2\sqrt{D_x}} - \eta \sqrt{t} \right) \right) \\
+ \exp (A_0x) \left( \frac{x}{2\sqrt{D_x}} + \eta \sqrt{t} \right) \\
- \frac{K_xp^*}{2B^*} \left( \exp (A_0x - B^*t) \text{erf} \left( \frac{x}{2\sqrt{D_x}} - \eta \sqrt{t} \right) \right) \\
+ \exp (A_0x - B^*t) \left( \frac{x}{2\sqrt{D_x}} + \eta \sqrt{t} \right) \\
+ 2 \exp (A_0x) \left( 1 - \exp (-B^*t) \right) \\
+ \frac{K_xq}{2AK_xC^*} \left( \exp (A_0x - C^*t) \text{erf} \left( \frac{x}{2\sqrt{D_x}} - E^* \sqrt{t} \right) \right) \\
+ \exp (A_0x - C^*t) \left( \frac{x}{2\sqrt{D_x}} + E^* \sqrt{t} \right) \\
+ 2 \exp (-A_0x) \left( 1 - \exp (-C^*t) \right). \tag{17} \]

where the complementary error function \( \text{erf} \left( x \right) = 1 - \text{erf} \left( x \right) = (2/\sqrt{\pi}) \int_0^x e^{-z^2} \, dz \), the real constants, \( \delta, \eta, B^*, C^*, P^*, A_0, A_1, A_2, A_3, A_4, A_5 \), and \( A_6 \) are given in the appendix.

3.2. Steady-State Solution. The steady-state solution is derived from (17) by taking limit \( t \to \infty \). Hence, pollutant concentrations in this state give

\[ X(x) = S - \frac{K_xq}{K_\alpha} \left( X_0 - S + \frac{K_xq}{K_\alpha} + A_0 \right) \exp (A_0x) \\
- \frac{K_xp^*}{B^*} \exp (A_0x) + \frac{K_xq}{2AK_xC^*A} \exp (-A_0x). \tag{18} \]

The downstream of DO concentration limit was calculated by \( x \to \infty \) and therefore gives

\[ X(x \to \infty, t \to \infty) = S - \frac{K_xq}{K_\alpha}. \tag{19} \]

This limit is the same result which was obtained by Pimpunchat et al. [10].

3.3. Analytical and Numerical Simulation. Numerical solutions are obtained by rearranging (15). Then, the numerical solutions must satisfy

\[ X_{m+1}^{n+1} = FX_m^n + GX_m^n + HX_{m-1}^n - (K_2\Delta t)p_m^n + f, \tag{20} \]

where \( F = (D_x\Delta t/\Delta x^2) - (v\Delta t/2\Delta x) \), \( G = 1 - (2D_x\Delta t/\Delta x^2) - (\alpha\Delta t/\Delta x) \), \( H = (D_x\Delta t/\Delta x^2) + (v\Delta t/2\Delta x) \), and \( f = akS/A \) for pollution concentration \( p_m^n \) to be evaluated by the following equation [12]:

**Table 1:** Variable and parameter values.

| Parameter | SI units |
|-----------|----------|
| \( L \) | 325* |
| \( D_x \) | 3,456,000* |
| \( D_w \) | 3,456,000* |
| \( v \) | 43,200* |
| \( A \) | 2100 |
| \( q \) | 0.06* |
| \( K_1 \) | 8.27*** |
| \( K_2 \) | 44.10** |
| \( k \) | 0.007**** |
| \( \alpha \) | 16.50** |
| \( S \) | 0.01* |

* [14]; ** [10]; *** based on the molecular weights in the chemical reaction \( K_1 = (3/16)K_2; *** \) estimated.

**Figure 2:** Analytical and numerical solutions of DO concentrations at different times (t)
The parameter values used in this model are the same as in [9], given by Table 1. The results are compared between the analytical and numerical solutions obtained by the Laplace transform technique and the finite difference technique, respectively. Figure 2 shows the variation in the longitudinal region 0 ≤ x ≤ 50 km at different times t = 0.05, t = 0.5, t = 1, and t → ∞ where step size ∆x = 0.1, Xo = S, Xi = 0.95 × 10⁻³ kg m⁻³, and q = 0.06 kg m⁻¹ day⁻¹.

The arbitrary constant of the exponential pollution source term (λ = 0.06289 day⁻¹) in (18) is assumed by the total rate of pollutant addition q being reduced by 5% along the river (L = 318 km), approximately [12]. The relative errors are calculated by (22), provided in Table 2. Their values appear acceptable between the analytical and numerical solutions. The maximum percentage relative error is less than 3 × 10⁻²%.

Figure 3 depicts the analytical and numerical solutions of DO concentrations by various values of the rate of pollutant addition (q) at t = 1 day and 0.06 ≤ q ≤ 0.48.

\[ P^{m+1}_m = \frac{B P^n_m + C P^n_{m+1} + E P^n_{m-1} + Q}{\Delta x^2} \]

(21)

where \( B = (D_p \Delta t/\Delta x^2) - (v \Delta t/2 \Delta x) \), \( C = 1 - (2D_p \Delta t/\Delta x^2) \) – \( K_1 \Delta t \), \( E = (D_p \Delta t/\Delta x^2) + (v \Delta t/2 \Delta x) \), and \( Q = q(1 - \exp(-\lambda x^m_i)) \Delta t/A \). The x and t meshes must be chosen to be \( D_p \Delta t/(\Delta x)^2 \leq 1/2 \) in order to ensure stability. In this study, the analytical and numerical solutions were compared by utilized relative error, which is assessed by

\[ \text{Relative error} = \frac{|P_{\text{analytical}} - P_{\text{numerical}}|}{P_{\text{analytical}}} \]  

(22)

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Figure 6: Behaviors of DO concentrations ($X/X_o$) at $t = 0.5$ days by various arbitrary constants of exponentially increasing pollution source terms ($1 \times 10^{-1} \leq \lambda \leq 1 \times 10^{-5}$ day$^{-1}$) with $q = 60$ kg km$^{-1}$ day$^{-1}$.

Table 3: Various $\lambda$ for $X/X_o$ concentrations at $t = 0.5$ days and $t \to \infty$.

| Exponentially increasing pollution source $L = 50$ km, $q = 60$, $X_i = 0.005$ | $X/X_o$ at $t = 0.5$ days | $X/X_o$ at $t \to \infty$ |
| --- | --- | --- |
| $1 \times 10^{-5}$ | 0.50196 | 0.99999 |
| $1 \times 10^{-4}$ | 0.501934 | 0.99996 |
| $1 \times 10^{-3}$ | 0.50171 | 0.99965 |
| $1 \times 10^{-2}$ | 0.49979 | 0.99690 |
| $1 \times 10^{-1}$ | 0.49474 | 0.98769 |

DO concentrations with various rates of pollutant addition along the river ($q$) at $t = 1$ day, $X_o = S$, $X_i = 0.95 \times 10^{-2}$ kg m$^{-3}$, and starting from $q = 0.06$ to $q = 0.48$ kg m$^{-1}$ day$^{-1}$. The concentrations decreasingly vary inversely proportional to $q$; $X$ decreases as $q$ increases. In 1 day, the concentration gradient will gradually decrease and greatly diminish when the distance is 35 kilometers. When the distance is long enough, the values converge to a positive constant. Figure 4 shows the concentration by various initial concentrations ($X_i$) at $1.5 \times 10^{-2} \leq X_i \leq 5 \times 10^{-3}$ at $t = 0.5$ and $q = 0.48$. The concentrations decreasingly vary obviously with $X_i$; $X$ decreases as $X_i$ decreases. Additionally, the DO concentration surface plot with $\Delta x = 0.1$ and $\Delta t = 0.01$ is depicted in Figure 5. The distinction of concentration is decreased slowly near the origin but is decreased rapidly far away, until converging to a positive constant when the distance is long enough. The rate of concentration decreases quite differently via $t$; it decreases rapidly at the beginning, when $t$ is very small ($t < 0.1$ approximately), and decreases more slowly later. The behavior in Figure 6 is a comparison of the DO concentrations between time $t = 0.5$ and $t \to \infty$ (the steady state) days by varying an arbitrary constant of exponential pollution source terms ($\lambda$). It is considered by default from $1 \times 10^{-5}$ to $1 \times 10^{-2}$ day$^{-1}$ by $X_i = 0.005$ and $X_o = S = 0.01$. From Table 3, concentrations decrease rapidly ($<5\%$) at the beginning; when entering into a steady state, they will diminish by an exceptionally small amount, not more than 1%.

4. Concluding Remarks

In this work, we used a mathematical model for water quality to analytically and numerically investigate dissolved oxygen concentrations in a river. This model was considered for the depletion of DO due to increased pollution degradation by the exponential form of the sources. The unsteady state solutions in 1D are proposed by using the Laplace transform technique and the explicit finite difference technique, for analytical and numerical solutions, respectively. The parameters that directly affect the DO concentration are the rate of pollutant addition along the river $q$ and the initial concentration $X_i$. It is found that the variation is proportional directly with $X_i$ and is inversely proportional with $q$. The values of both parameters are the result of the amount of pollutants in the river. Based on the results, this study is suitable for rivers which have pollution sources varying with a position where the downstream pollution sources are higher than upstream, as appears in the Tha Chin river, a distributary of the Chao Praya river in Thailand. These results are an observation of the reduction of DO concentrations without treatment or aeration to the water. Otherwise, if there is no sufficient planning or control of the amount of pollution emitted into the river, oxygen depletion will continue to occur and will certainly affect water quality.

Appendix

The real constants, $\delta, \eta, B^*, C^*, P^*, A_1, A_2, A_3, A_4, A_5, A_6, A_7, A_8, A^*$, and $E^*$ that were used in Equations (14), (17), and (18) are as follows:
\[ \delta = \frac{\nu}{2D_x}, \]
\[ \eta = \sqrt{\frac{\nu^2}{4D_x} + \frac{\alpha}{A}} \]
\[ B^* = \frac{\alpha}{A} - D_x A_1^2 + \nu A_1, \]
\[ C^* = \frac{\alpha}{A} - D_x \lambda^2 - \nu \lambda, \]
\[ P^* = P_0 - \frac{q}{AK_1} + \frac{q}{AK_3}, \]
\[ A_1 = \left( \gamma - \frac{\beta}{\sqrt{D_p}} \right), \]
\[ A_2 = \left( \delta - \frac{\eta}{\sqrt{D_z}} \right), \]
\[ A_3 = \left( \delta + \frac{\eta}{\sqrt{D_z}} \right), \]
\[ A_4 = \left( \delta - \frac{A^*}{\sqrt{D_z}} \right), \]
\[ A_5 = \left( \delta + \frac{A^*}{\sqrt{D_z}} \right), \]
\[ A_6 = \left( \delta - \frac{E^*}{\sqrt{D_z}} \right), \]
\[ A_7 = \left( \delta - \frac{E^*}{\sqrt{D_z}} \right), \]
\[ A_8 = \frac{K_2 P^*}{B^*} - \frac{K_1 q}{AK_3 C^*}, \]
\[ A^* = \sqrt{\eta^2 - B^*}, \]
\[ E^* = \sqrt{\eta^2 - C^*}. \]

**Data Availability**

The results of this study were obtained from a numerical technique compared with analytical solutions. The raw data was not used in the calculation of this matter. We plotted the trends of DO and BOD increase from the data from Mobile Application Tha Chin Water Quality, Regional Environment Office of Ministry of National Resources and Environment which was referred in the reference no. [5]. Accordingly, the researchers can access this data on the website.

**Conflicts of Interest**

The authors declare that they have no conflicts of interest.

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