Numerical simulations for reactive nitrogen compounds pollution measurements in a stream using Saulyev method

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Abstract. Nutrient pollution is one of most harmful environmental problems, and is caused by surplus nitrogen in water. This nitrogen concentration occurring in water can take several forms, such as organic nitrogen, ammonia, nitrite, nitrate, and dissolved nitrogen gas. Pollution levels can be measured via data collection; however, this is a rather difficult and complex process, and the results obtained widely deviate in term of measurement. A mathematical model can be used in complicated water-quality measurement. The advection-dispersion-reaction model provides a pollutant concentration field. In this research, there are five numerical models for nitrogen pollutant concentration measurement in a stream proposed: a total nitrogen dispersion model, an organic nitrogen dispersion model, an ammonia dispersion model, a nitrite dispersion model, and a nitrate dispersion model. The traditional Forward Time Central Space finite difference technique and the unconditionally explicit Saulyev technique are employed to obtain five approximated types of organic and inorganic nitrogen pollutant concentrations in each time and place. This paper proposes five forms of nitrogen pollutant measurement model for the unconditionally stable Saulyev method, so as to make it more accurate without incurring any significant loss of computational efficiency. The

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five approximated forms of pollutant concentrations obtained indicate that all models improve the nutrient pollution measurement process.

Keywords: numerical simulations, nitrogen compound, Saulyev technique.

1. Introduction

Water is a main factor in the survival of life on Earth. Water pollution is a global problem caused by global population growth and economic growth. It is an important problem affecting society and the environment. The main causes of this problem are human settlements, industries, and agriculture. One of the leading water pollution causes is nutrient pollution. Nutrients, such as nitrogen and phosphorus, are chemicals that flow into natural water, such as rivers, lakes, and coastal oceans, coming from either point or nonpoint sources. Nutrients are necessary for aquatic and coastal ecosystems such as plant growth. Major sources of nutrients are transportation, industry, urban activity, fertilizer, animal wastes, plant debris, and nitrogen transported from excess or effluent communities in soil to water sources [1].

Nitrogen is one of the essential contaminants of water. Nitrogen concentrations occurring in natural waters can be modified into a variety of organic and inorganic forms, five being organic nitrogen, ammonia, nitrite, nitrate, and dissolved nitrogen gas [2]. Due to dissolved nitrogen gas having no biological effect, this is ignored. Excess nitrogen in the water can occur in pollution in general, such as low oxygen concentrations in natural waters caused by nitrogen compound oxidation, or toxic substances found in aquatic animals and affecting human health. Nitrogen is seen as one of the key nutrients for eutrophication, public health matters, and aquatic and the other problems.

Mathematical models are widely used in explaining environmental processes such as chemical, biology, physical, and other processes; parabolic equations can be reasonably explained in mathematical models [3]. The advection and diffusion equation is a form of PDE parabolic equation which plays an important role in describing transport processes and has that obtained popularity in solving various problems, including environmental problems such as water quality measurement [4], [5], and [6], air quality measurement, and others. For the measurement of water quality, many researches have used these equations to measure concentrations occurring in natural water sources, such as rivers, and to compare computed values with real values; their compared yields are similar [5] and [6]. The finite difference method is one of the most efficient methods of problem solving in advection and diffusion equations, etc. They can be classified into two forms: explicit and implicit schemes [3]. Explicit schemes are simple to calculate, and have been used to present stability and accuracy properties. In [4], a water quality assessment of a non-uniform flow stream was conducted by using the Crank-Nicolson method, and the explicit finite difference schemes were proposed respectively. The forward Time Central Space (FTCS) and Saulyev schemes were used to determine water quality concentration. In [7], they were

implemented to measure air pollutant concentrations in an area under a sky train; three dimensional advection and diffusion equations were solved by using the explicit FTCS method, such that this method was used in two cases of wind inflow as the x direction and the $x-y$ directions. [8], described the measurement of water pollutant concentration control in a connected-pond reservoir that were connected two ponds using a hydrodynamic model and a steady-state pollutant dispersion model through a three different finite difference scheme as backward, forward, and central-in-space, with a steady-state pollutant dispersion model that formed a steady-state advection-diffusion equation, which was then used to perform water pollutant concentration level control and cost optimization.

Thus, the simple finite different methods are represented here as simple explicit schemes in the forms of the FTCS scheme and the Saulyev scheme [4]. Both schemes are used in calculating mathematical model as water quality models. When compared, two comparisons have shown that the Saulyev scheme is more efficient [4].

For implementation, we analyze nitrogen pollutant models from the advection-dispersion-reaction equation to estimate pollutant concentrations in terms of total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate concentrations. We take two numerical methods, the FTCS and the Saulyev methods, to compare with the analytical solution that forms the governing equation. We compute nitrogen pollutant models with two numerical methods to compare efficient solvability. We solve previous models with the Saulyev method by comparing different right boundary conditions.

2. Dispersion models

2.1 Advectiondiffusionreaction equation

In a stream water pollutant concentration measurement model, the governing equation is a one-dimensional advection-diffusion-reaction equation. A simplified representation, averaging the equation over the depths, as shown in [6], is

$$(2.1) \qquad \frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2} - f\left(C\right), \quad 0 \leq x \leq L, 0 < t \leq T,$$

with the initial condition :

$$(2.2) \qquad C\left(x,0\right) = k\left(x\right), \quad 0 \leq x \leq L,$$

and the boundary conditions :

$$(2.3) \qquad \begin{aligned} C\left(0,t\right) &= g\left(t\right), \quad 0 < t \leq T, \\ C\left(1,t\right) &= h\left(t\right), \quad 0 < t \leq T, \end{aligned}$$

where $C\left(x,t\right)$ is the concentration at the point x and at time t, D is the diffusion coefficient of nitrogen pollution, u is the velocity component, $f\left(C\right)$ is reaction to a sink or source terms, and $k\left(x\right), g\left(t\right)$ and $h\left(t\right)$ are given.

2.2 Nitrogen dispersion models

We consider the nitrogen pollutant concentration models in surface water by using a modified model for approximate concentrations of some nitrogen pollutants: the general nitrogen forms, total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate which play roles in nitrogen processes are described by the general knowledge of nitrogen [1] and [10].

$$(2.4) \qquad \text{ON} \xrightarrow{\text{ammonification}} \text{NH}_3 \xrightarrow{\text{nitrification}} \text{NO}_2 \xrightarrow{\text{nitrification}} \text{NO}_3$$
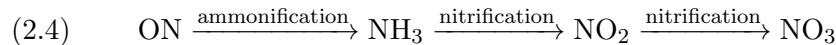
Nitrogen from wastewater is discharged from many sources, such as human, animal, industry, agriculture, and other sources. General discharged raw wastewater contains around $40-45$ % organic nitrogen; and about $55-60\%$ ammonia, with the sum of nitrates and nitrites making up about $0-5\%$ of the total nitrogen [12].

Therefore, different nitrogen pollutant concentrations are analyzed under reaction terms using five different nitrogen dispersion models, which were established by (2.1), and associated with (2.2) and (2.3). We consider these models to approximate nitrogen pollutant concentration behaviors that occur in natural water sources to be total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate. These models are described by the different dispersion models, such as the total nitrogen concentration model, the organic nitrogen concentration model, the ammonia concentration model, the nitrite concentration model, and the nitrate concentration model.

2.2.1 Total nitrogen dispersion model

The total nitrogen (TN) pollutant concentration measurement in a stream is described by the one-dimensional advection-diffusion-reaction equation.

$$(2.5) \qquad \frac{\partial C_1}{\partial t} = -u\frac{\partial C_1}{\partial x} + D_1\frac{\partial^2 C_1}{\partial x^2} - R_1\left(C_1\right) + Q, \quad 0 \le x \le 1, 0 < t \le 1,$$

the initial condition

$$(2.6) \qquad C_1\left(x,0\right) = k_1\left(x\right), \quad 0 \le x \le 1,$$

and the boundary conditions :

$$(2.7) \qquad \begin{aligned} C_1\left(0,t\right) &= g_1\left(t\right), \quad 0 < t \le 1, \\ C_1\left(1,t\right) &= h_1\left(t\right), \quad 0 < t \le 1, \end{aligned}$$

where u is water flow velocity, $C_1(x,t)$ is the total nitrogen concentration at the point x and time t, D_1 is the total nitrogen diffusion coefficient, R_1 is the reaction rate due to the degradation, Q is the inlet total nitrogen concentration due to sources, $k_1(x)$ is the potential total nitrogen concentration function along the stream, $g_1(t)$ is the total nitrogen concentration function at the discharge point, and $h_1(t)$ is the rate of change of the total nitrogen concentration with respect to distance at the end of the stream.

2.2.2 Organic nitrogen dispersion model

Most organic nitrogen (ON) pollutants are dissolved in living and nonliving forms from domestic wastes such as urea, uric acid, polypeptides and amino acids [11]. This model describes the organic nitrogen pollutant concentration behavior where the performance measurement concentration occurs under reaction term by the degradation of the organic nitrogen concentration in water, with consideration of the total nitrogen concentration.

The organic nitrogen (ON) pollutant concentration measurement in a stream is described by the one-dimensional advection-diffusion-reaction equation.

$$(2.8) \qquad \frac{\partial C_2}{\partial t} = -u \frac{\partial C_2}{\partial x} + D_2 \frac{\partial^2 C_2}{\partial x^2} + R_2 \left(R_1 C_1 \right), \quad 0 \leq x \leq 1, 0 < t \leq 1,$$

the initial condition

$$(2.9) \qquad C_2 \left(x, 0 \right) = k_2 \left(x \right), \quad 0 \leq x \leq 1,$$

and the boundary conditions :

$$(2.10) \qquad \begin{aligned} \frac{\partial C_2 \left(0, t \right)}{\partial t} &= g_2 \left(t \right), \quad 0 < t \leq 1, \\ \frac{\partial C_2 \left(1, t \right)}{\partial t} &= h_2 \left(t \right), \quad 0 < t \leq 1, \end{aligned}$$

where u is water flow velocity, $C_2(x, t)$ is the organic nitrogen concentration at the point x and time t, D_2 is the organic nitrogen diffusion coefficient, R_2 is the reaction rate due to the degradation, $k_2(x)$ is the potential organic nitrogen concentration function along the stream, $g_2(t)$ is the organic nitrogen concentration function at the discharge point, and $h_2(t)$ is the rate of change of the organic nitrogen concentration with respect to distance at the end of the stream.

2.2.3 Ammonia dispersion model

Ammonia (NH_3) occurs in organic nitrogen by the ammonification process, which gives ammonia (NH_3) and ammonium (NH_4^+). The mass of ammonia (NH_3) and ammonium (NH_4^+) are considered in terms of pH and temperature. Ammonia (NH_3) is toxic to aquatic life, whereas ammonium (NH_4^+), supports algae and aquatic plant growth. However, ammonia and ammonium are similar [11]. This model describes ammonia pollutant concentration behavior where the performance measurement concentration occurs under reaction term by the degradation of the ammonia pollutant concentration in water, with consideration of the total nitrogen concentration.

The ammonia (NH_3) pollutant concentration measurement in a stream is described by the one-dimensional advection-diffusion-reaction equation.

$$(2.11) \qquad \frac{\partial C_3}{\partial t} = -u \frac{\partial C_3}{\partial x} + D_3 \frac{\partial^2 C_3}{\partial x^2} + R_3 \left(R_1 C_1 \right), \quad 0 \leq x \leq 1, 0 < t \leq 1,$$

the initial condition

$$(2.12) \qquad C_3(x,0) = k_3(x), \quad 0 \le x \le 1,$$

and the boundary conditions :

$$(2.13) \qquad \begin{aligned} \frac{\partial C_3(0,t)}{\partial t} &= g_3(t), \quad 0 < t \le 1, \\ \frac{\partial C_3(1,t)}{\partial t} &= h_3(t), \quad 0 < t \le 1, \end{aligned}$$

where u is water flow velocity, $C_3(x,t)$ is the ammonia concentration at the point x and time t, D_3 is the ammonia diffusion coefficient, R_3 is the reaction rate due to the degradation, $k_3(x)$ is the potential ammonia concentration function along the stream, $g_3(t)$ is the ammonia concentration function at the discharge point, and $h_3(t)$ is the rate of change of the ammonia concentration with respect to distance at the end of the stream.

2.2.4 Nitrite dispersion model

The nitrite (NO_2) pollutant is oxidized by the nitrification process, such as to convert ammonia to nitrite. Nitrite is toxic to infants when at excessive levels [11]. This model describes nitrite pollutant concentration behavior where the performance measurement concentration occurs under reaction term by the degradation of the nitrite pollutant concentration in water, with consideration of the total nitrogen concentration.

The nitrite (NO_2) pollutant concentration measurement in a stream is described by the one-dimensional advection-diffusion-reaction equation.

$$(2.14) \qquad \frac{\partial C_4}{\partial t} = -u\frac{\partial C_4}{\partial x} + D_4\frac{\partial^2 C_4}{\partial x^2} + R_4(R_1 C_1), \quad 0 \le x \le 1, 0 < t \le 1,$$

the initial condition

$$(2.15) \qquad C_4(x,0) = k_4(x), \quad 0 \le x \le 1,$$

and the boundary conditions :

$$(2.16) \qquad \begin{aligned} \frac{\partial C_4(0,t)}{\partial t} &= g_4(t), \quad 0 < t \le 1, \\ \frac{\partial C_4(1,t)}{\partial t} &= h_4(t), \quad 0 < t \le 1, \end{aligned}$$

where u is water flow velocity, $C_4(x,t)$ is the nitrite concentration at the point x and time t, D_4 is the nitrite diffusion coefficient, R_4 is the reaction rate due to the degradation, $k_4(x)$ is the potential nitrite concentration function along the stream, $g_4(t)$ is the nitrite concentration function at the discharge point, and $h_4(t)$ is the rate of change of the nitrite concentration with respect to distance at the end of the stream.

2.2.5 Nitrate dispersion model

The nitrate (NO_3) pollutant is transformed from nitrite by the nitrification process and can convert to nitrite [11], which is toxic and hazardous to infants. This model describes nitrate pollutant concentration behavior where the performance measurement concentration occurs under reaction term by the degradation of the nitrate pollutant concentration in water, with consideration of the total nitrogen concentration.

The nitrate (NO_3) pollutant concentration measurement in a stream is described by the one-dimensional advection-diffusion-reaction equation.

$$(2.17) \qquad \frac{\partial C_5}{\partial t} = -u\frac{\partial C_5}{\partial x} + D_5\frac{\partial^2 C_5}{\partial x^2} + R_5\left(R_1 C_1\right), \quad 0 \le x \le 1, 0 < t \le 1,$$

the initial condition

$$(2.18) \qquad\qquad\qquad C_5\left(x, 0\right) = k_5\left(x\right), \quad 0 \le x \le 1,$$

and the boundary conditions :

$$(2.19) \qquad \begin{aligned} \frac{\partial C_5\left(0, t\right)}{\partial t} &= g_5\left(t\right), \quad 0 < t \le 1, \\ \frac{\partial C_5\left(1, t\right)}{\partial t} &= h_5\left(t\right), \quad 0 < t \le 1, \end{aligned}$$

where u is water flow velocity, $C_5(x, t)$ is the nitrate concentration at the point x and time t, D_5 is the nitrate diffusion coefficient, R_5 is the reaction rate due to the degradation, $k_5(x)$ is the potential nitrate concentration function along the stream, $g_5(t)$ is the nitrate concentration function at the discharge point, and $h_5(t)$ is the rate of change of the nitrate concentration with respect to distance at the end of the stream.

3. Numerical techniques for nitrogen dispersion models

This section presents the two numerical schemes of finite difference methods, the FTCS scheme and the Saulyev scheme, which are explicit schemes.

We can solve $C(x_i, t_n)$ or C_i^n at grid point (x_i, t_n) where $0 \le i \le M$ and $0 \le n \le N$ such that i and n are positive integers. Each node of x_i and t_n is separated by an equal grid on the x-range and t-range as the column of space and time, respectively, where $x_i = i\Delta x$, $i = 0, 1, 2, ..., M$, $t_n = n\Delta t$, $n = 0, 1, 2, ..., N$ and the values of $\Delta x > 0$ and $\Delta t > 0$ are the grid of space and time increments, respectively [4].

3.1 Forward Time Central Space technique applied to five forms of nitrogen measurement model

The FTCS scheme can be written as the discretization of time and space derivative term as follows [4]

$$
\begin{aligned}
\frac{\partial C}{\partial t} &= \frac{C_i^{n+1} - C_i^n}{\Delta t}, \\
\frac{\partial C}{\partial x} &= \frac{C_{i+1}^n - C_{i-1}^{n+1}}{2\Delta x}, \\
\text{and} \quad \frac{\partial^2 C}{\partial x^2} &= \frac{C_{i+1}^n - 2C_i^n + C_{i-1}^{n+1}}{(\Delta x)^2}.
\end{aligned}
$$
(3.1)

Substituting (3.1) into nitrogen dispersion models (the total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate measurement models) results in (2.5), (2.8), (2.11), (2.14), and (2.17), respectively.

Moreover, the FTCS has numerical stability that depends on the condition of the diffusion number (λ) and the advection number (γ) , as follows

$$
\begin{aligned}
\lambda &= \frac{D\Delta t}{(\Delta x)^2} < \frac{1}{2}, \\
\text{and} \quad \gamma_i^n &= \frac{u_i^n \Delta t}{\Delta x} < 1.
\end{aligned}
$$
(3.2)

These values depend on choosing a suitable grid time increment, as Δt is not of much high width.

3.1.1 Forward Time Central Space technique for the total nitrogen dispersion model

Taking (3.1) into (2.5), we obtain the discretization of total nitrogen dispersion model as

$$
\begin{aligned}
\frac{(C_1)_i^{n+1} - (C_1)_i^n}{\Delta t} =& -u_i^n \left(\frac{(C_1)_{i+1}^n - (C_1)_{i-1}^n}{2\Delta x} \right) \\
&+ D_1 \left(\frac{(C_1)_{i+1}^n - 2(C_1)_i^n + (C_1)_{i-1}^n}{(\Delta x)^2} \right) - R_1(C_1)_i^n + Q.
\end{aligned}
$$
(3.3)

Rearranging (3.3) leads to (3.4) for the FTCS solution, represented as

$$
\begin{aligned}
(C_1)_i^{n+1} =& \left(\frac{1}{2}\gamma_i^n + \lambda \right) (C_1)_{i-1}^n + (1 - R_1\Delta t - 2\lambda)(C_1)_i^n \\
&+ \left(\lambda - \frac{1}{2}\gamma_i^n \right) (C_1)_{i+1}^n + Q\Delta t,
\end{aligned}
$$
(3.4)

where $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma_i^n = \frac{u_i^n \Delta t}{\Delta x}$.

Substituting (3.1) into (2.7) and rearranging on the right-bound of the boundary condition, which is the derivative equation, we get (3.5).

The left boundary condition; $i = 0$,

$$C_1(0, t) = 1 = g_1(t),$$

and the right boundary condition; $i = M$,

(3.5)
$$\frac{\partial C_1(M, t)}{\partial x} = \frac{(C_1)^n_{M+1} - (C_1)^n_{M-1}}{\Delta x} = h_1(t),$$
$$(C_1)^n_{M+1} = 2h_1(t)\Delta x + (C_1)^n_{M-1}.$$

Substituting (3.5) into (3.4) leads to (3.6) of the right side equation, given as

$$(C_1)^{n+1}_M = 2\lambda(C_1)^n_{M-1} + 2h_1(t)\Delta x \left(\lambda - \frac{1}{2}\gamma^n_M\right)$$

(3.6)
$$+ (1 - R_1\Delta t - 2\lambda)(C_1)^n_M + Q\Delta t.$$

3.1.2 Forward Time Central Space technique for the organic nitrogen dispersion model

Likewise, substituting (3.1) into (2.8) leads to (3.7), written as

(3.7)
$$\frac{(C_2)^{n+1}_i - (C_2)^n_i}{\Delta t} = -u^n_i \left(\frac{(C_2)^n_{i+1} - (C_2)^n_{i-1}}{2\Delta x}\right)$$
$$+ D_2 \left(\frac{(C_2)^n_{i+1} - 2(C_2)^n_i + (C_2)^n_{i-1}}{(\Delta x)^2}\right) + R_2 R_1 (C_1)^n_i.$$

Rearranging (3.7) leads to (3.8) for the FTCS solution, represented as

$$(C_2)^{n+1}_i = \left(\frac{1}{2}\gamma^n_i + \lambda\right)(C_2)^n_{i-1} + (1 - 2\lambda)(C_2)^n_i$$

(3.8)
$$+ \left(\lambda - \frac{1}{2}\gamma^n_i\right)(C_2)^n_{i+1} + R_2 R_1 (C_1)^n_i \Delta t,$$

where $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma^n_i = \frac{u^n_i \Delta t}{\Delta x}$.

Substituting (3.1) into (2.10) and rearranging on the left and right-bound of the boundary condition of this model which are the derivative equations, we get (3.9).

The left boundary condition; $i = 0$,

$$\frac{\partial C_2(0, t)}{\partial x} = \frac{(C_2)^n_1 - (C_2)^n_{-1}}{2\Delta x} = g_2(t),$$
$$(C_2)^n_{-1} = (C_2)^n_1 - 2g_2(t)\Delta x,$$

and the right boundary condition; $i = M$,

(3.9)
$$\frac{\partial C_2(M, t)}{\partial x} = \frac{(C_2)^n_{M+1} - (C_2)^n_{M-1}}{2\Delta x} = h_2(t),$$
$$(C_2)^n_{M+1} = 2h_2(t)\Delta x + (C_2)^n_{M-1}.$$

Substituting (3.9) into (3.8) leads to the left and right side (3.10) and (3.11), respectively, given as follows

$$
\text{(3.10)} \quad (C_2)_0^{n+1} = 2\lambda(C_2)_1^n - 2g_2(t)\Delta x \left(\lambda + \frac{1}{2}\gamma_0^n \right) + (1 - 2\lambda)(C_2)_0^n
$$
$$
+ R_2 R_1 (C_1)_0^n \Delta t
$$

and

$$
\text{(3.11)} \quad (C_2)_M^{n+1} = 2\lambda(C_2)_{M-1}^n + 2h_2(t)\Delta x \left(\lambda - \frac{1}{2}\gamma_M^n \right) + (1 - 2\lambda)(C_2)_M^n
$$
$$
+ R_2 R_1 (C_1)_M^n \Delta t.
$$

3.1.3 Forward Time Central Space technique for the ammonia dispersion model

Likewise, substituting (3.1) into (2.11) leads to (3.12), written as

$$
\text{(3.12)} \quad \frac{(C_3)_i^{n+1} - (C_3)_i^n}{\Delta t} = -u_i^n \left(\frac{(C_3)_{i+1}^n - (C_3)_{i-1}^n}{2\Delta x} \right)
$$
$$
+ D_3 \left(\frac{(C_3)_{i+1}^n - 2(C_3)_i^n + (C_3)_{i-1}^n}{(\Delta x)^2} \right) + R_3 R_1 (C_1)_i^n.
$$

Rearranging (3.12) leads to (3.13), represented as

$$
(C_3)_i^{n+1} = \left(\frac{1}{2}\gamma_i^n + \lambda \right) (C_3)_{i-1}^n + (1 - 2\lambda)(C_3)_i^n + \left(\lambda - \frac{1}{2}\gamma_i^n \right) (C_3)_{i+1}^n
$$
$$
\text{(3.13)} \quad + R_3 R_1 (C_1)_i^n \Delta t,
$$

where $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma_i^n = \frac{u_i^n \Delta t}{\Delta x}$.

The left and right-bounds of the boundary conditions of this model are the derivative equations. Likewise, we can get (3.14) for the left and right sides, as below, from substituting (3.1) into (2.13) and rearranging these equations.

The left boundary condition; $i = 0$,

$$
\frac{\partial C_3(0, t)}{\partial x} = \frac{(C_3)_1^n - (C_3)_{-1}^n}{2\Delta x} = g_3(t),
$$
$$
(C_3)_{-1}^n = (C_3)_1^n - 2g_3(t)\Delta x,
$$

and the right boundary condition; $i = M$,

$$
\text{(3.14)} \quad \frac{\partial C_3(M, t)}{\partial x} = \frac{(C_3)_{M+1}^n - (C_3)_{M-1}^n}{2\Delta x} = h_3(t),
$$
$$
(C_3)_{M+1}^n = 2h_3(t)\Delta x + (C_3)_{M-1}^n.
$$

Substituting (3.14) into (3.13) which leads to the left and right side, (3.15) and (3.16), respectively, given as follows

$$
\text{(3.15)} \quad (C_3)_0^{n+1} = 2\lambda(C_3)_1^n - 2g_3(t)\Delta x \left(\lambda + \frac{1}{2}\gamma_0^n \right) + (1 - 2\lambda)(C_3)_0^n
$$
$$
+ R_3 R_1 (C_1)_0^n \Delta t
$$

and

$$(3.16) \quad (C_3)_M^{n+1} = 2\lambda(C_3)_{M-1}^n + 2h_3(t)\Delta x \left(\lambda - \frac{1}{2}\gamma_M^n\right) + (1 - 2\lambda)(C_3)_M^n$$
$$+ R_3 R_1 (C_1)_M^n \Delta t.$$

3.1.4 Forward Time Central Space technique for the nitrite dispersion model

Likewise, substituting (3.1) into (2.14) leads to (3.17), written as

$$(3.17) \quad \frac{(C_4)_i^{n+1} - (C_4)_i^n}{\Delta t} = -u_i^n \left(\frac{(C_4)_{i+1}^n - (C_4)_{i-1}^n}{2\Delta x}\right)$$
$$+ D_4 \left(\frac{(C_4)_{i+1}^n - 2(C_4)_i^n + (C_4)_{i-1}^n}{(\Delta x)^2}\right) + R_4 R_1 (C_1)_i^n.$$

Rearranging (3.17) leads to (3.18), represented as

$$(C_4)_i^{n+1} = \left(\frac{1}{2}\gamma_i^n + \lambda\right)(C_4)_{i-1}^n + (1 - 2\lambda)(C_4)_i^n$$
$$(3.18) \qquad\qquad + \left(\lambda - \frac{1}{2}\gamma_i^n\right)(C_4)_{i+1}^n + R_4 R_1 (C_1)_i^n \Delta t,$$

where $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma_i^n = \frac{u_i^n \Delta t}{\Delta x}$.

The left and right-bounds of the boundary conditions of this model are the derivative equations. Likewise, we can get (3.19) for the left and right sides, as below, from substituting (3.1) into (2.16) and rearranging these equations.

The left boundary condition; $i = 0$,

$$\frac{\partial C_4(0,t)}{\partial x} = \frac{(C_4)_1^n - (C_4)_{-1}^n}{2\Delta x} = g_4(t),$$
$$(C_4)_{-1}^n = (C_4)_1^n - 2g_4(t)\Delta x,$$

and the right boundary condition; $i = M$,

$$(3.19) \qquad \frac{\partial C_4(M,t)}{\partial x} = \frac{(C_4)_{M+1}^n - (C_4)_{M-1}^n}{2\Delta x} = h_4(t),$$
$$(C_4)_{M+1}^n = 2h_4(t)\Delta x + (C_4)_{M-1}^n.$$

Substituting (3.19) into (3.18) leads to the left and right side, (3.20) and (3.21), respectively, given as follows

$$(3.20) \quad (C_4)_0^{n+1} = 2\lambda(C_4)_1^n - 2g_4(t)\Delta x \left(\lambda + \frac{1}{2}\gamma_0^n\right) + (1 - 2\lambda)(C_4)_0^n$$
$$+ R_4 R_1 (C_1)_0^n \Delta t$$

and

$$(3.21) \quad (C_4)_M^{n+1} = 2\lambda(C_4)_{M-1}^n + 2h_4(t)\Delta x \left(\lambda - \frac{1}{2}\gamma_M^n\right) + (1 - 2\lambda)(C_4)_M^n$$
$$+ R_4 R_1 (C_1)_M^n \Delta t.$$

3.1.5 Forward Time Central Space technique for the nitrate dispersion model

Likewise, substituting (3.1) into (2.17) leads to (3.22), written as

$$
(3.22) \quad \frac{(C_5)_i^{n+1} - (C_5)_i^n}{\Delta t} = - u_i^n \left(\frac{(C_5)_{i+1}^n - (C_5)_{i-1}^n}{2\Delta x} \right)
$$
$$
+ D_5 \left(\frac{(C_5)_{i+1}^n - 2(C_5)_i^n + (C_5)_{i-1}^n}{(\Delta x)^2} \right) + R_5 R_1 (C_1)_i^n.
$$

Rearranging (3.22) leads to (3.23), represented as

$$
(C_5)_i^{n+1} = \left(\frac{1}{2}\gamma_i^n + \lambda \right) (C_5)_{i-1}^n + (1 - 2\lambda)(C_5)_i^n
$$
$$
(3.23) \qquad + \left(\lambda - \frac{1}{2}\gamma_i^n \right) (C_5)_{i+1}^n + R_5 R_1 (C_1)_i^n \Delta t,
$$

where $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma_i^n = \frac{u_i^n \Delta t}{\Delta x}$.

The left and right-bounds of the boundary conditions of this model are the derivative equations. Likewise, we can get (3.24) for the left and right sides, as below, from substituting (3.1) into (2.19) and rearranging these equations.

The left boundary condition; $i = 0$,

$$
\frac{\partial C_5(0, t)}{\partial x} = \frac{(C_5)_1^n - (C_5)_{-1}^n}{2\Delta x} = g_5(t),
$$
$$
(C_5)_{-1}^n = (C_5)_1^n - 2g_5(t)\Delta x,
$$

and the right boundary condition; $i = M$,

$$
(3.24) \quad \frac{\partial C_5(M, t)}{\partial x} = \frac{(C_5)_{M+1}^n - (C_5)_{M-1}^n}{2\Delta x} = h_5(t),
$$
$$
(C_5)_{M+1}^n = 2h_5(t)\Delta x + (C_5)_{M-1}^n.
$$

Substituting (3.24) into (3.23) leads to the left and right side, (3.25) and (3.26), respectively, given as follows

$$
(3.25) \quad (C_5)_0^{n+1} = 2\lambda(C_5)_1^n - 2g_5(t)\Delta x \left(\lambda + \frac{1}{2}\gamma_0^n \right) + (1 - 2\lambda)(C_5)_0^n
$$
$$
+ R_5 R_1 (C_1)_0^n \Delta t
$$

and

$$
(3.26) \quad (C_5)_M^{n+1} = 2\lambda(C_5)_{M-1}^n + 2h_5(t)\Delta x \left(\lambda - \frac{1}{2}\gamma_M^n \right) + (1 - 2\lambda)(C_5)_M^n
$$
$$
+ R_5 R_1 (C_1)_M^n \Delta t.
$$

3.2 Unconditionally stable Saulyev technique applied to five forms of nitrogen dispersion measurement model

Saulyev (1964) introduced asymmetric approximations for the parabolic equations that are widely used in environmental solving, such as advection and diffusion equations, etc. The solution is given to be an approximation that is explicit and has unconditional stability [13].

The Saulyev scheme can be written as the discretization of time, and space derivative term, as per [4]
where let $C(x,t)$ and u denote C_i^n and u_i^n then

$$
\begin{aligned}
\frac{\partial C}{\partial t} &= \frac{C_i^{n+1} - C_i^n}{\Delta t}, \\
\frac{\partial C}{\partial x} &= \frac{C_{i+1}^n - C_{i-1}^{n+1}}{2\Delta x}, \\
\text{and} \quad \frac{\partial^2 C}{\partial x^2} &= \frac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}.
\end{aligned}
$$

(3.27)

Substituting (3.27) into nitrogen dispersion models (the total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate measurement models) results in (2.5), (2.8), (2.11), (2.14), and (2.17), respectively.

3.2.1 Saulyev technique for the total nitrogen dispersion model

Likewise, substituting (3.27) into (2.5) leads to (3.28), written as

$$
\begin{aligned}
\frac{(C_1)_i^{n+1} - (C_1)_i^n}{\Delta t} = &- u_i^n \left(\frac{(C_1)_{i+1}^n - (C_1)_{i-1}^{n+1}}{2\Delta x} \right) \\
&+ D_1 \left(\frac{(C_1)_{i+1}^n - (C_1)_i^n - (C_1)_i^{n+1} + (C_1)_{i-1}^{n+1}}{(\Delta x)^2} \right) \\
&- R_1 (C_1)_i^n + Q.
\end{aligned}
$$

(3.28)

Rearranging (3.28) leads to (3.29), represented as

$$
\begin{aligned}
(C_1)_i^{n+1} = &\frac{1}{(1+\lambda)} \Bigg(\left(\frac{1}{2}\gamma_i^n + \lambda \right) (C_1)_{i-1}^{n+1} + (1 - \lambda - R_1 \Delta t)(C_1)_i^n \\
&+ \left(\lambda - \frac{1}{2}\gamma_i^n \right) (C_1)_{i+1}^n + Q\Delta t \Bigg),
\end{aligned}
$$

(3.29)

where $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma_i^n = \frac{u_i^n \Delta t}{\Delta x}$.

Substituting (3.27) into (2.7) and rearranging on the right-bound of the boundary condition, which is the derivative equation, we get (3.30).

The left boundary condition; $i = 0$,

$$C_1(0, t) = 1,$$

and the right boundary condition; $i = M$,

(3.30)
$$\frac{\partial C_1(M, t)}{\partial x} = \frac{(C_1)^n_{M+1} - (C_1)^n_{M-1}}{2\Delta x} = h_1(t),$$
$$(C_1)^n_{M+1} = 2h_1(t)\Delta x + (C_1)^n_{M-1}.$$

Substituting (3.30) into (3.29) leads to (3.31) of the right side equation, given as

(3.31)
$$(C_1)^{n+1}_i = \frac{1}{(1+\lambda)} \left(2\lambda(C_1)^{n+1}_{M-1} + (1 - \lambda - R_1\Delta t)(C_1)^n_M + 2h_1(t)\Delta x \right.$$
$$\left. \left(\lambda - \frac{1}{2}\gamma^n_M \right) + Q\Delta t \right).$$

3.2.2 Saulyev technique for the organic nitrogen dispersion model

Likewise, substituting (3.27) into (2.8) leads to (3.32), written as

(3.32)
$$\frac{(C_2)^{n+1}_i - (C_2)^n_i}{\Delta t} = - u^n_i \left(\frac{(C_2)^n_{i+1} - (C_2)^{n+1}_{i-1}}{2\Delta x} \right)$$
$$+ D_2 \left(\frac{(C_2)^n_{i+1} - (C_2)^n_i - (C_2)^{n+1}_i + (C_2)^{n+1}_{i-1}}{(\Delta x)^2} \right)$$
$$+ R_2 R_1 (C_1)^n_i.$$

Rearranging (3.32) leads to (3.33), represented as

(3.33)
$$(C_2)^{n+1}_i = \frac{1}{(1+\lambda)} \left(\left(\frac{1}{2}\gamma^n_i + \lambda \right) (C_2)^{n+1}_{i-1} + (1 - \lambda)(C_2)^n_i \right.$$
$$\left. + \left(\lambda - \frac{1}{2}\gamma^n_i \right) (C_2)^n_{i+1} + R_2 R_1 (C_1)^n_i \Delta t \right),$$

where $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma^n_i = \frac{u^n_i \Delta t}{\Delta x}$.

Substituting (3.27) into (2.10) and rearranging on the left and right-bound of the boundary condition of this model, which are the derivative equation, we get (3.34).

The left boundary condition; $i = 0$,

$$\frac{\partial C_2(0,t)}{\partial x} = \frac{(C_2)_1^n - (C_2)_{-1}^{n+1}}{2\Delta x} = g_2(t),$$
$$(C_2)_{-1}^n = (C_2)_1^{n+1} - 2g_2(t)\Delta x,$$

and the right boundary condition; $i = M$,

$$(3.34) \qquad \frac{\partial C_2(M,t)}{\partial x} = \frac{(C_2)_{M+1}^n - (C_2)_{M-1}^{n+1}}{2\Delta x} = h_2(t),$$
$$(C_2)_{M+1}^n = 2h_2(t)\Delta x + (C_2)_{M-1}^{n+1}.$$

Substituting (3.34) into (3.33) leads to the left and right side (3.35) and (3.36), respectively, given as follows

$$(3.35) \qquad (C_2)_0^{n+1} = \frac{1}{(1+\lambda)}\Bigg(2\lambda(C_2)_1^{n+1} + (1-\lambda)(C_2)_0^n - 2g_2(t)\Delta x$$
$$\left(\lambda + \frac{1}{2}\gamma_0^n\right) + R_2R_1(C_1)_0^n\Delta t\Bigg)$$

and

$$(3.36) \qquad (C_2)_M^{n+1} = \frac{1}{(1+\lambda)}\Bigg((2\lambda(C_2)_{M-1}^{n+1} + (1-\lambda)(C_2)_M^n + 2h_2(t)\Delta x$$
$$\left(\lambda - \frac{1}{2}\gamma_M^n\right) + R_2R_1(C_1)_M^n\Delta t\Bigg).$$

3.2.3 Saulyev technique for the ammonia dispersion model

Likewise, substituting (3.27) into (2.11) leads to (3.37), written as

$$(3.37) \qquad \frac{(C_3)_i^{n+1} - (C_3)_i^n}{\Delta t} = -u_i^n\left(\frac{(C_3)_{i+1}^n - (C_3)_{i-1}^{n+1}}{2\Delta x}\right)$$
$$+ D_3\left(\frac{(C_3)_{i+1}^n - (C_3)_i^n - (C_3)_i^{n+1} + (C_3)_{i-1}^{n+1}}{(\Delta x)^2}\right)$$
$$+ R_3R_1(C_1)_i^n.$$

Rearranging (3.37) leads to (3.38), represented as

$$(3.38) \qquad (C_3)_i^{n+1} = \frac{1}{(1+\lambda)}\Bigg(\left(\frac{1}{2}\gamma_i^n + \lambda\right)(C_3)_{i-1}^{n+1} + (1-\lambda)(C_3)_i^n$$
$$+ \left(\lambda - \frac{1}{2}\gamma_i^n\right)(C_3)_{i+1}^n + R_3R_1(C_1)_i^n\Delta t\Bigg),$$

where $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma_i^n = \frac{u_i^n \Delta t}{\Delta x}$.

The left and right-bounds of the boundary conditions of this model are the derivative equations. Likewise, we can get (3.39) for the left and right sides, as below, from substituting (3.27) into (2.13) and rearranging these equations.

The left boundary condition; $i = 0$,

$$\frac{\partial C_3(0,t)}{\partial x} = \frac{(C_3)_1^n - (C_3)_{-1}^{n+1}}{2\Delta x} = g_3(t),$$
$$(C_3)_{-1}^n = (C_3)_1^{n+1} - 2g_3(t)\Delta x,$$

and the right boundary condition; $i = M$,

(3.39)
$$\frac{\partial C_3(M,t)}{\partial x} = \frac{(C_3)_{M+1}^n - (C_3)_{M-1}^{n+1}}{2\Delta x} = h_3(t),$$
$$(C_3)_{M+1}^n = 2h_3(t)\Delta x + (C_3)_{M-1}^{n+1}.$$

Substituting (3.39) into (3.38) which leads to the left and right side (3.40) and (3.41), respectively, given as follows

(3.40)
$$(C_3)_0^{n+1} = \frac{1}{(1+\lambda)}\left(2\lambda(C_3)_1^{n+1} + (1-\lambda)(C_3)_0^n - 2g_3(t)\Delta x\left(\lambda + \frac{1}{2}\gamma_0^n\right) \right.$$
$$\left. + R_3 R_1 (C_1)_0^n \Delta t \right)$$

and

(3.41)
$$(C_3)_M^{n+1} = \frac{1}{(1+\lambda)}\left(2\lambda(C_3)_{M-1}^{n+1} + (1-\lambda)(C_3)_M^n + 2h_3(t)\Delta x\left(\lambda - \frac{1}{2}\gamma_M^n\right) \right.$$
$$\left. + R_3 R_1 (C_1)_M^n \Delta t \right).$$

3.2.4 Saulyev technique for the nitrite dispersion model

Likewise, substituting (3.27) into (2.14) leads to (3.42), written as

(3.42)
$$\frac{(C_4)_i^{n+1} - (C_4)_i^n}{\Delta t} = -u_i^n\left(\frac{(C_4)_{i+1}^n - (C_4)_{i-1}^{n+1}}{2\Delta x} \right)$$
$$+ D_4\left(\frac{(C_4)_{i+1}^n - (C_4)_i^n - (C_4)_i^{n+1} + (C_4)_{i-1}^{n+1}}{(\Delta x)^2} \right)$$
$$+ R_4 R_1 (C_1)_i^n.$$

Rearranging (3.42) which leads to (3.43), represented as

$$
(3.43) \quad
\begin{aligned}
(C_4)_i^{n+1} = & \frac{1}{(1+\lambda)} \Bigg(\left(\frac{1}{2}\gamma_i^n + \lambda \right) (C_4)_{i-1}^{n+1} + (1-\lambda)(C_4)_i^n \\
& + \left(\lambda - \frac{1}{2}\gamma_i^n \right) (C_4)_{i+1}^n + R_4 R_1 (C_1)_i^n \Delta t \Bigg),
\end{aligned}
$$

where $\lambda = \frac{D \Delta t}{(\Delta x)^2}$ and $\gamma_i^n = \frac{u_i^n \Delta t}{\Delta x}$.

The left and right-bounds of the boundary conditions of this model are the derivative equations. Likewise, we can get (3.44) for the left and right sides, as below, from substituting (3.27) into (2.16) and rearranging these equations.

The left boundary condition; $i = 0$,

$$
\begin{aligned}
\frac{\partial C_4(0,t)}{\partial x} = & \frac{(C_4)_1^n - (C_4)_{-1}^{n+1}}{2\Delta x} = g_4(t), \\
(C_4)_{-1}^n = & (C_4)_1^{n+1} - 2g_4(t)\Delta x,
\end{aligned}
$$

and the right boundary condition; $i = M$,

$$
(3.44) \quad
\begin{aligned}
\frac{\partial C_4(M,t)}{\partial x} = & \frac{(C_4)_{M+1}^n - (C_4)_{M-1}^{n+1}}{2\Delta x} = h_4(t), \\
(C_4)_{M+1}^n = & 2h_4(t)\Delta x + (C_4)_{M-1}^{n+1}.
\end{aligned}
$$

Substituting (3.44) into (3.43) leads to the left and right side (3.45) and (3.46), respectively, given as follows

$$
(3.45) \quad
\begin{aligned}
(C_4)_0^{n+1} = & \frac{1}{(1+\lambda)} \Bigg(2\lambda(C_4)_1^{n+1} + (1-\lambda)(C_4)_0^n - 2g_4(t)\Delta x \left(\lambda + \frac{1}{2}\gamma_0^n \right) \\
& + R_4 R_1 (C_1)_0^n \Delta t \Bigg)
\end{aligned}
$$

and

$$
(3.46) \quad
\begin{aligned}
(C_4)_M^{n+1} = & \frac{1}{(1+\lambda)} \Bigg(2\lambda(C_4)_{M-1}^{n+1} + (1-\lambda)(C_4)_M^n + 2h_4(t)\Delta x \left(\lambda - \frac{1}{2}\gamma_M^n \right) \\
& + R_4 R_1 (C_1)_M^n \Delta t \Bigg).
\end{aligned}
$$

3.2.5 Saulyev technique for the nitrate dispersion model

Likewise, substituting (3.27) into (2.17) leads to (3.47), written as

(3.47)
$$
\begin{aligned}
\frac{(C_5)_i^{n+1} - (C_5)_i^n}{\Delta t} =& -u_i^n \left(\frac{(C_5)_{i+1}^n - (C_5)_{i-1}^{n+1}}{2\Delta x} \right) \\
&+ D_5 \left(\frac{(C_5)_{i+1}^n - (C_5)_i^n - (C_5)_i^{n+1} + (C_5)_{i-1}^{n+1}}{(\Delta x)^2} \right) \\
&+ R_5 R_1 (C_1)_i^n.
\end{aligned}
$$

Rearranging (3.47) leads to (3.48), represented as

(3.48)
$$
\begin{aligned}
(C_5)_i^{n+1} =& \frac{1}{(1+\lambda)} \left(\left(\frac{1}{2}\gamma_i^n + \lambda \right) (C_5)_{i-1}^{n+1} + (1-\lambda)(C_5)_i^n \right. \\
&\left. + \left(\lambda - \frac{1}{2}\gamma_i^n \right) (C_5)_{i+1}^n + R_5 R_1 (C_1)_i^n \Delta t \right),
\end{aligned}
$$

where $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma_i^n = \frac{u_i^n \Delta t}{\Delta x}$.

The left and right-bounds of the boundary conditions of this model are the derivative equations. Likewise, we can get (3.49) for the left and right sides, as below, from substituting (3.27) into (2.19) and rearranging these equations.

The left boundary condition; $i = 0$,

$$
\begin{aligned}
\frac{\partial C_5(0,t)}{\partial x} =& \frac{(C_5)_1^n - (C_5)_{-1}^{n+1}}{2\Delta x} = g_5(t), \\
(C_5)_{-1}^n =& (C_5)_1^{n+1} - 2g_5(t)\Delta x,
\end{aligned}
$$

and the right boundary condition; $i = M$,

(3.49)
$$
\begin{aligned}
\frac{\partial C_5(M,t)}{\partial x} =& \frac{(C_5)_{M+1}^n - (C_5)_{M-1}^{n+1}}{2\Delta x} = h_5(t), \\
(C_5)_{M+1}^n =& 2h_5(t)\Delta x + (C_5)_{M-1}^{n+1}.
\end{aligned}
$$

Substituting (3.49) into (3.48) leads to the left and right side (3.50) and (3.51), respectively, given as follows

(3.50)
$$
\begin{aligned}
(C_5)_0^{n+1} =& \frac{1}{(1+\lambda)} \left(2\lambda(C_5)_1^{n+1} + (1-\lambda)(C_5)_0^n - 2g_5(t)\Delta x \left(\lambda + \frac{1}{2}\gamma_0^n \right) \right. \\
&\left. + R_5 R_1 (C_1)_0^n \Delta t \right)
\end{aligned}
$$

and

$$(C_5)_M^{n+1} = \frac{1}{(1+\lambda)}\left(2\lambda(C_5)_{M-1}^{n+1} + (1-\lambda)(C_5)_M^n + 2h_5(t)\Delta x\left(\lambda - \frac{1}{2}\gamma_M^n\right)\right.$$

(3.51)

$$\left. + R_5 R_1(C_1)_M^n \Delta t\right).$$

4. Numerical experiments

In the section, we implement analytical, FTCS, and Saulyev solutions for approximation in three experiments. The first experiment is an accuracy comparison of the numerical methods with an analytical solution. The second experiment is an efficiency comparison between the FTCS and Saulyev solutions of the nitrogen dispersion models. The last part is a performance simulation of the nitrogen dispersion models with the Saulyev method.

4.1 Numerical simulation of an ideal pollutant dispersion measurement

We compare effective methods between the analytical method and numerical solutions using the FTCS and Saulyev methods. We consider an analytical solution to the simplest case of the governing equation with defined initial and boundary conditions, taken from [9], as an example to compare with the two numerical solutions.

We perform all three cases by computing (2.1) without the term of reactive pollutant ($f(C) = 0$) with the analytical, FTCS, and Saulyev methods. All three cases are easily solvable where it is assumed that the stream length is 1 km, the performance over the entire time interval is [0,1], the velocity component (u) is 1 m/s, the diffusion coefficient (D) is 0.01 m^2/s, and the grid step size of space (Δx) and time (Δt) are 0.05 and 0.0025.

The initial and boundary conditions are given to follow (2.2) and (2.3), and are, respectively [9];

$$C(x,0) = k(x) = exp\left(-\frac{(x+0.5)^2}{0.00125}\right), \quad 0 \le x \le 1,$$

(4.1)

$$C(0,t) = g(t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}}exp\left(-\frac{(0.5-t)^2}{(0.00125 + 0.04t)}\right),$$

$$0 < t \le 1,$$

$$C(1,t) = h(t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}}exp\left(-\frac{(1.5-t)^2}{(0.00125 + 0.04t)}\right),$$

$$0 < t \le 1.$$

Performing (2.1) without the term of reactive pollutant leads to (4.2) for analytical solution, represented as follows [9]

(4.2)
$$C(x,t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}} exp\left(-\frac{(x + 0.5 - t)^2}{0.00125 + 0.04t}\right),$$
$$0 \leq x \leq 1, 0 < t \leq 1.$$

Conducting (2.1) without the term of reactive pollutant by using the FTCS scheme from (3.1), we get and rearrange (4.3), which leads to (4.4)

(4.3) $$\frac{C_i^{n+1} - C_i^n}{\Delta t} = -u_i^n\left(\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}\right) + D\left(\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2}\right),$$

and

(4.4) $$C_i^{n+1} = \left(\frac{1}{2}\gamma_i^n + \lambda\right)C_{i-1}^n + (1 - 2\lambda)C_i^n + \left(\lambda - \frac{1}{2}\gamma_i^n\right)C_{i+1}^n,$$

where $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma_i^n = \frac{u_i^n \Delta t}{\Delta x}$.

Performing (2.1) without the term of reactive pollutant by using the Saulyev scheme from (3.27), we get and rearrange (4.5), which leads to (4.6).

(4.5) $$\frac{C_i^{n+1} - C_i^n}{\Delta t} = -u_i^n\left(\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}\right) + D\left(\frac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}\right),$$

and

(4.6) $$C_i^{n+1} = \frac{1}{(1 + \lambda)}\left(\left(\lambda + \frac{1}{2}\gamma_i^n\right)C_{i-1}^n + (1 - \lambda)C_i^n + \left(\lambda - \frac{1}{2}\gamma_i^n\right)C_{i+1}^n\right),$$

where $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma_i^n = \frac{u_i^n \Delta t}{\Delta x}$.

Consider that (4.2), (4.4), and (4.6) associate with the initial and boundary condition from (4.1). We get the approximate values for all three cases as analytical, FTCS, and Saulyev solutions, respectively.

Hence, these solutions can be shown by graph in order to compare the accuracy assessment of the two numerical methods. Fig. 1 shows the result of two numerical solutions for comparison with the analytical solution at $C(0.5, t)$, which describe the approximate values of two numerical solutions near fixed points of the analytic solution, showing that the numerical solutions are best.

4.2 Numerical simulations of five forms of nitrogen pollutant concentration measurements

We consider here the experiment for comparing two numerical methods, the FTCS and Saulyev methods, with the application of nitrogen dispersion models in section 2.2. It is possible to use numerical methods to solve each case of the defined grid space (Δx) and time (Δt) increments.
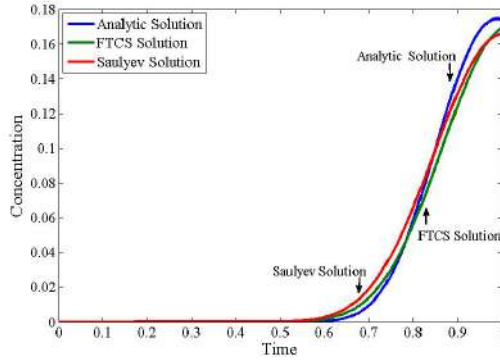
Figure 1: Comparison of concentrations (kg/m^3) of analytic, FTCS and Saulyev solutions at $C(0.5, t)$.

Table 1: Comparison Δx and Δt for computing nitrogen pollutant models of the total nitrogen with two numerical methods which are possible in the solving.

Δx	Δt	λ	γ	FTCS	SAULYEV
	0.1	0.25	0.05	stable	stable
0.2	0.05	0.125	0.025	stable	stable
	0.025	0.0625	0.0125	stable	stable
	0.0125	0.0313	0.00625	stable	stable
	0.1	1	0.1	unstable	stable
0.1	0.05	0.5	0.05	stable	stable
	0.025	0.25	0.025	stable	stable
	0.0125	0.125	0.0125	stable	stable
	0.1	4	0.2	unstable	stable
0.05	0.05	2	0.1	unstable	stable
	0.025	1	0.05	unstable	stable
	0.0125	0.5	0.025	stable	stable
	0.1	16	0.4	unstable	stable
0.025	0.05	8	0.2	unstable	stable
	0.025	4	0.1	unstable	stable
	0.0125	2	0.05	unstable	stable

For example, considering the concentration measurement of the nitrogen pollutant concentration in a stream at time t of total nitrogen (C_1), organic nitrogen (C_2), ammonia (C_3), nitrite (C_4), and nitrate (C_5) concentrations, assume that the stream reach is about 1 km, which is considered over the entire time interval [0,1]. This stream is surrounded by residential components. Wastewater is discharged into the stream, such that the wastewater contains nitrogen as the total nitrogen concentration form, which is everywhere throughout the stream,

is described by a interpolated function $C_1(x,0) = k_1(x) = 1 + x(1-x)$ kg/m^3 initially, this discharged pollutant concentration at the left side of the stream $(x = 0)$ is $C_1(0,t) = g_1(t) = 1$ kg/m^3 for all time and at $t = 0$, and the right side of the stream $(x = 1)$ is the rate of change of the total nitrogen concentration for releasing out $\frac{\partial C_1(1,t)}{\partial x} = h_1(t) = -0.001$ for all time and at $t = 0$. Organic nitrogen, ammonia, nitrite, and nitrate pollutant concentrations depend on the total nitrogen concentration, such that they are defined by the same values as there are pollutant concentrations everywhere throughout the stream, and are kept at $C_2(x,0) = C_3(x,0) = C_4(x,0) = C_5(x,0) = 0$ kg/m^3 initially, at the left side of the stream $(x = 0)$ is the rate of change of nitrogen pollutant concentration for releasing in as $\frac{\partial C_2(0,t)}{\partial x} = \frac{\partial C_3(0,t)}{\partial x} = \frac{\partial C_4(0,t)}{\partial x} = \frac{\partial C_5(0,t)}{\partial x} = 0$ for all time and at $t = 0$, and the right side of the stream is the rate of change of nitrogen pollutant concentration for releasing out as $\frac{\partial C_2(1,t)}{\partial x} = \frac{\partial C_3(1,t)}{\partial x} = \frac{\partial C_4(1,t)}{\partial x} = \frac{\partial C_5(1,t)}{\partial x} = -0.001$ for all time and at $t = 0$. The component of velocity is a constant as $u = 0.1$ m/s. This stream has approximate diffusion coefficients of total nitrogen (D_1), organic nitrogen (D_2), ammonia (D_3), nitrite (D_4), and nitrate (D_5) concentrations of 0.1, $0.85D_1$, $0.65D_1$, $0.45D_1$, and $0.3D_1$ m^2/s, respectively. The rates of degradation of total nitrogen (R_1), organic nitrogen (R_2), ammonia (R_3), nitrite (R_4), and nitrate (R_5) concentrations are 0.1, $0.85R_1$, $0.65R_1$, $0.45R_1$, and $0.3R_1$ s^{-1}, respectively. The inlet flow of the total nitrogen concentration into the stream is 0.001 m^2/s.

Start by computing the numerical solution equations (the FTCS and Saulyev methods). For the FTCS method, implement solution equatios as the total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate in section 3.1, which associate with setting parameter values. For the Saulyev method, implement solution equations as the total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate in section 3.2, which associate with setting parameter values.

Perform both methods for each Δx and Δt to compare each output of the numerical method that can be possible to measure for each case, as shown in Table 1.

From Table 1, we observe that it is possible to use the test to solve all of the cases for the Saulyev solutions. The FTCS solutions represent divergent yields and cannot be used in some cases. Therefore, the Saulyev method shows that is a consistent method for all cases under unconditional stability.

The FTCS method is impossible to compute if Δt has such large increases to not be satisfied for stability conditions which depend on λ and γ.

4.3　Numerical simulations of water-quality measurement in a stream with nitrogen pollutant concentration measurement using Saulyev method

According to the numerical computation of the nitrogen dispersion models, the FTCS method is impossible to use for the majority of cases. In the current section, we implement the Saulyev method with the nitrogen dispersion models.

This presents a comparative computation of nitrogen pollutant concentration for the different rates of change observed in them at the right boundary conditions, in order to explain the different nitrogen pollutant concentration behaviors.

Similarly, from the previous section, the same implementation of the Saulyev method is done with the concentration measurement of the nitrogen pollutant concentration in the stream at time t as the total nitrogen(C_1), organic nitrogen(C_2), ammonia (C_3), nitrite (C_4), and nitrate (C_5). Assume that the stream reach is about 1 km, which is considered over the entire time interval [0,1], some stream physical characteristics, initial and boundary conditions are similar, but some stream physical characteristics are different, such as the component of velocity depending on distance x, described by a function $u = 0.1 + x(1-x)(0.1)$ m/s. This stream has an approximate diffusion coefficient of the total nitrogen concentration (D_1) with a function $D_1 = 0.1 + (1 + x(1-x))(0.1)$ m^2/s, depending on distances. Furthermore, the grid space (Δx) and time (Δt) increments are defined by 0.00625 and 0.01, respectively.

We perform solution equations for the total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate with the Saulyev method in section 3.2, all five cases which associate with setting parameter values above and the previous section, by determining the different rates of change of nitrogen pollutant concentrations at right boundary conditions of -0.001, -0.002, -0.003, -0.004 and -0.005. Table 2 and 3 show each nitrogen pollutant concentration where the rates of change of nitrogen pollutant concentrations at the right boundary conditions of -0.001 and -0.005, respectively.

We observed that each measurement of all five cases gives each output of concentration in the same direction of the approximated value and each output of concentration in the cases of organic nitrogen, ammonia, nitrite, and nitrate obtained depend on the different defined rates of change of nitrogen pollutant concentrations at right boundary conditions.

5. Discussion

Consider that the given five graphs in Fig. 2 are examples from the nitrogen pollutant models in the case of the rate of change of nitrogen pollutant concentrations at the right boundary condition of -0.001. The graphs clearly show the effects of the increase or decrease in nitrogen pollutant concentrations in the stream, such that the total nitrogen pollutant concentration decreased continuously in Fig.2 (a), while the organic nitrogen, ammonia, nitrite and nitrate pollutant concentrations increased continuously in Fig. 2 (b)-(e). It can be explained that discharged wastewater consists of nitrogen pollutant concentrations, as the total nitrogen concentration, which is the origination concentration, can measure four different nitrogen pollutant concentrations (organic nitrogen, ammonia, nitrite, and nitrate) at many space points at various times. Fig. 3 compares each nitrogen pollutant concentration (organic nitrogen, ammonia, nitrite, and nitrate pollutant concentrations) from the total nitrogen concentra-

Figure 2: (a)The total nitrogen, (b)organic nitrogen, (c)ammonia, (d) nitrite, and (e)nitrate (kg/m^3) where the rate of change at the right boundary condition is -0.001.

tions by considering the different rates of change of nitrogen pollutant concentrations at right boundary conditions of -0.001, -0.002, -0.003, -0.004, and, -0.005, such that the different rates of change of nitrogen pollutant concentrations at the right boundary condition is similar, the organic nitrogen pollutant concentration is at a higher level, and the other pollutant concentrations (ammonia, nitrite, and nitrate) have high concentrations, respectively, following nature. Fig. 4

(a)

(b)

(c)

(d)

(e)
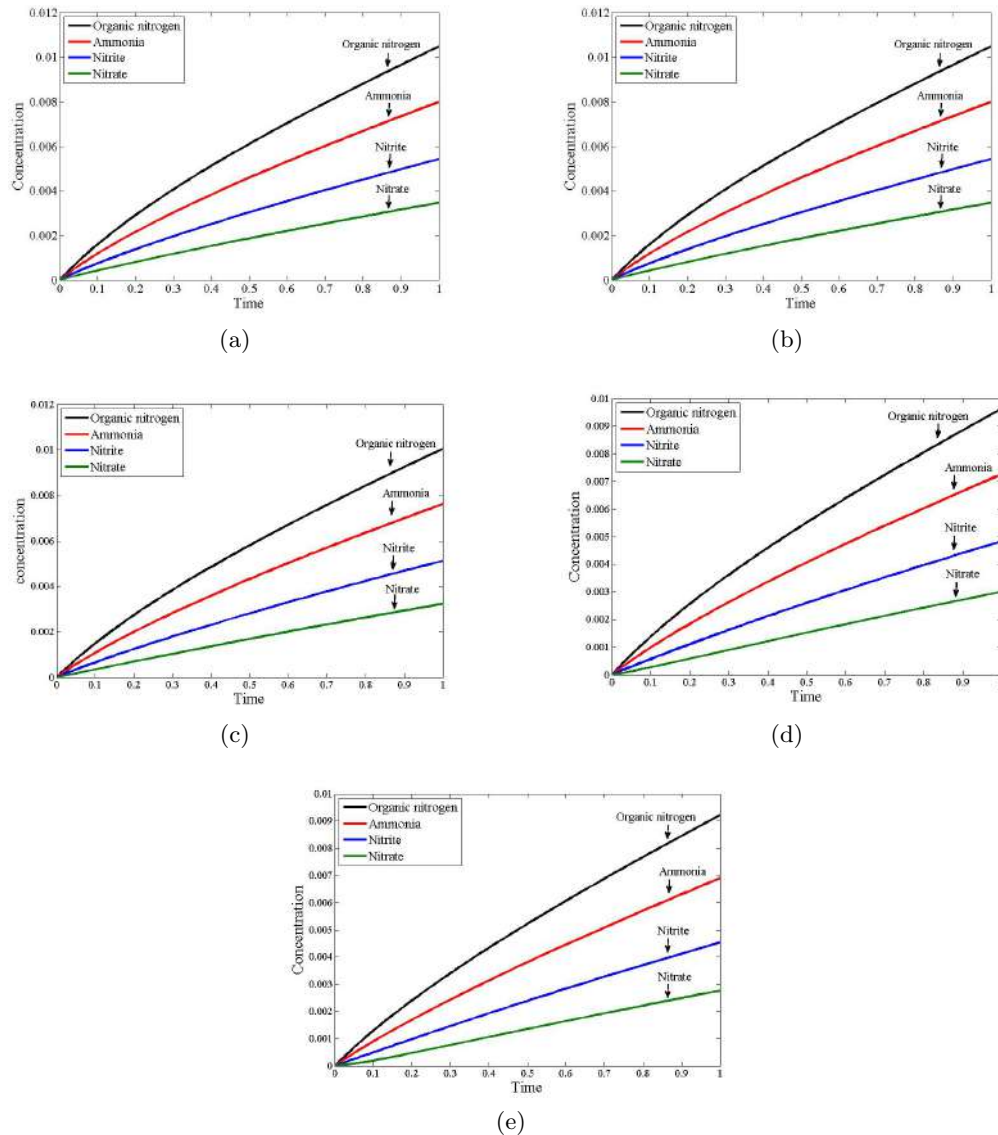
Figure 3: The organic nitrogen, ammonia, nitrite, and nitrate concentrations (kg/m^3) from the total nitrogen concentration in cases of the rates of change at right boundary condition of (a)-0.001, (b)-0.002, (c)-0.003, (d)-0.004, and (e)-0.005 at $C(1,t)$.

compares the different rates of change of nitrogen pollutant concentrations at right boundary conditions of -0.001, -0.002, -0.003, -0.004, and -0.005 such that they affect the pollutant concentration levels of each nitrogen pollutant concentration (the total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate pollutant concentrations). The difference of each nitrogen pollutant concentra-

(a)

(b)

(c)

(d)

(e)

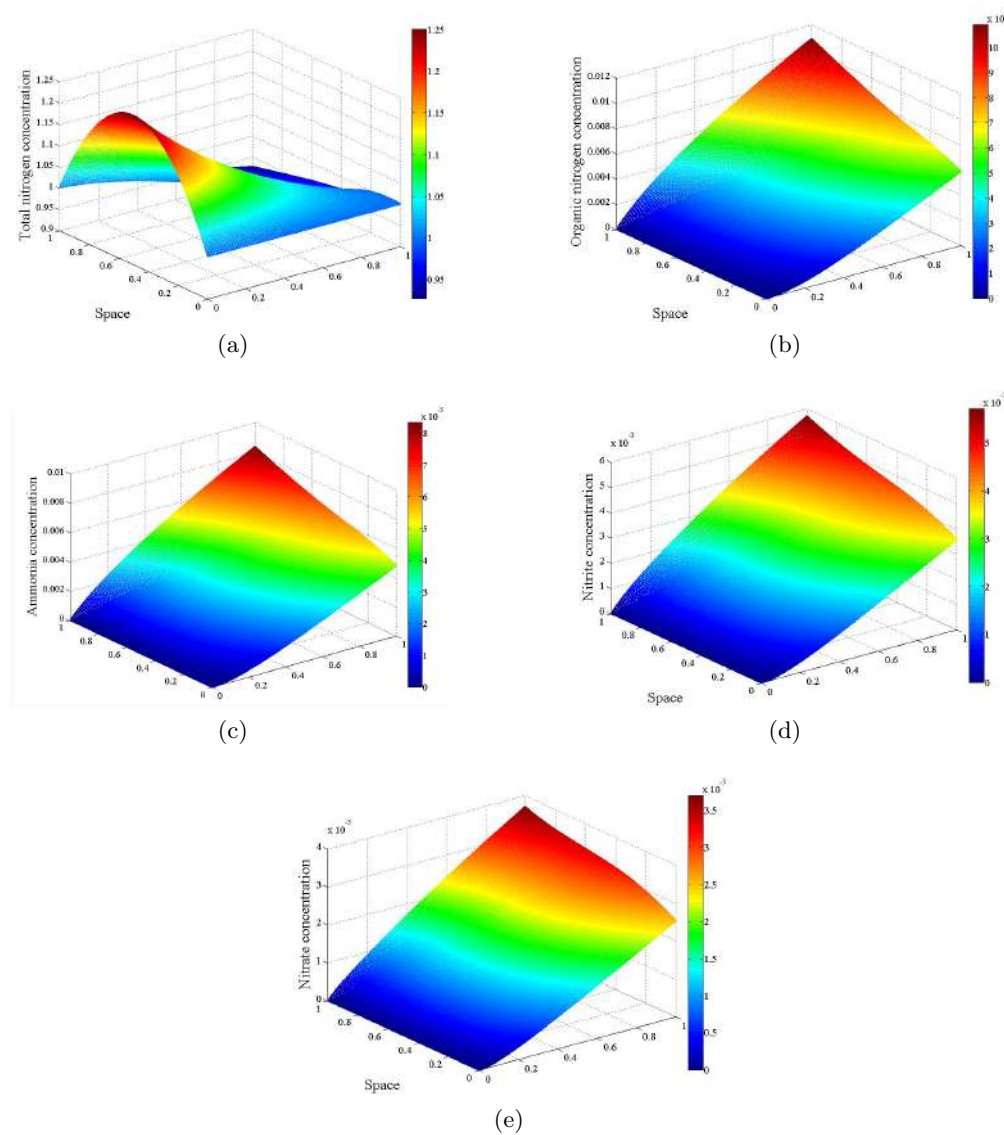Figure 4: Comparison (a) the total nitrogen, (b) organic nitrogen, (c) ammonia, (d) nitrite, and (e) nitrate (kg/m^3) when the rates of change at the right boundary condition are -0.001, -0.002, -0.003, -0.004, and -0.005 at $C(1,t)$.

tion between the rates of change at right boundary conditions at $C(1,t)$ have equal pollutant concentration values, which shown in Table 4. Observe that if the rates of change of nitrogen pollutant concentrations have low values to high values, the nitrogen pollutant concentration levels will also have low values to high values respectively.

(a)

$t \setminus x$	0	0.2	0.4	0.6	0.8	1
0	1	1.1600	1.2400	1.2400	1.1600	1
0.2	1	1.1112	1.1620	1.1465	1.0616	1.0112
0.4	1	1.0734	1.0991	1.0689	1.0058	0.9930
0.6	1	1.0429	1.0470	1.0034	0.9860	0.9693
0.8	1	1.0177	1.0031	0.9766	0.9635	0.9467
1	1	0.9965	0.9702	0.9582	0.9430	0.9273

(b)

$t \setminus x$	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.5422	1.1541	1.5746	1.8371	1.9462	3.0696
0.4	1.6457	2.5138	3.1438	3.5373	3.9721	5.3720
0.6	2.9711	3.9580	4.6862	5.1254	6.0974	7.3600
0.8	4.3962	5.4335	6.1916	6.9160	7.9936	9.1780
1	5.8637	6.9113	7.6932	8.6747	9.7592	10.8905

(c)

$t \setminus x$	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.4918	1.0041	1.3282	1.5092	1.5594	2.3043
0.4	1.4213	2.1222	2.605	2.8789	3.1126	4.0544
0.6	2.4970	3.2809	3.8376	4.1442	4.7102	5.5914
0.8	3.6337	4.4507	5.0295	5.4828	6.1653	7.0068
1	4.7942	5.6159	6.1984	6.812	7.5319	8.3428

(d)

$t \setminus x$	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.4172	0.8025	1.0171	1.1166	1.1187	1.5024
0.4	1.1281	1.6371	1.9618	2.1187	2.1853	2.6907
0.6	1.9180	2.4801	2.8581	3.0372	3.2616	3.763
0.8	2.7389	3.3215	3.7170	3.9480	4.2688	4.7613
1	3.5708	4.1553	4.5481	4.8565	5.2251	5.7072

(e)

$t \setminus x$	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.3335	0.6017	0.7295	0.7752	0.7561	0.9103
0.4	0.8445	1.1932	1.3956	1.4732	1.4590	1.6760
0.6	1.3949	1.7786	2.0202	2.1125	2.1570	2.3872
0.8	1.9602	2.3576	2.6145	2.723	2.8245	3.0587
1	2.5303	2.9292	3.1857	3.3267	3.4648	3.6994

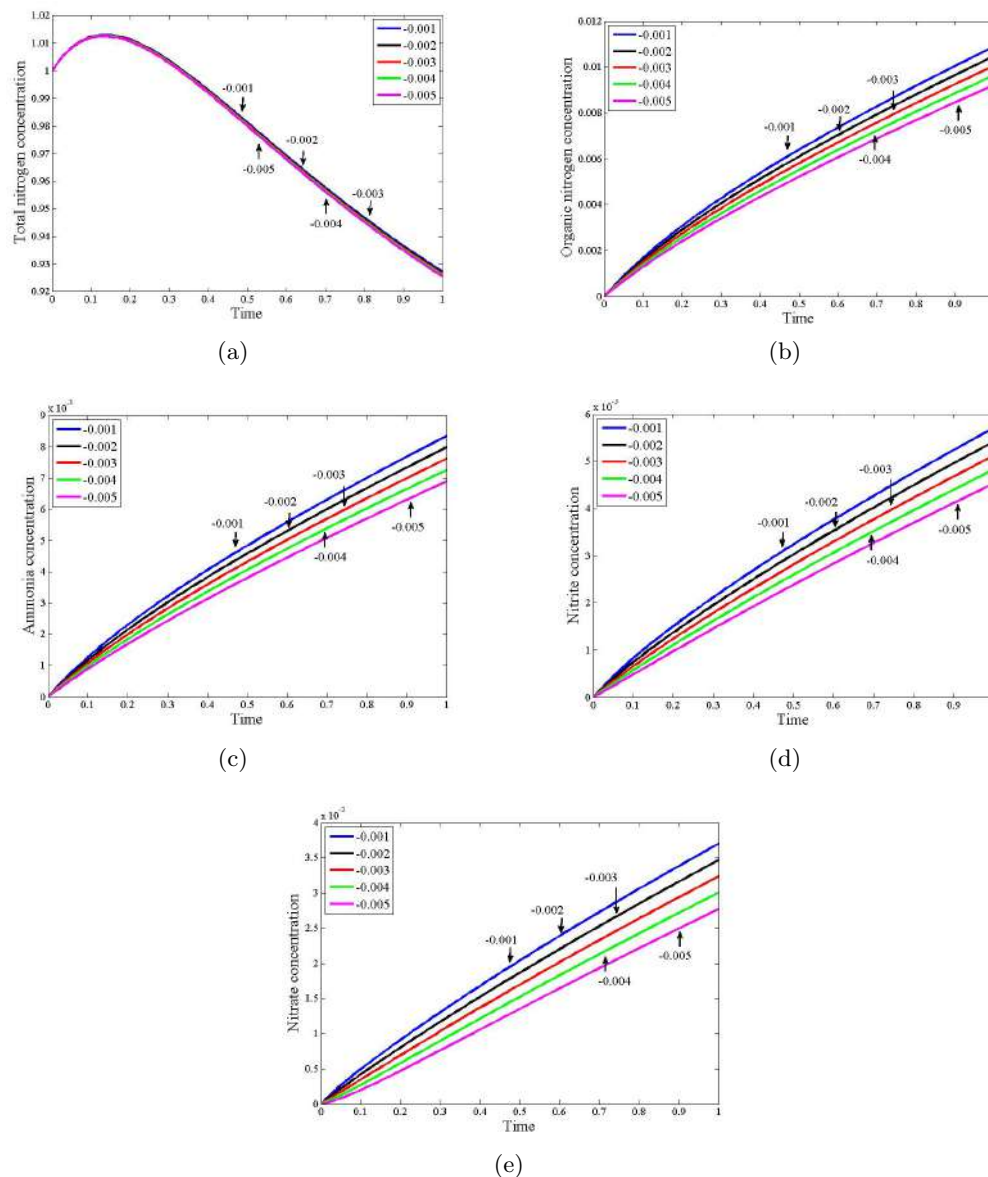Table 2. (a) The total nitrogen, (b) organic nitrogen, (c) ammonia, (d) nitrite, and (e) nitrate, (kg/m^3) where the rate of change at the right boundary condition is -0.001 such that there are Δx=0.00625 and Δt=0.01.

6. Conclusion

In this study, the nitrogen pollutant concentration models in a stream, the total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate concentrations, are considered. These models show that each nitrogen pollutant concentration behavior, such as the total nitrogen concentration, affects the measurement of various pollutant concentrations of nitrogen, such as the organic nitrogen,

(a)

$t \backslash x$	0	0.2	0.4	0.6	0.8	1
0	1	1.1600	1.2400	1.2400	1.1600	1
0.2	1	1.1112	1.1620	1.1465	1.0616	1.0105
0.4	1	1.0734	1.0991	1.0689	1.0056	0.9919
0.6	1	1.0429	1.0470	1.0034	0.9855	0.9679
0.8	1	1.0177	1.0031	0.9764	0.9628	0.9451
1	1	0.9965	0.9702	0.9578	0.9421	0.9255

(b)

$t \backslash x$	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.5422	1.1541	1.5746	1.8371	1.9462	2.3966
0.4	1.6457	2.5138	3.1438	3.5373	3.8069	4.3332
0.6	2.9711	3.9580	4.6862	5.1254	5.6310	6.064
0.8	4.3962	5.4335	6.1916	6.7568	7.3045	7.6775
1	5.8637	6.9113	7.6716	8.3508	8.8875	9.2172

(c)

$t \backslash x$	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.4918	1.0041	1.3282	1.5092	1.5594	1.6906
0.4	1.4213	2.1222	2.6050	2.8789	2.9834	3.1357
0.6	2.4970	3.2809	3.8376	4.1442	4.3456	4.4593
0.8	3.6337	4.4507	5.0295	5.3777	5.6233	5.7045
1	4.7942	5.6159	6.1871	6.5895	6.8423	6.8966

(d)

$t \backslash x$	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.4172	0.8025	1.0171	1.1166	1.1187	0.9729
0.4	1.1281	1.6371	1.9618	2.1187	2.1017	1.9249
0.6	1.9180	2.4801	2.8581	3.0372	3.0172	2.8312
0.8	2.7389	3.3215	3.717	3.8967	3.8967	3.6969
1	3.5708	4.1553	4.5447	4.7367	4.7447	4.5310

(e)

$t \backslash x$	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.3335	0.6017	0.7295	0.7752	0.7561	0.4709
0.4	0.8445	1.1932	1.3956	1.4732	1.4151	1.0574
0.6	1.3949	1.7786	2.0202	2.1125	2.0141	1.6426
0.8	1.9602	2.3576	2.6145	2.7048	2.5964	2.2139
1	2.5303	2.9292	3.1852	3.2761	3.1626	2.7709

Table 3. (a) The total nitrogen, (b) organic nitrogen, (c) ammonia, (d) nitrite, and (e) nitrate, (kg/m^3) where the rate of change at the right boundary condition is -0.005 such that there are Δx=0.00625 and Δt=0.01.

ammonia, nitrite, and nitrate. The solution performance of these models can be shown by using the numerical methods (the FTCS and Saulyev methods), which are explicit schemes. Both methods are in good agreement with the analytic solution but they have differences under conditions, such that the FTCS method can solve problems under a stability condition, while the Saulyev method be able to solve many scenarios without the limitation of stability conditions. The Saulyev method gives good agreement approximated solutions without stability

(a)

$t \setminus rates$	-0.001 and -0.002	-0.002 and -0.003	-0.003 and -0.004	-0.004 and -0.005
		$(\times 10^{-3})$		
0	0	0	0	0
0.2	1.7636	1.7636	1.7636	1.7636
0.4	2.7637	2.7637	2.7637	2.7637
0.6	3.4577	3.4577	3.4577	3.4577
0.8	3.9962	3.9962	3.9962	3.9962
1	4.4401	4.4401	4.4401	4.4401

(b)

$t \setminus rates$	-0.001 and -0.002	-0.002 and -0.003	-0.003 and -0.004	-0.004 and -0.005
		$(\times 10^{-4})$		
0	0	0	0	0
0.2	1.6824	1.6824	1.6824	1.6824
0.4	2.5970	2.5970	2.5970	2.5970
0.6	3.2400	3.2400	3.2400	3.2400
0.8	3.7513	3.7513	3.7513	3.7513
1	4.1833	4.1833	4.1833	4.1833

(c)

$t \setminus rates$	-0.001 and -0.002	-0.002 and -0.003	-0.003 and -0.004	-0.004 and -0.005
		$(\times 10^{-4})$		
0	0	0	0	0
0.2	1.5341	1.5341	1.5341	1.5341
0.4	2.2966	2.2966	2.2966	2.2966
0.6	2.8301	2.8301	2.8301	2.8301
0.8	3.2557	3.2557	3.2557	3.2557
1	3.6156	3.6156	3.6156	3.6156

(d)

$t \setminus rates$	-0.001 and -0.002	-0.002 and -0.003	-0.003 and -0.004	-0.004 and -0.005
		$(\times 10^{-4})$		
0	0	0	0	0
0.2	1.3237	1.3237	1.3237	1.3237
0.4	1.9145	1.9145	1.9145	1.9145
0.6	2.3296	2.3296	2.3296	2.3296
0.8	2.6610	2.6610	2.6610	2.6610
1	2.9404	2.9404	2.9404	2.9404

(e)

$t \setminus rates$	-0.001 and -0.002	-0.002 and -0.003	-0.003 and -0.004	-0.004 and -0.005
		$(\times 10^{-4})$		
0	0	0	0	0
0.2	1.0985	1.0985	1.0985	1.0985
0.4	1.5463	1.5463	1.5463	1.5463
0.6	1.8617	1.8617	1.8617	1.8617
0.8	2.1119	2.1119	2.1119	2.1119
1	2.3214	2.3214	2.3214	2.3214

Table 4. Comparison each two rates of change at $C(1,t)$ right boundary condition at of (a) the total nitrogen, (b) organic nitrogen, (c) ammonia, (d) nitrite, and (e) nitrate concentrations (kg/m^3) such that there are Δx=0.00625 and Δt=0.01.

limitation. It is a good method for several realistic scenarios. In the simulation, we can see that the total nitrogen pollutant controlling gives better overall water-quality levels than another nitrogen pollutant compounds controlling.

References

[1] J. O. Helgesen, *Surface-Water-Quality Assessment of the Lower Kansas River Basin, Kansas and Nebraska Results of Investigations, 1987-90: National Water-Quality Assessment*, United States Government Printing Office, Washington, 1996, 55-56.

[2] R. F. Weiner and R. A. Matthews, *Environmental Engineering,*4th ed., USA : Elsevier Science, 2003, 97-99.

[3] Q. Feng, *Application Of Alternating Group Explicit Method For Parabolic Equations*, WSEAS Transactions on Information Science and Applications, 6 (2009), 1216-1225.

[4] N. Pochai, *A numerical treatment of nondimensional form of water quality model in a nonuniform flow stream using Saulyev scheme*, Mathematical Problems in Engineering, 491317 (2011), 1-15.

[5] S. A. Mirbagheri, M. Abaspour and K.H. Zamani, *Mathematical modeling of water quality in river systems. Case study : Jajrood river in Tehran Iran*, European Water 27/28 (2009), 31-41.

[6] S. Marsili-Libelli and E. Giusti, *Water quality modelling for small river basins*, Environmental Modelling & Software, 23 (2008), 451-463.

[7] W. Kraychang and N. Pochai, *Implicit finite difference simulation of water pollution control in a connected reservoir system*, IAENG International Journal of Applied Mathematics, 46 (2016), 47-57.

[8] K. Suebyat and N. Pochai, *A numerical simulation of a three-dimensional air quality model in an area under a Bangkok sky train platform using an explicit finite difference scheme*, IAENG International Journal of Applied Mathematics, 47 (2017), 471-476.

[9] M. Dehghan, *Weighted finite difference techniques for the one-dimensional advection diffusion equation*, Applied Mathematics and Computation, 147 (2004), 307-319.

[10] D. A. Chin, *Water-quality engineering in natural systems :fate and transport processes in the water environment*, 2nd ed., John Wiley & Sons, Hoboken, New Jersey, USA, 2013, 39-42.

[11] C. N. Sawyer, P. L. McCarty and G. F. Parkin, *Chemistry for Environmental Engineering and Science*, 5th ed., The McGraw-Hill Companies, 2003, 631-646.

[12] L. K. Wang, Y. Hung and N. K. Shammas, *Advanced Physicochemical Treatment Processes*, Humana Press, Totowa, New Jersey, USA, 2006, 47-48.

[13] L. Lapidus and G. F. Pinder, *Numerical solution of partial differential equations in science and engineering*, Wiley-Interscience, 1999, 192-199.