ตัวแบบเชิงคณิตศาสตร์ของการวัดสารประกอบไนโตรเจนที่มีกลไกกำจัดในแม่น้ำ

MATHEMATICAL MODELS OF NITROGEN COMPOUND MEASUREMENT WITH REMOVAL MECHANISM IN A RIVER

อารีรัตน์ ว่องก๊ก
AREERAT VONGKOK

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A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENT FOR THE DEGREE OF DOCTOR OF PHILOSOPHY IN DEPARTMENT OF APPLIED MATHEMATICS

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หัวข้อวิทยานิพนธ์	ตัวแบบเชิงคณิตศาสตร์ของการวัดสารประกอบไนโตรเจนที่มีกลไกกำจัดในแม่น้ำ
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บทคัดย่อ

มลพิษจากสารประกอบไนโตรเจนเป็นปัญหาทางสิ่งแวดล้อมที่เกิดขึ้นโดยทั่วไป หากแหล่งน้ำต่างๆ ได้รับปริมาณของสารประกอบไนโตรเจนเกินความจำเป็นแล้วนั้น จะเกิดผลกระทบต่อแหล่งน้ำ เช่นปรากฏการณ์ยูโทรฟิเคชัน ซึ่งเป็นอันตรายต่อสุขภาพของมนุษย์ สัตว์น้ำและสัตว์เลี้ยงในปศุสัตว์ ดังนั้นการกำจัดไนโตรเจนทางธรรมชาติที่เป็นมิตรกับสิ่งแวดล้อม เป็นวิธีหนึ่งที่จะช่วยลดปริมาณของสารประกอบไนโตรเจนได้เพื่อควบคุมปริมาณนั้นให้อยู่ในเกณฑ์มาตรฐาน ตัวแบบเชิงคณิตศาสตร์ของการวัดสารประกอบไนโตรเจนที่มีกลไกกำจัดในแม่น้ำนั้น ได้ถูกนำเสนอด้วยสมการการพา การแพร่และปฏิกิริยา แบบหนึ่งมิติ สมการเหล่านี้ใช้วิธีผลต่างอันตะชัดแจ้ง หรือ/และการประมาณค่าในช่วงกำลังสามที่ใช้กับเงื่อนไขค่าเริ่มต้นและขอบเขตในการแก้ปัญหา

คำสำคัญ: สารประกอบไนโตรเจน, ตัวแบบเชิงคณิตศาสตร์, สมการการพา การแพร่และปฏิกิริยา, วิธีผลต่างอันตะชัดแจ้ง, การประมาณค่าในช่วง

Thesis Title	Mathematical Models of Nitrogen Compound Measurement with Removal Mechanism in a River
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Abstract

Nitrogen conpound pollution is environmental problem that occur generally. If several water souces have received amount of nitrogen conpounds over necessity, then they will occur effect aganist water souces such as eutrophication which bring harm to human health, aquatic animals, and livestock animal health. Therefore, natural nitrogen removal which be eco-friendly is one technique that can reduce amount of nitrogen conpounds in order to control those amount under standard rules. Mathematical models of nitrogen compound measurement with removal mechanism in a river are proposed by one-dimensional advection-diffusion-reaction equations. They were solved by explicit Saulyev technique or/and cubic spline interpolation to initial and left boundary conditions.

Keywords: Nitrogen conpound, Mathematical model, Advection-diffusion-reaction equation, Saulyev technique, cubic spline interpolation.

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Areerat Vongkok

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Chapter 1
Introduction

1.1 The nitrogen compound pollution problem and its mathematical measurement

Water plays an important role against living beings on the Earth. Water indicate abundance, culture and economic prosperity and nowadays, due to increased population and socio-economic development lead to economical extensions. These bring into increased requirement for using more natural resources continuously but the most users that are the lack of responsibility or consciousness as well with effect's occurrences of water environment. They discharge wastewater into surface water sources. Although, our world will been developed a good way forward but water pollution problems that still exist continuously. In Thailand, the main sources of wastewater come from different sorts such as domestic (67%), industry (32.5%), and agriculture (0.5%) wastewaters [1].

Nitrogen compound is one of pollutants that is contaminated into surface water sources such that this substance has many forms such as organic nitrogen, ammonia, nitrite, and nitrate. Microbial activities can convert nitrogen to cycle that are organic nitrogen to ammonia by ammonification, ammonia to nitrite and nitrite to nitrate by nitrification, and nitrite and nitrate to nitrogen gases by denitrification [2]. Nitrogen enrichment over demands in surface water affect to occur nitrogen pollution that lead to algae bloom or eutrophication. This phenomenon is causes of changing on aquatic ecosystems such as reduced oxygen concentrations, residues of toxicants in aquatic animals, death of aquatic animals and plants, etc., moreover these substances affect against human and animal health such as the blue-baby syndrome in infants, toxicants on livestock. Therefore, the nitrogen removal will help reduce and control nitrogen level in aquatic ecosystem in order to enter environmental balance or water quality standard rule. The nitrogen removal systems are developed many technological alternatives such that microbial agents is one of alternatives that is interesting. It can restore aquatic ecosystem by bioremediation to be eco-friendly [3].

Due to data collection of various pollutants or substances at any places and time in order to observe behavior of those substances in water sources that are complicated, expensive, and cumbersome. Mathematical tool such as mathematical model that is numerical model which can help describe flow dynamic and mass transport processes at any places and time. This model is described by physical, biological, and chemical processes. Numerical methods are one popular tool that are brought to use for solving such as finite difference, finite volume, finite element

methods, etc. Finite difference method is simple method against using to solve problems [4-6]. Moreover, interpolation techniques are efficient technique computationally, they can approximate functions from data set that known values [7-9].

For implementation, we will propose the advection- dispersion- reaction equation in one-dimensional dispersion models of the nitrogen pollutant and the nitrogen pollutant with removal mechanism, such as the total nitrogen, organic nitrogen, ammonia, nitrite, nitrate, total nitrogen with removal mechanism, and nitrogen remover concentrations. We will also represent efficiency of the approximate solutions by comparing with analytical solutions. We will perform these one-dimensional dispersion models using the Saulyev scheme and Saulyev scheme associated with cubic spline interpolation to the boundary conditions, and then compare the performance of the nitrogen pollutant and nitrogen pollutant with removal mechanism in cases of the different rates of change at the right boundary condition.

1.2 Literature review

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 [4]. The advection and diffusion equation is a form of PDE parabolic equation which plays an important roles in describing transport processes and has obtained popularity in solving various problems, including environmental problems such as water quality measurement [5], [10], and [11], 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 [10] and [11]. 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 [4]. In [5], a water quality assessment of a non-uniform flow river 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 [12], the mathematical model of a one-dimensional advection-diffusion-reaction equation for explaining the mass transport of pollutants and suspended matter in a river or canal was performed by using the Saulyev technique with quadratic interpolated initial-boundary conditions and compared with analytical solution. The results were similar. [6], 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. In [13], 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.

The cubic spline interpolation method is used for results of piecewise linear third-order equations continuously through each defined data point such that they are approximate values at any point between data points [7] which have first and second derivatives to be continuous. It is used in various applications, such as in [8] to compare the efficiency of both cubic spline interpolation and Piecewise Cubic Hermite Spline (PCHIP); there, petroleum engineering data and the defined three functions for interpolation were used, and then error analysis of both methods from defined functions was considered. The cubic spline was shown to be better than the other method. In [14], cubic spline interpolation was applied to the shape of a child's teeth for producing orthodontic arch wires that were individually suitable.

1.3 Objectives of the study

1) To propose mathematical models of the nitrogen compound measurement with removal mechanism.
2) To propose efficient finite difference method.
3) To propose an interpolation technique to initial and left boundary conditions for approximation function from data sets.
4) To consider reaction that occur with the nitrogen compound and the removed nitrogen compound associate with the remover along a river in any time and places.
5) To propose effect of the different rates of change between the river and their environment.

1.4 Scope of the thesis

1) We will consider advection- diffusion- reaction equations for nitrogen compound model and modified model of nitrogen compound with removal mechanism in a river, they consist of the total nitrogen, organic nitrogen, ammonia, nitrite, nitrate, and nitrogen remover.
2) The finite difference methods are considered for approximation solving.
3) The interpolation methods are considered for approximation boundary conditions in models.
4) The simulation are given by each model that are considered to associate with proposed techniques.
5) We will consider the different rates of change at the boundary conditions that affect against the levels of various substances.
6) The levels of various substances are given from approximation that they can adopt for utilization in water source management.

1.5 Plan of the thesis

The thesis explains the numerical models of nitrogen compound and nitrogen compound with removal mechanism. They are showed in form of one-dimensional advection-diffusion-reaction equations that are described with physical, chemical and biological processes. The numerical techniques are efficient which are used for simulation of flow dynamic and interested substance mass levels in transport process in a river.

The first part will study and review the basic knowledges and researches about the nitrogen process, numerical models and performance establish one-dimensional advection-diffusion-reaction equations and defined domains in thesis.

The second part will study the numerical techniques for solving the advection-diffusion-reaction equations such as finite difference methods, unconditionally explicit Saulyev finite difference methods, and applying the other one technique with cubic spline interpolation.

The third part will establish one-dimensional advection- diffusion-reaction equations which have two groups of models such as nitrogen compound and nitrogen compound with removal mechanism models and defined domains.

The forth part is the approximation of nitrogen compound model by using finite difference methods, and then comparing the different rates of change at boundary conditions.

Finally, to be the approximation of nitrogen compound with removal mechanism models by using unconditionally explicit Saulyev finite difference methods

with cubic spline interpolation to boundary conditions, and then comparing also the different rates of change at boundary conditions.

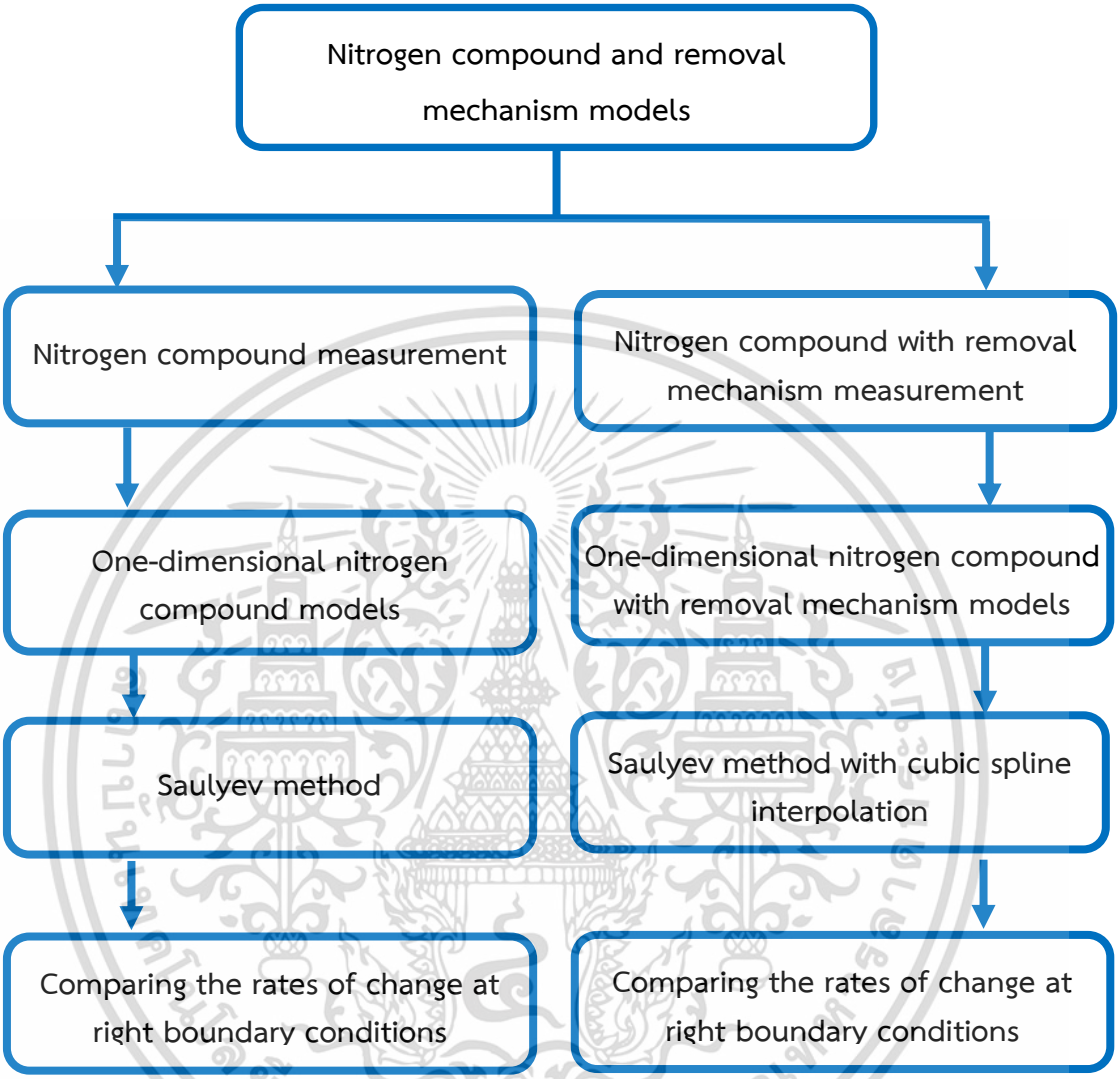


Figure 1.1 Flow chart of the thesis process

1.6 Benefits of the thesis

This proposed study in thesis is to develop the mathematical models for simulation nitrogen compound and nitrogen compound with natural removal mechanism that occur in a river. These simulations can represent the behaviors of goal substance flow and mass at any places and time which are performed by the proposed techniques. Those techniques have received acceptance that are efficient, reliable and accurate for application to use in realistic scenarios. This study can take to apply for water resources management guide in natural water sources in order to prevent the nitrogen compound pollution or algae bloom or eutrophication phenomenon.

Chapter 2
Nitrogen Compounds, Concentration Models and Solving Methods

In this chapter, describe characteristics of nitrogen compound which has five forms in water resources. The nitrogen remover that is eco-friendly. Effects of nitrogen pollution that affect against health risk, the environment and the economy. Surface water quality standard in Thailand that explain classification of water bodies from water usage and required water quality standard parameters. Mathematical model of advection diffusion reaction equation that is basic transport equation from patail differential equation and numerical methods for problem-solving solutions.

2.1 The nitrogen compound

The nitrogen compound in surface water which has the general forms, total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate which play roles in nitrogen processes are described by the general knowledge of nitrogen [4] and [15].

$$\mathrm{ON} \xrightarrow{ammonification} \mathrm{NH_3} \xrightarrow{nitrification} \mathrm{NO_2} \xrightarrow{nitrification} \mathrm{NO_3} \tag{2.1}$$

2.1.1 Total nitrogen

The total nitrogen (TN) is the sum of all nitrogen forms such that organic nitrogen, ammonia, nitrite, and nitrate [16].

2.1.2 Organic nitrogen

Most organic nitrogen (ON) are dissolved in living and nonliving forms from domestic wastes such as urea, uric acid, polypeptides and amino acids [17].

2.1.3 Ammonia

Ammonia $(\mathrm{NH_3})$ occurs in organic nitrogen by the ammonification process, which gives ammonia $(\mathrm{NH_3})$ and ammonium $(\mathrm{NH_4^+})$. The mass of ammonia $(\mathrm{NH_3})$ and ammonium $(\mathrm{NH_4^+})$ are considered in terms of pH and temperature. Ammonia $(\mathrm{NH_3})$ is toxic to aquatic life, whereas ammonium $(\mathrm{NH_4^+})$, supports algae and aquatic plant growth. However, ammonia and ammonium are similar [17].

2.1.4 Nitrite

The nitrite (NO_2) is oxidized by the nitrification process, such as to convert ammonia to nitrite. Nitrite is toxic to infants when at excessive levels [17].

2.1.5 Nitrate

The nitrate (NO_3) is transformed from nitrite by the nitrification process and can convert to nitrite [17], which is toxic and hazardous to infants.

2.2 The nitrogen remover

Microbial technology is one of the processes for the utilization of beneficial microorganisms as microbial agents for biological degradation. They consist of several species, such as yeasts, enzymes, bacillus, micrococcus, photosynthetic bacteria, nitrifying bacteria, denitrifying bacteria, lactic acid bacteria, bacterium pseudoanthracis, actinomycetes, acetobacter, photosynthesizing bacteria, actinomycetes, fermenting fungi, etc. [3,18], which have different biodegradation abilities, pollutant removal mechanisms, and symbiotic relationships, when used in suitable proportions. Using selected microorganisms depends on pollutant removal objectives. The microorganisms can solve water pollution efficiently by self-mechanisms in natural water systems and eco-friendly cleaning. For instance, microbial agents have been studied for nitrogen removal, such as effective microorganisms (EM) [19-23], HP-RPe-3 [3], etc. They are able to degrade or remove total nitrogen (organic nitrogen, ammonia, nitrite, and nitrate) and adapt stable degradation processes in aquatic nitrogen process efficiently.

2.3 Effects of nitrogen pollution

Nitrogen which is discharged into many water sources occur from animal, industrial, human, agricultural, and other sources; raw domestic wastewater that is discharged contains many concentrations of nitrogen compounds, such as 40-45% organic nitrogen, 55-60% ammonia, and the sum of nitrate and nitrite 0-5% of the total nitrogen [24]. Nowadays, nitrogen-concentrationed water is also increasing, following various factors such as the development of countries, population growth, and socioeconomic progress.

Excessive nitrogen in water can cause the most serious aquatic ecological problems for the surface waters, health risks and bring many economic losses.

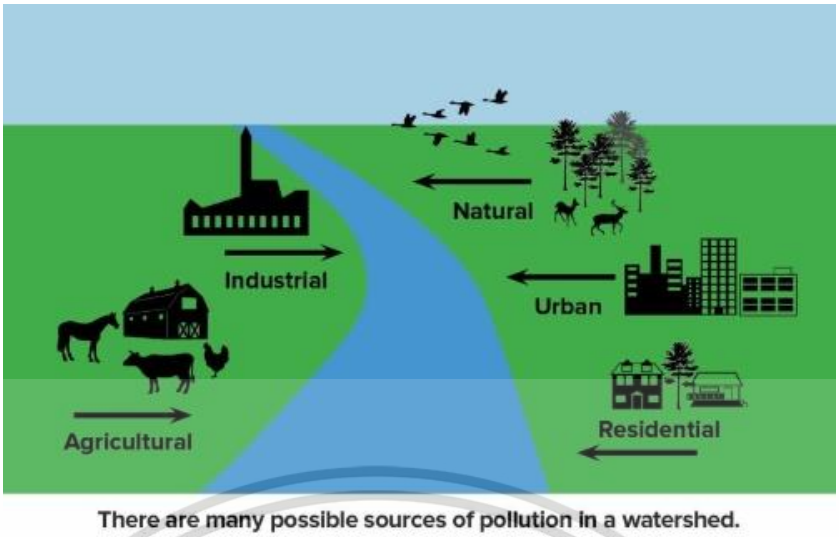


Figure 2.1 Wastewater from many sources
(https://www.dec.ny.gov/chemical/94150.html)

2.3.1 Risks to human and animal health

Nitrogen can lead to harmful algal blooms such as cyanobacteria or blue-green algae. They can produce chemicals that to be poisonous which can cause for illness or death in livestock, pets, wildlife, humans. Other symtoms from toxics or poisons are skin irritation or rash, diarrhea, cramps and vomiting to fainting, numbness, dizziness, tingling, paralysis, etc [25].

2.3.2 The environment

Increased nitrogen in water sources may lead to nitrogen pollution which can unbalance the aquatic ecosystem in water and poor water quality. Nitrogen is an essential nutrient that can cause an increase of algal blooms in Figure 2.2. They can lead to hypoxia, affecting biological diversity, reduced fish and other animal populations, decreased water transparency, noxious fumes, odor, discolored water, unsightliness.

2.3.3 The economy

Nitrogen pollution can affect socio-economic impact which make loss of money for entrepreneurial income, management of the aquatic environment and public health. The tourism industry lose income from recreational activities such as fishing, boating, etc. Contaminated water that make an economic loss to the livestock system. Fishery industries are faced with contaminated fish and decreasing fish population. Contaminated drinking water must lose costs to purify water. The pollution affect

against human health which is a loss for the healthcare costs. Country must lose butget for aquatic environmental management and public health.

(a) (b)

Figure 2.2 (a) Algae bloom in river (b) Water oxygen depletion (https://www.epa.gov/nutrientpollution/issue#main-content and https://www.waterworld.com/drinking-water/treatment/article/16193850/the-bluegreen-monster-how-harmful-algal-blooms-are-increasing-costs-risks-for-wtps)

2.4 Surface water quality standard in Thailand

Based on geographical characteristics, Thailand can be divided into 25 river basins. The average of annual rainfall for the country is about 1,700 mm. The total annual rainfall of all river basins is about 800,000 million m^3 of which 75 % of the amount is lost through evaporation, evatranspiration and the remaining 25 % (200,000 million m^3) is in rivers, rivers, and reservoirs. Thus, the available water quantity was about 3,300 m^3 per capita per year (Office of National Water Resources Committee, 4000) [26].

The water quality standard had been defined in 1994. Surface water quality standards have been defined 28 items under dividng classification of water bodies which have five classes by considering water usage in Table 2.1. The General Water Quality Index was defined as an indicator to promote public understanding of water quality, which was calculated with the values of eight parameters eight parameters (pH, DO, BOD, TS, FCB, NO_3, TP, SS). These standards represent the national minimum standards [27].

Table 2.1 Surface water quality standard classification

Class	Description/Condition	Beneficial Use
Class 1	Natural water resources without wastewater from any activities	Water is safe for consumption, sanitized, and appropriate for propagation and ecosystem conservation.
Class 2	Very clean freshwater surface water resource	Water resources for conservation, fishery, swimming, water recreation and consumption (with basic treatment).
Class 3	Medium clean fresh surface water resources Water resources	Water resources for agriculture and consumtion (with general treatment)
Class 4	Fairly clean fresh surface water resources	Water resources for industrial work and consumption (with special treatment).
Class 5	Sources which are not classified into classes 1-4	Water resources for transportation.

Table 2.2 Surface Water Quality Standard in Thailand

Parameter	Units	Statistics	Standard Value for Class[1)]					Methods for Examination
			Class 1	Class 2	Class 3	Class 4	Class 5	
1. Colour,Odour and Taste			n	n'	n'	n'	-	-
2. Temperature	C°	-	n	n'	n'	n'	-	Thermometer
3. pH	-	-	n	5-9	5-9	5-9	-	Electrometric pH Meter
4. Dissolved Oxygen (DO)[2/]	mg/l	P20	n	6.0	4.0	2.0	-	Azide Modification
5. BOD (5 days, 20°C)	mg/l	P80	n	1.5	2.0	4.0	-	Azide Modification at 20°C , 5 days
6. Total Coliform Bacteria	MPN/100 ml	P80	n	5,000	20,000	-	-	Multiple Tube Fermentation Technique
7. Fecal Coliform Bateria	MPN/ 100 ml	P80	n	1,000	4,000	-	-	Multiple Tube Fermentation Technique
8. NO_3 -N	mg/l	-	n	5.0			-	Cadmium Reduction
9. NH_3 -N	mg/l	-	n	0.5			-	Distillation Nesslerization
10. Phenols	mg/l	-	n	0.005			-	Distillation, 4-Amino antipyrene

Table 2.2 (Continued)

Parameter	Units	Statistics	Standard Value for Class[1)]					Methods for Examination
			Class 1	Class 2	Class 3	Class 4	Class 5	
11. Copper (Cu)	mg/l	-	n		0.1		-	Atomic Absorption - Direct Aspiration
12. Nickle (Ni)	mg/l	-	n		0.1		-	Atomic Absorption - Direct Aspiration
13. Manganese (Mn)	mg/l	-	n		1.0		-	Atomic Absorption - Direct Aspiration
14. Zinc (Zn)	mg/l	-	n		1.0		-	Atomic Absorption - Direct Aspiration
15. Cadmium (Cd)	mg/l	-	n		0.005* 0.05**		-	Atomic Absorption - Direct Aspiration
16. Chromium Hexavalent	mg/l	-	n		0.05		-	Atomic Absorption - Direct Aspiration
17. Lead (Pb)	mg/l	-	n		0.05		-	Atomic Absorption - Direct Aspiration
18. Total Mercury (Total Hg)	mg/l	-	n		0.002		-	Atomic Absorption- Cold Vapour Technique
19. Arsenic (As)	mg/l	-	n		0.01		-	Atomic Absorption - Direct Aspiration
20. Cyanide (Cyanide)	mg/l	-	n		0.005		-	Pyridine-Barbituric Acid
21. Radioactivity - Alpha - Beta	Becqurel /l	-	n		0.1 1.0		-	Gas-Chromatography
22. Total Organochlorine Pesticides	mg/l	-	n		0.05		-	Gas-Chromatography
23. DDT	µg/l	-	n		1.0		-	Gas-Chromatography
24. Alpha-BHC	µg/l	-	n		0.02		-	Gas-Chromatography
25. Dieldrin	µg/l	-	n		0.1		-	Gas-Chromatography
26. Aldrin	µg/l	-	n		0.1		-	Gas-Chromatography
27. Heptachlor & Heptachlore-poxide	µg/l	-	n		0.2		-	Gas-Chromatography
28. Endrin	µg/l	-	n		None		-	Gas-Chromatography

Remark : [1)] DO value is minimum value

P = Percentile value

n = naturally

n'= naturally but changing not more than 3° C

* = when water hardness not more than 100 mg/l as $CaCO_3$

** = when water hardness more than 100 mg/l as $CaCO_3$

Based on Standard Methods for the Examination of Water and Wastewater recommended by APHA : American Public Health Association, AWWA : American Water Works Association and WPCF : Water Pollution Control Federation.

Notification of the National Environmental Board, No. 8, B.E. 2537 (1994), issued under the Enhancement and Conservation of National Environmental Quality Act B.E.2535 (1992) , published in the Royal Government Gazette, Vol. 111, Part 16, dated February 24, B.E.2537 (1994) [28].

The Water Quality Index (WQI) indicates the general water quality, derived from five water quality parameters, namely Dissolved Oxygen (DO), Biochemical Oxygen Demand (BOD), Total Coliform Bacteria (TCB), Faecal Coliform Bacteria (FCB), and Ammonia – Nitrogen (NH_3 -N). The index is between 0 – 100, classifying the quality as excellent (91 – 100), good (71 – 90), fair (61 – 70), poor (31 – 60), and very poor (0 – 30).

2.5 Advection-diffusion-reaction equation (ADRE)

We consider the parabolic equation. The mathematical model describing the transport and diffusion processes is a one-dimensional advection-diffusion-reaction equation (ADRE) [10].

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2} - f(C,x,t), \quad \text{for all } (x,t) \in (0,L)\times(0,T), \tag{2.2}$$

the initial condition:

$$C(x,0) = k(x),\ 0 \le x \le L, \tag{2.3}$$

and boundary conditions:

$$\begin{aligned} C(0,t) &= g(t), \quad 0 < t \le T, \\ C(L,t) &= h(t), \quad 0 < t \le T, \end{aligned} \tag{2.4}$$

where L is the length of a river segment, T is the stationary time of simulation, $C(x,t)$ is the concentration at the point x and at time t, D is the diffusion coefficient of nitrogen pollution, u is the velocity component, $f(C,x,t)$ is a linear function dua to chemical reaction, pollution sink or pollution source, and $k(x)$, $g(t)$ and $h(t)$ are given.

2.6 Numerical techniques

We present 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 [5].

2.6.1 Forward Time Central Space technique

The FTCS scheme can be written as the discretization of time and space derivative term as follows [5]

$$\frac{\partial C}{\partial t} = \frac{C_i^{n+1} - C_i^n}{\Delta t}, \qquad (2.5)$$

$$\frac{\partial C}{\partial x} = \frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x},$$

and $$\frac{\partial^2 C}{\partial x^2} = \frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2}.$$

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

$$\lambda = \frac{D\Delta t}{(\Delta x)^2} < \frac{1}{2} \qquad (2.6)$$

and $$\gamma_i^n = \frac{u_i^n \Delta t}{\Delta x} < 1.$$

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

2.6.2 Unconditionally stable Saulyev technique

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 [29].

The Saulyev scheme can be written as the discretization of time, and space derivative term, as per [5]

where let $C(x,t)$ and u denote C_i^n and u_i^n then

$$\frac{\partial C}{\partial t} = \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad \frac{\partial C}{\partial x} = \frac{C_{i+1}^n - C_{i-1}^{n+1}}{2\Delta x}, \quad \text{and} \quad \frac{\partial^2 C}{\partial x^2} = \frac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}. \tag{2.7}$$

2.7 Cubic Spline Interpolation

The cubic spline interpolation method provides a piecewise polynomial approximation obtained by considering a unique cubic equation of each subinterval, such that they have the necessary conditions as first and second derivatives of a cubic spline which are continuous [30-31].

Suppose $(x_0, y_0), (x_1, y_1), (x_2, y_2), ..., (x_n, y_n)$ are each pair of nodes which all have $n+1$ pairs of nodes where $a = x_0 < x_1 < ... < x_n = b$. The function $S(x)$ is approximated between each pair of nodes, which is called a cubic spline, if there exist n cubic polynomials that satisfies these conditions.

1) $S(x)$ is a cubic polynomial at each subinterval $[x_i, x_{i+1}]$ where $i = 0, 1, ..., n-1$

$$S_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3, \tag{2.8}$$

a_i, b_i, c_i, and d_i are unknown constant coefficients of each cubic polynomial,

2) $S_{i+1}(x_{i+1}) = S_i(x_{i+1})$ where $i = 0, 1, ..., n-2$, (2.9)

3) $S'_{i+1}(x_{i+1}) = S'_i(x_{i+1})$ where $i = 0, 1, ..., n-2$, (2.10)

4) $S''_{i+1}(x_{i+1}) = S''_i(x_{i+1})$ where $i = 0, 1, ..., n-2$, (2.11)

5) One of sets of boundary conditions is satisfied according to this condition as

(i) $S''(x_0) = S''(x_n) = 0$ (natural boundary), (2.12)

(ii) $S'(x_0) = y'_0$ and $S'(x_n) = y'_n$ (clamped boundary). (2.13)

For the natural boundary conditions, there are n linear equations for coefficients $c_0, c_1, c_2, ..., c_n$ so we can solve the solution of c_i from a tridiagonal linear system $T\mathbf{x} = \mathbf{b}$, where T is a tridiagonal matrix of $n \times n$ as follows

$$T=\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ h_0 & 2(h_0+h_1) & h_1 & \ddots & \ddots & 0 \\ 0 & h_1 & 2(h_1+h_2) & h_2 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & h_{n-2} & 2(h_{n-2}+h_{n-1}) & h_{n-1} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \tag{2.14}$$

$$\mathbf{b}=\begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{n-1} \\ \alpha_n \end{bmatrix}=\begin{bmatrix} 0 \\ \frac{3}{h_1}(a_2-a_1)-\frac{3}{h_0}(a_1-a_0) \\ \vdots \\ \frac{3}{h_{n-1}}(a_n-a_{n-1})-\frac{3}{h_{n-2}}(a_{n-1}-a_{n-2}) \\ 0 \end{bmatrix}, \tag{2.15}$$

and $$\mathbf{x}=\begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{bmatrix}. \tag{2.16}$$

Then $\mathbf{b}$ and $\mathbf{x}$ are the vectors dimension of n,

$$h_i=x_{i+1}-x_i, \tag{2.17}$$

$$\alpha_i=\frac{3}{h_i}(a_{i+1}-a_i)-\frac{3}{h_{i-1}}(a_i-a_{i-1}) \text{ for } i=1,2,...,n-1. \tag{2.18}$$

$a_i, b_i,$ and d_i can be calculated by the following these equations

$$a_i=y_i \text{ where } i=0,1,...,n, \tag{2.19}$$

$$b_i=\frac{(a_{i+1}-a_i)}{h_i}-\frac{h_i(c_{i+1}-2c_i)}{3} \text{ where } i=0,1,...,n-1, \tag{2.20}$$

and $$d_i=\frac{(c_{i+1}-c_i)}{3h_i} \text{ where } i=0,1,...,n-1. \tag{2.21}$$

The results of coefficients can always be written in the form of cubic function on $[x_i, x_{i+1}]$ where $i=0,1,...,n-1.$ as

$$S_i(x)=a_i+b_i(x-x_i)+c_i(x-x_i)^2+d_i(x-x_i)^3. \tag{2.22}$$

Chapter 3

Numerical Simulations for Reactive Nitrogen Compounds Pollution Measurements in a River Using Saulyev Method

This chapter proposes 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 theses models with the Saulyev method by comparing different right boundary conditions.

3.1 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 [2] and [15].

$$\begin{array}{ccccccc} & & & & TN & & \\ & & & & \Downarrow & & \\ ON & \xrightarrow{ammonification} & NH_3 & \xrightarrow{nitrification} & NO_2 & \xrightarrow{nitrification} & NO_3 \end{array} \tag{3.1}$$

Therefore, different nitrogen pollutant concentrations are analyzed under reaction terms using five different nitrogen dispersion models, which were established by (2.2), and associated with (2.3) and (2.4). 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.

3.1.1 Total nitrogen dispersion model

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

$$\frac{\partial C_1}{\partial t} = -u\frac{\partial C_1}{\partial x} + D_1\frac{\partial^2 C_1}{\partial x^2} - R_1(C_1) + Q, \quad \text{for all } (x,t)\in(0,L)\times(0,T), \tag{3.2}$$

the initial condition:

$$C_1(x,0) = k_1(x), \quad 0 \le x \le L, \tag{3.3}$$

and the boundary conditions:

$$\begin{aligned} &C_1(0,t) = g_1(t), \quad 0 < t \le T, \\ &\frac{\partial C_1(L,t)}{\partial x} = h_1(t), \ 0 < t \le T, \end{aligned} \tag{3.4}$$

where L is the length of a river segment, T is the stationary time of simulation, 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 river, $g_1(t)$ 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 river.

3.1.2 Organic nitrogen dispersion model

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

$$\frac{\partial C_2}{\partial t} = -u\frac{\partial C_2}{\partial x} + D_2\frac{\partial^2 C_2}{\partial x^2} + R_2(R_1C_1), \quad \text{for all } (x,t)\in(0,L)\times(0,T), \tag{3.5}$$

the initial condition:

$$C_2(x,0) = k_2(x), \quad 0 \le x \le T, \tag{3.6}$$

and the boundary conditions:

$$\begin{aligned} &\frac{\partial C_2(0,t)}{\partial x} = g_2(t), \quad 0 < t \le T, \\ &\frac{\partial C_2(L,t)}{\partial x} = h_2(t), \quad 0 < t \le T, \end{aligned} \tag{3.7}$$

where L is the length of a river segment, T is the stationary time of simulation, 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 river, $g_2(t)$ 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 river.

3.1.3 Ammonia dispersion model

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

$$\frac{\partial C_3}{\partial t} = -u\frac{\partial C_3}{\partial x} + D_3\frac{\partial^2 C_3}{\partial x^2} + R_3(R_1C_1), \quad \text{for all } (x,t)\in(0,L)\times(0,T), \tag{3.8}$$

the initial condition:

$$C_3(x,0) = k_3(x), \quad 0 \le x \le L, \tag{3.9}$$

and the boundary conditions:

$$\begin{aligned} \frac{\partial C_3(0,t)}{\partial x} &= g_3(t), \quad 0 < t \le T, \\ \frac{\partial C_3(L,t)}{\partial x} &= h_3(t), \quad 0 < t \le T, \end{aligned} \tag{3.10}$$

where L is the length of a river segment, T is the stationary time of simulation, 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 river, $g_3(t)$ 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 river.

3.1.4 Nitrite dispersion model

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

$$\frac{\partial C_4}{\partial t} = -u\frac{\partial C_4}{\partial x} + D_4\frac{\partial^2 C_4}{\partial x^2} + R_4(R_1C_1), \quad \text{for all } (x,t)\in(0,L)\times(0,T), \tag{3.11}$$

the initial condition:

$$C_4(x,0) = k_4(x), \quad 0 \le x \le L, \tag{3.12}$$

and the boundary conditions:

$$\frac{\partial C_4(0,t)}{\partial x} = g_4(t), \quad 0 < t \le T, \\ \frac{\partial C_4(L,t)}{\partial x} = h_4(t), \quad 0 < t \le T, \tag{3.13}$$

where L is the length of a river segment, T is the stationary time of simulation, 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 river, $g_4(t)$ 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 river.

3.1.5 Nitrate dispersion model

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

$$\frac{\partial C_5}{\partial t} = -u\frac{\partial C_5}{\partial x} + D_5\frac{\partial^2 C_5}{\partial x^2} + R_5(R_1C_1), \text{ for all } (x,t) \in (0,L)\times(0,T), \tag{3.14}$$

the initial condition:

$$C_5(x,0) = k_5(x), \quad 0 \le x \le L, \tag{3.15}$$

and the boundary conditions:

$$\frac{\partial C_5(0,t)}{\partial x} = g_5(t), \quad 0 < t \le T, \\ \frac{\partial C_5(L,t)}{\partial x} = h_5(t), \quad 0 < t \le T, \tag{3.16}$$

where L is the length of a river segment, T is the stationary time of simulation, 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 river, $g_5(t)$ 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 river.

3.2 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 [5].

3.2.1 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 [5]

$$\frac{\partial C}{\partial t} = \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad \frac{\partial C}{\partial x} = \frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}, \quad \text{and} \quad \frac{\partial^2 C}{\partial x^2} = \frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2}. \tag{3.17}$$

Substituting (3.17) into nitrogen dispersion models (the total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate measurement models) results in (3.2), (3.5), (3.8) (3.11), and (3.14), respectively.

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

$$\lambda = \frac{D\Delta t}{(\Delta x)^2} < \frac{1}{2} \tag{3.18}$$

and $$\gamma_i^n = \frac{u_i^n \Delta t}{\Delta x} < 1.$$

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

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

Taking (3.17) into (3.2), we obtain the discretization of total nitrogen dispersion model as

$$\frac{(C_1)_i^{n+1}-(C_1)_i^n}{\Delta t}=-u_i^n\left(\frac{(C_1)_{i+1}^n-(C_1)_{i-1}^n}{2\Delta x}\right)+D_1\left(\frac{(C_1)_{i+1}^n-2(C_1)_i^n+(C_1)_{i-1}^n}{(\Delta x)^2}\right) \qquad (3.19)$$
$$-R_1(C_1)_i^n+Q.$$

Rearranging (3.19) leads to (3.20) for the FTCS solution, represented as

$$(C_1)_i^{n+1}=\left(\frac{1}{2}\gamma_i^n+\lambda\right)(C_1)_{i-1}^n+(1-R_1\Delta t-2\lambda)(C_1)_i^n+\left(\lambda-\frac{1}{2}\gamma_i^n\right)(C_1)_{i+1}^n+Q\Delta t. \qquad (3.20)$$

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

Substituting (3.17) into (3.4) and rearranging on the right-bound of the boundary condition, which is the derivative equation, we get (3.21).

The left boundary condition; $i=0$,

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

and the right boundary condition; $i=M$, (3.21)

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

$$(C_1)_{M+1}^n=2h_1(t)\Delta x+(C_1)_{M-1}^n.$$

Substituting (3.21) into (3.20) leads to (3.22) of the right side equation, given as

$$(C_1)_M^{n+1}=2\lambda(C_1)_{M-1}^n+2h_1(t)\Delta x\left(\lambda-\frac{1}{2}\gamma_M^n\right)+(1-R_1\Delta t-2\lambda)(C_1)_M^n+Q\Delta t\ , \qquad (3.22)$$

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

Likewise, substituting (3.17) into (3.5) leads to (3.23), written as

$$\frac{(C_2)_i^{n+1}-(C_2)_i^n}{\Delta t}=-u_i^n\left(\frac{(C_2)_{i+1}^n-(C_2)_{i-1}^n}{2\Delta x}\right)+D_2\left(\frac{(C_2)_{i+1}^n-2(C_2)_i^n+(C_2)_{i-1}^n}{(\Delta x)^2}\right) \\ +R_2R_1(C_1)_i^n. \tag{3.23}$$

Rearranging (3.23) leads to (3.24) for the FTCS solution, represented as

$$(C_2)_i^{n+1}=\left(\frac{1}{2}\gamma_i^n+\lambda\right)(C_2)_{i-1}^n+(1-2\lambda)(C_2)_i^n+\left(\lambda-\frac{1}{2}\gamma_i^n\right)(C_2)_{i+1}^n \\ +R_2\,R_1(C_1)_i^n\Delta t\,, \tag{3.24}$$

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

Substituting (3.17) into (3.7) and rearranging on the left and right-bound of the boundary conditions of this model, which are the derivative equations, we get (3.25).

The left boundary condition; $i=0$,

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

and the right boundary condition; $i=M$, (3.25)

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

Substituting (3.25) into (3.24) leads to the left and right side (3.26) and (3.27), respectively, given as follows

$$(C_2)_0^{n+1}=2\lambda(C_2)_1^n-2g_2(t)\Delta x\left(\lambda+\frac{1}{2}\gamma_0^n\right)+(1-2\lambda)(C_2)_0^n \\ +R_2\,R_1(C_1)_0^n\Delta t \tag{3.26}$$

and

$$(C_2)_M^{n+1}=2\lambda(C_2)_{M-1}^n+2h_2(t)\Delta x\left(\lambda-\frac{1}{2}\gamma_M^n\right)+(1-2\lambda)(C_2)_M^n \\ +R_2\,R_1(C_1)_M^n\Delta t. \tag{3.27}$$

3.2.1.3 Forward Time Central Space technique for the ammonia dispersion model

Likewise, substituting (3.17) into (3.8) leads to (3.28), written as

$$\frac{(C_3)_i^{n+1}-(C_3)_i^n}{\Delta t}=-u_i^n\left(\frac{(C_3)_{i+1}^n-(C_3)_{i-1}^n}{2\Delta x}\right) +D_3\left(\frac{(C_3)_{i+1}^n-2(C_3)_i^n+(C_3)_{i-1}^n}{(\Delta x)^2}\right)+R_3R_1(C_1)_i^n. \tag{3.28}$$

Rearranging (3.28) leads to (3.29), for the FTCS solution, represented as

$$(C_3)_i^{n+1}=\left(\frac{1}{2}\gamma_i^n+\lambda\right)(C_3)_{i-1}^n+(1-2\lambda)(C_3)_i^n+\left(\lambda-\frac{1}{2}\gamma_i^n\right)(C_3)_{i+1}^n +R_3R_1(C_1)_i^n\Delta t \tag{3.29}$$

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 (3.30) for the left and right sides, as below, from substituting (3.17) into (3.10) 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; $i=M$, (3.30)

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

Substituting (3.30) into (3.29) leads to the left and right side, (3.31) and (3.32), respectively, given as follows

$$(C_3)_0^{n+1}=2\lambda(C_3)_1^n-2g_3(t)\Delta x\left(\lambda+\frac{1}{2}\gamma_0^n\right)+(1-2\lambda)(C_3)_0^n +R_3R_1(C_1)_0^n\Delta t \tag{3.31}$$

and

$$(C_3)_M^{n+1} = 2\lambda(C_3)_{M-1}^n + 2h_3(t)\Delta x\left(\lambda - \frac{1}{2}\gamma_M^n\right) + (1-2\lambda)(C_3)_M^n + R_3R_1(C_1)_M^n\Delta t. \quad (3.32)$$

3.2.1.4 Forward Time Central Space technique for the nitrite dispersion model

Likewise, substituting (3.17) into (3.11) leads to (3.33), written as

$$\frac{(C_4)_i^{n+1} - (C_4)_i^n}{\Delta t} = -u_i^n\left(\frac{(C_4)_{i+1}^n - (C_4)_{i-1}^n}{2\Delta x}\right) + D_4\left(\frac{(C_4)_{i+1}^n - 2(C_4)_i^n + (C_4)_{i-1}^n}{(\Delta x)^2}\right) + R_4R_1(C_1)_i^n. \quad (3.33)$$

Rearranging (3.33) leads to (3.34), for the FTCS solution, represented as

$$(C_4)_i^{n+1} = \left(\frac{1}{2}\gamma_i^n + \lambda\right)(C_4)_{i-1}^n + (1-2\lambda)(C_4)_i^n + \left(\lambda - \frac{1}{2}\gamma_i^n\right)(C_4)_{i+1}^n + R_4R_1(C_1)_i^n\Delta t \quad (3.34)$$

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 (3.35) for the left and right sides, as below, from substituting (3.17) into (3.13) 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; $i = M$, (3.35)

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

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

Substituting (3.35) into (3.34) leads to the left and right side, (3.36) and (3.37), respectively, given as follows

$$(C_4)_0^{n+1} = 2\lambda(C_4)_1^n - 2g_4(t)\Delta x\left(\lambda + \frac{1}{2}\gamma_0^n\right) + (1-2\lambda)(C_4)_0^n + R_4 R_1 (C_1)_0^n \Delta t \tag{3.36}$$

and

$$(C_4)_M^{n+1} = 2\lambda(C_4)_{M-1}^n + 2h_4(t)\Delta x\left(\lambda - \frac{1}{2}\gamma_M^n\right) + (1-2\lambda)(C_4)_M^n + R_4 R_1 (C_1)_M^n \Delta t. \tag{3.37}$$

3.2.1.5 Forward Time Central Space technique for the nitrate dispersion model

Likewise, substituting (3.17) into (3.14) leads to (3.38), written as

$$\frac{(C_5)_i^{n+1} - (C_5)_i^n}{\Delta t} = -u_i^n\left(\frac{(C_5)_{i+1}^n - (C_5)_{i-1}^n}{2\Delta x}\right) + D_5\left(\frac{(C_5)_{i+1}^n - 2(C_5)_i^n + (C_5)_{i-1}^n}{(\Delta x)^2}\right) + R_5 R_1 (C_1)_i^n. \tag{3.38}$$

Rearranging (3.38) leads to (3.39), for the FTCS solution, represented as

$$(C_5)_i^{n+1} = \left(\frac{1}{2}\gamma_i^n + \lambda\right)(C_5)_{i-1}^n + (1-2\lambda)(C_5)_i^n + \left(\lambda - \frac{1}{2}\gamma_i^n\right)(C_5)_{i+1}^n + R_5 R_1 (C_1)_i^n \Delta t \tag{3.39}$$

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 (3.40) for the left and right sides, as below, from substituting (3.17) into (3.16) 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; $i = M$, (3.40)

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

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

Substituting (3.40) into (3.39) leads to the left and right side, (3.41) and (3.42), respectively, given as follows

$$(C_5)_0^{n+1} = 2\lambda(C_5)_1^n - 2g_5(t)\Delta x\left(\lambda + \frac{1}{2}\gamma_0^n\right) + (1-2\lambda)(C_5)_0^n + R_5 R_1 (C_1)_0^n \Delta t \tag{3.41}$$

and

$$(C_4)_M^{n+1} = 2\lambda(C_4)_{M-1}^n + 2h_4(t)\Delta x\left(\lambda - \frac{1}{2}\gamma_M^n\right) + (1-2\lambda)(C_4)_M^n + R_4 R_1 (C_1)_M^n \Delta t. \tag{3.42}$$

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

The Saulyev scheme can be written as the discretization of time and space derivative term, as per [5]

where let $C(x,t)$ and u denote C_i^n and u_i^n then

$$\frac{\partial C}{\partial t} = \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad \frac{\partial C}{\partial x} = \frac{C_{i+1}^n - C_{i-1}^{n+1}}{2\Delta x}, \tag{3.43}$$

and $\dfrac{\partial^2 C}{\partial x^2} = \dfrac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}$.

Substituting (3.43) into nitrogen dispersion models (the total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate measurement models) results in (3.2), (3.5), (3.8), (3.11), and (3.14), respectively.

3.2.2.1 Saulyev technique for the total nitrogen dispersion model

Likewise, substituting (3.43) into (3.2) leads to (3.44), written as

$$\frac{(C_1)_i^{n+1} - (C_1)_i^n}{\Delta t} = -u_i^n\left(\frac{(C_1)_{i+1}^n - (C_1)_{i-1}^{n+1}}{2\Delta x}\right) + D_1\left(\frac{(C_1)_{i+1}^n - (C_1)_i^n - (C_1)_i^{n+1} + (C_1)_{i-1}^{n+1}}{(\Delta x)^2}\right) - R_1(C_1)_i^n + Q. \tag{3.44}$$

Rearranging (3.44) leads to (3.45), represented as

$$(C_1)_i^{n+1} = \frac{1}{(1+\lambda)}\left(\begin{array}{l}\left(\frac{1}{2}\gamma_i^n + \lambda\right)(C_1)_{i-1}^{n+1} + (1-\lambda-R_1\Delta t)(C_1)_i^n + \left(\lambda - \frac{1}{2}\gamma_i^n\right)(C_1)_{i+1}^n \\ +Q\Delta t\end{array}\right) \quad (3.45)$$

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

Substituting (3.43) into (3.4) and rearranging on the right-bound of the boundary condition, which is the derivative equation, we get (3.46).

The left boundary condition; $i = 0$,

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

and the right boundary condition; $i = M$, (3.46)

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

$$(C_1)_{M+1}^n = 2h_1(t)\Delta x + (C_1)_{M-1}^n.$$

Substituting (3.46) into (3.45) leads to (3.47) of the right side equation, given as

$$(C_1)_i^{n+1} = \frac{1}{(1+\lambda)}\left(\begin{array}{l}2\lambda(C_1)_{M-1}^{n+1} + (1-\lambda-R_1\Delta t)(C_1)_M^n \\ +2h_1(t)\Delta x\left(\lambda - \frac{1}{2}\gamma_M^n\right) + Q\Delta t\end{array}\right). \quad (3.47)$$

3.2.2.2 Saulyev technique for the organic nitroge dispersion model

Likewise, substituting (3.43) into (3.5) leads to (3.48), written as

$$\begin{aligned}\frac{(C_2)_i^{n+1} - (C_2)_i^n}{\Delta t} &= -u_i^n\left(\frac{(C_2)_{i+1}^n - (C_2)_{i-1}^{n+1}}{2\Delta x}\right) \\ &\quad + D_2\left(\frac{(C_2)_{i+1}^n - (C_2)_i^n - (C_2)_i^{n+1} + (C_2)_{i-1}^{n+1}}{(\Delta x)^2}\right) + R_2 R_1 (C_1)_i^n.\end{aligned} \quad (3.48)$$

Rearranging (3.48) leads to (3.49), represented as

$$(C_2)_i^{n+1} = \frac{1}{(1+\lambda)}\left(\begin{array}{l}\left(\frac{1}{2}\gamma_i^n + \lambda\right)(C_2)_{i-1}^{n+1} + (1-\lambda)(C_2)_i^n + \left(\lambda - \frac{1}{2}\gamma_i^n\right)(C_2)_{i+1}^n \\ +R_2\, R_1 (C_1)_i^n \Delta t\end{array}\right) \quad (3.49)$$

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

Substituting (3.43) into (3.7) and rearranging on the left and right-bound of the boundary conditions of this model, which are the derivative equation, we get (3.50).

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; $i=M$, (3.50)

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

Substituting (3.50) into (3.49) leads to the left and right side (3.51) and (3.52), respectively, given as follows

$$(C_2)_0^{n+1}=\frac{1}{(1+\lambda)}\left(\begin{array}{l}2\lambda(C_2)_1^{n+1}+(1-\lambda)(C_2)_0^n-2g_2(t)\Delta x\left(\lambda+\frac{1}{2}\gamma_0^n\right)\\+R_2R_1(C_1)_0^n\Delta t\end{array}\right) \quad (3.51)$$

and

$$(C_2)_M^{n+1}=\frac{1}{(1+\lambda)}\left(\begin{array}{l}2\lambda(C_2)_{M-1}^{n+1}+(1-\lambda)(C_2)_M^n+2h_2(t)\Delta x\left(\lambda-\frac{1}{2}\gamma_M^n\right)\\+R_2R_1(C_1)_M^n\Delta t\end{array}\right). \quad (3.52)$$

3.2.2.3 Saulyev technique for the ammonia dispersion model

Likewise, substituting (3.43) into (3.8) leads to (3.53), written as

$$\begin{aligned}\frac{(C_3)_i^{n+1}-(C_3)_i^n}{\Delta t}=&-u_i^n\left(\frac{(C_3)_{i+1}^n-(C_3)_{i-1}^{n+1}}{2\Delta x}\right)\\&+D_3\left(\frac{(C_3)_{i+1}^n-(C_3)_i^n-(C_3)_i^{n+1}+(C_3)_{i-1}^{n+1}}{(\Delta x)^2}\right)+R_3R_1(C_1)_i^n.\end{aligned} \quad (3.53)$$

Rearranging (3.53) leads to (3.54), represented as

$$(C_3)_i^{n+1}=\frac{1}{(1+\lambda)}\left(\begin{array}{l}\left(\frac{1}{2}\gamma_i^n+\lambda\right)(C_3)_{i-1}^{n+1}+(1-\lambda)(C_3)_i^n+\left(\lambda-\frac{1}{2}\gamma_i^n\right)(C_3)_{i+1}^n\\+R_3R_1(C_1)_i^n\Delta t\end{array}\right) \quad (3.54)$$

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 (3.55) for the left and right sides, as below, from substituting (3.43) into (3.10) 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; $i=M$, (3.55)

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

Substituting (3.55) into (3.54) leads to the left and right side (3.56) and (3.57), respectively, given as follows

$$(C_3)_0^{n+1}=\frac{1}{(1+\lambda)}\left(\begin{array}{l}2\lambda(C_3)_1^{n+1}+(1-\lambda)(C_3)_0^n-2g_3(t)\Delta x\left(\lambda+\frac{1}{2}\gamma_0^n\right)\\+R_3R_1(C_1)_0^n\Delta t\end{array}\right), \tag{3.56}$$

and

$$(C_3)_M^{n+1}=\frac{1}{(1+\lambda)}\left(\begin{array}{l}2\lambda(C_3)_{M-1}^{n+1}+(1-\lambda)(C_3)_M^n+2h_3(t)\Delta x\left(\lambda-\frac{1}{2}\gamma_M^n\right)\\+R_3R_1(C_1)_M^n\Delta t\end{array}\right). \tag{3.57}$$

3.2.2.4 Saulyev technique for the nitrite dispersion model

Likewise, substituting (3.43) into (3.11) leads to (3.58), written as

$$\begin{aligned}\frac{(C_4)_i^{n+1}-(C_4)_i^n}{\Delta t}=&-u_i^n\left(\frac{(C_4)_{i+1}^n-(C_4)_{i-1}^{n+1}}{2\Delta x}\right)\\&+D_4\left(\frac{(C_4)_{i+1}^n-(C_4)_i^n-(C_4)_i^{n+1}+(C_4)_{i-1}^{n+1}}{(\Delta x)^2}\right)+R_4R_1(C_1)_i^n.\end{aligned} \tag{3.58}$$

Rearranging (3.58) which leads to (3.59), represented as

$$(C_4)_i^{n+1}=\frac{1}{(1+\lambda)}\left(\begin{array}{l}\left(\frac{1}{2}\gamma_i^n+\lambda\right)(C_4)_{i-1}^{n+1}+(1-\lambda)(C_4)_i^n+\left(\lambda-\frac{1}{2}\gamma_i^n\right)(C_4)_{i+1}^n\\+R_4R_1(C_1)_i^n\Delta t\end{array}\right) \tag{3.59}$$

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 (3.60) for the left and right sides, as below, from substituting (3.43) into (3.13) and rearranging these equations.

The left boundary condition; $i = 0$,

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

and the right boundary condition; $i = M$, (3.60)

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

Substituting (3.60) into (3.59) leads to the left and right side (3.61) and (3.62), respectively, given as follows

$$(C_4)_0^{n+1} = \frac{1}{(1+\lambda)}\left(\begin{array}{l} 2\lambda(C_4)_1^{n+1} + (1-\lambda)(C_4)_0^n - 2g_4(t)\Delta x\left(\lambda + \frac{1}{2}\gamma_0^n\right) \\ +R_4 R_1 (C_1)_0^n \Delta t \end{array}\right) \quad (3.61)$$

and

$$(C_4)_M^{n+1} = \frac{1}{(1+\lambda)}\left(\begin{array}{l} 2\lambda(C_4)_{M-1}^{n+1} + (1-\lambda)(C_4)_M^n + 2h_4(t)\Delta x\left(\lambda - \frac{1}{2}\gamma_M^n\right) \\ +R_4 R_1 (C_1)_M^n \Delta t \end{array}\right). \quad (3.62)$$

3.2.2.5 Saulyev technique for the nitrate dispersion model

Likewise, substituting (3.43) into (3.14) leads to (3.63), written as

$$\begin{aligned} \frac{(C_5)_i^{n+1} - (C_5)_i^n}{\Delta t} &= -u_i^n\left(\frac{(C_5)_{i+1}^n - (C_5)_{i-1}^{n+1}}{2\Delta x}\right) \\ &\quad + D_5\left(\frac{(C_5)_{i+1}^n - (C_5)_i^n - (C_5)_i^{n+1} + (C_5)_{i-1}^{n+1}}{(\Delta x)^2}\right) + R_5 R_1 (C_1)_i^n. \end{aligned} \quad (3.63)$$

Rearranging (3.63) leads to (3.64), represented as

$$(C_5)_i^{n+1} = \frac{1}{(1+\lambda)}\begin{pmatrix}\left(\frac{1}{2}\gamma_i^n + \lambda\right)(C_5)_{i-1}^{n+1} + (1-\lambda)(C_5)_i^n + \left(\lambda - \frac{1}{2}\gamma_i^n\right)(C_5)_{i+1}^n \\ +R_5\, R_1 (C_1)_i^n \Delta t\end{pmatrix} \quad (3.64)$$

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 (3.65) for the left and right sides, as below, from substituting (3.43) into (3.16) and rearranging these equations.

The left boundary condition; $i = 0$,

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

and the right boundary condition; $i = M$, (3.65)

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

Substituting (3.65) into (3.64) leads to the left and right side (3.66) and (3.67), respectively, given as follows

$$(C_5)_0^{n+1} = \frac{1}{(1+\lambda)}\begin{pmatrix}2\lambda(C_5)_1^{n+1} + (1-\lambda)(C_5)_0^n - 2g_5(t)\Delta x\left(\lambda + \frac{1}{2}\gamma_0^n\right) \\ +R_5\, R_1 (C_1)_0^n \Delta t\end{pmatrix} \quad (3.66)$$

and

$$(C_5)_M^{n+1} = \frac{1}{(1+\lambda)}\begin{pmatrix}2\lambda(C_5)_{M-1}^{n+1} + (1-\lambda)(C_5)_M^n - 2h_5(t)\Delta x\left(\lambda - \frac{1}{2}\gamma_M^n\right) \\ +R_5\, R_1 (C_1)_M^n \Delta t\end{pmatrix} \quad (3.67)$$

3.3 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.

3.3.1 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 boundaryconditions, taken from [32], as an example to compare with the two numerical solutions.

We perform all three cases by computing (2.2) without the term of reactive pollutant $(f(C,x,t)=0)$ with the analytical, FTCS, and Saulyev methods. All three cases are easily solvable where it is assumed that the river 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 (2.3) and (2.4), and are, respectively [32];

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

and (3.68)

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

$$C(1,t)=h(t)=\frac{0.025}{\sqrt{0.000625+0.02t}}\exp\left(-\frac{(1.5-t)^2}{(0.00125+0.04t)}\right),\ 0<t\le 1.$$

Performing (2.2) without the term of reactive pollutant leads to (3.69) for analytical solution, represented as follows [32]

$$C(x,t)=\frac{0.025}{\sqrt{0.000625+0.02t}}\exp\left(-\frac{(x+0.5-t)^2}{(0.00125+0.04t)}\right),\quad 0<x<1,\ 0<t\le 1, \tag{3.69}$$

Conducting (2.2) without the term of reactive pollutant by using the FTCS scheme from (3.17), we get and rearrange (3.70), which leads to (3.71).

$$\frac{C_i^{n+1}-C_i^n}{\Delta t}=-u_i^n\left(\frac{C_{i+1}^n-C_{i-1}^n}{2\Delta x}\right)+D\left(\frac{C_{i+1}^n-2C_i^n+C_{i-1}^n}{(\Delta x)^2}\right) \tag{3.70}$$

and

$$C_i^{n+1} = \left(\frac{1}{2}\gamma_i^n + \lambda\right)C_{i-1}^n + (1-2\lambda)C_i^n + \left(\lambda - \frac{1}{2}\gamma_i^n\right)C_{i+1}^n \tag{3.71}$$

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

Performing (2.2) without the term of reactive pollutant by using the Saulyev scheme from (3.43), we get and rearrange (3.72), which leads to (3.73).

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = -u_i^n\left(\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}\right) + D\left(\frac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}\right) \tag{3.72}$$

and

$$C_i^{n+1} = \frac{1}{(1+\lambda)}\left(\left(\lambda + \frac{1}{2}\gamma_i^n\right)C_{i-1}^n + (1-\lambda)C_i^n + \left(\lambda - \frac{1}{2}\gamma_i^n\right)C_{i+1}^n\right) \tag{3.73}$$

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

Consider that (3.69), (3.71), and (3.73) associate with the initial and boundary condition from (3.68). 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. Figure 3.1 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.

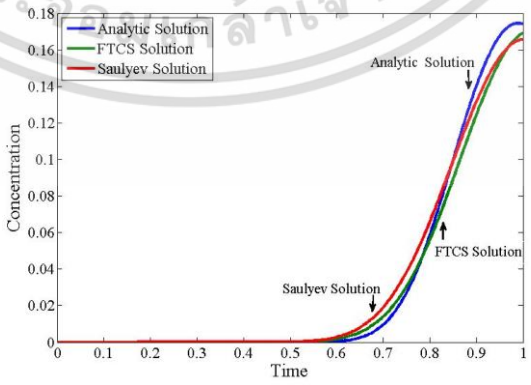


Figure 3.1 Comparison of concentrations (kg/m^3) of analytic, FTCS and Saulyev solutions at $C(0.5,t)$

3.3.2 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 3.1. It is possible to use numerical methods to solve each case of the defined grid space (Δx) and time (Δt) increments.

For example, considering the concentration measurement of the nitrogen pollutant concentration in a river 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 river reach is about 1 km, which is considered over the entire time interval [0,1]. This river is surrounded by residential components. Wastewater is discharged into the river, such that the wastewater contains nitrogen as the total nitrogen concentration form, which is everywhere throughout the river, is described by an 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 river $(x=0)$ 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 river $(x=1)$ 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 river, 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 river $(x=0)$ 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 river $(x=1)$ 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 river 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 (Q) into the river is 0.001 m^2/s.

Start by computing the numerical solution equations (the FTCS and Saulyev methods). For the FTCS method, implement solution equations with the total nitrogen,

organic nitrogen, ammonia, nitrite, and nitrate in section 3.2.1, 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 3.2.2, 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 3.1.

From Table 3.1, 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.

Table 3.1 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
0.4000	0.1000	0.2500	0.0500	stable	stable
	0.0500	0.1250	0.0250	stable	stable
	0.0250	0.0625	0.0125	stable	stable
	0.0125	0.0313	0.0063	stable	stable
0.1000	0.1000	1.0000	0.1000	unstable	stable
	0.0500	0.5000	0.0500	stable	stable
	0.0250	0.2500	0.0250	stable	stable
	0.0125	0.1250	0.0125	stable	stable
0.0500	0.1000	4.0000	0.2000	unstable	stable
	0.0500	2.0000	0.1000	unstable	stable
	0.0250	1.0000	0.0500	unstable	stable
	0.0125	0.5000	0.0250	stable	stable
0.0250	0.1000	16.0000	0.4000	unstable	stable
	0.0500	8.0000	0.2000	unstable	stable
	0.0250	4.0000	0.1000	unstable	stable
	0.0125	2.0000	0.0500	unstable	stable

3.3.3 Numerical simulations of water-quality measurement in a river 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 river 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 river reach is about 1 km, which is considered over the entire time interval [0,1]; some river physical characteristics, initial and boundary conditions are similar, but some river 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 river 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 3.2.2, 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. Tables 3.2 and 3.3 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.

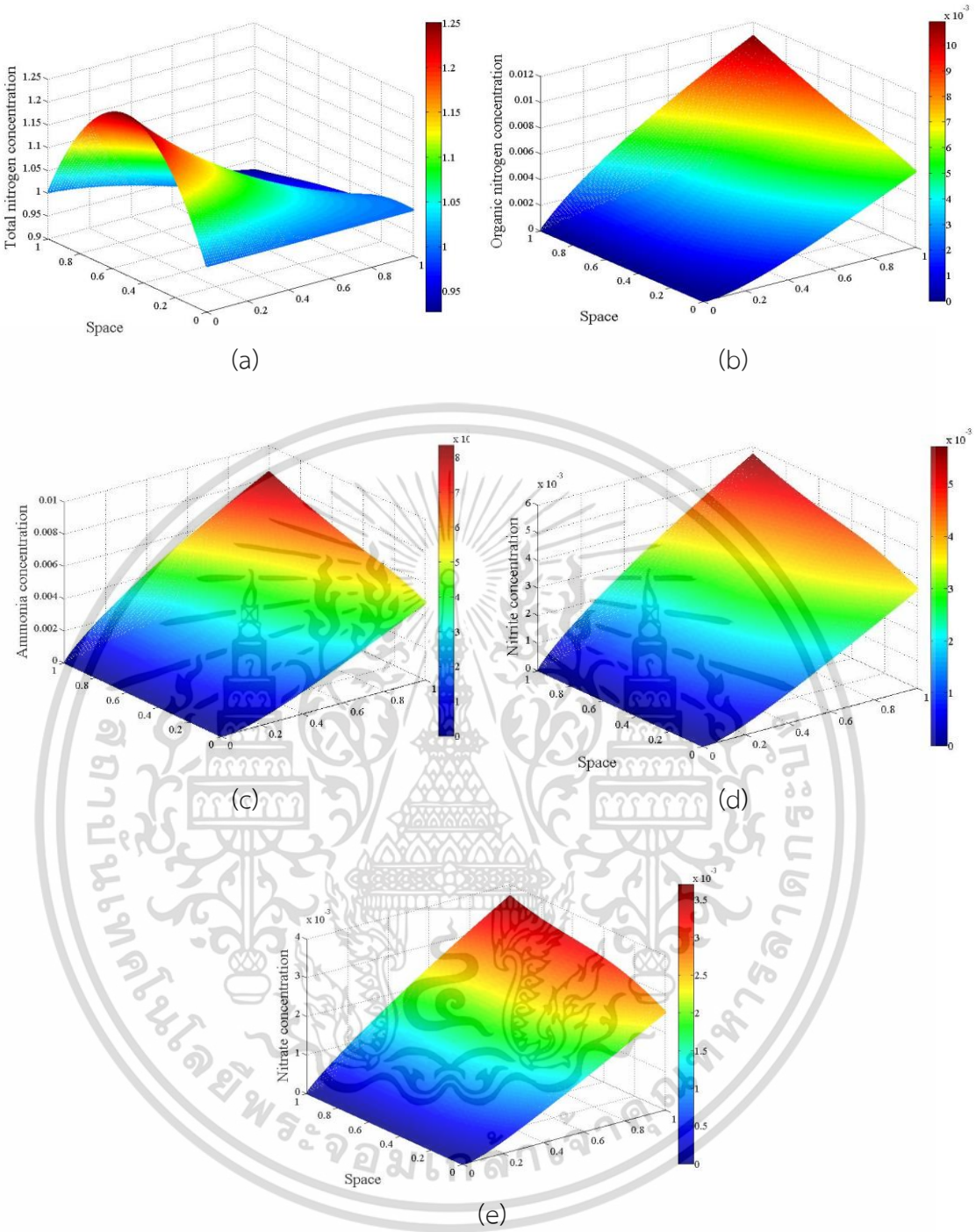


Figure 3.2 (a) The total nitrogen, (b) organic nitrogen, (c) ammonia, (d) nitrite, and (e) nitrate (kg/m^3) where the rate of change at the right boundary condition is -0.001

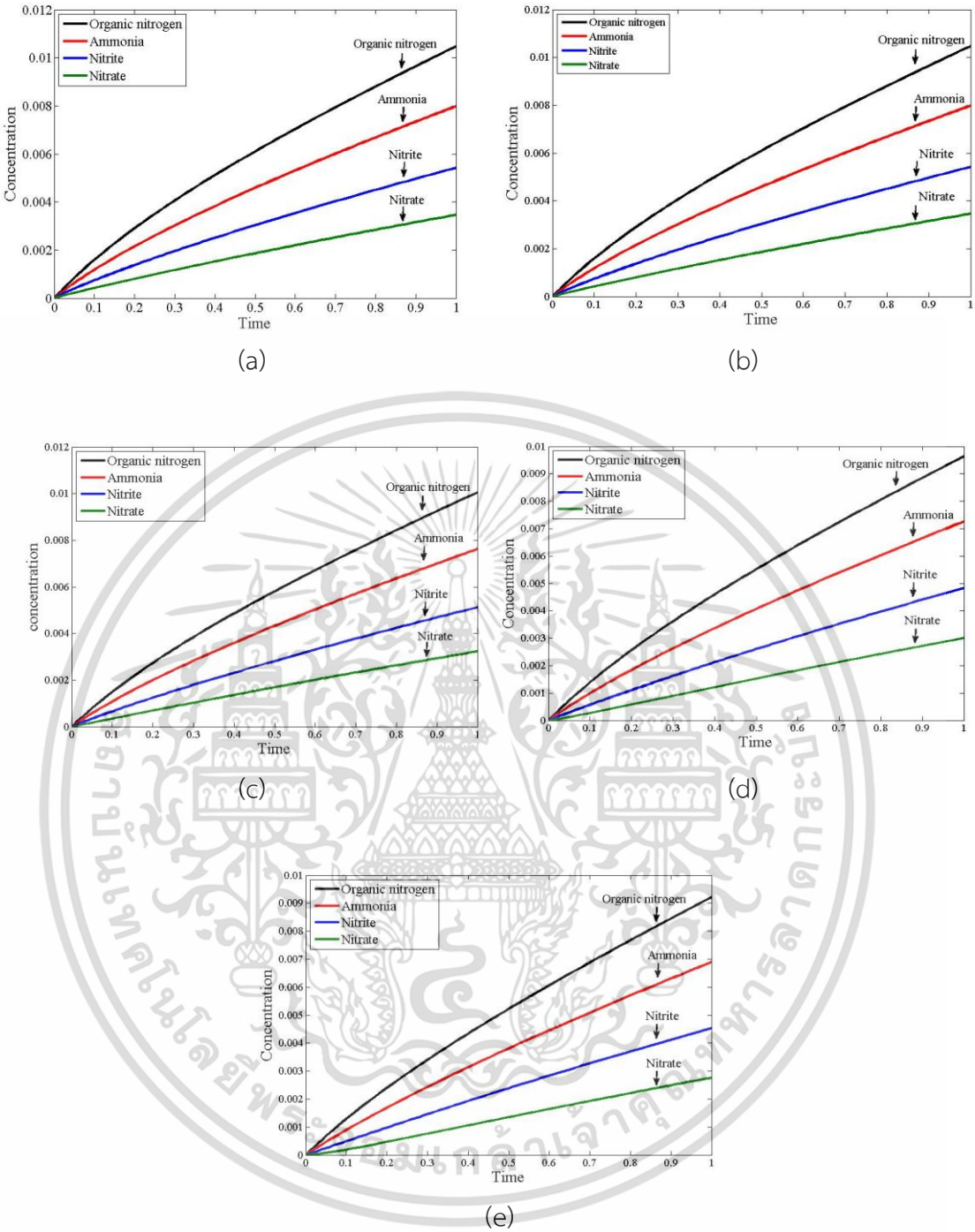


Figure 3.3 The organic nitrogen, ammonia, nitrite, and nitrate concentrations (kg/m^3) from the total nitrogen concentration in cases of the rates of change at right boundary condition of (a) -0.001, (b) -0.002, (c) -0.003, (d) -0.004, and (e) -0.005 at $C(1,t)$

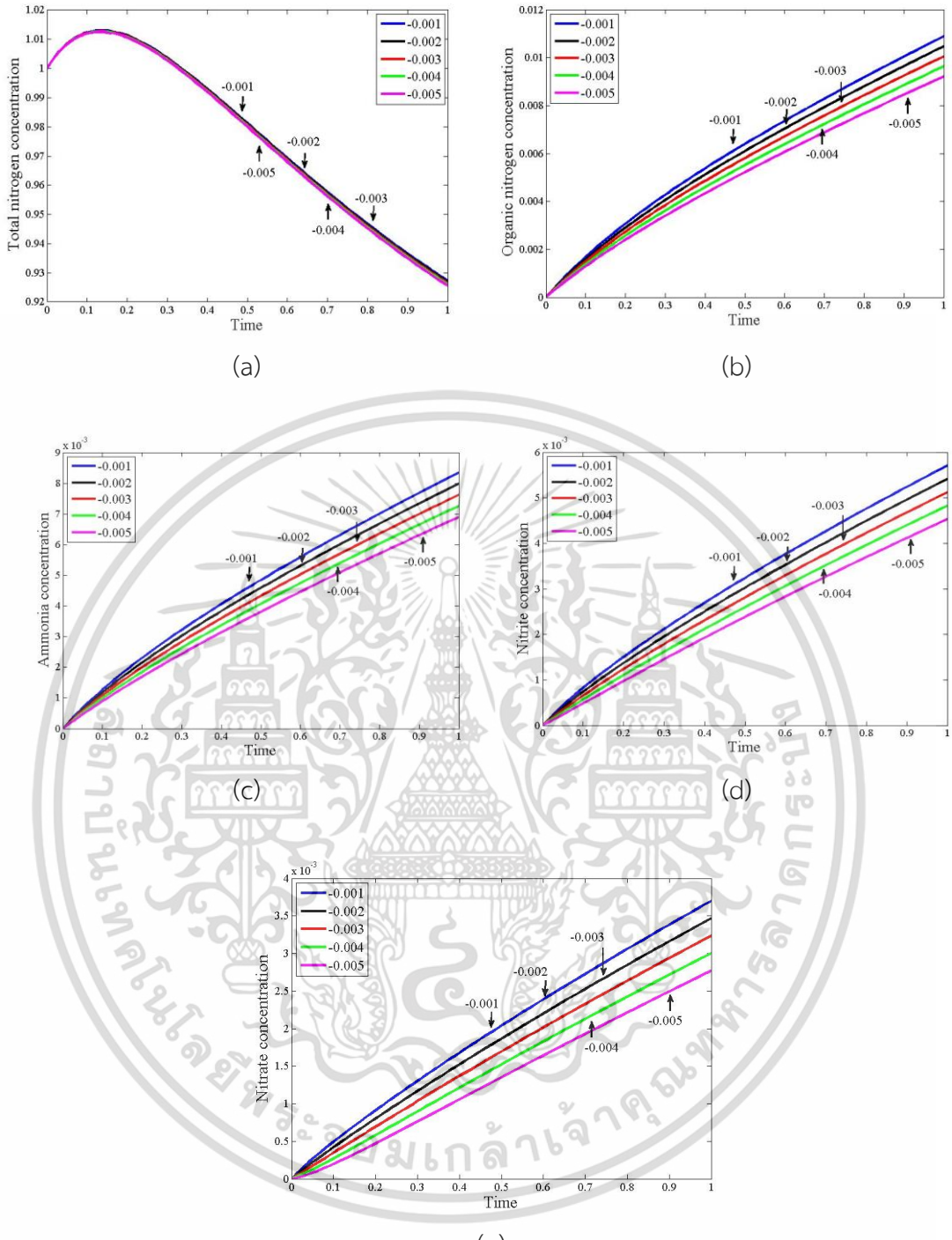


Figure 3.4 Comparison (a) the total nitrogen, (b) the organic nitrogen, (c) ammonia, (d) nitrite, and (e) nitrate (kg/m^3) when the rates of change at the right boundary condition are -0.001, -0.002, -0.003, -0.004, and -0.005 at $C(1,t)$

Table 3.2 (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 $\Delta x = 0.00625$ and $\Delta t = 0.01$

(a)

t / 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 / 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 / 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	2.6050	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	6.8120	7.5319	8.3428

Table 3.2 (Continued)

(d)

t / 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	3.7630
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 / 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 3.3 (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 $\Delta x = 0.00625$ and $\Delta t = 0.01$

(a)

t / 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 / 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	6.0640
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 / 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	2.605	2.8789	2.9834	3.1357
0.6	2.497	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

Table 3.3 (Continued)

(d)

t / 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	1.918	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	4.531

(e)

t / 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 3.4 Comparison each two rates of change at right boundary condition at $C(1,t)$ of (a) the total nitrogen, (b) organic nitrogen, (c) ammonia, (d) nitrite, and (e) nitrate concentrations (kg/m^3) such that there are $\Delta x = 0.00625$ and $\Delta t = 0.01$

(a)

t	-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	-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	-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

Table 3.4 (Continued)

(d)

t	-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	-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

3.4 Discussions

Consider that the given five graphs in Figure 3.2 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 river, such that the total nitrogen pollutant concentration decreased continuously in Figure 3.2 (a), while the organic nitrogen, ammonia, nitrite and nitrate pollutant concentrations increased continuously in Figure 3.2 (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. Figure 3.3 compares each nitrogen pollutant concentration (organic nitrogen, ammonia, nitrite, and nitrate pollutant concentrations) from the total nitrogen concentrations 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 other rates of change of nitrogen pollutant concentrations at the right boundary condition are 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. Figure 3.4 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), with the difference of each nitrogen pollutant concentration between the rates of change at right boundary conditions at $C(1,t)$ have equal pollutant concentration values, which shown in Table 3.4. 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.

Chapter 4

Numerical Models of Nitrogen Compound Measurements in a River with Removal Mechanism Using Saulyev Technique with Cubic Spline Interpolation

This chapter proposes the advection-dispersion-reaction equation in one-dimensional dispersion models of the nitrogen pollutant and the nitrogen remover in nitrogen removal mechanisms, such as the total nitrogen, organic nitrogen, ammonia, nitrite, nitrate, and nitrogen remover concentrations. We represent efficiency of the approximate solutions by comparing the Saulyev scheme with cubic spline interpolation to the initial and boundary conditions with the analytical solution through the advection-diffusion equation. We perform these one-dimensional dispersion models using the Saulyev scheme associated with cubic spline interpolation to the initial and left boundary conditions, and then compare the performance of the nitrogen pollutant and nitrogen remover in cases of the different rates of change at the right boundary condition.

4.1 Nitrogen and their nitrogen pollutant compounds dispersion models

Nitrogen in the aquatic environment can be classified in two main forms, organic compound and inorganic compound (ammonia, nitrite, and nitrate). They perform reactions in nature processes as [2] and [15]

$$\begin{array}{c} \text{TN} \\ \Downarrow \\ \text{ON} \xrightarrow{\textit{ammonification}} \text{NH}_3 \xrightarrow{\textit{nitrification}} \text{NO}_2 \xrightarrow{\textit{nitrification}} \text{NO}_3 \end{array} \tag{4.1}$$

4.1.1 Total nitrogen dispersion model

The one-dimensional advection-diffusion-reaction equation can describe the total nitrogen pollutant concentration in a river as follows;

$$\frac{\partial C_1}{\partial t} = -u\frac{\partial C_1}{\partial x} + D_1\frac{\partial^2 C_1}{\partial x^2} - R_1 C_1 - Q_1, \quad \text{for all } (x,t) \in (0,L)\times(0,T), \tag{4.2}$$

the initial condition:

$$C_1(x,0) = k_1(x), \quad 0 \le x \le L, \tag{4.3}$$

and the boundary conditions:

$$\begin{aligned} &C_1(0,t) = g_1(t), \quad 0 < t \le T, \\ &\frac{\partial C_1(L,t)}{\partial x} = h_1(t), \quad 0 < t \le T. \end{aligned} \tag{4.4}$$

Then, the length of a river segmen is L, the stationary time of simulation is T, the water flow velocity is u, the total nitrogen concentration at the point x and time t is $C_1(x,t)$, the total nitrogen diffusion coefficient is D_1, the reaction rate due to the degradation of the total nitrogen is R_1, the inlet total nitrogen concentration due to sources is Q_1, the potential total nitrogen concentration function along the river is $k_1(x)$, the total nitrogen concentration function at the discharge point is $g_1(t)$, and the rate of change of the total nitrogen concentration with respect to distance at the end of the river is $h_1(t)$.

4.1.2 Organic nitrogen dispersion model

The one-dimensional advection-diffusion-reaction equation can describe organic nitrogen pollutant concentration in a river by considering the association with the degradation of the total nitrogen concentration as follows;

$$\frac{\partial C_2}{\partial t} = -u\frac{\partial C_2}{\partial x} + D_2\frac{\partial^2 C_2}{\partial x^2} + R_2(R_1C_1), \quad \text{for all } (x,t) \in (0,L)\times(0,T), \tag{4.5}$$

the initial condition:

$$C_2(x,0) = k_2(x), \quad 0 \le x \le L, \tag{4.6}$$

and the boundary conditions:

$$\begin{aligned} &\frac{\partial C_2(0,t)}{\partial x} = g_2(t), \quad 0 < t \le T, \\ &\frac{\partial C_2(L,t)}{\partial x} = h_2(t), \quad 0 < t \le T. \end{aligned} \tag{4.7}$$

Then, the length of a river segmen is L, the stationary time of simulation is T, the water flow velocity is u, the organic nitrogen concentration at the point x and time t is $C_2(x,t)$, the organic nitrogen diffusion coefficient is D_2, the reaction rate due to the degradation is R_2, the potential organic nitrogen concentration function along the river is $k_2(x)$, the organic nitrogen concentration function at the discharge point is $g_2(t)$, and the rate of change of the organic nitrogen concentration with respect to distance at the end of the river is $h_2(t)$.

4.1.3 Ammonia dispersion model

The one-dimensional advection-diffusion-reaction equation can describe ammonia pollutant concentration in a river by considering the association with the degradation of the ammonia concentration as follows;

$$\frac{\partial C_3}{\partial t} = -u\frac{\partial C_3}{\partial x} + D_3\frac{\partial^2 C_3}{\partial x^2} + R_3(R_1C_1), \text{ for all } (x,t)\in(0,L)\times(0,T), \tag{4.8}$$

the initial condition:

$$C_3(x,0) = k_3(x), \quad 0 \le x \le L, \tag{4.9}$$

and the boundary conditions:

$$\begin{aligned} \frac{\partial C_3(0,t)}{\partial x} &= g_3(t), \quad 0 < t \le T, \\ \frac{\partial C_3(L,t)}{\partial x} &= h_3(t), \quad 0 < t \le T. \end{aligned} \tag{4.10}$$

Then, the length of a river segmen is L, the stationary time of simulation is T, the water flow velocity is u, the ammonia concentration at the point x and time t is $C_3(x,t)$, the ammonia diffusion coefficient is D_3, the reaction rate due to the degradation is R_3, the potential ammonia concentration function along the river is $k_3(x)$, the ammonia concentration function at the discharge point is $g_3(t)$, and the rate of change of the ammonia concentration with respect to distance at the end of the river is $h_3(t)$.

4.1.4 Nitrite dispersion model

The one-dimensional advection-diffusion-reaction equation can describe nitrite pollutant concentration in a river by considering the association with the degradation of the total nitrogen concentration as follows;

$$\frac{\partial C_4}{\partial t} = -u\frac{\partial C_4}{\partial x} + D_4\frac{\partial^2 C_4}{\partial x^2} + R_4(R_1C_1), \quad \text{for all } (x,t)\in(0,L)\times(0,T), \tag{4.11}$$

the initial condition:

$$C_4(x,0) = k_4(x), \quad 0 \le x \le L, \tag{4.12}$$

and the boundary conditions:

$$\begin{aligned} \frac{\partial C_4(0,t)}{\partial x} &= g_4(t), \quad 0 \le t \le T, \\ \frac{\partial C_4(L,t)}{\partial x} &= h_4(t), \quad 0 \le t \le T. \end{aligned} \tag{4.13}$$

Then, the length of a river segmen is L, the stationary time of simulation is T, the water flow velocity is u, the nitrite concentration at the point x and time t is $C_4(x,t)$, the nitrite diffusion coefficient is D_4, the reaction rate due to the degradation is R_4, the potential nitrite concentration function along the river is $k_4(x)$, the nitrite concentration function at the discharge point is $g_4(t)$, and the rate of change of the nitrite concentration with respect to distance at the end of the river is $h_4(t)$.

4.1.5 Nitrate dispersion model

The one-dimensional advection-diffusion-reaction equation can describe nitrate pollutant concentration in a river by considering the association with the degradation of the total nitrogen concentration as follows;

$$\frac{\partial C_5}{\partial t} = -u\frac{\partial C_5}{\partial x} + D_5\frac{\partial^2 C_5}{\partial x^2} + R_5(R_1C_1), \quad \text{for all } (x,t)\in(0,L)\times(0,T), \tag{4.14}$$

the initial condition:

$$C_5(x,0) = k_5(x), \quad 0 \le x \le L, \tag{4.15}$$

and the boundary conditions:

$$\begin{aligned} &\frac{\partial C_5(0,t)}{\partial x} = g_5(t), \quad 0 < t \le T, \\ &\frac{\partial C_5(L,t)}{\partial x} = h_5(t), \quad 0 < t \le T. \end{aligned} \tag{4.16}$$

Then, the length of a river segmen is L, the stationary time of simulation is T, the water flow velocity is u, the nitrate concentration at the point x and time t is $C_5(x,t)$, the nitrate diffusion coefficient is D_5, the reaction rate due to the degradation is R_5, the potential nitrate concentration function along the river is $k_5(x)$, the nitrate concentration function at the discharge point is $g_5(t)$, and the rate of change of the nitrate concentration with respect to distance at the end of the river is $h_5(t)$.

4.2 Dispersion model of nitrogen remover

The one-dimensional advection-diffusion-reaction equation can describe the nitrogen remover concentration in a river as follows;

$$\frac{\partial C_6}{\partial t} = -u\frac{\partial C_6}{\partial x} + D_6\frac{\partial^2 C_6}{\partial x^2} - R_6C_6 - Q_6, \text{ for all } (x,t)\in(0,L)\times(0,T), \tag{4.17}$$

the initial condition:

$$C_6(x,0) = k_6(x), \quad 0 \le x \le L, \tag{4.18}$$

and the boundary conditions:

$$C_6(0,t) = g_6(t), \quad 0 < t \le T,$$
$$\frac{\partial C_6(L,t)}{\partial x} = h_6(t), \quad 0 < t \le T. \tag{4.19}$$

Then, the length of a river segmen is L, the stationary time of simulation is T, the water flow velocity is u, the nitrogen remover concentration at the point x and time t is $C_6(x,t)$, the nitrogen remover diffusion coefficient is D_6, the reaction rate due to the degradation is R_6, the inlet for the nitrogen remover concentration due to sources is Q_6, the potential nitrogen remover concentration function along the river is $k_6(x)$, the nitrogen remover concentration function at the discharge point is $g_6(t)$, and the rate of change of the nitrogen remover concentration with respect to distance at the end of the river is $h_6(t)$. The nitrogen remover could be eliminate the total nitrogen.

4.3 Total nitrogen with removal mechanism dispersion model

Nitrogen removal mechanisms from contaminated water can remove, convert, and control the occurrence of nitrogen pollution. Microbial agents have been researched which can remove nitrogen efficiently in water sources. These removers can lead to good water quality.

$$\begin{array}{ccccccc} & & & \overset{degradation}{\rightarrow} & \textbf{\textit{nitrogen remover}} & & \\ & & \mathrm{TN} & & \Downarrow & & \\ \mathrm{ON} & \overset{ammonification}{\rightarrow} & \mathrm{NH_3} & \overset{nitrification}{\rightarrow} & \mathrm{NO_2} & \overset{nitrification}{\rightarrow} & \mathrm{NO_3} \end{array} \tag{4.20}$$

The total nitrogen with removal mechanism of nitrogen remover in a river can be described by the one-dimensional advection-diffusion-reaction equation as follows;

$$\frac{\partial C_1}{\partial t} = -u\frac{\partial C_1}{\partial x} + D_1\frac{\partial^2 C_1}{\partial x^2} - R_1C_1 - R_6'C_6 - Q_1, \text{ for all } (x,t) \in (0,L)\times(0,T), \tag{4.21}$$

where $R_6' = r_6R_6$,

the initial condition:

$$C_1(x,0) = k_1(x), \quad 0 \le x \le L, \tag{4.22}$$

and the boundary conditions:

$$C_1(0,t) = g_1(t), \quad 0 < t \le T.$$
$$\frac{\partial C_1(L,t)}{\partial x} = h_1(t), \quad 0 < t \le T, \tag{4.23}$$

Then, the length of a river segmen is L, the stationary time of simulation is T, the water flow velocity is u, the total nitrogen concentration at the point x and time t is $C_1(x,t)$, the total nitrogen diffusion coefficient is D_1, the reaction rate due to the degradation of the total nitrogen and nitrogen remover for removing the total nitrogen are R_1 and R_6' respectively, the proportion of degradation rate of the total nitrogen remover for removing the total nitrogen is r_6, the inlet for total nitrogen concentration due to sources is Q_1, the potential total nitrogen concentration function along the river is $k_1(x)$, the total nitrogen concentration function at the discharge point is $g_1(t)$, and the rate of change of the total nitrogen concentration with respect to distance at the end of the river is $h_1(t)$.

4.4 Numerical techniques

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

We can approximate $C(x_i,t_n)$ or C_i^n at grid point (x_i,t_n) where $0 \le i \le M$ and $0 \le n \le N$ for all positive integers of i and n .Each node has an equal grid on the x- range and t- range such that x_i and t_n run through a plane of space and time, respectively, where $x_i = i\Delta x$ and $t_n = n\Delta t$ by space and time increments are $\Delta x > 0$ and $\Delta t > 0$, respectively.

4.4.1 Unconditionally stable Saulyev technique applied to six forms of dispersion measurement models of nitrogen removal mechanism

The Saulyev scheme is used to solve a parabolic PDE in one dimension, which depends on time and space derivative terms, and can be written in these forms [4]:

Let $C(x,t)$ and u be defined as C_i^n and u_i^n then

$$\frac{\partial C}{\partial t} = \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad \frac{\partial C}{\partial x} = \frac{C_{i+1}^n - C_{i-1}^{n+1}}{2\Delta x}, \quad \text{and} \quad \frac{\partial^2 C}{\partial x^2} = \frac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}. \tag{4.24}$$

Substituting (4.24) into nitrogen (the total nitrogen with removal mechanism, organic nitrogen, ammonia, nitrite, and nitrate (and the nitrogen remover dispersion models in (4.21), (4.5), (4.8), (4.11), (4.14), and (4.17), respectively.

4.4.1.1 Saulyev technique for the total nitrogen with removal mechanism dispersion model

Substituting (4.24) into (4.21), we can write the discretization of total nitrogen dispersion model in the following way:

$$\begin{aligned}\frac{(C_1)_i^{n+1}-(C_1)_i^n}{\Delta t} &= -u_i^n\left(\frac{(C_1)_{i+1}^n-(C_1)_{i-1}^{n+1}}{2\Delta x}\right)\\ &\quad +D_1\left(\frac{(C_1)_{i+1}^n-(C_1)_i^n-(C_1)_i^{n+1}+(C_1)_{i-1}^{n+1}}{(\Delta x)^2}\right)\\ &\quad -R_1(C_1)_i^n-R_6'(C_6)_i^n-Q_1,\end{aligned} \tag{4.25}$$

where $R_6' = r_6 R_6$,

The above equation gives a solution to become

$$(C_1)_i^{n+1} = \frac{1}{(1+\lambda)}\left(\begin{aligned}&\left(\frac{1}{2}\gamma_i^n+\lambda\right)(C_1)_{i-1}^{n+1}+(1-\lambda-R_1\Delta t)(C_1)_i^n\\ &+\left(\lambda-\frac{1}{2}\gamma_i^n\right)(C_1)_{i+1}^n-R_6'(C_6)_i^n\Delta t-Q_1\Delta t\end{aligned}\right) \tag{4.26}$$

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

Substituting (4.24) into (4.23), we can write and rearrange the discretization of the right-boundary condition, which is the derivative equation; then, we have (4.27).

The left boundary condition; $i=0$,

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

and the right boundary condition; $i=M$, (4.27)

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

$$(C_1)_{M+1}^n = 2h_1(t)\Delta x+(C_1)_{M-1}^n.$$

Substituting (4.27) into (4.26), the right-side equation gives a solution to become

$$(C_1)_M^{n+1} = \frac{1}{(1+\lambda)}\left(\begin{aligned}&2\lambda(C_1)_{M-1}^{n+1}+(1-\lambda-R_1\Delta t)(C_1)_M^n\\ &+2h_1(t)\Delta x\left(\lambda-\frac{1}{2}\gamma_M^n\right)-R_6'(C_6)_i^n\Delta t-Q_1\Delta t\end{aligned}\right). \tag{4.28}$$

4.4.1.2 Saulyev technique for the organic nitrogen dispersion model

Substituting)4.24(into (4.5), we can write the discretization of the organic nitrogen dispersion model in the following way:

$$\begin{aligned}\frac{(C_2)_i^{n+1}-(C_2)_i^n}{\Delta t} &= -u_i^n\left(\frac{(C_2)_{i+1}^n-(C_2)_{i-1}^{n+1}}{2\Delta x}\right)\\ &\quad +D_2\left(\frac{(C_2)_{i+1}^n-(C_2)_i^n-(C_2)_i^{n+1}+(C_2)_{i-1}^{n+1}}{(\Delta x)^2}\right)\\ &\quad +R_2R_1(C_1)_i^n.\end{aligned} \tag{4.29}$$

The above equation gives a solution to become

$$(C_2)_i^{n+1}=\frac{1}{(1+\lambda)}\left(\begin{array}{l}\left(\frac{1}{2}\gamma_i^n+\lambda\right)(C_2)_{i-1}^{n+1}+(1-\lambda)(C_2)_i^n\\ +\left(\lambda-\frac{1}{2}\gamma_i^n\right)(C_2)_{i+1}^n+R_2\,R_1(C_1)_i^n\Delta t\end{array}\right) \tag{4.30}$$

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

Substituting (4.24) into (4.7), we can write and rearrange the discretization of the left-right boundary conditions, which are the derivative equations; then, we have (4.31).

The left boundary condition; $i=0$,

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

and the right boundary condition; $i=M$, (4.31)

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

Substituting (4.31) into (4.30), the left and right-side equations give solutions to become

$$(C_2)_0^{n+1}=\frac{1}{(1+\lambda)}\left(\begin{array}{l}2\lambda(C_2)_1^{n+1}+(1-\lambda)(C_2)_0^n-2g_2(t)\Delta x\left(\lambda+\frac{1}{2}\gamma_0^n\right)\\ +R_2\,R_1(C_1)_0^n\Delta t\end{array}\right) \tag{4.32}$$

and

$$(C_2)_M^{n+1} = \frac{1}{(1+\lambda)}\left(\begin{array}{l} 2\lambda(C_2)_{M-1}^{n+1} + (1-\lambda)(C_2)_M^n + 2h_2(t)\Delta x\left(\lambda - \frac{1}{2}\gamma_M^n\right) \\ +R_2\, R_1 (C_1)_M^n \Delta t \end{array}\right). \tag{4.33}$$

4.4.1.3 Saulyev technique for the ammonia dispersion model

Similarly, substituting (4.24) into (4.8), we can write the discretization of the ammonia dispersion model in the following way:

$$\begin{aligned} \frac{(C_3)_i^{n+1} - (C_3)_i^n}{\Delta t} &= -u_i^n\left(\frac{(C_3)_{i+1}^n - (C_3)_{i-1}^{n+1}}{2\Delta x}\right) \\ &\quad + D_3\left(\frac{(C_3)_{i+1}^n - (C_3)_i^n - (C_3)_i^{n+1} + (C_3)_{i-1}^{n+1}}{(\Delta x)^2}\right) \\ &\quad + R_3\, R_1 (C_1)_i^n. \end{aligned} \tag{4.34}$$

The above equation gives a solution to become

$$(C_3)_i^{n+1} = \frac{1}{(1+\lambda)}\left(\begin{array}{l} \left(\frac{1}{2}\gamma_i^n + \lambda\right)(C_3)_{i-1}^{n+1} + (1-\lambda)(C_3)_i^n \\ +\left(\lambda - \frac{1}{2}\gamma_i^n\right)(C_3)_{i+1}^n + R_3\, R_1 (C_1)_i^n \Delta t \end{array}\right) \tag{4.35}$$

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

Substituting (4.24) into (4.10), we can write and rearrange the discretization of the left-right boundary conditions, which are the derivative equations; then, we have (4.36).

The left boundary condition; $i = 0$,

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

and the right boundary condition; $i = M$, (4.36)

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

Substituting (4.36) into (4.35), the left and right-side equations give solutions to become

$$(C_3)_0^{n+1} = \frac{1}{(1+\lambda)}\begin{pmatrix} 2\lambda(C_3)_1^{n+1} + (1-\lambda)(C_3)_0^n - 2g_3(t)\Delta x\left(\lambda + \frac{1}{2}\gamma_0^n\right) \\ +R_3\, R_1 (C_1)_0^n \Delta t \end{pmatrix}, \tag{4.37}$$

and

$$(C_3)_M^{n+1} = \frac{1}{(1+\lambda)}\begin{pmatrix} 2\lambda(C_3)_{M-1}^{n+1} + (1-\lambda)(C_3)_M^n + 2h_3(t)\Delta x\left(\lambda - \frac{1}{2}\gamma_M^n\right) \\ +R_3\, R_1 (C_1)_M^n \Delta t \end{pmatrix}. \tag{4.38}$$

4.4.1.4 Saulyev technique for the nitrite dispersion model

Similarly, substituting (4.24) into (4.11), we can write the discretization of the nitrite dispersion model in the following way:

$$\begin{aligned} \frac{(C_4)_i^{n+1} - (C_4)_i^n}{\Delta t} &= -u_i^n \left(\frac{(C_4)_{i+1}^n - (C_4)_{i-1}^{n+1}}{2\Delta x} \right) \\ &\quad + D_4 \left(\frac{(C_4)_{i+1}^n - (C_4)_i^n - (C_4)_i^{n+1} + (C_4)_{i-1}^{n+1}}{(\Delta x)^2} \right) \\ &\quad + R_4\, R_1 (C_1)_i^n . \end{aligned} \tag{4.39}$$

The above equation gives a solution to become

$$(C_4)_i^{n+1} = \frac{1}{(1+\lambda)}\begin{pmatrix} \left(\frac{1}{2}\gamma_i^n + \lambda\right)(C_4)_{i-1}^{n+1} + (1-\lambda)(C_4)_i^n \\ +\left(\lambda - \frac{1}{2}\gamma_i^n\right)(C_4)_{i+1}^n + R_4\, R_1 (C_1)_i^n \Delta t \end{pmatrix} \tag{4.40}$$

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

Substituting (4.24) into (4.13), we can write and rearrange the discretization of the left-right boundary conditions, which are the derivative equations; then, we have (4.41).

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; $i = M$, (4.41)

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

Substituting (4.41) into (4.40), the left and right-side equations give solutions to become

$$(C_4)_0^{n+1} = \frac{1}{(1+\lambda)}\left(\begin{array}{l} 2\lambda(C_4)_1^{n+1} + (1-\lambda)(C_4)_0^n - 2g_4(t)\Delta x\left(\lambda + \frac{1}{2}\gamma_0^n\right) \\ +R_4\, R_1 (C_1)_0^n \Delta t \end{array}\right) \tag{4.42}$$

and

$$(C_4)_M^{n+1} = \frac{1}{(1+\lambda)}\left(\begin{array}{l} 2\lambda(C_4)_{M-1}^{n+1} + (1-\lambda)(C_4)_M^n + 2h_4(t)\Delta x\left(\lambda - \frac{1}{2}\gamma_M^n\right) \\ +R_4\, R_1 (C_1)_M^n \Delta t \end{array}\right). \tag{4.43}$$

4.4.1.5 Saulyev technique for the nitrate dispersion model

Similarly, substituting (4.24) into (4.14), we can write the discretization of the nitrate dispersion model in the following way:

$$\begin{aligned} \frac{(C_5)_i^{n+1} - (C_5)_i^n}{\Delta t} &= -u_i^n\left(\frac{(C_5)_{i+1}^n - (C_5)_{i-1}^{n+1}}{2\Delta x}\right) \\ &\quad + D_5\left(\frac{(C_5)_{i+1}^n - (C_5)_i^n - (C_5)_i^{n+1} + (C_5)_{i-1}^{n+1}}{(\Delta x)^2}\right) \\ &\quad + R_5\, R_1 (C_1)_i^n. \end{aligned} \tag{4.44}$$

The above equation gives a solution to become

$$(C_5)_i^{n+1} = \frac{1}{(1+\lambda)}\left(\begin{array}{l} \left(\frac{1}{2}\gamma_i^n + \lambda\right)(C_5)_{i-1}^{n+1} + (1-\lambda)(C_5)_i^n \\ +\left(\lambda - \frac{1}{2}\gamma_i^n\right)(C_5)_{i+1}^n + R_5\, R_1 (C_1)_i^n \Delta t \end{array}\right) \tag{4.45}$$

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

Substituting (4.24) into (4.16), we can write and rearrange the discretization of the left-right boundary conditions, which are the derivative equations; then, we have (4.46).

The left boundary condition; $i = 0$,

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

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

and the right boundary condition; $i = M$, (4.46)

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

Substituting (4.46) into (4.45), the left and right-side equations give solutions to become

$$(C_5)^{n+1}_0 = \frac{1}{(1+\lambda)}\left(\begin{array}{l} 2\lambda(C_5)^{n+1}_1 + (1-\lambda)(C_5)^n_0 - 2g_5(t)\Delta x\left(\lambda + \frac{1}{2}\gamma^n_0\right) \\ +R_5\, R_1 (C_1)^n_0 \Delta t \end{array}\right) \tag{4.47}$$

and

$$(C_5)^{n+1}_M = \frac{1}{(1+\lambda)}\left(\begin{array}{l} 2\lambda(C_5)^{n+1}_{M-1} + (1-\lambda)(C_5)^n_M + 2h_5(t)\Delta x\left(\lambda - \frac{1}{2}\gamma^n_M\right) \\ +R_5\, R_1 (C_5)^n_M \Delta t \end{array}\right). \tag{4.48}$$

4.4.1.6 Saulyev technique for the nitrogen remove dispersion model

Similarly, substituting (4.24) into (4.17), we can write the discretization of the nitrogen remover dispersion model in the following way:

$$\begin{aligned} \frac{(C_6)^{n+1}_i - (C_6)^n_i}{\Delta t} = -u^n_i &\left(\frac{(C_6)^n_{i+1} - (C_6)^{n+1}_{i-1}}{2\Delta x}\right) \\ &+D_6\left(\frac{(C_6)^n_{i+1} - (C_6)^n_i - (C_6)^{n+1}_i + (C_6)^{n+1}_{i-1}}{(\Delta x)^2}\right) \\ &-R_6(C_6)^n_i - Q_6. \end{aligned} \tag{4.49}$$

The above equation gives a solution to become

$$(C_6)^{n+1}_i = \frac{1}{(1+\lambda)}\left(\begin{array}{l} \left(\frac{1}{2}\gamma^n_i + \lambda\right)(C_6)^{n+1}_{i-1} + (1-\lambda - R_6\Delta t)(C_6)^n_i \\ +\left(\lambda - \frac{1}{2}\gamma^n_i\right)(C_6)^n_{i+1} - Q_6\,\Delta t \end{array}\right) \tag{4.50}$$

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

Substituting (4.24) into (4.19), we can write and rearrange the discretization of the right boundary condition, which is the derivative equation; then, we have (4.51).

The left boundary condition; $i = 0$,

$$C_6(0,t) = g_6(t),$$

and the right boundary condition; $i = M$, (4.51)

$$\frac{\partial C_6(M,t)}{\partial x} = \frac{(C_6)_{M+1}^n - (C_6)_{M-1}^{n+1}}{2\Delta x} = h_6(t),$$

$$(C_6)_{M+1}^n = 2h_6(t)\Delta x + (C_6)_{M-1}^{n+1}.$$

Substituting) 4.51 (into) 4.50(, the right-side equation gives a solution to become

$$(C_6)_M^{n+1} = \frac{1}{(1+\lambda)}\begin{pmatrix} 2\lambda(C_6)_{M-1}^{n+1} + (1-\lambda - R_6\Delta t)(C_6)_M^n \\ +2h_6(t)\Delta x\left(\lambda - \frac{1}{2}\gamma_M^n\right) - Q_6\Delta t \end{pmatrix}. \quad (4.52)$$

4.5 Numerical experiments

In this section, we conduct numerical experiments in two cases, by considering a numerical simulation of the efficiency method, the Saulyev solution with the cubic spline interpolation of the initial and boundary conditions, and compare it with an analytical solution; the other experiment shows a numerical simulation of the nitrogen dispersion models with a numerical method; the Saulyev solution with the cubic spline interpolation of the initial and left boundary conditions.

4.5.1 Numerical simulation of an ideal pollutant dispersion measurement

We focus on an effective numerical method that can provide numerical solutions and perform a numerical simulation of the advection-diffusion equation which is without reaction term of the pollutant concentration form (2.2), that is $(f(C,x,t) = 0)$, by comparing between the analytical solution and numerical solution .This simple experiment considers the case of a river length of 1 km, a time interval of]0,1[, a river velocity (u) of 1 m/s, a pollutant diffusion coefficient (D) of 0.01 m^2/s, and step sizes in space (Δx) and time (Δt) of 0.05 km and 0.0025 s, respectively; the initial and boundary conditions are defined that satisfy (2.2) and (2.3) as follows [32];

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

$$C(0,t) = g(t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}} \exp\left(-\frac{(0.5-t)^2}{(0.00125 + 0.04t)}\right),\ 0 < t \le 1, \quad (4.53)$$

$$C(L,t) = h(t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}}$$

and

$$\exp\left(-\frac{(1.5-t)^2}{(0.00125+0.04t)}\right),\ 0 < t \le 1.$$

To solve (2.2), without reaction term, we have (4.54), the analytical solution [32].

$$C(x,t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}} \exp\left(-\frac{(x+0.5-t)^2}{(0.00125+0.04t)}\right),\ 0 < x < 1,\ 0 < t \le 1. \tag{4.54}$$

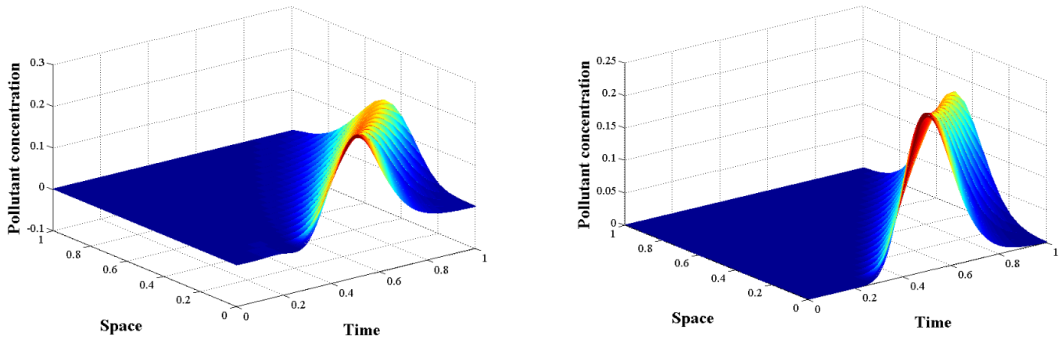
Then, we use (2.2), also without reaction term, by using the Saulyev scheme from (4.24), we have (4.55), which is the numerical solution.

$$C_i^{n+1} = \frac{1}{(1+\lambda)}\left(\left(\lambda + \frac{1}{2}\gamma_i^n\right)C_{i-1}^n + (1-\lambda)C_i^n + \left(\lambda - \frac{1}{2}\gamma_i^n\right)C_{i+1}^n\right) \tag{4.55}$$

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

To consider these solutions as analytical solutions (4.53) - (4.54), and Saulyev solution (4.55), are associated with cubic spline interpolation to the initial and boundary conditions, such that the defined nodes of cubic spline interpolation to the initial and left-right boundary conditions are the nodes of 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, and 1 at node values of analytical solution on $C(x,0)$, $C(0,t)$, and $C(1,t)$ .We assume that these node values are the collected pollutant concentration data of each distance and time in a river.

Both of the pollutant concentration solutions are shown in Figure 4.1. They are compared to the pollutant concentrations of initial $C(x,0)$, left boundary $C(0,t)$, right boundary $C(1,t)$ conditions, and $C(0.5,t)$ in Figure 4.2, which give the root mean square errors in Table 4.1.



(a) (b)

Figure 4.1 The pollutant concentrations (kg/m^3) of (a) the Saulyev with cubic spline interpolation solution and (b) analytical solution

Table 4.1 The root mean square errors of pollutant concentration of Saulyev with cubic spline interpolation solutions to the left boundary $C(0,t)$, right boundary $C(1,t)$ conditions and $C(0.5,t)$ by comparison with analytical solution

Time/Space (s)/(km)	$C(0,t)$	$C(1,t)$ (kg/m^3)	$C(0.5,t)$
0.1	2.84×10^{-14}	4.14×10^{-25}	-1.33×10^{-9}
0.2	2.19×10^{-5}	0	-5.35×10^{-7}
0.3	1.50×10^{-2}	0	-9.01×10^{-6}
0.4	1.51×10^{-1}	-2.65×10^{-23}	-2.29×10^{-5}
0.5	2.41×10^{-1}	9.53×10^{-22}	1.03×10^{-4}
0.6	1.50×10^{-1}	2.60×10^{-15}	2.61×10^{-3}
0.7	5.27×10^{-2}	6.50×10^{-11}	1.91×10^{-2}
0.8	1.29×10^{-2}	7.72×10^{-8}	6.61×10^{-2}
0.9	2.50×10^{-3}	1.16×10^{-5}	1.32×10^{-1}
1	4.06×10^{-4}	4.06×10^{-4}	1.66×10^{-1}
RMSE	2.60×10^{-3}	2.30×10^{-5}	5.34×10^{-3}

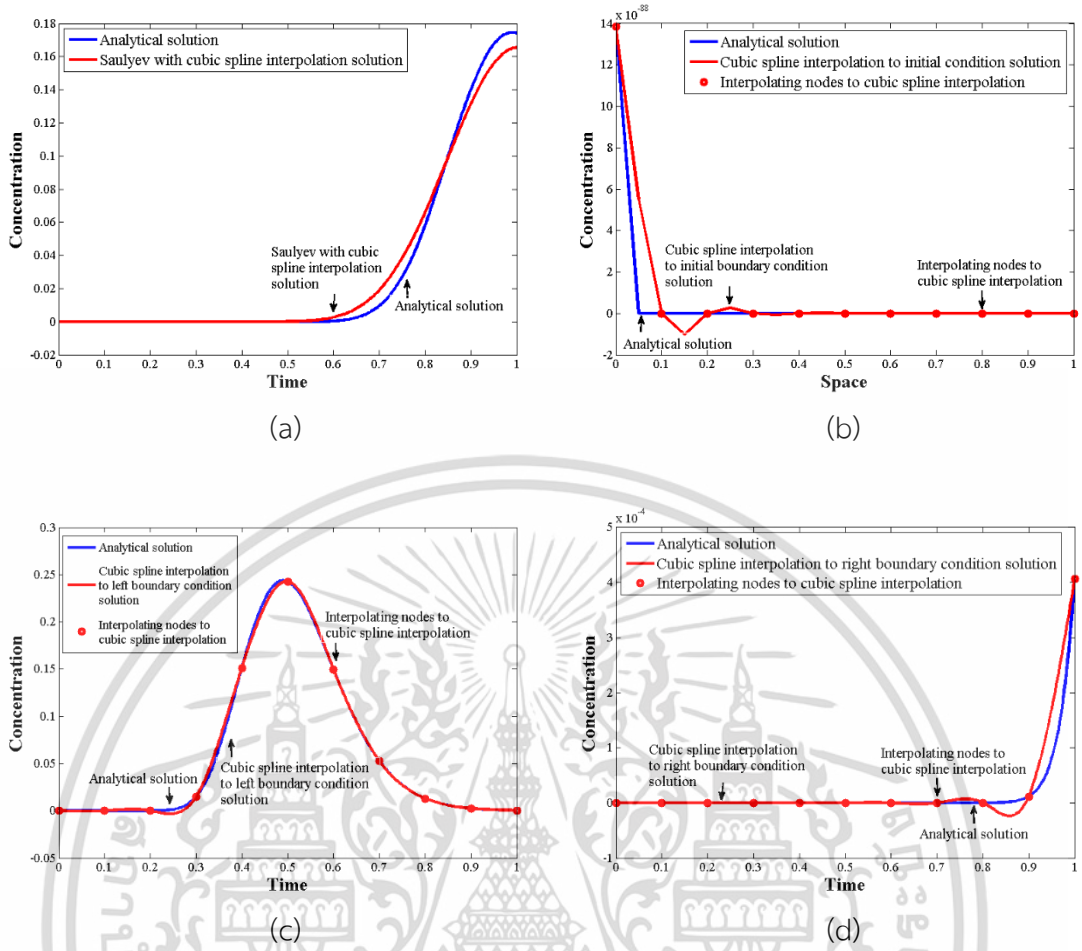


Figure 4.2 Comparison of pollutant concentrations (kg/m^3) of (a) analytical and Saulyev with cubic spline interpolation solutions at $C(0.5,t)$, analytical and cubic spline interpolation solutions to (b) the initial $C(x,0)$, (c) left boundary $C(0,t)$,and (d) right boundary $C(1,t)$ conditions

4.5.2 Numerical simulations of water-quality measurement in a river with nitrogen pollutant with removal mechanism and nitrogen remover concentration measurements by using the Saulyev technique with cubic spline interpolation to the initial and left boundary conditions

According to the numerical method, the previous part can provide a solution efficiently and, therefore, we perform numerical simulations of the nitrogen dispersion models with this numerical method, the Saulyev technique with cubic spline interpolation to the initial and left boundary conditions. These numerical simulations show dynamics in each nitrogen pollutant that occur in a river, where this river has had nitrogen removal by microbial agents .In the case study experiment, we focus on different nitrogen pollutants and nitrogen removers for the different rates of change at the right boundary .

We have used nitrogen dispersion models in a river at time t, such as the The total nitrogen with removal mechanism (C_1), organic nitrogen (C_2), ammonia (C_3), nitrite (C_4), nitrate (C_5), and nitrogen remover (C_6). Assume that a river is considered that has a length of 1 km by the performance at time interval of $[0,1]$. It is flanked by many houses and agricultural areas, and the upstream area has many houses. Wastewater is drained and irrigated into it, which consists of nitrogen concentration in several forms. The river is of low fluidity.

We will consider the behaviors of nitrogen pollutants and nitrogen removers in the river in the case of five simulations .We have determined parameter settings that are possible values of each case; then, consider the different rates of change of substances at the right boundary condition of each case, such as -0.001, -0.002,- 0.003, -0.004, and -0.005, respectively, as follows;

4.5.2.1 Simulation 1

A stream has a velocity (u) that depends on the function of $u(x)=0.1+x(1-x)(0.1)$ m/s. The approximated diffusion coefficients (D) of each substance are $D_1(x)=0.1+(1+x(1-x))(0.1)$, $D_2=0.85D_1$, $D_3=0.65D_1$, $D_4=0.45D_1$, $D_5=0.3D_1$, and $D_6=0.9$ m^2/s. The rates of degradation (R) of each substance are $R_1=0.1$, $R_2=0.85R_1$, $R_3=0.65R_1$, $R_4=0.45R_1$, $R_5=0.3R_1$, and $R_6=0.9$ s^{-1}. The inflow rates (Q) of each substance are $Q_1=0.001$ and $Q_6=0.001$ m^2/s. The grid space (Δx) and time (Δt) increments are defined by 0.00625 km and 0.01 s, respectively.

The total nitrogen with removal mechanism is determined from collected data along the length of the river, explained by the nodes of space of 0, 0.2, 0.4, 0.6, 0.8, and 1 km at node values of concentration on function $C_1(x,0)=1+x(1-x)$ kg/m^3, and follows the time at $x=0$ which is explained by the nodes of 0, 0.2, 0.4, 0.6, 0.8, and 1 s at node values of concentration on function $C_1(0,t)=1+e^{-t}\sin t$ kg/m^3. The rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_1(1,t)}{\partial x}=$ -0.001 for all times and at $t=0$.

The organic nitrogen concentration is initially released along the length of the river of $C_2(x,0)=0$ kg/m^3. There are a rate of change of concentration at $x=0$ that is constant for draining, in which $\frac{\partial C_2(0,t)}{\partial x}=0$ for all times and at $t=0$, and the rate of change of concentration at $x=1$ that is decreasing for draining out, which is $\frac{\partial C_2(1,t)}{\partial x}=$

-0.001 for all times and at $t=0$.

The ammonia concentration is initially released along the length of the river of $C_3(x,0)=0$ kg/m^3 .The rate of change of concentration at $x=0$ is constant for draining, in which $\frac{\partial C_3(0,t)}{\partial x}=0$ for all times and at $t=0$, and the rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_3(1,t)}{\partial x}$ = -0.001 for all times and at $t=0$.

The nitrite concentration is initially released along the length of the river of $C_4(x,0)=0$ kg/m^3 .The rate of change of concentration at $x=0$ is constant for draining, in which $\frac{\partial C_4(0,t)}{\partial x}=0$ for all time and at $t=0$, and the rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_4(1,t)}{\partial x}$ = -0.001 for all times and at $t=0$.

The nitrate concentration is initially released along the length of the river of $C_5(x,0)=0$ kg/m^3 .The rate of change of concentration at $x=0$ is constant for draining, in which $\frac{\partial C_5(0,t)}{\partial x}=0$ for all times and at $t=0$, and the rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_5(1,t)}{\partial x}$ = -0.001 for all times and at $t=0$.

The nitrogen remover is determined by collected data along the length of the river from released nitrogen remover on the upstream side, which can be explained by the nodes of space of 0, 0.2, 0.4, 0.6, 0.8, and 1 km at node values of concentration on function $C_6(x,0)=0.1|\cos x|$ kg/m^3, and to follow the time at $x=0$ which can be explained by the nodes of 0, 0.2, 0.4, 0.6, 0.8, and 1 s at node values of concentration on function $C_6(0,t)=0.1e^{-t}$ kg/m^3 .The rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_6(1,t)}{\partial x}$ = -0.001 for all times and at $t=0$.

4.5.2.2 Simulation 2

A stream has a velocity (u) that depends on the function of $u(x)=0.1+x(1-x)(0.1)$ m/s. The approximated diffusion coefficients (D) of each substance are $D_1(x)=0.1+(1+x(1-x))(0.1)$, $D_2=0.85D_1$, $D_3=0.65D_1$, $D_4=0.45D_1$, $D_5=0.3D_1$, and $D_6=0.9$ m^2/s .The rates of degradation (R) of each substance are $R_1=0.1$, $R_2=0.85R_1$, $R_3=0.65R_1$, $R_4=0.45R_1$, $R_5=0.3R_1$, and R_6 = 0.9 s^{-1} .The inflow rates (Q) of each substance are $Q_1=0.001$ and $Q_6=0.001$ m^2/s .

The grid space (Δx) and time (Δt) increments are defined by 0.00625 km and 0.01 s, respectively .

The total nitrogen with removal mechanism is determined from collected data along the length of the river, explained by the nodes of space of 0, 0.2, 0.4, 0.6, 0.8, and 1 km at node values of concentration on function $C_1(x,0) = 1 + x(1-x)$ kg/m^3, and follows the time at $x = 0$ which is explained by the nodes of 0, 0.2, 0.4, 0.6, 0.8, and 1 s at node values of concentration on function $C_1(0,t) = 1 + e^{-t}\sin t$ kg/m^3 .The rate of change of concentration at $x = 1$ is decreasing for draining out, which is $\frac{\partial C_1(1,t)}{\partial x}$ = -0.002 for all times and at $t = 0$.

The organic nitrogen concentration is initially released along the length of the river of $C_2(x,0) = 0$ kg/m^3 .There are a rate of change of concentration at $x = 0$ that is constant for draining, in which $\frac{\partial C_2(0,t)}{\partial x} = 0$ for all times and at $t = 0$, and the rate of change of concentration at $x = 1$ that is decreasing for draining out, which is $\frac{\partial C_2(1,t)}{\partial x}$ = -0.002 for all times and at $t = 0$.

The ammonia concentration is initially released along the length of the river of $C_3(x,0) = 0$ kg/m^3 .The rate of change of concentration at $x = 0$ is constant for draining, in which $\frac{\partial C_3(0,t)}{\partial x} = 0$ for all times and at $t = 0$, and the rate of change of concentration at $x = 1$ is decreasing for draining out, which is $\frac{\partial C_3(1,t)}{\partial x}$ = -0.002 for all times and at $t = 0$.

The nitrite concentration is initially released along the length of the river of $C_4(x,0) = 0$ kg/m^3 .The rate of change of concentration at $x = 0$ is constant for draining, in which $\frac{\partial C_4(0,t)}{\partial x} = 0$ for all time and at $t = 0$, and the rate of change of concentration at $x = 1$ is decreasing for draining out, which is $\frac{\partial C_4(1,t)}{\partial x}$ = -0.002 for all times and at $t = 0$.

The nitrate concentration is initially released along the length of the river of $C_5(x,0) = 0$ kg/m^3 .The rate of change of concentration at $x = 0$ is constant for draining, in which $\frac{\partial C_5(0,t)}{\partial x} = 0$ for all times and at $t = 0$, and the rate of change of concentration at $x = 1$ is decreasing for draining out, which is $\frac{\partial C_5(1,t)}{\partial x}$ = -0.002 for all times and at $t = 0$.

The nitrogen remover is determined by collected data along the length of the river from released nitrogen remover on the upstream side, which can be explained

by the nodes of space of 0, 0.2, 0.4, 0.6, 0.8, and 1 km at node values of concentration on function $C_6(x,0)=0.1|\cos x|$ kg/m^3, and to follow the time at $x=0$ which can be explained by the nodes of 0, 0.2, 0.4, 0.6, 0.8, and 1 s at node values of concentration on function $C_6(0,t)=0.1e^{-t}$ kg/m^3 .The rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_6(1,t)}{\partial x}$ =-0.002 for all times and at $t=0$.

4.5.2.3 Simulation 3

A stream has a velocity (u) that depends on the function of $u(x)=0.1+x(1-x)(0.1)$ m/s. The approximated diffusion coefficients (D) of each substance are $D_1(x)=0.1+(1+x(1-x))(0.1)$, $D_2=0.85D_1$, $D_3=0.65D_1$, $D_4=0.45D_1$, $D_5=0.3D_1$, and $D_6=0.9$ m^2/s . The rates of degradation (R) of each substance are $R_1=0.1$, $R_2=0.85R_1$, $R_3=0.65R_1$, $R_4=0.45R_1$, $R_5=0.3R_1$, and $R_6=$ 0.9 s^{-1} .The inflow rates (Q) of each substance are $Q_1=0.001$ and $Q_6=0.001$ m^2/s . The grid space (Δx) and time (Δt) increments are defined by 0.00625 km and 0.01 s, respectively.

The total nitrogen with removal mechanism is determined from collected data along the length of the river, explained by the nodes of space of 0, 0.2, 0.4, 0.6, 0.8, and 1 km at node values of concentration on function $C_1(x,0)=1+x(1-x)$ kg/m^3, and follows the time at $x=0$ which is explained by the nodes of 0, 0.2, 0.4, 0.6, 0.8, and 1 s at node values of concentration on function $C_1(0,t)=1+e^{-t}\sin t$ kg/m^3 .The rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_1(1,t)}{\partial x}$ = -0.003 for all times and at $t=0$.

The organic nitrogen concentration is initially released along the length of the river of $C_2(x,0)=0$ kg/m^3 .There are a rate of change of concentration at $x=0$ that is constant for draining, in which $\frac{\partial C_2(0,t)}{\partial x}=0$ for all times and at $t=0$, and the rate of change of concentration at $x=1$ that is decreasing for draining out, which is $\frac{\partial C_2(1,t)}{\partial x}$ = -0.003 for all times and at $t=0$.

The ammonia concentration is initially released along the length of the river of $C_3(x,0)=0$ kg/m^3 .The rate of change of concentration at $x=0$ is constant for draining, in which $\frac{\partial C_3(0,t)}{\partial x}=0$ for all times and at $t=0$, and the rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_3(1,t)}{\partial x}$ =-0.003 for all times and at $t=0$.

The nitrite concentration is initially released along the length of the river of $C_4(x,0)=0$ kg/m^3 .The rate of change of concentration at $x=0$ is constant for draining, in which $\frac{\partial C_4(0,t)}{\partial x}=0$ for all time and at $t=0$, and the rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_4(1,t)}{\partial x}$ = -0.003 for all times and at $t=0$.

The nitrate concentration is initially released along the length of the river of $C_5(x,0)=0$ kg/m^3 .The rate of change of concentration at $x=0$ is constant for draining, in which $\frac{\partial C_5(0,t)}{\partial x}=0$ for all times and at $t=0$, and the rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_5(1,t)}{\partial x}$ = -0.003 for all times and at $t=0$.

The nitrogen remover is determined by collected data along the length of the river from released nitrogen remover on the upstream side, which can be explained by the nodes of space of 0, 0.2, 0.4, 0.6, 0.8, and 1 km at node values of concentration on function $C_6(x,0)=0.1|\cos x|$ kg/m^3, and to follow the time at $x=0$ which can be explained by the nodes of 0, 0.2, 0.4, 0.6, 0.8, and 1 s at node values of concentration on function $C_6(0,t)=0.1e^{-t}$ kg/m^3 .The rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_6(1,t)}{\partial x}$ = -0.003 for all times and at $t=0$.

4.5.2.4 Simulation 4

A stream has a velocity (u) that depends on the function of $u(x)=0.1+x(1-x)(0.1)$ m/s. The approximated diffusion coefficients (D) of each substance are $D_1(x)=0.1+(1+x(1-x))(0.1)$, $D_2=0.85D_1$, $D_3=0.65D_1$, $D_4=0.45D_1$, $D_5=0.3D_1$, and $D_6=0.9$ m^2/s .The rates of degradation (R) of each substance are $R_1=0.1$, $R_2=0.85R_1$, $R_3=0.65R_1$, $R_4=0.45R_1$, $R_5=0.3R_1$, and R_6 = 0.9 s^{-1} .The inflow rates (Q) of each substance are $Q_1=0.001$ and $Q_6=0.001$ m^2/s . The grid space (Δx) and time (Δt) increments are defined by 0.00625 km and 0.01 s, respectively.

The total nitrogen with removal mechanism is determined from collected data along the length of the river, explained by the nodes of space of 0, 0.2, 0.4, 0.6, 0.8, and 1 km at node values of concentration on function $C_1(x,0)=1+x(1-x)$ kg/m^3, and follows the time at $x=0$ which is explained by the nodes of 0, 0.2, 0.4, 0.6, 0.8, and 1 s at node values of concentration on function $C_1(0,t)=1+e^{-t}\sin t$ kg/m^3 .The rate of change of concentration at $x=1$ is decreasing for draining out, which

is $\frac{\partial C_1(1,t)}{\partial x} =$ -0.004 for all times and at $t=0$.

The organic nitrogen concentration is initially released along the length of the river of $C_2(x,0)=0$ kg/m^3 .There are a rate of change of concentration at $x=0$ that is constant for draining, in which $\frac{\partial C_2(0,t)}{\partial x}=0$ for all times and at $t=0$, and the rate of change of concentration at $x=1$ that is decreasing for draining out, which is $\frac{\partial C_2(1,t)}{\partial x} =$ -0.004 for all times and at $t=0$.

The ammonia concentration is initially released along the length of the river of $C_3(x,0)=0$ kg/m^3 .The rate of change of concentration at $x=0$ is constant for draining, in which $\frac{\partial C_3(0,t)}{\partial x}=0$ for all times and at $t=0$, and the rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_3(1,t)}{\partial x}=$ -0.004 for all times and at $t=0$.

The nitrite concentration is initially released along the length of the river of $C_4(x,0)=0$ kg/m^3 .The rate of change of concentration at $x=0$ is constant for draining, in which $\frac{\partial C_4(0,t)}{\partial x}=0$ for all time and at $t=0$, and the rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_4(1,t)}{\partial x}=$ -0.004 for all times and at $t=0$.

The nitrate concentration is initially released along the length of the river of $C_5(x,0)=0$ kg/m^3 .The rate of change of concentration at $x=0$ is constant for draining, in which $\frac{\partial C_5(0,t)}{\partial x}=0$ for all times and at $t=0$, and the rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_5(1,t)}{\partial x}=$ -0.004 for all times and at $t=0$.

The nitrogen remover is determined by collected data along the length of the river from released nitrogen remover on the upstream side, which can be explained by the nodes of space of 0, 0.2, 0.4, 0.6, 0.8, and 1 km at node values of concentration on function $C_6(x,0)=0.1|\cos x|$ kg/m^3, and to follow the time at $x=0$ which can be explained by the nodes of 0, 0.2, 0.4, 0.6, 0.8, and 1 s at node values of concentration on function $C_6(0,t)=0.1e^{-t}$ kg/m^3 .The rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_6(1,t)}{\partial x}=$ -0.004 for all times and at $t=0$.

4.5.2.5 Simulation 5

A stream has a velocity (u) that depends on the function of $u(x)=0.1+x(1-x)(0.1)$ m/s. The approximated diffusion coefficients (D) of each substance are $D_1(x)=0.1+(1+x(1-x))(0.1)$, $D_2=0.85D_1$, $D_3=0.65D_1$, $D_4=0.45D_1$, $D_5=0.3D_1$, and $D_6=0.9$ m^2/s. The rates of degradation (R) of each substance are $R_1=0.1$, $R_2=0.85R_1$, $R_3=0.65R_1$, $R_4=0.45R_1$, $R_5=0.3R_1$, and $R_6=0.9$ s^{-1}. The inflow rates (Q) of each substance are $Q_1=0.001$ and $Q_6=0.001$ m^2/s. The grid space (Δx) and time (Δt) increments are defined by 0.00625 km and 0.01 s, respectively.

The total nitrogen with removal mechanism is determined from collected data along the length of the river, explained by the nodes of space of 0, 0.2, 0.4, 0.6, 0.8, and 1 km at node values of concentration on function $C_1(x,0)=1+x(1-x)$ kg/m^3, and follows the time at $x=0$ which is explained by the nodes of 0, 0.2, 0.4, 0.6, 0.8, and 1 s at node values of concentration on function $C_1(0,t)=1+e^{-t}\sin t$ kg/m^3. The rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_1(1,t)}{\partial x}=$ -0.005 for all times and at $t=0$.

The organic nitrogen concentration is initially released along the length of the river of $C_2(x,0)=0$ kg/m^3. There are a rate of change of concentration at $x=0$ that is constant for draining, in which $\frac{\partial C_2(0,t)}{\partial x}=0$ for all times and at $t=0$, and the rate of change of concentration at $x=1$ that is decreasing for draining out, which is $\frac{\partial C_2(1,t)}{\partial x}=$ -0.005 for all times and at $t=0$.

The ammonia concentration is initially released along the length of the river of $C_3(x,0)=0$ kg/m^3. The rate of change of concentration at $x=0$ is constant for draining, in which $\frac{\partial C_3(0,t)}{\partial x}=0$ for all times and at $t=0$, and the rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_3(1,t)}{\partial x}=$ -0.005 for all times and at $t=0$.

The nitrite concentration is initially released along the length of the river of $C_4(x,0)=0$ kg/m^3. The rate of change of concentration at $x=0$ is constant for draining, in which $\frac{\partial C_4(0,t)}{\partial x}=0$ for all time and at $t=0$, and the rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_4(1,t)}{\partial x}=$ -0.005 for all times and at $t=0$.

The nitrate concentration is initially released along the length of the river of $C_5(x,0)=0$ kg/m^3 .The rate of change of concentration at $x=0$ is constant for draining, in which $\frac{\partial C_5(0,t)}{\partial x}=0$ for all times and at $t=0$, and the rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_5(1,t)}{\partial x}$ =-0.005 for all times and at $t=0$.

The nitrogen remover is determined by collected data along the length of the river from released nitrogen remover on the upstream side, which can be explained by the nodes of space of 0, 0.2, 0.4, 0.6, 0.8, and 1 km at node values of concentration on function $C_6(x,0)=0.1|\cos x|$ kg/m^3, and to follow the time at $x=0$ which can be explained by the nodes of 0, 0.2, 0.4, 0.6, 0.8, and 1 s at node values of concentration on function $C_6(0,t)=0.1e^{-t}$ kg/m^3 .The rate of change of concentration at $x=1$ is decreasing for draining out, which is $\frac{\partial C_6(1,t)}{\partial x}$ =-0.005 for all times and at $t=0$.

The performance of the approximation solutions of simulations 1 to 5 are approximated by using the Saulyev technique associated with cubic spline interpolation of the initial and left boundary conditions. They can represent the approximated solutions of each substance at $C(1,t)$ to follow simulation 1 and 5 which are shown in Tables 4.2 and 4.3.

Table 4.2 The solutions of simulation 1 for (a) total nitrogen with removal mechanism, (b) organic nitrogen, (c) ammonia, (d) nitrite, (e) nitrate, and (f) nitrogen remover (kg/m^3) where the rate of change at the right boundary condition is -0.001

(a)

t / x	0	0.2	0.4	0.6	0.8	1
0	1	1.160	1.240	1.240	1.160	1
0.2	1.163	1.213	1.224	1.185	1.081	1.035
0.4	1.261	1.246	1.214	1.142	1.054	1.049
0.6	1.310	1.260	1.199	1.106	1.065	1.057
0.8	1.322	1.256	1.175	1.103	1.070	1.061
1	1.310	1.235	1.151	1.101	1.071	1.060

(b)

t / x	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.570	1.216	1.637	1.890	1.986	3.122
0.4	1.808	2.755	3.383	3.743	4.133	5.595
0.6	3.358	4.454	5.173	5.548	6.469	7.852
0.8	5.061	6.223	6.962	7.601	8.655	10.008
1	6.827	8.002	8.754	9.660	10.760	12.095

(c)

t / x	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.518	1.058	1.380	1.550	1.588	2.339
0.4	1.565	2.328	2.800	3.039	3.230	4.208
0.6	2.832	3.699	4.234	4.475	4.984	5.939
0.8	4.200	5.110	5.656	6.021	6.655	7.605
1	5.606	6.522	7.061	7.585	8.278	9.224

Table 4.2 (Continued)

(d)

t / x	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.440	0.846	1.055	1.144	1.136	1.521
0.4	1.247	1.798	2.104	2.228	2.260	2.780
0.6	2.186	2.802	3.149	3.266	3.438	3.974
0.8	3.184	3.826	4.178	4.325	4.587	5.133
1	4.201	4.846	5.185	5.400	5.715	6.267

(e)

t / x	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.353	0.634	0.755	0.792	0.766	0.920
0.4	0.938	1.311	1.493	1.542	1.503	1.725
0.6	1.599	2.014	2.220	2.261	2.263	2.507
0.8	2.294	2.725	2.934	2.971	3.019	3.275
1	2.998	3.430	3.631	3.689	3.768	4.033

(f)

t / x	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-2})$			
0	10	9.801	9.211	8.253	6.967	5.403
0.2	8.187	7.857	7.154	6.146	4.849	4.307
0.4	6.703	6.218	5.439	4.388	3.474	3.462
0.6	5.488	4.892	4.046	2.982	2.868	2.844
0.8	4.493	3.808	2.908	2.430	2.431	2.397
1	3.679	2.918	2.133	2.149	2.123	2.081

Table 4.3 The solutions of simulation 5 for (a) total nitrogen with removal mechanism, (b) organic nitrogen, (c) ammonia, (d) nitrite, (e) nitrate, and (f) nitrogen remover (kg/m^3) where the rate of change at the right boundary condition is -0.005

(a)

t / x	0	0.2	0.4	0.6	0.8	1
0	1	1.160	1.240	1.240	1.160	1
0.2	1.163	1.213	1.224	1.185	1.081	1.034
0.4	1.261	1.246	1.214	1.142	1.054	1.048
0.6	1.310	1.260	1.199	1.106	1.065	1.056
0.8	1.322	1.256	1.175	1.103	1.070	1.059
1	1.310	1.235	1.151	1.101	1.070	1.058

(b)

t / x	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.570	1.216	1.637	1.890	1.986	2.449
0.4	1.808	2.755	3.383	3.743	3.967	4.556
0.6	3.358	4.454	5.173	5.548	6.003	6.556
0.8	5.061	6.223	6.962	7.442	7.966	8.508
1	6.827	8.002	8.733	9.336	9.889	10.422

(c)

t / x	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.518	1.058	1.380	1.550	1.588	1.725
0.4	1.565	2.328	2.800	3.039	3.101	3.290
0.6	2.832	3.699	4.234	4.475	4.620	4.807
0.8	4.200	5.110	5.656	5.916	6.113	6.303
1	5.606	6.522	7.050	7.362	7.589	7.778

Table 4.3 (Continued)

(d)

t / x	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.440	0.846	1.055	1.144	1.136	0.992
0.4	1.247	1.798	2.104	2.228	2.176	2.014
0.6	2.186	2.802	3.149	3.266	3.193	3.042
0.8	3.184	3.826	4.178	4.274	4.215	4.069
1	4.201	4.846	5.182	5.281	5.234	5.092

(e)

t / x	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-3})$			
0	0	0	0	0	0	0
0.2	0.353	0.634	0.755	0.792	0.766	0.480
0.4	0.938	1.311	1.493	1.542	1.459	1.106
0.6	1.599	2.014	2.220	2.261	2.120	1.762
0.8	2.294	2.725	2.934	2.953	2.791	2.431
1	2.998	3.430	3.631	3.638	3.466	3.105

(f)

t / x	0	0.2	0.4	0.6	0.8	1
			$(\times 10^{-2})$			
0	10	9.801	9.211	8.253	6.967	5.403
0.2	8.187	7.857	7.154	6.146	4.849	4.211
0.4	6.703	6.218	5.439	4.388	3.440	3.280
0.6	5.488	4.892	4.046	2.982	2.756	2.584
0.8	4.493	3.808	2.908	2.373	2.248	2.067
1	3.679	2.918	2.121	2.028	1.876	1.688

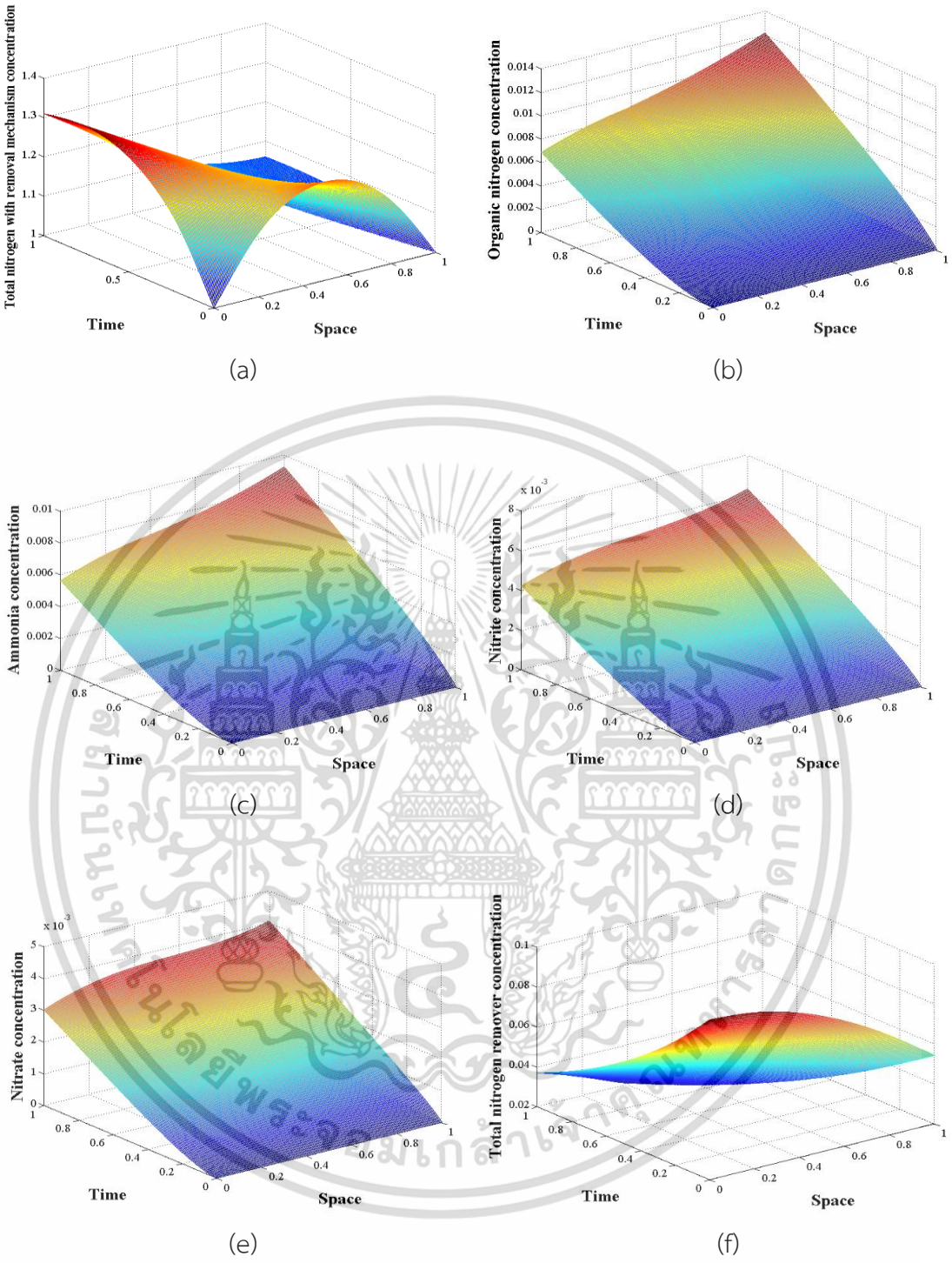
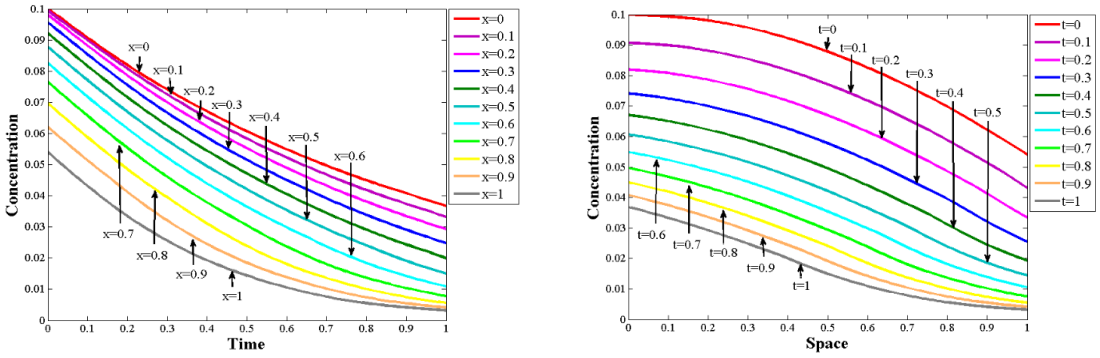
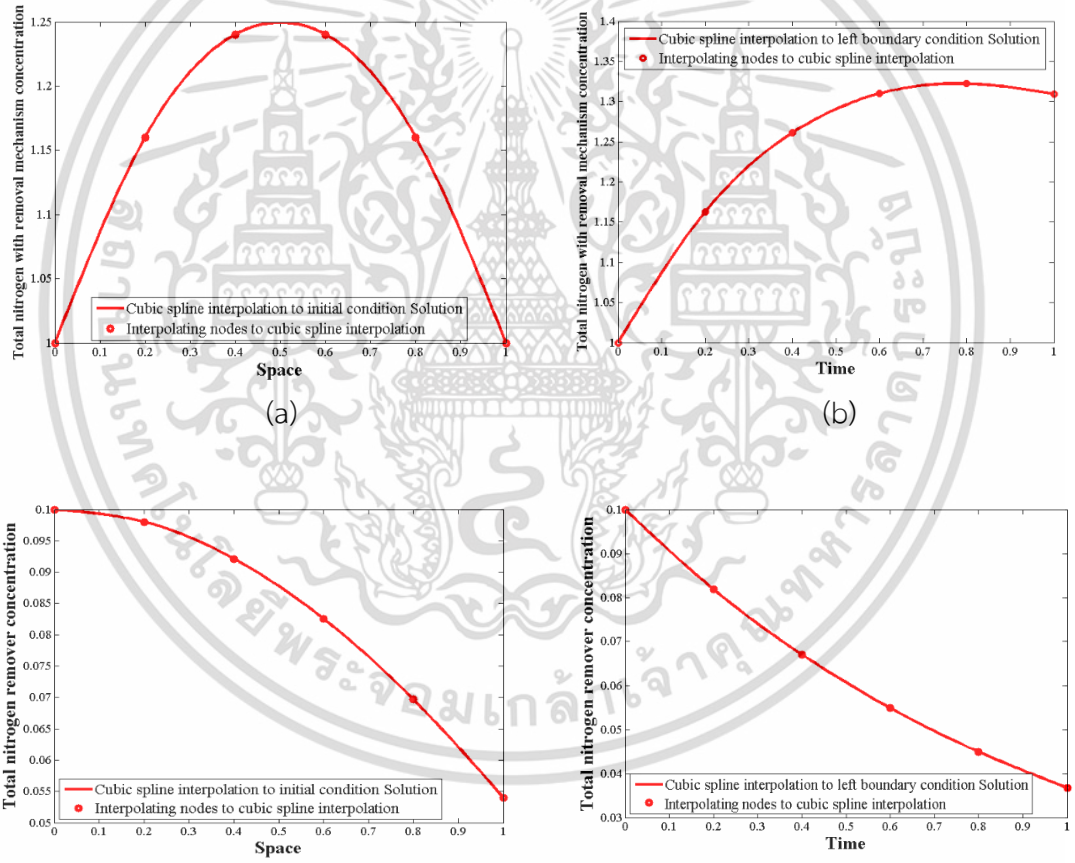


Figure 4.3 The solutions of simulation 1 of (a) total nitrogen with removal mechanism, (b) organic nitrogen, (c) ammonia, (d) nitrite, (e) nitrate, and (f) nitrogen remover (kg/m^3) where the rate of change at the right boundary condition is -0.001



(a) (b)

Figure 4.4 The solutions of simulation 1 for nitrogen remover (kg/m^3) that are distributed on (a) time and (b) space in cases of the rate of change at the right boundary condition of -0.001



(a) (b)

(c) (d)

Figure 4.5 The solutions of simulation 1 where cubic spline interpolation is applied to the initial and left boundary condition solutions of (a)-(b) the total nitrogen with removal mechanism and (c)-(d) nitrogen remover (kg/m^3) in cases of the rate of change of concentration at the right boundary condition of -0.001

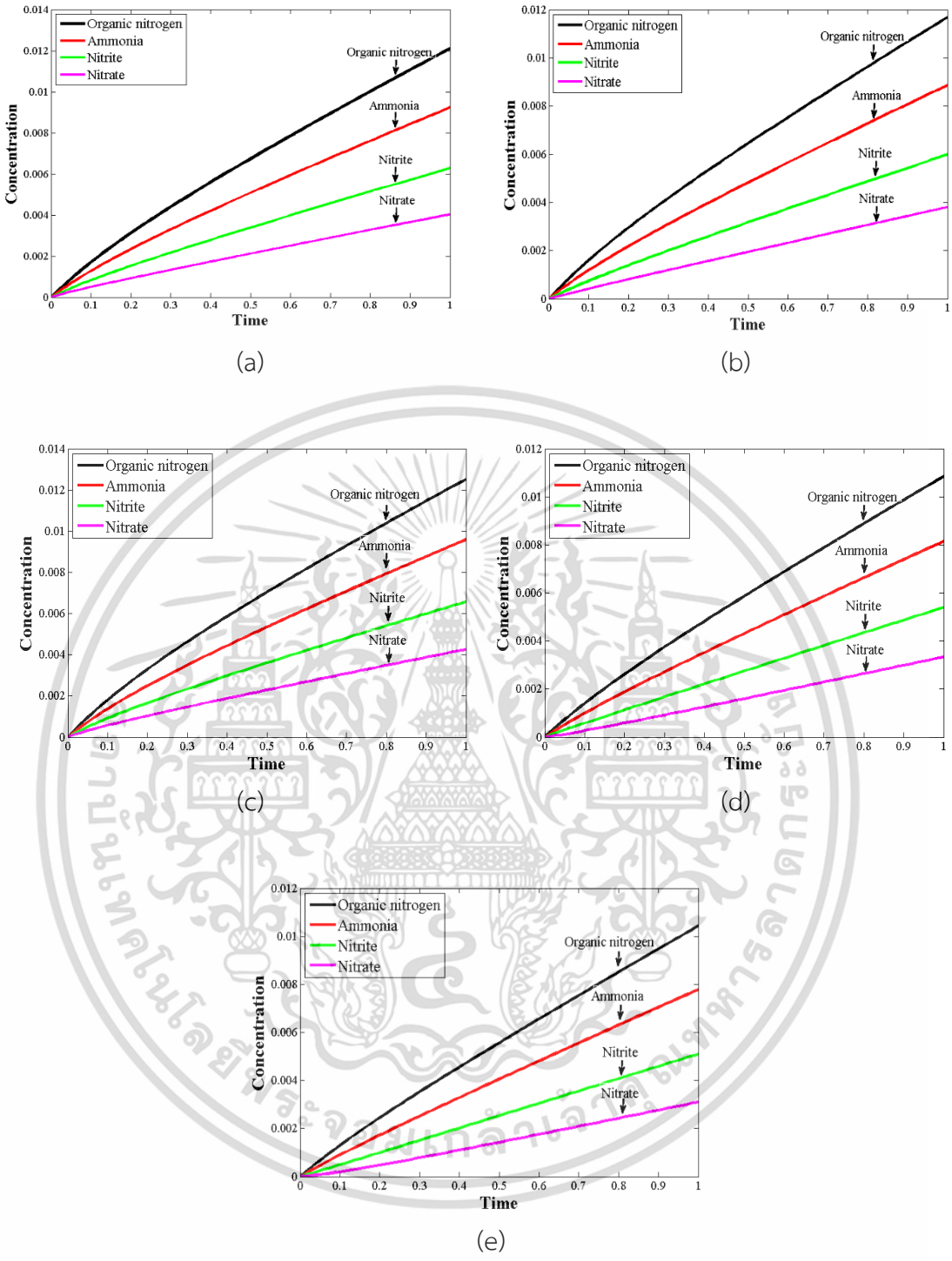


Figure 4.6 The solutions of simulation 1 to 5 for organic nitrogen, ammonia, nitrite, and nitrate concentrations (kg/m^3) from the total nitrogen with removal mechanism in cases of the rates of change at right boundary condition of (a) -0.001, (b) -0.002, (c) -0.003, (d) -0.004, and (e) -0.005 at $C(1,t)$

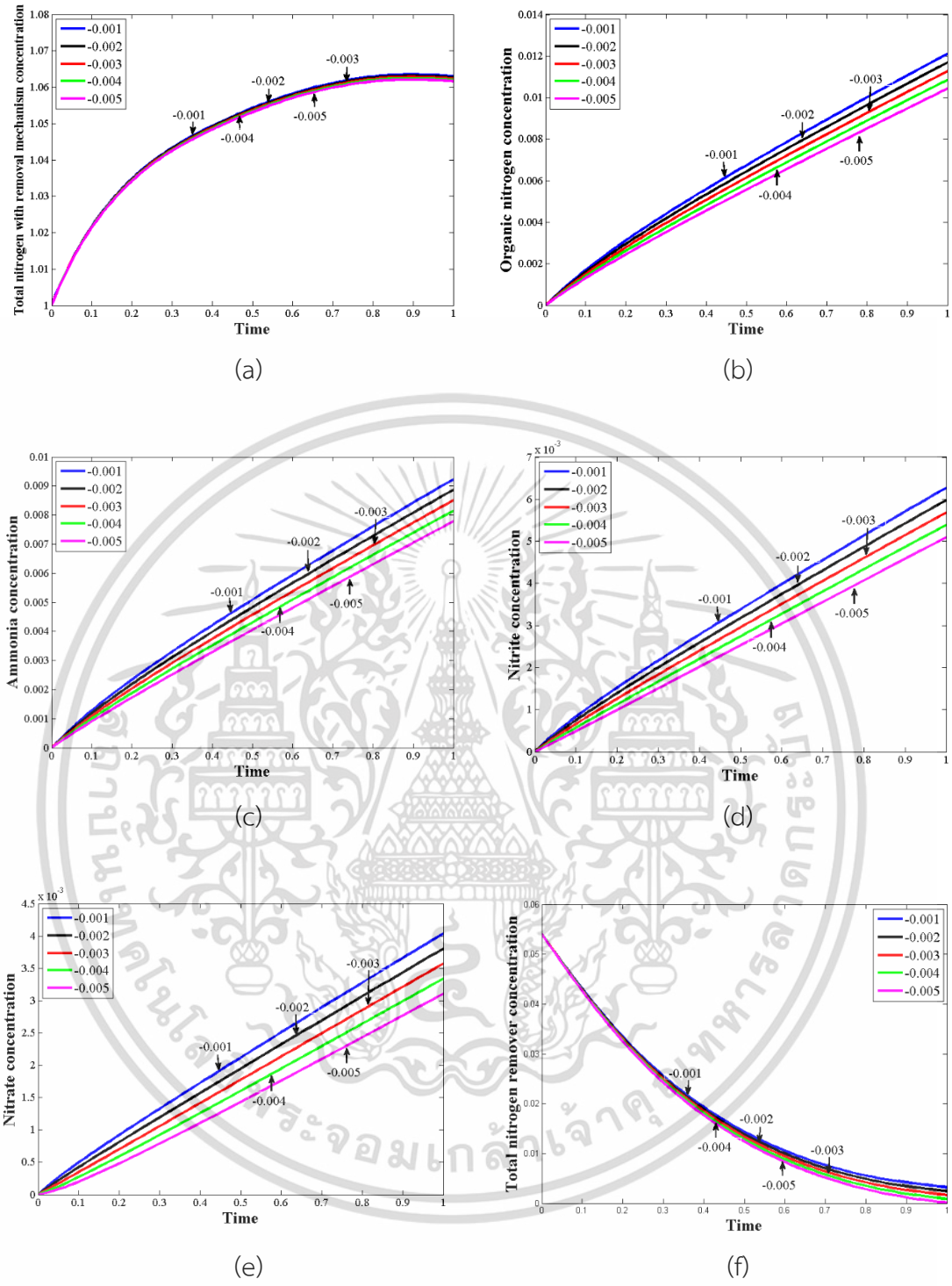


Figure 4.7 Comparison the solutions of simulation 1 to 5 for each same-substance of (a) total nitrogen with removal mechanism, (b) organic nitrogen, (c) ammonia, (d) nitrite, (e) nitrate, and (f) nitrogen remover (kg/m^3) where the rates of change are different at the right boundary condition of -0.001, -0.002, -0.003, -0.004, and -0.005, respectively, at $C(1,t)$

4.6 Discussion

The given graphs from the simulated experiment in Figures 4.1 - 4.2 show pollutant concentrations by using the Saulyev technique with cubic spline interpolation of the initial and boundary conditions are effectively close to the analytical solutions. Observe that the root mean square errors from Table 4.1 give values approaching zero. All of the values shown demonstrate that this technique is significantly good. Tables 4.2-4.3 show approximated values in the cases of rates of change of each substance at the right boundary conditions of -0.001 and -0.005, respectively; they are in the same direction, and the other cases of the rates of change at the right boundary conditions of -0.002, -0.003 and -0.004 which have approximated values that also are similar to the rates of change of -0.001 and -0.005. Figures 4.3 - 4.4 show the effect of the nitrogen pollutant in the nitrogen removal mechanism, and nitrogen remover, in the case of the rate of change at the right boundary condition of -0.001. The approximated concentrations show that the total nitrogen and nitrogen remover levels decrease continuously due to decomposition. The total nitrogen with removal mechanism that is still leftover has been transformed into organic nitrogen, ammonia, nitrite, and nitrate pollutant concentrations. They increase continuously to follow the nitrogen process in natural water sources. Figure 4.5 shows the solutions of cubic spline interpolation of the initial and left boundary conditions of the total nitrogen and nitrogen remover, which are effective for approximation from collected data from each place or time. Figure 4.6 compares the organic nitrogen, ammonia, nitrite, and nitrate pollutant concentrations when the rates of change at the right boundary condition are -0.001, -0.002, -0.003, -0.004, and -0.005. The organic nitrogen pollutant concentration occurs at a higher level, and the other pollutant concentrations (ammonia, nitrite, and nitrate) have high concentrations in which it is possible to follow the natural process. These simulations follow a similar pattern. Figure 4.7 shows a comparison of concentration levels of each pollutant concentration of nitrogen and nitrogen remover at the different rates of change of concentration at the right boundary conditions of -0.001, -0.002, -0.003, -0.004, and -0.005, respectively, and demonstrates that the highest reduction rate of 0.005 occurs with the lowest nitrogen pollutant (organic nitrogen, ammonia, nitrite, and nitrate) and nitrogen remover, and the lowest reduction rate of 0.001 occurs with the highest nitrogen pollutant and nitrogen remover.

Chapter 5
Conclusion

In this study, the nitrogen pollutant concentration models in a river, 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, 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 limitation. It is a good method for several realistic scenarios.

In numerical models of nitrogen compound measurements in a river with removal mechanism using Saulyev technique with cubic spline interpolation, nitrogen pollutant) total nitrogen, organic nitrogen, ammonia, nitrite, and nitrate (and nitrogen remover models in a river are proposed. The Saulyev technique with cubic spline interpolation to the initial and left boundary conditions is introduced . The proposed technique gives accurately approximated solutions when compared with the analytical solution. The total nitrogen concentration can be removed by the nitrogen remover. The overall water-quality when the removal mechanism is activated that is better than the unpurified system. Removing the total nitrogen concentration can control the other pollutant concentrations, such as the organic nitrogen, ammonia, nitrite, and nitrate concentrations. These models give reliable approximated solutions to follow the foundation removal mechanism.

In the simulation, we can see that the total nitrogen pollutant controlling gives better overall water-quality levels than another nitrogen pollutant compounds controlling. These simulations can be applied in order to implement water resource management in other realistic problems.

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Academic Publications

1. Areerat Vongkok and Nopparat Pochai. 2019 " Numerical simulations for reactive nitrogen compounds pollution measurements in a stream using Saulyev method" *Italian Journal of Pure and Applied Mathematics*: (accepted)
2. Areerat Vongkok and Nopparat Pochai. 2019 "Numerical models of nitrogen compound measurements in a stream with removal mechanism using Saulyev technique with cubic spline interpolation" *Journal of Interdisciplinary Mathematics*: (accepted)