

NUMERICAL COMPUTATION FOR ONE-DIMENSIONAL
WATER QUALITY MODEL IN A RIVER USING
SEVERAL FINITE DIFFERENCE METHODS



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

DEPARTMENT OF MATHEMATICS

FACULTY OF SCIENCE

KING MONGKUT'S INSTITUTE OF TECHNOLOGY LADKRABANG

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Thesis Title	Numerical Computation for One-Dimensional Water Quality Model in a River Using Several Finite Difference Methods
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Abstract

Water pollution is one of the most important environmental problems. The major water sources are contaminated with dirt and undesirable substances which affects quality of life and economic and social developments.

In this research, mathematical models of water quality measurement, the hydrodynamic model and the dispersion model are introduced. The hydrodynamic model provides the velocity and elevation of water flow. The dispersion model describes the concentration pollutants. The hydrodynamical and dispersion models are formulated in one-dimensional equations. We first calculate the velocity fields of flow form. The velocity field is used as the input of the dispersion model. Several finite difference methods are proposed to solve the dispersion model. The explicit methods, the implicit methods, the Crank-Nicolson methods, the modified Siemieniuch-Gladwell methods, the four points explicit upwind methods, the third order Crank-Nicolson methods, the four points implicit upwind methods, the explicit upwind methods, and the Lax-Wendroff methods are used to find the pollutant concentration. The numerical simulation indicates that the proposed finite difference methods give difference aspects of each problem concerned in the study.

Keywords : hydrodynamic model, dispersion model, water-quality, finite difference methods, river

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Piyada Phosri

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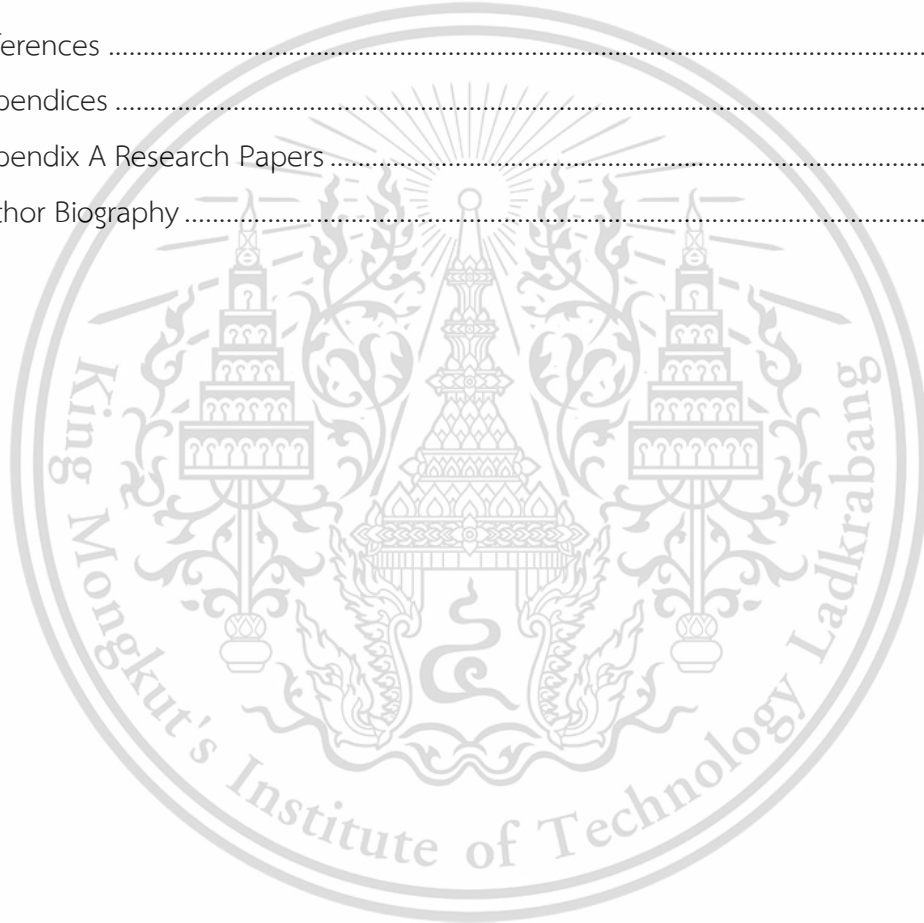
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Chapter 1

Introduction

1.1 The water pollution problem

Nowadays, when talking about the environment, people often experience anxiety. This is due to the current environment having deteriorated and heavy pollution being created. Whether it is due to water pollution, air pollution, noise pollution, or even soil pollution, when a toxic environment occurs, it will affect the health of the body and mind of humans; day by day, various pollution problems tend to increase.

Currently, water pollution is one of the most important environmental problems in a country when compared to other forms of pollution. Water pollution often occurs in big cities. A country's major water sources are contaminated with dirt and substances. This pollution makes it impossible to make full use of the water source, which affects quality of life and economic and social development.

Water pollution is mainly caused by sewage from residences, which often contains organic substances as well. Such wastewater is often the cause of the black color and putrid odor of water with toxic residues, such as water from agricultural sources that contain fertilizer, and pesticides, effluents containing heavy metals contaminated by industrial plants, etc. These substances will accumulate in the food chain orbit of aquatic animals and subsequently affect humans.

From the above problems, it is found that the various effects of water pollution are numerous. These days, the increases in industrial occupation and number of peoples are the principal reasons for the quality of water used being deteriorated. Therefore, if we know the value of the concentration of pollution that is from sources of emissions, such as from littering down river, we might be able to control the concentration of water pollution in that area and prevent it from exceeding the standard. As has already been mentioned, we recognize that the importance of water pollution, so it is interesting to study.

1.2 Literature review

Mathematical simulation is an important method to detect water quality assumption in a considered area. The numerical solution technique is a finite difference method which may be easily applied to mathematical simulation flow and transport modeling. The theory and solution techniques of the finite-difference method can be found in many textbooks [1–6]. There are many examples of using the numerical scheme for approximating direction advection-diffusion equation (ADE) by using the finite difference method. In [7], a two - dimensional advection-diffusion equation was solved by using the split-operator method. In [8], two-dimensional diffusion with an integral condition was solved by using the explicit finite difference method. The numerical test was obtained by using standard forward time central space (FTCS) method and fully explicit technique to give acceptable results and to suggest convergence to the exact solution.

[9] developed and compared for solution a one-dimensional advection-diffusion equation with a constant coefficient, with comparison of the errors associated with the equations, and provided a means to develop more accurate finite difference schemes. [10] presented a one-dimensional advection-diffusion equation with the finite differences method using implicit spreadsheet simulation (ADEISS), for use with the backward time central space (BTCS), upwind and Crank–Nicolson schemes. The numerical results of the Crank–Nicolson scheme was in good agreement with the analytical solution. [11] studied the numerical solution of the advection-diffusion equation with a third-order upwind scheme by using spreadsheet simulation (ADE-TUSS). The solution of the advection-diffusion equation could be obtained for explicit, implicit, and Crank–Nicolson schemes by only changing the values of the temporal weighted parameter. The results showed that use of the high-order schemes in the spreadsheet simulation was very applicable for the numerical solution of the advection-diffusion equation, and the Crank–Nicolson scheme was in good agreement with the analytical solution. [12-14] proposed the higher-order upwind difference be used for the convective terms of the convection-diffusion equation.

[15-16] the finite element method to solve a one-dimensional convection-diffusion equation. [17] used a non-linear hydrodynamic model to simulate the water current and the elevation in a uniform reservoir, with the Lax–Wendroff technique

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being used to approximate the solutions for optimal control of water treatment in the system to achieve minimum cost. [18] presented a numerical simulation of a one-dimensional advection-diffusion-reaction equation with boundary condition functions by using the Saul'yev finite difference technique. The numerical result was dependable. [19] showed two mathematical models used to simulate pollution; the first was a hydrodynamic model that provided the velocity field and elevation of a water flow by using the Crank–Nicolson method, and the second was a dispersion model. The governing equation was a one-dimensional advection-dispersion–reaction equation that gave the pollutant concentration using the Crank–Nicolson method. [20] used the finite difference scheme to solve and identify the effect of non-uniform water flows in a stream. Two mathematical models were used to simulate pollution; the first was a hydrodynamic model gave the velocity field and elevation of a water flow by using the Crank-Nicolson method, and the second was an advection-dispersion-reaction that gave the pollutant concentration to obtain explicit schemes, the forward time central space and Saul'yev schemes.

[21] developed a new scheme that guaranteed the positivity of the solutions for a one advection-diffusion-reaction equation in one spatial dimension. [22] simulated water quality by two mathematical models for one-dimensional equations. The first model was a hydrodynamic model that provided the velocity field and the elevation of water using the Crank-Nicolson method, which input of values of velocity of the second model. The second model was an advection-dispersion-reaction model that gave pollutant concentration using traditional MacCormack method and the modified MacCormack method. The results of the MacCormack modified method were more accurate than the compared traditional MacCormack method. [23] focused on one-dimensional water quality by using two models, a hydrodynamic model (WHYSWESS-HD) and an advection-dispersion-reaction model. The results showed a good water quality model when compared with to that relying on MIKE 11. [24] proposed an analytical solution for the non-dimensional equation of a two-dimensional hydrodynamic model with generalized boundary condition and initial conditions; this model explained the elevation of water in an open uniform reservoir.

Recently, [25] simulated a one-dimensional equation for water quality in a non-uniform flow stream by using two models. The first model was a hydrodynamic model that provided the velocity field and the water elevation; the Crank-Nicolson

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methods were used. The second model was an advection-diffusion-reaction model that provided the pollutant concentrations; a new fourth-order scheme and a Saulyev scheme was used. The results of the new fourth-order scheme coupled to the Saulyev method was more accurate when compared with traditional methods.

1.3 Objectives of the thesis

- 1) To simulate the water current of a river by using a hydrodynamic model.
- 2) To apply the advection-diffusion-reaction equation of a dispersion model to describe water pollutant concentration by using finite difference methods.
- 3) To apply the hydrodynamic model and advection-diffusion-reaction equation to water pollutant measurement by using finite difference methods.
- 4) To simulate and approximate the numerical solution of water current and water pollutant concentration by using the proposed finite difference methods.

1.4 Scopes of the thesis

- 1) To find the numerical solutions of advection-diffusion-reaction equations by using finite difference methods.
- 2) To consider a dimensionless equation of the hydrodynamic model.
- 3) To calculate the approximated pollutant concentration only in a one-dimensional domain in space.
- 4) To compare the calculated solutions of the water quality model by explicit and implicit methods.

1.5 Plan of the thesis

The thesis describes the mathematical modeling of water pollution measurement. We divide this into two, which are the water quality measurements in a uniform flow stream and in a non-uniform flow stream. There are two mathematical models used to simulate water quality in uniform flow stream and pollutant concentration proposed. There are two mathematical models used to simulate water quality in non-uniform flow systems; the first is a hydrodynamic model that provides the velocity field and the elevation of water. The second is a dispersion model that

gives the pollutant concentration field. A couple of models are formulated in one-dimensional equations. At each step, the calculated flow velocity fields of the first model are input into the second model as the field data.

The first part of the description gives details of the basic knowledge about shallow water and a mathematical model for water quality, measurement, and control, by defining the domain of a problem in the thesis and domain of the study case.

The second part studies a numerical method for solving a one-dimensional hydrodynamic model and a one-dimensional dispersion model.

The third part is the computation of the velocity of water and elevation of water for the hydrodynamic model. In this process of simulation, we consider in one dimension and use the Crank-Nicolson technique for solving the velocity of water and elevation of water.

The fourth part is computation of water pollutant concentration related to the dispersion model. We input the velocity of water from the hydrodynamic into the dispersion model. In this process of simulation, we use several finite difference methods for solving the concentration of pollution.

Finally, we propose the concentration of pollution and compare numerical solutions from several finite difference methods in one-dimensional advection-dispersion-reaction.

Moreover, in this thesis, the research is divided into 3 works. In work 1, we are inspired by Dehghan [9] in 2004 and Karahan [11] in 2007, in which velocity of water is assumed to be constant and does not have chemical reactions in the advection-diffusion equation, but in our work, it is assumed that there are chemical reaction term in the advection-diffusion equation; see figure 1.2. Work 2 was inspired by Dehghan [9] in 2004 and Karahan [11] in 2007, but our work assumes that there are chemical reaction terms in the advection-diffusion equation, and we also find the velocity of water that can be interpolated from the hydrodynamic model; see figure 1.3. Work 3 was inspired by Dehghan [9] in 2004 and continues from work 2. We assume that there are chemical reaction terms in the advection-diffusion equation, that velocity of water can be interpolated from the hydrodynamic model, and there is no stability computational aspect but, in work 3, we obtain more computational stability; see figure 1.4.

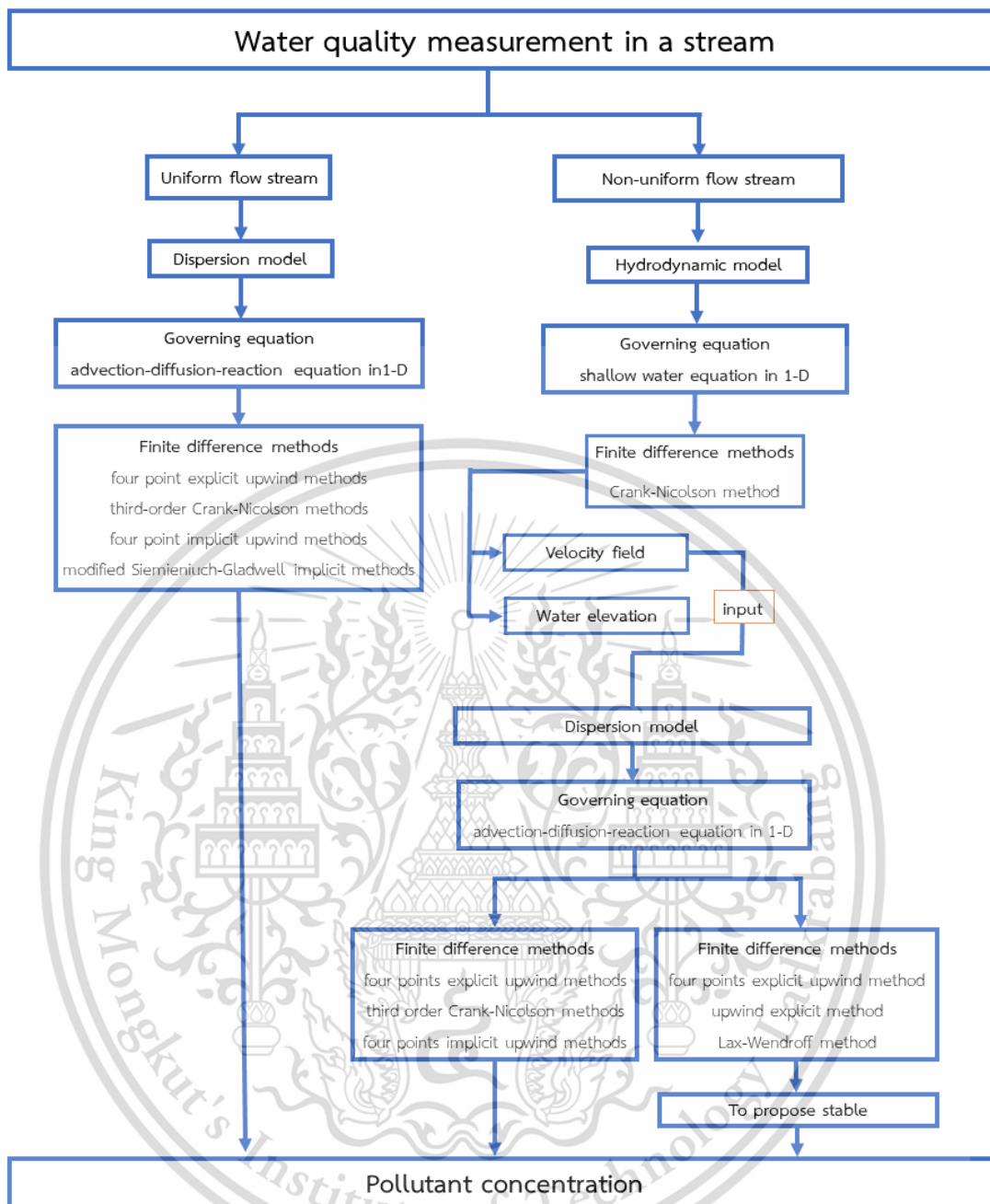


Figure 1.1 Plan of the thesis

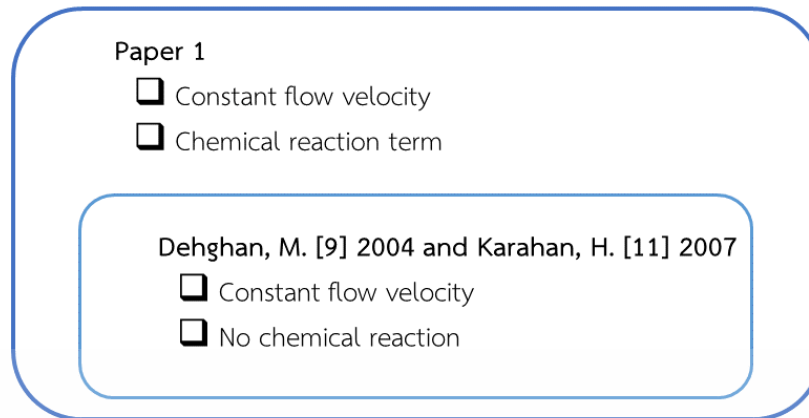


Figure 1.2 Scope of work 1

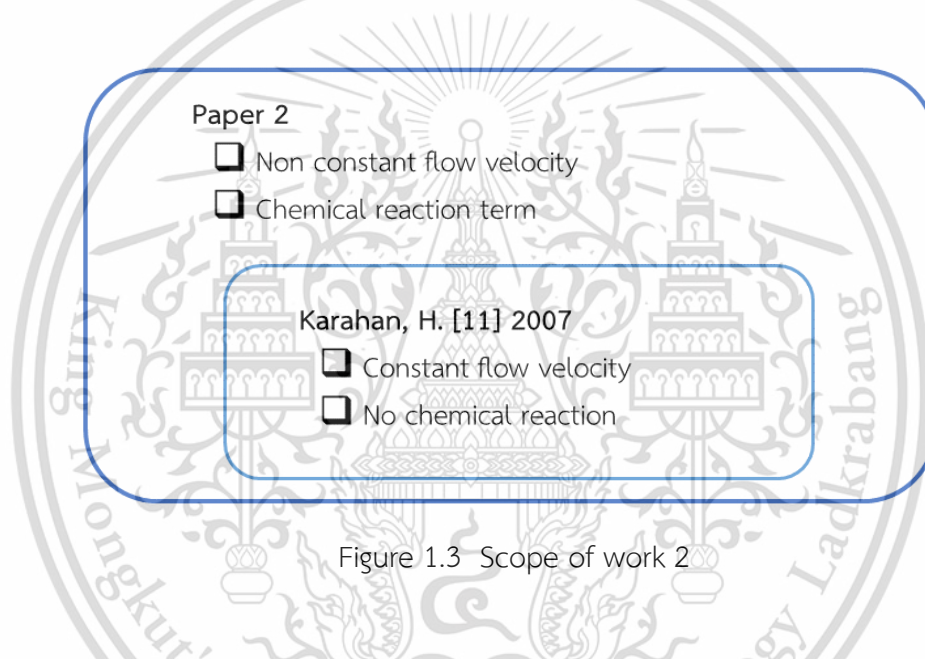


Figure 1.3 Scope of work 2

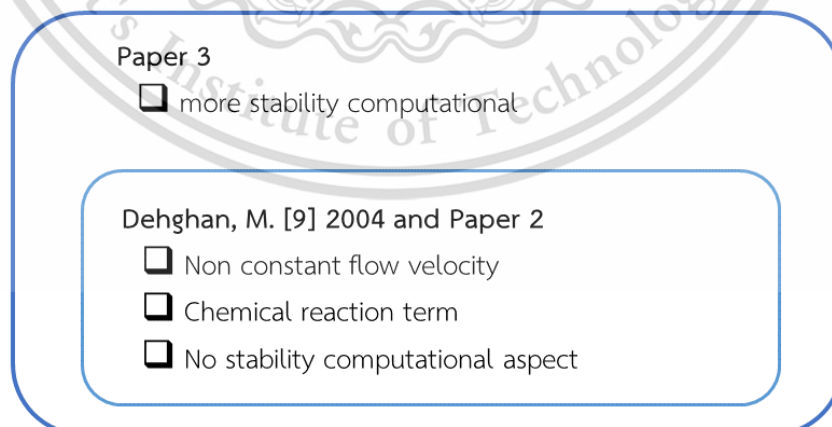


Figure 1.4 Scope of work 3

1.6 Expected results

- 1) To apply a model for water pollution assessment water quality.
- 2) To predict the occurrence of water pollution problems.
- 3) To develop mathematical models for real-world problems.

The contexts of the chapters of this thesis are as follows:

In chapter 2 (basic concepts and preliminaries), a preliminary, one-dimensional hydrodynamic model, the governing equations of water pollution concentration corresponding to the finite difference approximations, and the model of a one-dimensional advection-diffusion-reaction equation are presented.

In chapter 3 (water quality measurement model in a uniform flow stream), the finite difference techniques are introduced for calculating water pollutant concentration. The one-dimensional advection-diffusion-reaction equation is solved by using the explicit methods, the implicit methods, the Crank-Nicolson methods, and the modified Siemieniuch-Gladwell methods. In this chapter, we compare the approximate solution of water pollutant concentrations with the analytical solution.

Chapter 4 (water quality measurement model in a non-uniform flow stream) is divided into two sections. Firstly, a numerical simulation of a one-dimensional hydrodynamic model, using the Crank-Nicolson methods to describe the elevation of water and velocity of water, is presented. Secondly, numerical simulation of a one-dimensional water pollution measurement model is obtained, using the four points explicit upwind methods, the third order Crank-Nicolson methods, the four points implicit upwind methods for section 4.2, and the four points explicit upwind methods, the explicit upwind methods, and the Lax-Wendroff methods for section 4.3.

Chapter 5 (discussion and conclusion) discusses the numerical simulation of the one-dimensional water quality model in chapter 3. The discussion of the numerical simulation of the one-dimensional hydrodynamic model and the numerical simulation of the one-dimensional dispersion model in chapter 4 for sections 4.2 and sections 4.3, is presented.

Chapter 2

Basic Concepts and Preliminaries

2.1 Water pollution

2.1.1 Definition of water pollution



Figure 2.1 Water Pollution

(<https://inwfile.com/s-cf/4csc0g.jpg>)

Some specific definitions of water pollution are given, as per the following:

The Environment Act of 1980 defines water pollution as “Any direct or indirect alteration of the physical, thermal, chemical, biological, or radioactive properties of any part of the environment by discharge, emission or deposit of wastes so as to affect any beneficial use adversely or to cause a condition which is hazardous to public health, safety or welfare of animals, birds, wildlife, aquatic life or to plants of every description.”

The National Institute of Environmental Health Sciences defines water pollution as “any contamination of water with chemicals or other foreign substances that are detrimental to human, plant, or animal health.”

The World Health Organization (WHO) has defined water pollution as “inclusion of any foreign material either from natural or other sources into a water body, thereby changing the natural qualities of water and making it unusable for its intended purpose.”

The Environmental Pollution Center defines water pollution as “the presence in groundwater of toxic chemicals and biological agents that exceed what is naturally found in the water and may pose a threat to human health and/or the environment.”

2.1.2 Substances that cause water pollution

2.1.2.1 Biological agents are organisms that cause wastewater or deterioration, such as bacteria, protozoa, or viruses in the water. Examples include *Vibrio*, which causes cholera, *Shigella*, which is the cause of dysentery, typhoid, enteritis, etc. Algae will grow in water sources that have a lot of nutrients. Algae multiplies rapidly, causing death to and the rotting of aquatic animals, which in turn causes sewage and water sources to lack oxygen.

2.1.2.2 Organic substances are waste from the food industry, such as sugar factories, flour, beer, slaughterhouses, canned food factories, etc. It also includes waste from houses. The wastes released are proteins, carbohydrates, and fats.

2.1.2.3 Inorganic substances include water containing nitrates and phosphate salts from agriculture; high levels of nitrates and phosphates help algae and aquatic plants grow and multiply rapidly.

2.1.2.4 Heavy metal is found in water sources and includes arsenic, lead, mercury, cadmium, zinc, chromium, nickel, manganese, etc. For example, in Thailand, people in Ron Phibun district, Nakhon Si Thammarat Province, were exposed to black fever, because the drinking water contained high quantities of arsenic.

2.1.2.5 Surface float suspensions and sediments- surface-water floats are oil, oil stains, and other substances, some of which are flammable. Therefore, these cause danger to aquatic animals; in addition, they also block light from entering the water and prevent oxygen from being able to spread. Examples are leaves, twigs, foam sheets, plastic bags, cans, and suspensions.

2.1.2.6 Radioactive substances include uranium, strontium, cesium, iodine, etc. Such radioactive substances can pass into the water by various methods, such as follow:

- from the production of uranium
- from washing the clothes of radioactivity laboratory personnel
- from waste from a radioactivity laboratory
- from waste from hospitals that has been examined and treated by

radioactivity

- from water from atomic power plants
- from radioactive dust caused by nuclear weapons experiments.

2.1.3 Effects of water pollution

The important effects of water pollution consist of those affecting human health and the environment.

2.1.3.1 Public health wastewater is a source of disease spread. It causes outbreaks of diseases such as cholera and typhoid, and allows for mosquito breeding grounds, which are carriers of many diseases.

2.1.3.2 In fisheries, water pollution causes various aquatic animal decreases until they may eventually become extinct, because they cannot live and breed normally due to the oxygen used in respiration.

2.1.3.3 Consumption water that has a lot of additives must add more dirt removal systems to produce standardized water. This causes a higher cost of quality water for consumer use.

2.1.3.4 In agriculture, the wastewater is acidic and alkaline, and is not suitable for cultivation in most parts. In addition, such water may be toxic to pets in agricultural areas.

2.1.3.5 Water pollution destroys natural beauty, affecting human mental health.

2.1.4 Sources of water pollution

Sources of pollution that affect water quality in water sources can be divided into 2 major types, which are point sources and non-point sources.

2.1.4.1 Point sources are localized sources such as community sources, industrial factories, wastewater from community sources, discharged wastewater from dwellings, etc. For example, discharged wastewater from washing clothes contains an amount of mineral phosphates. Common detergents cause plants to grow and cover a lot of water, resulting in the oxygen in the air being unable to dissolve, causing wastewater and aquatic animals to die, as well as littering the river. Industrial wastewater is created from the raw material washing process. Production processes such as factory cleaning include wastewater that has not been treated or wastewater which is still not in accordance with the industrial effluent standards. The composition

of wastewater from industrial plants is different. It depends on the effluent flow rate, type, and size of the factory. Examples of point sources are shown in figure 2.2.



Figure 2.2 Water pollution from industrial wastewater
(https://usercontent2.hubstatic.com/8789343_f520.jpg)

2.1.4.2 Non-point sources include wastewater from agricultural activities and Animal husbandry. The wastewater from cultivation is high in nitrogen, phosphorus, potassium, and various toxic substances. Most impurities are found in the form of organic matter. Examples of non-point sources are shown in figure 2.3.



Figure 2.3 Water pollution from agricultural activities
(https://upload.wikimedia.org/wikipedia/commons/thumb/9/95/Runoff_of_soil_%26_fertilizer.jpg/1024px-Runoff_of_soil_%26_fertilizer.jpg)

2.1.5 The characteristics of water pollution

The characteristics of water pollutant can be divided into 3 parts. Polluted water has different water quality components from good water. These components can be separated into 3 major characteristics, which are as follows:

2.1.5.1 Physical characteristics mean the characteristics of water pollution that can be perceived by the five senses. There are important physical indicators, such as the following:

- Temperature is one of the factors that directly and indirectly influence the life of aquatic animals.

- Color checking of water is sometimes popular, due to being able to provide a rough overview of the production capacity, environment, and suspended solids contained in the water source.

- The turbidity of water will show how much of a suspended substance is present. Suspensions contain materials such as fine soil, organic matter, inorganic substances plankton, and small organisms; these substances will spread and prevent light from penetrating the water.

- Odors from wastewater are usually gases which are caused by the decomposition of organic substances in the wastewater.

- Taste can be an indicator, as natural clean water has no taste. The taste of water is different due to the presence of organic or inorganic substances, such as brackish water. This is because a large amount of chloride salt is dissolved in the water.

2.1.5.2 Chemical characteristics refer to the characteristics of water pollution caused by the presence of chemicals in the water that causes chemical conditions in the water. There are important chemical image indices which are the following:

- Conductivity is a characteristic of water that indicates the desire for water to flow.

- Potential of Hydrogen ion value (pH) in natural water has a pH value between 6.5 - 8.5; the difference in pH depends on the characteristics of many landscapes and the environment.

- Dissolved Oxygen (DO) means the value that indicates the amount of dissolved oxygen in the water. Oxygen is very important to aquatic life. In natural water sources, dissolved oxygen is between 5 - 7 milligrams per liter.

- Biochemical Oxygen Demand (BOD) is a value that indicates the amount of oxygen that is used to decompose organic species. The BOD measurement is also used for water quality monitoring in rivers and canals.

- Chemical Oxygen Demand (COD) is a value that indicates the amount of oxygen needed to oxidize organic matter in water. COD is therefore an indicator of water pollution as well as BOD.

2.1.5.3 Biological characteristics mean the characteristics of water pollution caused by the presence of any type of organism mixed in water and which can be toxic to humans and aquatic animals. Biological indicators include phytoplankton, bacteria that cause communicable diseases through water and food, viruses, fungi, and various helminths.

2.2 Finite difference approximations

We introduce the finite difference expression and describe the basic concepts and methods for approximating solutions. A typical grid point is given by $x_i = i\Delta x$, $i = 0, 1, 2, \dots, M$, and $t_n = n\Delta t$, $n = 0, 1, 2, \dots, N$, where Δx and Δt are the grid spacing or grid size or step size in the space and time coordinates, respectively, and i , and n are integers. Note that $h = \Delta x$ and approximate $C(x_i, t_n)$ by C_i^n , value of the difference approximation of $C(x, t)$. The derivatives of the function are approximated using a Taylor series.

The finite difference time grid:

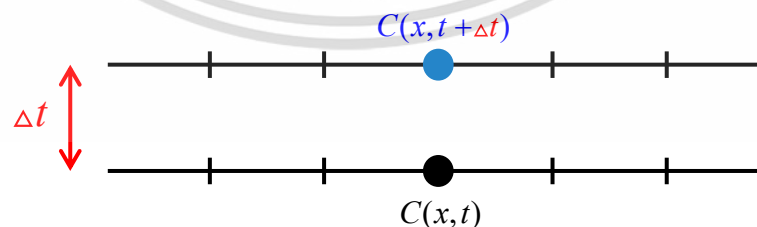


Figure 2.4 The time grid of finite difference

The finite difference space grid:

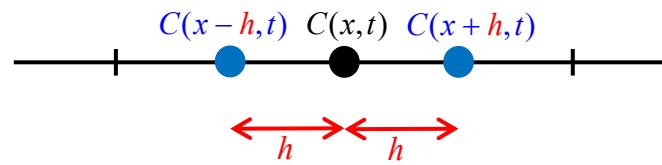


Figure 2.5 The space grid of finite difference

The Taylor series for a function $C(x, t)$:

$$C_{i+1} = C_i + h \frac{\partial C}{\partial x} + \frac{h^2}{2!} \frac{\partial^2 C}{\partial x^2} + \frac{h^3}{3!} \frac{\partial^3 C}{\partial x^3} + \frac{h^4}{4!} \frac{\partial^4 C}{\partial x^4} + \frac{h^5}{5!} \frac{\partial^5 C}{\partial x^5} + \dots, \quad (2.1)$$

$$C_{i-1} = C_i - h \frac{\partial C}{\partial x} + \frac{h^2}{2!} \frac{\partial^2 C}{\partial x^2} - \frac{h^3}{3!} \frac{\partial^3 C}{\partial x^3} + \frac{h^4}{4!} \frac{\partial^4 C}{\partial x^4} - \frac{h^5}{5!} \frac{\partial^5 C}{\partial x^5} + \dots, \quad (2.2)$$

2.2.1 Forward difference in space

From equation (2.1) and rearranging equation to isolate the first derivative,

$$\begin{aligned} h \frac{\partial C}{\partial x} &= C_{i+1} - C_i - \frac{h^2}{2!} \frac{\partial^2 C}{\partial x^2} - \frac{h^3}{3!} \frac{\partial^3 C}{\partial x^3} - \frac{h^4}{4!} \frac{\partial^4 C}{\partial x^4} - \dots, \\ \frac{\partial C}{\partial x} &= \frac{C_{i+1} - C_i}{h} + \left(-\frac{h}{2!} \frac{\partial^2 C}{\partial x^2} - \frac{h^2}{3!} \frac{\partial^3 C}{\partial x^3} - \frac{h^3}{4!} \frac{\partial^4 C}{\partial x^4} - \dots \right), \\ \frac{\partial C}{\partial x} &= \frac{C_{i+1} - C_i}{h} + O(h), \\ \frac{\partial C}{\partial x} &\approx \frac{C_{i+1} - C_i}{\Delta x}. \end{aligned} \quad (2.3)$$

2.2.2 Backward difference in space

From equation (2.2) and rearranging this equation to isolate the second derivative,

$$\begin{aligned} h \frac{\partial C}{\partial x} &= C_i - C_{i-1} + \frac{h^2}{2!} \frac{\partial^2 C}{\partial x^2} - \frac{h^3}{3!} \frac{\partial^3 C}{\partial x^3} + \frac{h^4}{4!} \frac{\partial^4 C}{\partial x^4} - \dots, \\ \frac{\partial C}{\partial x} &= \frac{C_i - C_{i-1}}{h} + \left(\frac{h}{2!} \frac{\partial^2 C}{\partial x^2} - \frac{h^2}{3!} \frac{\partial^3 C}{\partial x^3} + \frac{h^3}{4!} \frac{\partial^4 C}{\partial x^4} - \dots \right), \\ \frac{\partial C}{\partial x} &= \frac{C_i - C_{i-1}}{h} + O(h), \\ \frac{\partial C}{\partial x} &\approx \frac{C_i - C_{i-1}}{\Delta x}. \end{aligned} \quad (2.4)$$

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2.2.3 Central difference in space for first derivative

Subtracting the second equation from the first equation [equation (2.1) - equation (2.2)],

$$\begin{aligned}
 C_{i+1} - C_{i-1} &= 2h \frac{\partial C}{\partial x} + \frac{2h^3}{3!} \frac{\partial^3 C}{\partial x^3} + \frac{2h^5}{5!} \frac{\partial^5 C}{\partial x^5} + \dots, \\
 2h \frac{\partial C}{\partial x} &= C_{i+1} - C_{i-1} - \frac{2h^3}{3!} \frac{\partial^3 C}{\partial x^3} - \frac{2h^5}{5!} \frac{\partial^5 C}{\partial x^5} - \dots, \\
 \frac{\partial C}{\partial x} &= \frac{C_{i+1} - C_{i-1}}{2h} + \left(-\frac{h^2}{3!} \frac{\partial^3 C}{\partial x^3} - \frac{h^4}{5!} \frac{\partial^5 C}{\partial x^5} - \dots \right), \\
 \frac{\partial C}{\partial x} &= \frac{C_{i+1} - C_{i-1}}{2h} + O(h^2), \\
 \frac{\partial C}{\partial x} &\approx \frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}.
 \end{aligned} \tag{2.5}$$

2.2.4 Central difference in space for second derivative

Adding the second equation to the first equation [equation (2.1) + equation (2.2)],

$$\begin{aligned}
 C_{i+1} + C_{i-1} &= 2C_i + \frac{2h^2}{2!} \frac{\partial^2 C}{\partial x^2} + \frac{2h^4}{4!} \frac{\partial^4 C}{\partial x^4} + \dots, \\
 \frac{2h^2}{2!} \frac{\partial^2 C}{\partial x^2} &= C_{i+1} + C_{i-1} - 2C_i - \frac{2h^4}{4!} \frac{\partial^4 C}{\partial x^4} - \dots, \\
 \frac{\partial^2 C}{\partial x^2} &= \frac{C_{i+1} - 2C_i + C_{i-1}}{h^2} + \left(-\frac{2h^2}{4!} \frac{\partial^4 C}{\partial x^4} - \dots \right), \\
 \frac{\partial^2 C}{\partial x^2} &= \frac{C_{i+1} - 2C_i + C_{i-1}}{h^2} + O(h^2), \\
 \frac{\partial^2 C}{\partial x^2} &\approx \frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2}.
 \end{aligned} \tag{2.6}$$

2.2.5 Forward difference in space for first derivative

From equation (2.1) and substituting forward difference in space,

$$\begin{aligned}
 h \frac{\partial C}{\partial x} &= C_{i+1} - C_i - \frac{h^2}{2!} \frac{\partial^2 C}{\partial x^2} - \frac{h^3}{3!} \frac{\partial^3 C}{\partial x^3} - \frac{h^4}{4!} \frac{\partial^4 C}{\partial x^4} - \dots, \\
 \frac{\partial C}{\partial x} &= \frac{C_{i+1} - C_i}{h} - \frac{h}{2!} \frac{\partial^2 C}{\partial x^2} + \left(-\frac{h^2}{3!} \frac{\partial^3 C}{\partial x^3} - \frac{h^3}{4!} \frac{\partial^4 C}{\partial x^4} - \dots \right), \\
 \frac{\partial C}{\partial x} &= \frac{C_{i+1} - C_i}{h} - \frac{h}{2!} \frac{\partial^2 C}{\partial x^2} + O(h^2), \\
 \frac{\partial C}{\partial x} &\approx \frac{C_{i+1} - C_i}{h} - \frac{h}{2!} \frac{\partial}{\partial x} \left(\frac{C_{i+1} - C_i}{h} \right) + O(h^2),
 \end{aligned}$$

$$\begin{aligned}
\frac{\partial C}{\partial x} &\approx \frac{C_{i+1} - C_i}{h} - \frac{1}{2} \frac{\partial}{\partial x} (C_{i+1} - C_i) + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{C_{i+1} - C_i}{h} - \frac{1}{2} \left(\frac{C_{i+2} - C_{i+1}}{h} - \frac{C_{i+1} - C_i}{h} \right) + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{C_{i+1} - C_i}{h} - \left(\frac{C_{i+2} - C_{i+1} - C_{i+1} - C_i}{2h} \right) + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{C_{i+1} - C_i}{h} - \left(\frac{C_{i+2} - 2C_{i+1} - C_i}{2h} \right) + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{2C_{i+1} - 2C_i - C_{i+2} + 2C_{i+1} - C_i}{2h} + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{-3C_i + 4C_{i+1} - C_{i+2}}{2h} + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{-3C_{i,j,k}^n + 4C_{i+1}^n - C_{i+2}^n}{2\Delta x}.
\end{aligned} \tag{2.7}$$

2.2.6 Backward difference in space for first derivative

From equation (2.2) and substituting backward difference in space,

$$\begin{aligned}
h \frac{\partial C}{\partial x} &= C_i - C_{i-1} + \frac{h^2}{2!} \frac{\partial^2 C}{\partial x^2} - \frac{h^3}{3!} \frac{\partial^3 C}{\partial x^3} + \frac{h^4}{4!} \frac{\partial^4 C}{\partial x^4} - \dots, \\
\frac{\partial C}{\partial x} &= \frac{C_i - C_{i-1}}{h} + \frac{h}{2!} \frac{\partial^2 C}{\partial x^2} + \left(-\frac{h^2}{3!} \frac{\partial^3 C}{\partial x^3} + \frac{h^3}{4!} \frac{\partial^4 C}{\partial x^4} - \dots \right), \\
\frac{\partial C}{\partial x} &= \frac{C_i - C_{i-1}}{h} + \frac{h}{2!} \frac{\partial^2 C}{\partial x^2} + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{C_i - C_{i-1}}{h} + \frac{h}{2!} \frac{\partial}{\partial x} \left(\frac{C_i - C_{i-1}}{h} \right) + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{C_i - C_{i-1}}{h} + \frac{1}{2} \frac{\partial}{\partial x} (C_i - C_{i-1}) + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{C_i - C_{i-1}}{h} + \frac{1}{2} \left(\frac{C_i - C_{i-1}}{h} - \frac{C_{i-1} - C_{i-2}}{h} \right) + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{C_i - C_{i-1}}{h} + \left(\frac{C_i - C_{i-1} - C_{i-1} + C_{i-2}}{2h} \right) + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{C_i - C_{i-1}}{h} + \left(\frac{C_i - 2C_{i-1} + C_{i-2}}{2h} \right) + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{2C_i - 2C_{i-1} + C_i - 2C_{i-1} + C_{i-2}}{2h} + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{C_{i-2} - 4C_{i-1} + 3C_i}{2h} + O(h^2), \\
\frac{\partial C}{\partial x} &\approx \frac{C_{i-2}^n - 4C_{i-1}^n + 3C_i^n}{2\Delta x}.
\end{aligned} \tag{2.8}$$

2.2.7 Forward difference in space for second derivative

From forward difference in space,

$$\begin{aligned}
 \frac{\partial^2 C}{\partial x^2} &= \frac{\partial}{\partial x} \left(\frac{\partial C}{\partial x} \right), \\
 \frac{\partial^2 C}{\partial x^2} &\approx \frac{\partial}{\partial x} \left(\frac{C_{i+1} - C_i}{\Delta x} \right), \\
 \frac{\partial^2 C}{\partial x^2} &\approx \frac{1}{\Delta x} \left(\frac{C_{i+2} - C_{i+1}}{\Delta x} - \frac{C_{i+1} - C_i}{\Delta x} \right), \\
 \frac{\partial^2 C}{\partial x^2} &\approx \frac{1}{\Delta x} \left(\frac{C_{i+2} - C_{i+1} - C_{i+1} + C_i}{\Delta x} \right), \\
 \frac{\partial^2 C}{\partial x^2} &\approx \frac{1}{\Delta x} \left(\frac{C_{i+2} - 2C_{i+1} + C_i}{\Delta x} \right), \\
 \frac{\partial^2 C}{\partial x^2} &\approx \frac{C_i^n - 2C_{i+1}^n + C_{i+2}^n}{(\Delta x)^2}. \tag{2.9}
 \end{aligned}$$

2.2.8 Backward difference in space for second derivative

From backward difference in space,

$$\begin{aligned}
 \frac{\partial^2 C}{\partial x^2} &= \frac{\partial}{\partial x} \left(\frac{\partial C}{\partial x} \right), \\
 \frac{\partial^2 C}{\partial x^2} &\approx \frac{\partial}{\partial x} \left(\frac{C_i - C_{i-1}}{\Delta x} \right), \\
 \frac{\partial^2 C}{\partial x^2} &\approx \frac{1}{\Delta x} \left(\frac{C_{i-2} - 4C_{i-1} + 3C_i}{2\Delta x} - \frac{C_{i-3} - 4C_{i-2} + 3C_{i-1}}{2\Delta x} \right), \\
 \frac{\partial^2 C}{\partial x^2} &\approx \frac{1}{\Delta x} \left(\frac{C_{i-2} - 4C_{i-1} + 3C_i - C_{i-3} + 4C_{i-2} - 3C_{i-1}}{2\Delta x} \right), \\
 \frac{\partial^2 C}{\partial x^2} &\approx \frac{1}{\Delta x} \left(\frac{3C_i - 7C_{i-1} + 5C_{i-2} - C_{i-3}}{2\Delta x} \right), \\
 \frac{\partial^2 C}{\partial x^2} &\approx \frac{3C_i^n - 7C_{i-1}^n + 5C_{i-2}^n - C_{i-3}^n}{2(\Delta x)^2}. \tag{2.10}
 \end{aligned}$$

2.2.9 Two backward difference in space for second derivative

From backward difference in space,

$$\begin{aligned}
 \frac{\partial^2 C}{\partial x^2} &= \frac{\partial}{\partial x} \left(\frac{\partial C}{\partial x} \right), \\
 \frac{\partial^2 C}{\partial x^2} &\approx \frac{\partial}{\partial x} \left(\frac{C_i - C_{i-1}}{\Delta x} \right), \\
 \frac{\partial^2 C}{\partial x^2} &\approx \frac{1}{\Delta x} \left(\frac{C_i - C_{i-1}}{\Delta x} - \frac{C_{i-3} - 4C_{i-2} + 3C_{i-1}}{2\Delta x} \right),
 \end{aligned}$$

$$\begin{aligned}
\frac{\partial^2 C}{\partial x^2} &\approx \frac{1}{\Delta x} \left(\frac{2C_i - 2C_{i-1} - C_{i-3} + 4C_{i-2} - 3C_{i-1}}{2\Delta x} \right), \\
\frac{\partial^2 C}{\partial x^2} &\approx \frac{1}{\Delta x} \left(\frac{2C_i - 5C_{i-1} + 4C_{i-2} - C_{i-3}}{2\Delta x} \right), \\
\frac{\partial^2 C}{\partial x^2} &\approx \left(\frac{2C_i^n - 5C_{i-1}^n + 4C_{i-2}^n - C_{i-3}^n}{2(\Delta x)^2} \right).
\end{aligned} \tag{2.11}$$

2.3 The one-dimensional hydrodynamic model

The one-dimensional hydrodynamic model describes water current and elevation by using a system of shallow water equations as the conservation of mass and conservation of momentum. It is obtained by integrating the Navier-Stokes equations over the flow depth under the assumptions as hydrostatic pressure distribution and small bottom slope. The governing equation of the hydrodynamic describes the behavior of the reservoir. Figure 2.6 shows a shallow water system.

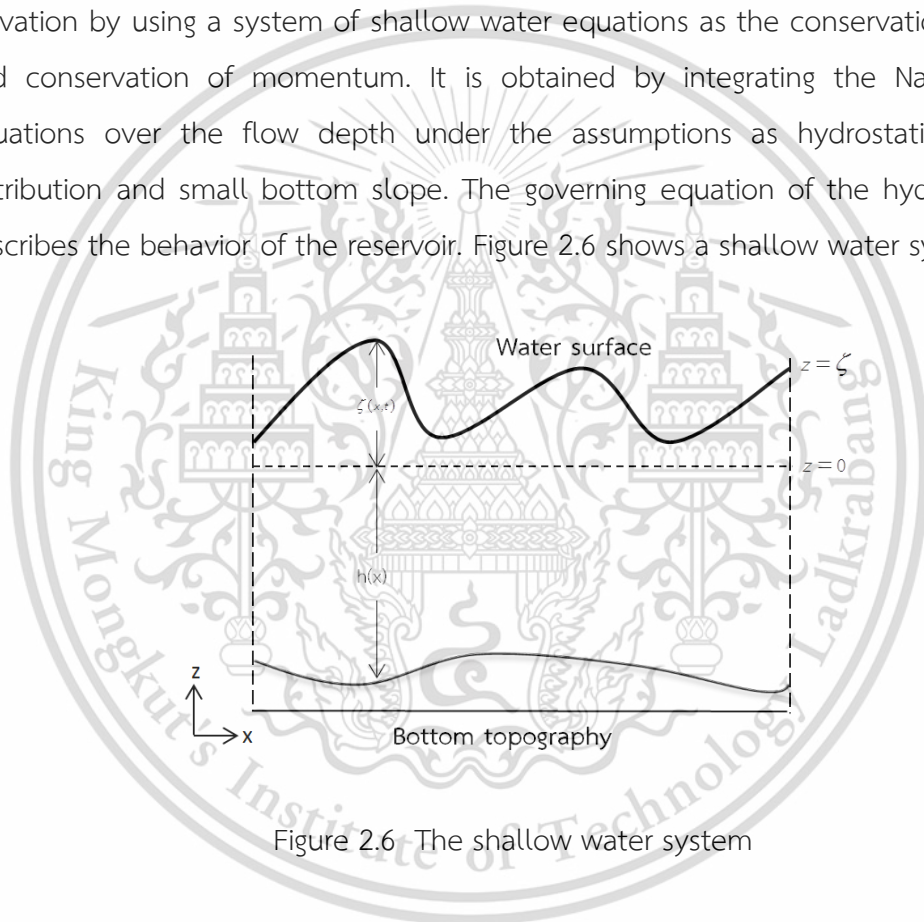


Figure 2.6 The shallow water system

We derive a simple form of the one-dimensional hydrodynamic by assuming the continuity and momentum balance; that is, we assume that the Coriolis, shearing stresses, and surface wind are small [19, 28-29] and h is a flat bottom topography [26]. We obtain the one-dimensional shallow water equations as follows:

$$\frac{\partial \zeta}{\partial t} + \frac{\partial}{\partial x} [(h + \zeta)u] = 0, \tag{2.12}$$

$$\frac{\partial u}{\partial t} + g \frac{\partial \zeta}{\partial x} = 0, \tag{2.13}$$

where x is the longitudinal distance along a stream (m), time t (s),
 $h(x)$ is the depth measured from the mean water to the bed of the reservoir (m),
 $\zeta(x,t)$ is the elevation from the mean water level to the temporary water surface (m/s),
 g is the acceleration due to gravity,
 $u(x,t)$ are the velocity components in x direction (m/s),

for all $(x,t) \in [0,L] \times [0,T]$. We assume that h is a constant and $\zeta \ll h$. Then equations (2.12) – (2.13) become;

$$\frac{\partial \zeta}{\partial t} + h \frac{\partial u}{\partial x} = 0, \quad (2.14)$$

$$\frac{\partial u}{\partial t} + g \frac{\partial \zeta}{\partial x} = 0. \quad (2.15)$$

2.4 A one-dimensional dispersion model

2.4.1 Mass transfer

2.4.2.1 Advection

Advection is the transfer of heat or cold in the atmosphere by the flow in the horizontal movement of an air mass. Advection, in general, moves matter from one position in space to another. The transportation of matter by the advection shown in figure 2.7.

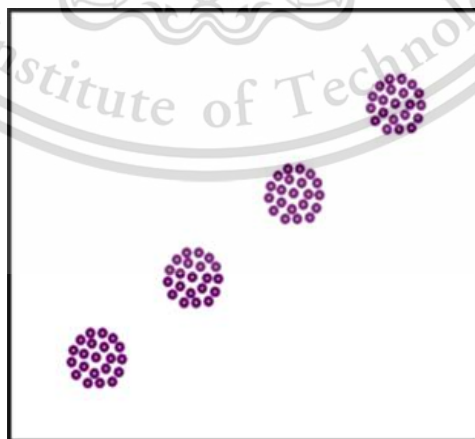


Figure 2.7 The transport by advection

2.4.2.2 Diffusion

Diffusion is the movement or the spread of mass in air or dissolved substances. Diffusion, in general, moves matter from regions of higher concentration to regions of lower concentration. The movement of mass will mix until they are evenly distributed in the concentration. The transportation of matter by diffusion shown in figure 2.8.

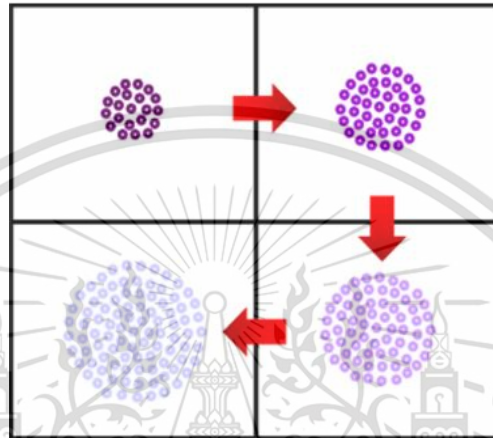


Figure 2.8 The transport by diffusion

2.4.2.3 Advection-diffusion (Dispersion)

Advection-diffusion is a system in which particles are dispersed continuously. It is the transfer of particles inside a system, due to two processes, the combination of the advection and diffusion. The transportation of matter by dispersion are shown in figure 2.9.

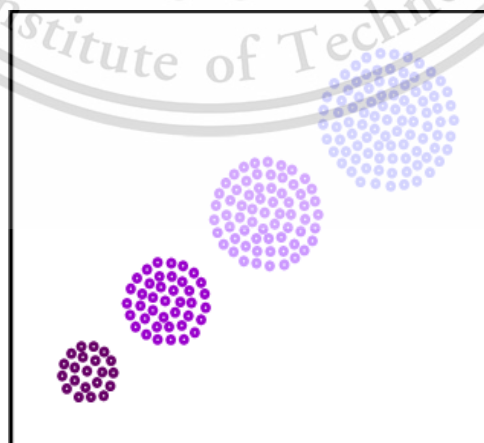


Figure 2.9 The transportation of dispersion

2.4.2.4 Reactions

Reactions refer to the mass gained or lost by transformations of the substances within the volume. Reactions either add mass, by changing another constituent into the substance being modeled, or remove mass, by transforming the substance into another constituent. The reaction is shown in figure 2.10.

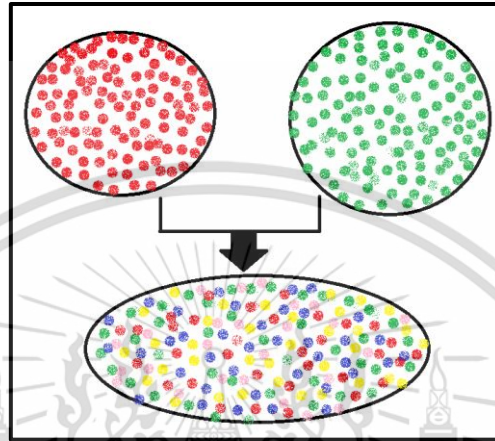


Figure 2.10 Reaction

2.4.2 Fluid flow

Fluid is a substance that can move or flow continuously when treated with a shear force which is parallel to the plane in which the fluid flows, regardless of the size of the shear.

2.4.2.1 Characteristics of fluid flow

Fluid flow is divided into 2 characteristics.

1. Laminar flow, or consistent flow, is a form of flow in which fluid particles move in an orderly manner. There is no mixing between the fluid layers in flow characteristics like this. In general, it occurs with high viscosity fluids and low velocity flows, or where the diameter of the pipe that the fluid flows through is very large when compared to the amount of fluid flowing inside the pipe.

2. Turbulent flow, or disorderly flow, generally occurs with low viscosity fluids and high velocity flows, or where the diameter of the pipe that the fluid flows through is small compared to the amount of fluid flowing inside the pipe. Fluid flow patterns have unpredictable directions and speeds and there is a mixture of fluid layers while moving. Laminar flow and turbulent flow are shown in figure 2.11.

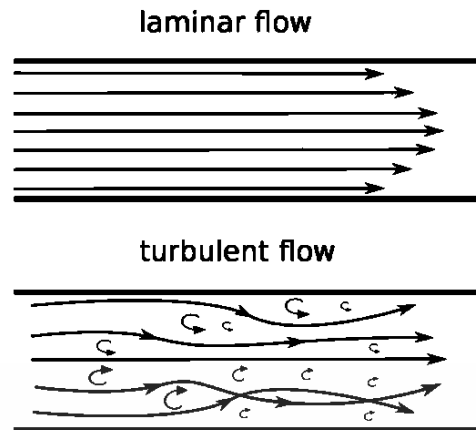


Figure 2.11 The turbulent flow and the laminar flow
 (https://diffzi.com/wp-content/uploads/2018/11/Laminar-Flow-vs.-Turbulent-Flow-768x701.png)

2.4.2.2 Reynolds number

The Reynolds number (Re) is a number that shows the relationship between fluid properties that change with temperature and pressure. It is determined by

$$Re = \frac{\rho UL}{\mu} = \frac{UL}{\nu}, \quad (2.16)$$

where

U is velocity (m/s),

L is characteristic linear dimension (m),

μ is dynamic viscosity of fluid (kg/m),

ν is kinematic viscosity (m^2/s),

ρ is density of the fluid (kg/m^3).

Fluids flowing in turbulent tubes have high Reynolds numbers, with the Reynolds number crisis as an indicator of the change in fluid flow characteristics:

- If the Reynolds number is less than or equal to 2000 ($Re \leq 2000$), the fluid will have a laminar flow.
- If the Reynolds number is greater than or equal to 4000 ($Re \geq 4000$), the fluid will have turbulent flow characteristics.

2.4.3 Governing equation for one-dimensional dispersion model

The concentration of water pollutants can be described by the advection-diffusion-reaction equation (ADREs). A simplified representation, by averaging the equation over the depth, is shown in [9, 20, 26-27, 30-31],

$$\frac{\partial C}{\partial t} + V \cdot \nabla C = \nabla \cdot (\bar{K} \otimes \nabla C) - KC, \quad (2.17)$$

where $C(x,t)$ is the water pollutant concentration at point x and at time t (kg/m^3). $\nabla = \frac{\partial}{\partial x} \vec{i}$ is matrix multiplication. The vector V is the velocity field (m/s), \bar{K} is dispersion tensor (m^2/s) and K describes the chemical reaction being creating or destroying. Therefore equation (2.17), can be rearranged as follows:

$$\begin{aligned} \frac{\partial C}{\partial t} + V \cdot \left(\frac{\partial}{\partial x} \vec{i} \right) C(x) &= \left(\frac{\partial}{\partial x} \vec{i} \right) \cdot \left(\bar{K} \otimes \left(\frac{\partial}{\partial x} \vec{i} \right) C(x) \right) - KC \\ \frac{\partial C}{\partial t} + V(u) \cdot \left(\frac{\partial C}{\partial x} \right) &= \left(\frac{\partial}{\partial x} \vec{i} \right) \cdot \left(K(x) \otimes \left(\frac{\partial C}{\partial x} \right) \right) - KC, \\ \frac{\partial C}{\partial t} + \left(u \frac{\partial C}{\partial x} \right) &= \left(\frac{\partial}{\partial x} \vec{i} \right) \cdot \left(K_x \frac{\partial C}{\partial x} \right) - KC, \\ \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} &= \frac{\partial}{\partial x} \left(K_x \frac{\partial C}{\partial x} \right) - KC, \\ \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} &= K_x \frac{\partial^2 C}{\partial x^2} - KC. \end{aligned} \quad (2.18)$$

We set $D = K_x$. Then, the one-dimensional advection-diffusion-reaction equation in equation (2.18) can be written as,

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2} - KC, \quad (2.19)$$

where $u(x,t)$ is the velocity in x direction (m/s),

D is the diffusion coefficient (m^2/s),

K is the mass decay rate,

with the potential pollutant concentration as the initial condition,

$$C(x,0) = f(x), \quad 0 \leq x \leq L, \quad (2.20)$$

and the released pollutant concentration on the left boundary and the right boundary,

$$C(0,t) = g(t), \quad 0 < t \leq T, \quad (2.21)$$

$$C(L,t) = h(t), \quad 0 < t \leq T, \quad (2.22)$$

where $f(t), g(t), h(t)$ are known functions. The domain for one-dimensional equations are illustrated in figure 2.12; we consider domain only the x -direction.

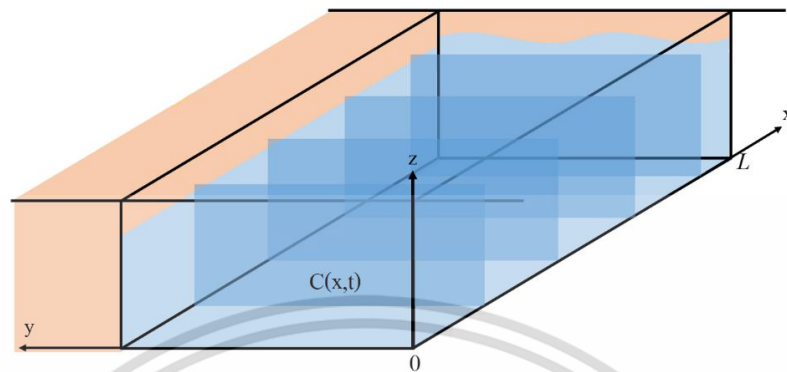


Figure 2.12 The domain for one-dimensional equations

Moreover, we consider the domain on two-dimensional and three-dimensional equations, seen in figure 2.13 and figure 2.14, respectively. From figure 2.13, we can see that, for two-dimensional equations consider domain in the x -direction and the y -direction. From figure 2.14, we consider domain in the x -direction, the y -direction, and the z -direction.

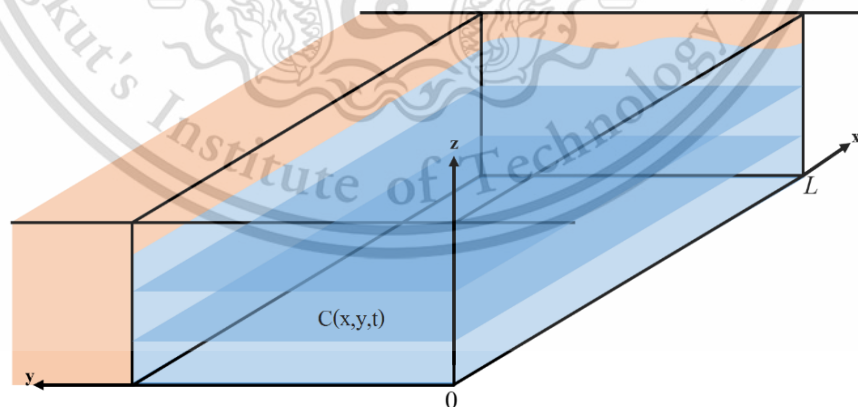


Figure 2.13 The domain for two-dimensional equations

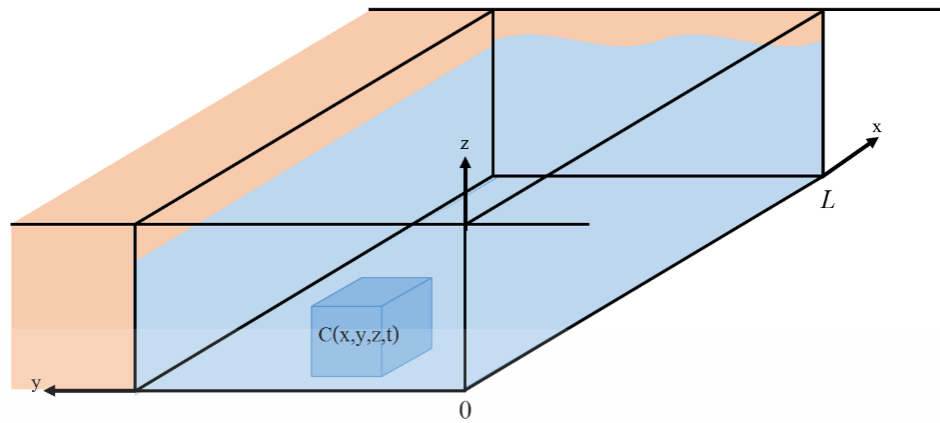


Figure 2.14 The domain for three-dimensional equations



Chapter 3

Water Quality Measurement Model in a Uniform Flow Stream

In this chapter, the numerical computations of a water-quality model in a uniform flow stream are proposed. The governing equation, which is a one-dimensional advection-diffusion-reaction equation, is approximated by using a finite difference technique. The explicit methods, the implicit methods, the Crank-Nicolson methods, and modified Siemieniuch-Gladwell methods are used to approximate the pollutant concentration at each point at all times on a uniform flow stream. The accuracy of the proposed computation technique is compared with the analytical and approximated solutions shown in the examples.

3.1 The finite difference techniques of the third-order upwind schemes

From [10], we get the following discretization, with the time derivative $t = n\Delta t$ by using forward-difference,

$$\frac{\partial C}{\partial t} \approx \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad (3.1)$$

to approximate the advective term in the advection-diffusion-reaction equation which incorporate temporal weight parameter, (ϕ) , near the left boundary, for $i = 2$,

$$u \frac{\partial C}{\partial x} \approx \frac{u}{6\Delta x} \left[\phi(-11C_i^{n+1} + 18C_{i+1}^{n+1} - 9C_{i+2}^{n+1} + 2C_{i+3}^{n+1}) + (1-\phi)(-11C_i^n + 18C_{i+1}^n - 9C_{i+2}^n + 2C_{i+3}^n) \right], \quad (3.2)$$

interior nodes of the solution domain, for $i = 3, \dots, M-2$,

$$u \frac{\partial C}{\partial x} \approx \frac{u}{6\Delta x} \left[\phi(C_{i-2}^{n+1} - 6C_{i-1}^{n+1} + 3C_i^{n+1} + 2C_{i+1}^{n+1}) + (1-\phi)(C_{i-2}^n - 6C_{i-1}^n + 3C_i^n + 2C_{i+1}^n) \right], \quad (3.3)$$

near right boundary, for $i = M-1$,

$$u \frac{\partial C}{\partial x} \approx \frac{u}{6\Delta x} \left[\phi(-2C_{i-3}^{n+1} + 9C_{i-2}^{n+1} - 18C_{i-1}^{n+1} + 11C_i^{n+1}) + (1-\phi)(-2C_{i-3}^n + 9C_{i-2}^n - 18C_{i-1}^n + 11C_i^n) \right], \quad (3.4)$$

and to approximate the diffusive term by using central-difference scheme,

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$$D \frac{\partial^2 C}{\partial x^2} \approx \frac{D}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n], \quad (3.5)$$

Next, we can assume each term by substituting equations (3.1–3.5) into equation (2.19) and, by incorporating temporal weight parameter, we obtain the computed solution as follows.

Near the left boundary for $i = 2$, we substitute equations (3.1–3.2) and equation (3.5) into equation (2.19) and, rearranging, we have

$$\begin{aligned} & \frac{C_i^{n+1} - C_i^n}{\Delta t} + \frac{u}{6\Delta x} \left\{ \phi(-11C_i^{n+1} + 18C_{i+1}^{n+1} - 9C_{i+2}^{n+1} + 2C_{i+3}^{n+1}) \right. \\ & \left. + (1-\phi)(-11C_i^n + 18C_{i+1}^n - 9C_{i+2}^n + 2C_{i+3}^n) \right\} \\ & = \frac{D}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n] - KC_i^n, \\ & C_i^{n+1} - C_i^n + \frac{u(\Delta t)}{6\Delta x} \left\{ \phi(-11C_i^{n+1} + 18C_{i+1}^{n+1} - 9C_{i+2}^{n+1} + 2C_{i+3}^{n+1}) \right. \\ & \left. + (1-\phi)(-11C_i^n + 18C_{i+1}^n - 9C_{i+2}^n + 2C_{i+3}^n) \right\} \\ & = \frac{D(\Delta t)}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n] - K(\Delta t)C_i^n, \\ & C_i^{n+1} - C_i^n + \frac{1}{6}Cr \left\{ \phi(-11C_i^{n+1} + 18C_{i+1}^{n+1} - 9C_{i+2}^{n+1} + 2C_{i+3}^{n+1}) \right. \\ & \left. + (1-\phi)(-11C_i^n + 18C_{i+1}^n - 9C_{i+2}^n + 2C_{i+3}^n) \right\} \\ & = \frac{Cr}{Pe} [C_{i-1}^n - 2C_i^n + C_{i+1}^n] - K(\Delta t)C_i^n, \\ & C_i^{n+1} - C_i^n - \frac{11}{6}Cr\phi C_i^{n+1} + \frac{18}{6}Cr\phi C_{i+1}^{n+1} - \frac{9}{6}Cr\phi C_{i+2}^{n+1} + \frac{2}{6}Cr\phi C_{i+3}^{n+1} \\ & - \frac{11}{6}Cr(1-\phi)C_i^n + \frac{18}{6}Cr(1-\phi)C_{i+1}^n - \frac{9}{6}Cr(1-\phi)C_{i+2}^n + \frac{2}{6}Cr(1-\phi)C_{i+3}^n \\ & = \frac{Cr}{Pe} C_{i-1}^n - 2\frac{Cr}{Pe} C_i^n + \frac{Cr}{Pe} C_{i+1}^n - K(\Delta t)C_i^n, \\ & \left[1 - \frac{11}{6}Cr\phi \right] C_i^{n+1} + 3Cr\phi C_{i+1}^{n+1} - \frac{3}{2}Cr\phi C_{i+2}^{n+1} + \frac{1}{2}Cr\phi C_{i+3}^{n+1} \\ & = \frac{Cr}{Pe} C_{i-1}^n - 2\frac{Cr}{Pe} C_i^n + \frac{Cr}{Pe} C_{i+1}^n - K(\Delta t)C_i^n + C_i^n + \frac{11}{6}Cr(1-\phi)C_i^n \\ & - 3Cr(1-\phi)C_{i+1}^n + \frac{3}{2}Cr(1-\phi)C_{i+2}^n - \frac{1}{3}Cr(1-\phi)C_{i+3}^n, \\ & \left[1 - \frac{11}{6}Cr\phi \right] C_i^{n+1} + 3Cr\phi C_{i+1}^{n+1} - \frac{3}{2}Cr\phi C_{i+2}^{n+1} + \frac{1}{2}Cr\phi C_{i+3}^{n+1} \\ & = \frac{Cr}{Pe} C_{i-1}^n + \left[1 - 2\frac{Cr}{Pe} - K(\Delta t) + \frac{11}{6}Cr(1-\phi) \right] C_i^n \\ & + \left[\frac{Cr}{Pe} - 3Cr(1-\phi) \right] C_{i+1}^n + \frac{3}{2}Cr(1-\phi)C_{i+2}^n - \frac{1}{3}Cr(1-\phi)C_{i+3}^n. \end{aligned} \quad (3.6)$$

Interior node for $i = 3, \dots, M - 2$, we substitute equation (3.1), equation (3.3), and equation (3.5) into equation (2.19), and we get

$$\begin{aligned}
& \frac{C_i^{n+1} - C_i^n}{\Delta t} + \frac{u}{6\Delta x} \left\{ \phi (C_{i-2}^{n+1} - 6C_{i-1}^{n+1} + 3C_i^{n+1} + 2C_{i+1}^{n+1}) \right. \\
& \left. + (1-\phi)(C_{i-2}^n - 6C_{i-1}^n + 3C_i^n + 2C_{i+1}^n) \right\} \\
& = \frac{D}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n] - KC_i^n, \\
& C_i^{n+1} - C_i^n + \frac{u(\Delta t)}{6\Delta x} \left\{ \phi (C_{i-2}^{n+1} - 6C_{i-1}^{n+1} + 3C_i^{n+1} + 2C_{i+1}^{n+1}) \right. \\
& \left. + (1-\phi)(C_{i-2}^n - 6C_{i-1}^n + 3C_i^n + 2C_{i+1}^n) \right\} \\
& = \frac{D(\Delta t)}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n] - K(\Delta t)C_i^n, \\
& C_i^{n+1} - C_i^n + \frac{1}{6}Cr\phi C_{i-2}^{n+1} - Cr\phi C_{i-1}^{n+1} + \frac{1}{2}Cr\phi C_i^{n+1} + \frac{1}{3}Cr\phi C_{i+1}^{n+1} \\
& + \frac{1}{6}Cr(1-\phi)C_{i-2}^n - Cr(1-\phi)C_{i-1}^n + \frac{1}{2}Cr(1-\phi)C_i^n \\
& + \frac{1}{3}Cr(1-\phi)C_{i+1}^n \\
& = \frac{Cr}{Pe} C_{i-1}^n - 2\frac{Cr}{Pe} C_i^n + \frac{Cr}{Pe} C_{i+1}^n - K(\Delta t)C_i^n, \\
& \frac{1}{6}Cr\phi C_{i-2}^{n+1} - Cr\phi C_{i-1}^{n+1} + \left[1 + \frac{1}{2}Cr\phi \right] C_i^{n+1} + \frac{1}{3}Cr\phi C_{i+1}^{n+1} \\
& + \frac{1}{6}Cr(1-\phi)C_{i-2}^n - Cr(1-\phi)C_{i-1}^n + \frac{1}{2}Cr(1-\phi)C_i^n \\
& + \frac{1}{3}Cr(1-\phi)C_{i+1}^n \\
& = \frac{Cr}{Pe} C_{i-1}^n - 2\frac{Cr}{Pe} C_i^n + \frac{Cr}{Pe} C_{i+1}^n - K(\Delta t)C_i^n - C_i^n, \\
& \frac{1}{6}Cr\phi C_{i-2}^{n+1} - Cr\phi C_{i-1}^{n+1} + \left[1 + \frac{1}{2}Cr\phi \right] C_i^{n+1} + \frac{1}{3}Cr\phi C_{i+1}^{n+1} \\
& = \frac{Cr}{Pe} C_{i-1}^n - 2\frac{Cr}{Pe} C_i^n + \frac{Cr}{Pe} C_{i+1}^n - K(\Delta t)C_i^n + C_i^n \\
& - \frac{1}{6}Cr(1-\phi)C_{i-2}^n + Cr(1-\phi)C_{i-1}^n - \frac{1}{2}Cr(1-\phi)C_i^n \\
& - \frac{1}{3}Cr(1-\phi)C_{i+1}^n, \\
& \frac{1}{6}Cr\phi C_{i-2}^{n+1} - Cr\phi C_{i-1}^{n+1} + \left[1 + \frac{1}{2}Cr\phi \right] C_i^{n+1} + \frac{1}{3}Cr\phi C_{i+1}^{n+1} \\
& = -\frac{1}{6}Cr(1-\phi)C_{i-2}^n + \left[\frac{Cr}{Pe} + Cr(1-\phi) \right] C_{i-1}^n \\
& + \left[1 - K(\Delta t) - 2\frac{Cr}{Pe} - \frac{1}{2}Cr(1-\phi) \right] C_i^n \\
& + \left[\frac{Cr}{Pe} - \frac{1}{3}Cr(1-\phi) \right] C_{i+1}^n.
\end{aligned} \tag{3.7}$$

Near the right boundary for $i = M - 1$, we substitute equation (3.1), equation (3.4), and equation (3.5) into equation (2.19), and we have

$$\begin{aligned}
& \frac{C_i^{n+1} - C_i^n}{\Delta t} + \frac{u}{6\Delta x} \left\{ \phi \left(-2C_{i-3}^{n+1} + 9C_{i-2}^{n+1} - 18C_{i-1}^{n+1} + 11C_i^{n+1} \right) \right. \\
& \left. + (1-\phi) \left(-2C_{i-3}^n + 9C_{i-2}^n - 18C_{i-1}^n + 11C_i^n \right) \right\} \\
& = \frac{D}{(\Delta x)^2} \left[C_{i-1}^n - 2C_i^n + C_{i+1}^n \right] - KC_i^n, \\
& C_i^{n+1} - C_i^n + \frac{u(\Delta t)}{6\Delta x} \left\{ \phi \left(-2C_{i-3}^{n+1} + 9C_{i-2}^{n+1} - 18C_{i-1}^{n+1} + 11C_i^{n+1} \right) \right. \\
& \left. + (1-\phi) \left(-2C_{i-3}^n + 9C_{i-2}^n - 18C_{i-1}^n + 11C_i^n \right) \right\} \\
& = \frac{D(\Delta t)}{(\Delta x)^2} \left[C_{i-1}^n - 2C_i^n + C_{i+1}^n \right] - K(\Delta t)C_i^n, \\
& C_i^{n+1} - C_i^n - 2\frac{1}{6}Cr\phi C_{i-3}^{n+1} + 9\frac{1}{6}Cr\phi C_{i-2}^{n+1} - 18\frac{1}{6}Cr\phi C_{i-1}^{n+1} + 11\frac{1}{6}Cr\phi C_i^{n+1} \\
& - 2\frac{1}{6}Cr(1-\phi)C_{i-3}^n + 9\frac{1}{6}Cr(1-\phi)C_{i-2}^n - 18\frac{1}{6}Cr(1-\phi)C_{i-1}^n \\
& + 11\frac{1}{6}Cr(1-\phi)C_i^n \\
& = \frac{Cr}{Pe}C_{i-1}^n - 2\frac{Cr}{Pe}C_i^n + \frac{Cr}{Pe}C_{i+1}^n - K(\Delta t)C_i^n, \\
& C_i^{n+1} - \frac{1}{3}Cr\phi C_{i-3}^{n+1} + \frac{3}{2}Cr\phi C_{i-2}^{n+1} - 3Cr\phi C_{i-1}^{n+1} + \frac{11}{6}Cr\phi C_i^{n+1} \\
& - \frac{1}{3}Cr(1-\phi)C_{i-3}^n + \frac{3}{2}Cr(1-\phi)C_{i-2}^n - 3Cr(1-\phi)C_{i-1}^n + \frac{11}{6}Cr(1-\phi)C_i^n \\
& = \frac{Cr}{Pe}C_{i-1}^n - 2\frac{Cr}{Pe}C_i^n + \frac{Cr}{Pe}C_{i+1}^n - K(\Delta t)C_i^n + C_i^n, \\
& -\frac{1}{3}Cr\phi C_{i-3}^{n+1} + \frac{3}{2}Cr\phi C_{i-2}^{n+1} - 3Cr\phi C_{i-1}^{n+1} + \left[1 + \frac{11}{6}Cr\phi \right] C_i^{n+1} \\
& = \frac{Cr}{Pe}C_{i-1}^n - 2\frac{Cr}{Pe}C_i^n + \frac{Cr}{Pe}C_{i+1}^n - K(\Delta t)C_i^n + C_i^n \\
& + \frac{1}{3}Cr(1-\phi)C_{i-3}^n - \frac{3}{2}Cr(1-\phi)C_{i-2}^n + 3Cr(1-\phi)C_{i-1}^n \\
& - \frac{11}{6}Cr(1-\phi)C_i^n, \\
& -\frac{1}{3}Cr\phi C_{i-3}^{n+1} + \frac{3}{2}Cr\phi C_{i-2}^{n+1} - 3Cr\phi C_{i-1}^{n+1} + \left[1 + \frac{11}{6}Cr\phi \right] C_i^{n+1} \\
& = \frac{1}{3}Cr(1-\phi)C_{i-3}^n - \frac{3}{2}Cr(1-\phi)C_{i-2}^n + \left[\frac{Cr}{Pe} + 3Cr(1-\phi) \right] C_{i-1}^n \quad (3.8) \\
& + \left[1 - 2\frac{Cr}{Pe} - \frac{11}{6}Cr(1-\phi) - K(\Delta t) \right] C_i^n + \frac{Cr}{Pe}C_{i+1}^n,
\end{aligned}$$

where $Cr = \frac{u(\Delta t)}{(\Delta x)}$ and $Pe = \frac{u(\Delta x)}{D}$.

3.1.1 The upwind explicit methods

From equations (3.6 – 3.8) substituting $\phi = 0$, we then have near the left boundary,

$$C_i^{n+1} = \frac{Cr}{Pe} C_{i-1}^n + \left[1 - 2 \frac{Cr}{Pe} - K(\Delta t) + \frac{11}{6} Cr \right] C_i^n + \left(\frac{Cr}{Pe} - 3Cr \right) C_{i+1}^n + \frac{3}{2} Cr C_{i+2}^n - \frac{1}{3} Cr C_{i+3}^n, \quad (3.9)$$

at interior node,

$$C_i^{n+1} = -\frac{1}{6} Cr C_{i-2}^n + \left[\frac{Cr}{Pe} + Cr \right] C_{i-1}^n + \left[1 - K(\Delta t) - 2 \frac{Cr}{Pe} - \frac{1}{2} Cr \right] C_i^n + \left[\frac{Cr}{Pe} - \frac{1}{3} Cr \right] C_{i+1}^n, \quad (3.10)$$

near the right boundary,

$$C_i^{n+1} = \frac{1}{3} Cr C_{i-3}^n - \frac{3}{2} Cr C_{i-2}^n + \left[\frac{Cr}{Pe} + 3Cr \right] C_{i-1}^n + \left[1 - 2 \frac{Cr}{Pe} - \frac{11}{6} Cr - K(\Delta t) \right] C_i^n + \frac{Cr}{Pe} C_{i+1}^n, \quad (3.11)$$

3.1.2 The Crank-Nicolson methods

From equations (3.6) – (3.8) substituting $\phi = 0.5$, we then have near the left boundary,

$$\begin{aligned} & \left[1 - \frac{11}{6} Cr\phi \right] C_i^{n+1} + \frac{3}{2} Cr\phi C_{i+1}^{n+1} - \frac{3}{4} Cr\phi C_{i+2}^{n+1} + \frac{1}{4} Cr\phi C_{i+3}^{n+1} \\ &= \frac{Cr}{Pe} C_{i-1}^n + \left[1 - 2 \frac{Cr}{Pe} - K(\Delta t) + \frac{11}{12} Cr \right] C_i^n + \left(\frac{Cr}{Pe} - \frac{3}{2} Cr \right) C_{i+1}^n \\ &+ \frac{3}{4} Cr C_{i+2}^n - \frac{1}{6} Cr C_{i+3}^n, \end{aligned} \quad (3.12)$$

at interior node,

$$\begin{aligned} & \frac{1}{12} Cr C_{i-2}^{n+1} - \frac{1}{2} Cr C_{i-1}^{n+1} + \left[1 + \frac{1}{4} Cr \right] C_i^{n+1} + \frac{1}{6} Cr C_{i+1}^{n+1} \\ &= -\frac{1}{12} Cr C_{i-2}^n + \left[\frac{Cr}{Pe} + \frac{1}{2} Cr \right] C_{i-1}^n \\ &+ \left[1 - K(\Delta t) - 2 \frac{Cr}{Pe} - \frac{1}{4} Cr \right] C_i^n + \left[\frac{Cr}{Pe} - \frac{1}{6} Cr \right] C_{i+1}^n, \end{aligned} \quad (3.13)$$

near the right boundary,

$$\begin{aligned}
& -\frac{1}{6}CrC_{i-3}^{n+1} + \frac{3}{4}CrC_{i-2}^{n+1} - \frac{3}{2}CrC_{i-1}^{n+1} + \left[1 + \frac{11}{12}Cr\right]C_i^{n+1} \\
& = \frac{1}{6}CrC_{i-3}^n - \frac{3}{4}CrC_{i-2}^n + \left[\frac{Cr}{Pe} + \frac{3}{2}Cr\right]C_{i-1}^n \\
& + \left[1 - 2\frac{Cr}{Pe} - \frac{11}{12}Cr - K(\Delta t)\right]C_i^n + \frac{Cr}{Pe}C_{i+1}^n.
\end{aligned} \tag{3.14}$$

3.1.3 The upwind implicit methods

From equations (3.6 – 3.8) substituting $\phi=1$, we then have near the left boundary,

$$\begin{aligned}
& \left[1 - \frac{11}{6}Cr\right]C_i^{n+1} + 3CrC_{i+1}^{n+1} - \frac{3}{2}CrC_{i+2}^{n+1} + \frac{1}{2}CrC_{i+3}^{n+1} \\
& = \frac{Cr}{Pe}C_{i-1}^n + \left[1 - 2\frac{Cr}{Pe} - K(\Delta t)\right]C_i^n + \frac{Cr}{Pe}C_{i+1}^n,
\end{aligned} \tag{3.15}$$

at interior node,

$$\begin{aligned}
& \frac{1}{6}CrC_{i-2}^{n+1} - CrC_{i-1}^{n+1} + \left[1 + \frac{1}{2}Cr\right]C_i^{n+1} + \frac{1}{3}CrC_{i+1}^{n+1} \\
& = \frac{Cr}{Pe}C_{i-1}^n + \left[1 - K(\Delta t) - 2\frac{Cr}{Pe}\right]C_i^n + \frac{Cr}{Pe}C_{i+1}^n,
\end{aligned} \tag{3.16}$$

near the right boundary,

$$\begin{aligned}
& -\frac{1}{3}CrC_{i-3}^{n+1} + \frac{3}{2}CrC_{i-2}^{n+1} - 3CrC_{i-1}^{n+1} + \left[1 + \frac{11}{6}Cr\right]C_i^{n+1} \\
& = \frac{Cr}{Pe}C_{i-1}^n + \left[1 - 2\frac{Cr}{Pe} - K(\Delta t)\right]C_i^n + \frac{Cr}{Pe}C_{i+1}^n.
\end{aligned} \tag{3.17}$$

3.2 The modified Siemieniuch-Gladwell implicit methods

The modified Siemieniuch-Gladwell technique [9] for solving the one-dimensional advection-diffusion-reaction equation (2.19) is as the following:

$$\begin{aligned}
\frac{\partial C}{\partial t} & \approx \left[\frac{2\frac{Cr}{Pe} - Cr}{4} \right] \left(\frac{C_{i-1}^{n+1} - C_{i-1}^n}{\Delta t} \right) + \left[\frac{2 - 2\frac{Cr}{Pe} + Cr}{2} \right] \left(\frac{C_i^{n+1} - C_i^n}{\Delta t} \right) \\
& + \left[\frac{2\frac{Cr}{Pe} - Cr}{4} \right] \left(\frac{C_{i+1}^{n+1} - C_{i+1}^n}{\Delta t} \right),
\end{aligned} \tag{3.18}$$

$$\frac{\partial C}{\partial x} \approx \left(\frac{C_{i+1}^n - C_{i-1}^n}{4\Delta x} \right) + \left(\frac{C_{i+1}^{n+1} - C_{i-1}^{n+1}}{4\Delta x} \right), \tag{3.19}$$

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$$\frac{\partial^2 C}{\partial t^2} \approx \frac{1}{2} \left(\frac{C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2} \right) + \frac{1}{2} \left(\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} \right), \quad (3.20)$$

substituting equations (3.18 - 3.20) into equation (2.19), and rearranging, we have,

$$\begin{aligned} & \left[\frac{2\frac{Cr}{Pe} - Cr}{4} \left(\frac{C_{i-1}^{n+1} - C_{i-1}^n}{\Delta t} \right) + \left[\frac{2 - 2\frac{Cr}{Pe} + Cr}{2} \left(\frac{C_i^{n+1} - C_i^n}{\Delta t} \right) \right. \right. \\ & \left. \left. + \left[\frac{2\frac{Cr}{Pe} - Cr}{4} \left(\frac{C_{i+1}^{n+1} - C_{i+1}^n}{\Delta t} \right) + u \left[\left(\frac{C_{i+1}^n - C_{i-1}^n}{4\Delta x} \right) + \left(\frac{C_{i+1}^{n+1} - C_{i-1}^{n+1}}{4\Delta x} \right) \right] \right] \right. \\ & \left. = D \left[\frac{1}{2} \left(\frac{C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2} \right) + \frac{1}{2} \left(\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} \right) \right] - KC_i^n, \end{aligned}$$

$$\begin{aligned} & \frac{1}{4(\Delta t)} \left[2\frac{Cr}{Pe} - Cr \right] (C_{i-1}^{n+1} - C_{i-1}^n) + \frac{1}{2(\Delta t)} \left[2 - 2\frac{Cr}{Pe} + Cr \right] (C_i^{n+1} - C_i^n) \\ & + \frac{1}{4(\Delta t)} \left[2\frac{Cr}{Pe} - Cr \right] (C_{i+1}^{n+1} - C_{i+1}^n) + \frac{u}{4\Delta x} (C_{i+1}^n - C_{i-1}^n + C_{i+1}^{n+1} - C_{i-1}^{n+1}) \\ & = \frac{D}{2(\Delta x)^2} (C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1} + C_{i+1}^n - 2C_i^n + C_{i-1}^n) - KC_i^n, \end{aligned}$$

$$\begin{aligned} & \left[2\frac{Cr}{Pe} - Cr \right] (C_{i-1}^{n+1} - C_{i-1}^n) + \left[4 - 4\frac{Cr}{Pe} + 2Cr \right] (C_i^{n+1} - C_i^n) \\ & + \left[2\frac{Cr}{Pe} - Cr \right] (C_{i+1}^{n+1} - C_{i+1}^n) + \frac{u(\Delta t)}{\Delta x} (C_{i+1}^n - C_{i-1}^n + C_{i+1}^{n+1} - C_{i-1}^{n+1}) \\ & = \frac{2D(\Delta t)}{(\Delta x)^2} (C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1} + C_{i+1}^n - 2C_i^n + C_{i-1}^n) \\ & - 4K(\Delta t)C_i^n, \end{aligned}$$

$$\begin{aligned} & \left[2\frac{Cr}{Pe} - Cr \right] C_{i-1}^{n+1} - \left[2\frac{Cr}{Pe} - Cr \right] C_{i-1}^n + \left[4 - 4\frac{Cr}{Pe} + 2Cr \right] C_i^{n+1} \\ & - \left[4 - 4\frac{Cr}{Pe} + 2Cr \right] C_i^n + \left[2\frac{Cr}{Pe} - Cr \right] C_{i+1}^{n+1} - \left[2\frac{Cr}{Pe} - Cr \right] C_{i+1}^n + CrC_{i+1}^n \\ & - CrC_{i-1}^n + CrC_{i+1}^{n+1} - CrC_{i-1}^{n+1} \\ & = 2\frac{Cr}{Pe} C_{i+1}^{n+1} - 4\frac{Cr}{Pe} C_i^{n+1} + 2\frac{Cr}{Pe} C_{i-1}^{n+1} + 2\frac{Cr}{Pe} C_{i+1}^n - 4\frac{Cr}{Pe} C_i^n \\ & + 2\frac{Cr}{Pe} C_{i-1}^n - 4K(\Delta t)C_i^n, \end{aligned}$$

$$\begin{aligned} & \left[2\frac{Cr}{Pe} - 2Cr \right] C_{i-1}^{n+1} - \left[2\frac{Cr}{Pe} - 2Cr \right] C_{i-1}^n + \left[4 - 4\frac{Cr}{Pe} + 2Cr \right] C_i^{n+1} \\ & - \left[4 - 4\frac{Cr}{Pe} + 2Cr \right] C_i^n + 2\frac{Cr}{Pe} C_{i+1}^{n+1} - 2\frac{Cr}{Pe} C_{i+1}^n \\ & = 2\frac{Cr}{Pe} C_{i+1}^{n+1} - 4\frac{Cr}{Pe} C_i^{n+1} + 2\frac{Cr}{Pe} C_{i-1}^{n+1} + 2\frac{Cr}{Pe} C_{i+1}^n - 4\frac{Cr}{Pe} C_i^n \\ & + 2\frac{Cr}{Pe} C_{i-1}^n - 4K(\Delta t)C_i^n, \end{aligned}$$

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$$\begin{aligned}
& \left[2\frac{Cr}{Pe} - 2Cr \right] C_{i-1}^{n+1} + \left[4 - 4\frac{Cr}{Pe} + 2Cr \right] C_i^{n+1} + 2\frac{Cr}{Pe} C_{i+1}^{n+1} - 2\frac{Cr}{Pe} C_{i+1}^{n+1} \\
& + 4\frac{Cr}{Pe} C_i^{n+1} - 2\frac{Cr}{Pe} C_{i-1}^{n+1} \\
& = 2\frac{Cr}{Pe} C_{i+1}^n - 4\frac{Cr}{Pe} C_i^n + 2\frac{Cr}{Pe} C_{i-1}^n - 4K(\Delta t) C_i^n \\
& + \left[2\frac{Cr}{Pe} - 2Cr \right] C_{i-1}^n + \left[4 - 4\frac{Cr}{Pe} + 2Cr \right] C_i^n + 2\frac{Cr}{Pe} C_{i+1}^n, \\
& - 2Cr C_{i-1}^{n+1} + [4 + 2Cr] C_i^{n+1} \\
& = \left[4\frac{Cr}{Pe} - 2Cr \right] C_{i-1}^n + \left[4 - 8\frac{Cr}{Pe} + 2Cr - 4K(\Delta t) \right] C_i^n \\
& + 4\frac{Cr}{Pe} C_{i+1}^n, \\
& - Cr C_{i-1}^{n+1} + [2 + Cr] C_i^{n+1} \\
& = \left[2\frac{Cr}{Pe} - Cr \right] C_{i-1}^n + \left[2 - 4\frac{Cr}{Pe} + Cr - 2K(\Delta t) \right] C_i^n \quad (3.21) \\
& + 2\frac{Cr}{Pe} C_{i+1}^n,
\end{aligned}$$

for all $1 \leq i < M-1$ and $0 \leq n \leq N$, where $Cr = \frac{u(\Delta t)}{(\Delta x)}$ and $Pe = \frac{u(\Delta x)}{D}$.

At left boundary, where $i = 0$, then equation (3.21) has unknown value. We can approximate $C_{i-1}^{n+1} \approx C_i^{n+1}$, $C_{i-1}^n \approx C_i^n$ and, substituting them into equation (3.21), we obtain

$$\begin{aligned}
- Cr C_i^{n+1} + [2 + Cr] C_i^{n+1} &= \left[2\frac{Cr}{Pe} - Cr \right] C_i^n \\
& + \left[2 - 4\frac{Cr}{Pe} + Cr - 2K(\Delta t) \right] C_i^n + 2\frac{Cr}{Pe} C_{i+1}^n, \\
2C_i^{n+1} &= \left[2 - 2\frac{Cr}{Pe} - 2K(\Delta t) \right] C_i^n + 2\frac{Cr}{Pe} C_{i+1}^n. \quad (3.22)
\end{aligned}$$

At right boundary, where $i = M$, then equation (3.21) has unknown value. We can approximate $C_{i+1}^{n+1} \approx C_i^{n+1}$, $C_{i+1}^n \approx C_i^n$ and substituting them into equation (3.21), we obtain

$$\begin{aligned}
- Cr C_{i-1}^{n+1} + [2 + Cr] C_i^{n+1} &= \left[2\frac{Cr}{Pe} - 2Cr \right] C_{i-1}^n \\
& + \left[2 - 4\frac{Cr}{Pe} + Cr - 2K(\Delta t) \right] C_i^n + 2\frac{Cr}{Pe} C_i^n,
\end{aligned}$$

$$\begin{aligned}
-CrC_{i-1}^{n+1} + [2 + Cr]C_i^{n+1} = & \left[2 \frac{Cr}{Pe} - 2Cr \right] C_{i-1}^n \\
& + \left[2 - 2 \frac{Cr}{Pe} + Cr - 2K(\Delta t) \right] C_i^n,
\end{aligned} \tag{3.23}$$

3.3 Numerical experiments and results

There are two simulations for approximation the pollinating concentration at each point at all times on a uniform flow stream with analytical solution by using the upwind explicit methods equations (3.9 - 3.11), the Crank-Nicolson methods equations (3.12 - 3.14), the upwind implicit methods equations (3.15 - 3.17), and the modified Siemieniuch-Gladwell methods equations (3.21 - 3.23) in an advection-diffusion-reaction equation (2.19). For simulation A and simulation B, we show some simulations by using initial and boundary conditions from [9] – [11] and [11] – [12], respectively.

The solution domain of the problem is covered by a mesh of grid point $x(x_i, t_n)$ by $x_i = i\Delta x$, $i = 0, 1, 2, \dots, M$, and $t_n = n\Delta t$, $n = 0, 1, 2, \dots, N$, where x_i and t_n are parallel to the space and time coordinate axes. We can approximate $C(x_i, t_n)$ by C_i^n , value of the difference approximation of $C(x, t)$. The constant spatial and time increment grid-spacings are $\Delta x = L/M$ and $\Delta t = T/N$.

3.3.1 Simulation A

We approximate the pollutant concentration [11]

$$c(x, t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}} \exp \left[-\frac{(x + 0.5 - t)^2}{(0.00125 + 0.004t)} \right] \tag{3.24}$$

with the initial condition,

$$c(x, 0) = \exp \left[-\frac{(x + 0.5)^2}{0.00125} \right], \tag{3.25}$$

the left boundary condition,

$$c(0, t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}} \exp \left[-\frac{(0.5 - t)^2}{(0.00125 + 0.004t)} \right], \tag{3.26}$$

and the right boundary condition,

$$c(1, t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}} \exp \left[-\frac{(1.5 - t)^2}{(0.00125 + 0.004t)} \right]. \tag{3.27}$$

In the analysis conducted in this simulation, the various parameters used are $D=0.01$ (m^2/s), $u=1$ (m/s). The stream is meshed into 50 elements with the space step and time steps as $\Delta x=0.02$ m and $\Delta t=0.002$ s, respectively.

The comparison of approximated solution levels after 1 second has passed of the explicit methods, the Crank-Nicolson methods, the implicit methods, and the modified Siemieniuch-Gladwell methods with an advection-diffusion-reaction equation is shown in tables 3.1 - 3.6 and figures 3.1 - 3.6. Figure 3.1 shows that the water pollutant concentrations from various finite difference methods with $K=0$. Figure 3.2 shows that the water pollutant concentrations from various finite difference methods with $K=-0.05$. Figure 3.3 shows that the water pollutant concentrations from various finite difference methods with $K=-0.2$. Figure 3.4 shows that the water pollutant concentrations from various finite difference methods with $K=0.05$. Figure 3.5 shows that the water pollutant concentrations from various finite difference methods with $K=0.2$ and figure 3.6 shows that the water pollutant concentrations from various finite difference methods with $K=1$.

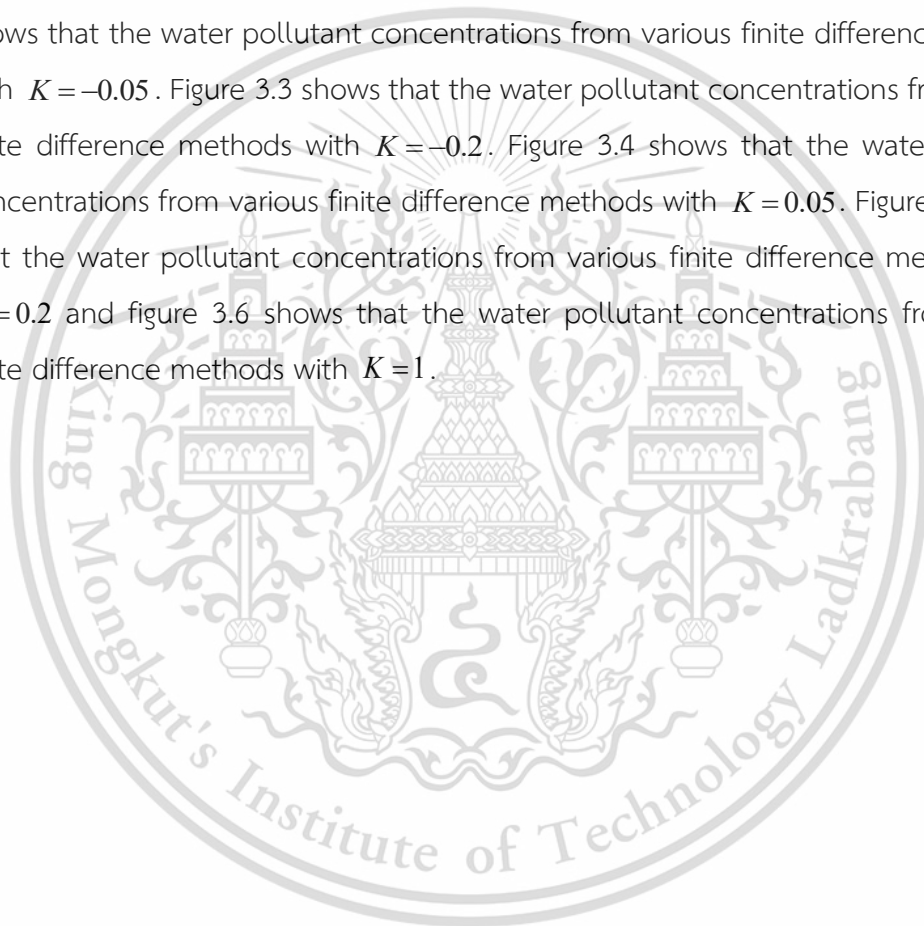


Table 3.1 The water pollutant concentration at $T=1$ for $K = -0.05$

Solution technique	Concentration (kg / m^3)										
	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
Explicit	0.000406	0.003385	0.018659	0.065392	0.142262	0.187282	0.144763	0.063166	0.014691	0.001653	0.000406
Implicit	0.000406	0.003361	0.018474	0.062210	0.129532	0.167233	0.133530	0.065392	0.019328	0.003351	0.000406
Crank-Nicolson	0.000406	0.003326	0.018141	0.058737	0.117647	0.149500	0.122514	0.065397	0.022838	0.005208	0.000406
Siemieniuch-Gladwell	0.000406	0.003501	0.019702	0.068194	0.141744	0.177657	0.137057	0.066920	0.021305	0.004554	0.000406

Table 3.2 The water pollutant concentration at $T=1$ for $K = -0.2$

Solution technique	Concentration (kg / m^3)										
	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
Explicit	0.000406	0.003464	0.019445	0.069096	0.151915	0.201607	0.156784	0.068716	0.016031	0.001806	0.000406
Implicit	0.000406	0.003410	0.018924	0.062064	0.125558	0.160833	0.132665	0.071199	0.024977	0.005718	0.000406
Crank-Nicolson	0.000406	0.003442	0.019264	0.065738	0.138284	0.179970	0.144613	0.071176	0.021121	0.003674	0.000406
Siemieniuch-Gladwell	0.000406	0.003581	0.020528	0.072069	0.151402	0.191282	0.148459	0.072820	0.023265	0.004986	0.000406

Table 3.3 The water pollutant concentration at $T=1$ for $K=0$

Solution technique	Concentration (kg / m^3)										
	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
Explicit	0.000406	0.003359	0.018404	0.064204	0.139186	0.182741	0.140966	0.061418	0.014270	0.001604	0.000406
Implicit	0.000406	0.003299	0.017888	0.057669	0.115125	0.145906	0.119308	0.063570	0.022166	0.005049	0.000406
Crank-Nicolson	0.000406	0.003334	0.018219	0.061078	0.126742	0.163194	0.130029	0.063571	0.018765	0.003250	0.000406
Siemieniuch-Gladwell	0.000406	0.003475	0.019434	0.066952	0.138667	0.173337	0.133456	0.065062	0.020690	0.004418	0.000406
Analytical	0.000406	0.003599	0.019642	0.066010	0.136603	0.174078	0.136603	0.066010	0.019642	0.003599	0.000406

Table 3.4 The water pollutant concentration at $T=1$ for $K=0.05$

Solution technique	Concentration (kg / m^3)										
	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
Explicit	0.000406	0.003333	0.018154	0.063038	0.136179	0.178312	0.137270	0.059718	0.013861	0.001557	0.000406
Implicit	0.000406	0.003307	0.017967	0.059968	0.124014	0.159254	0.126621	0.061801	0.018218	0.003153	0.000406
Crank-Nicolson	0.000406	0.003272	0.017638	0.056622	0.112658	0.142399	0.116186	0.061795	0.021515	0.004894	0.000406
Siemieniuch-Gladwell	0.000406	0.003449	0.019171	0.065733	0.135658	0.169125	0.129951	0.063256	0.020092	0.004286	0.000406

Table 3.5 The water pollutant concentration at $T=1$ for $K=0.2$

Solution technique	Concentration (kg / m^3)										
	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
Explicit	0.000406	0.003258	0.017424	0.059674	0.127552	0.165668	0.126759	0.054899	0.012703	0.001425	0.000406
Implicit	0.000406	0.003193	0.016913	0.053597	0.105578	0.132382	0.107307	0.056763	0.019673	0.004458	0.000406
Crank-Nicolson	0.000406	0.003230	0.017235	0.056763	0.116186	0.148005	0.116929	0.056782	0.016672	0.002876	0.000406
Siemieniuch-Gladwell	0.000406	0.003372	0.018403	0.062212	0.127028	0.157100	0.119984	0.058136	0.018400	0.003915	0.000406

Table 3.6 The water pollutant concentration at $T=1$ for $K=1$

Solution technique	Concentration (kg / m^3)										
	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
Explicit	0.000406	0.002888	0.014035	0.044649	0.090158	0.112096	0.082979	0.035075	0.007981	0.000887	0.000406
Implicit	0.000406	0.002807	0.013551	0.041568	0.076406	0.090235	0.069339	0.034930	0.011565	0.002711	0.000406
Crank-Nicolson	0.000406	0.002850	0.013840	0.042445	0.082216	0.100285	0.076549	0.036173	0.010395	0.001764	0.000406
Siemieniuch-Gladwell	0.000406	0.002994	0.014829	0.046483	0.089629	0.106168	0.078483	0.037093	0.011517	0.002414	0.000406

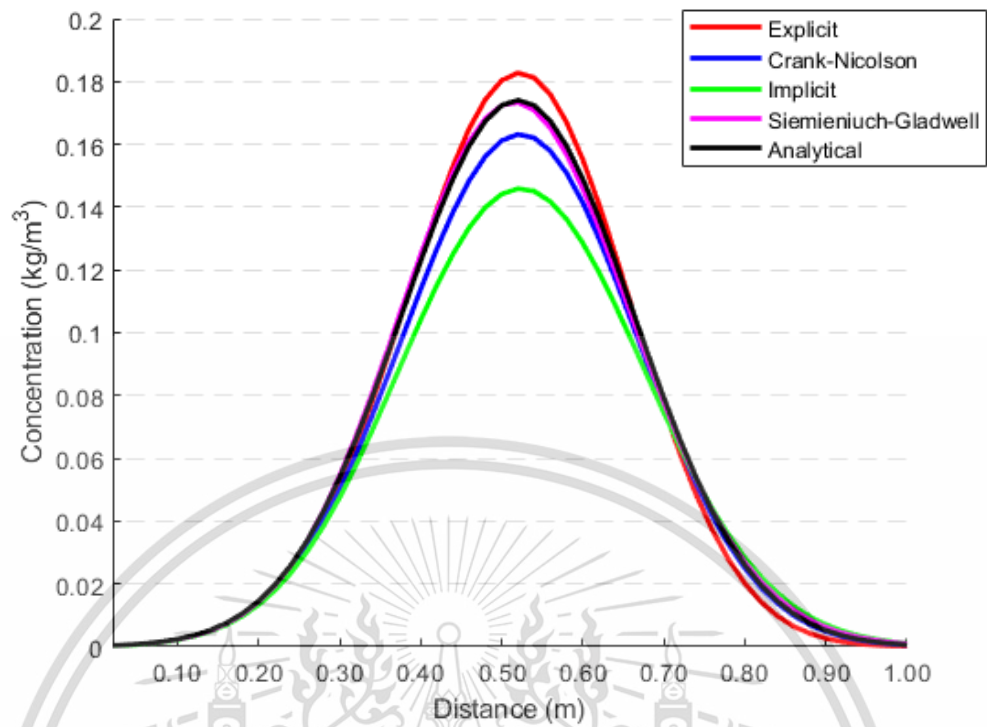


Figure 3.1 Comparison of numerical solutions techniques at $T=1$ for $K=0$

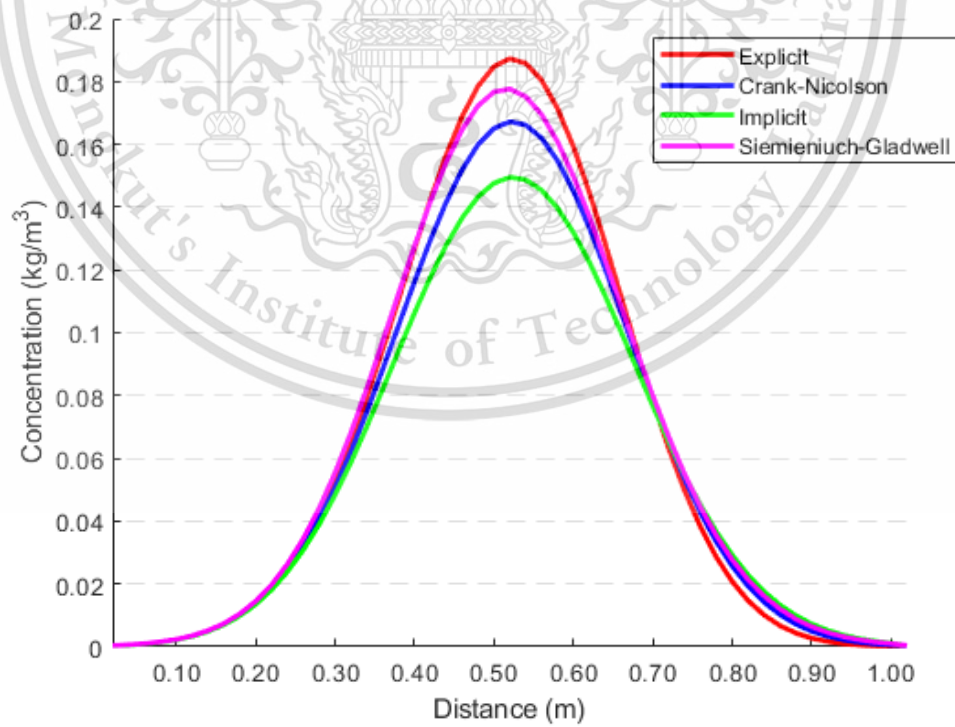


Figure 3.2 Comparison of numerical solutions techniques at $T=1$ for $K=-0.05$

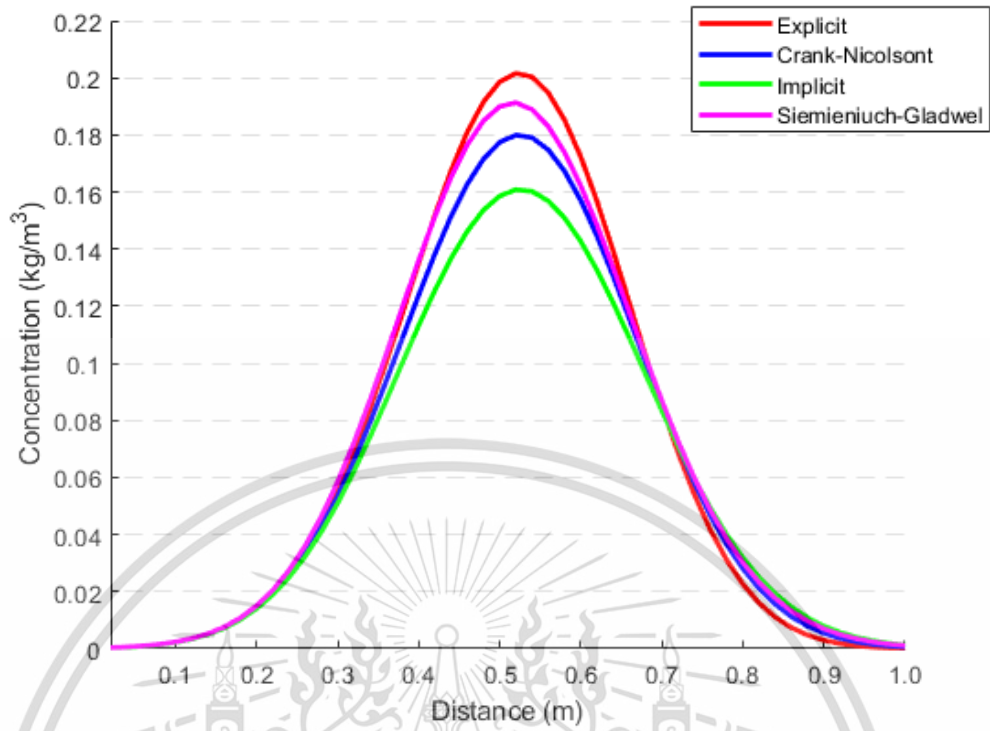


Figure 3.3 Comparison of numerical solutions techniques at $T=1$ for $K=-0.2$

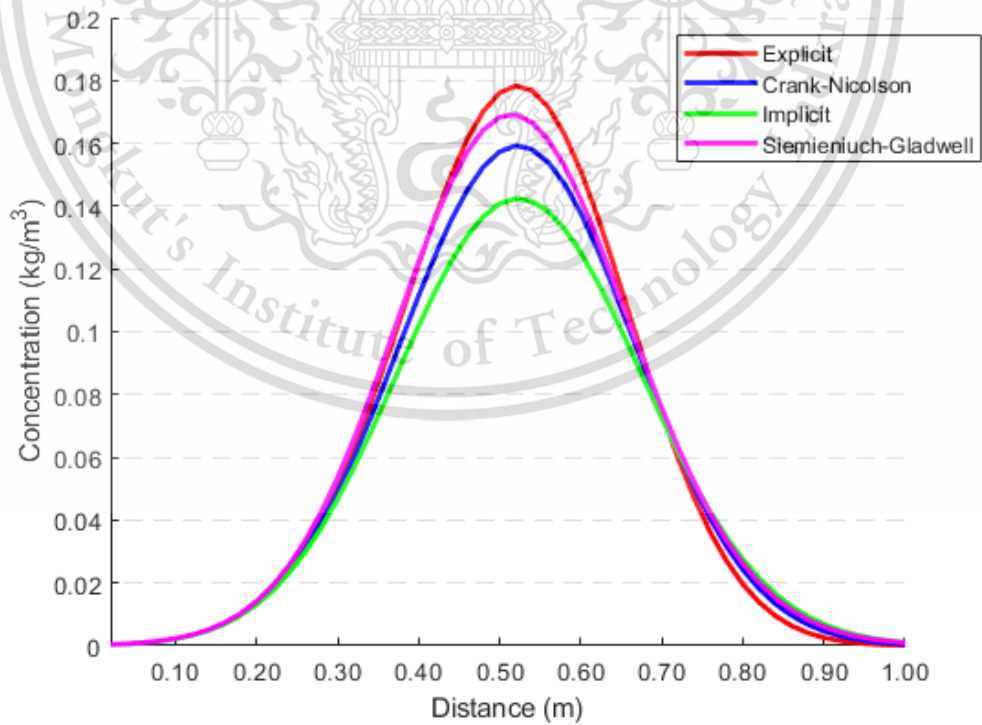


Figure 3.4 Comparison of numerical solutions techniques at $T=1$ for $K=0.05$

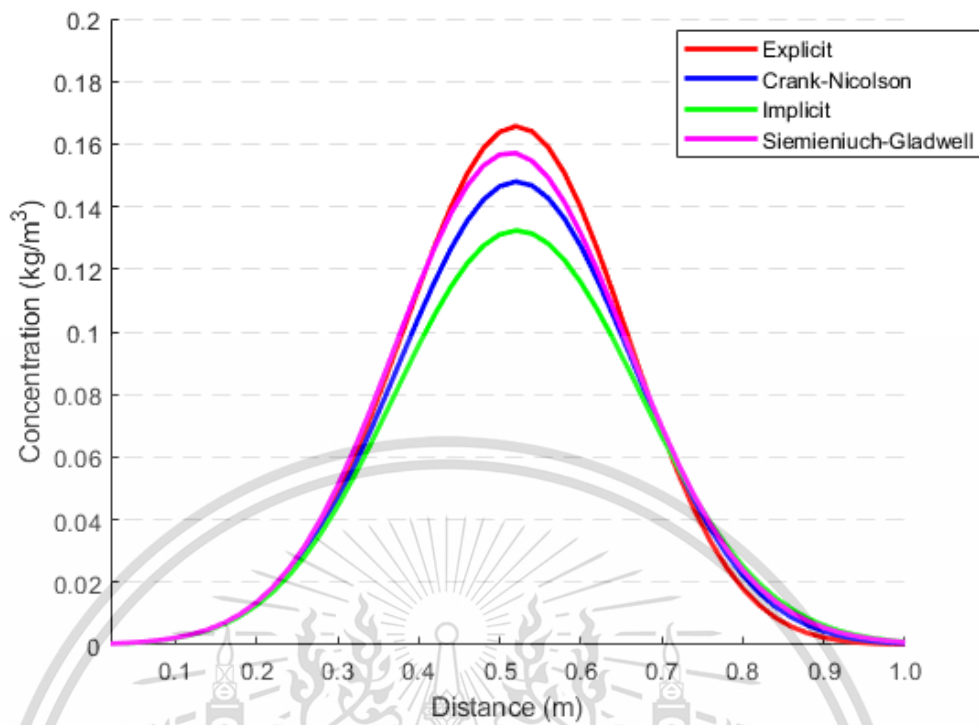


Figure 3.5 Comparison of numerical solutions techniques at $T=1$ for $K=0.2$

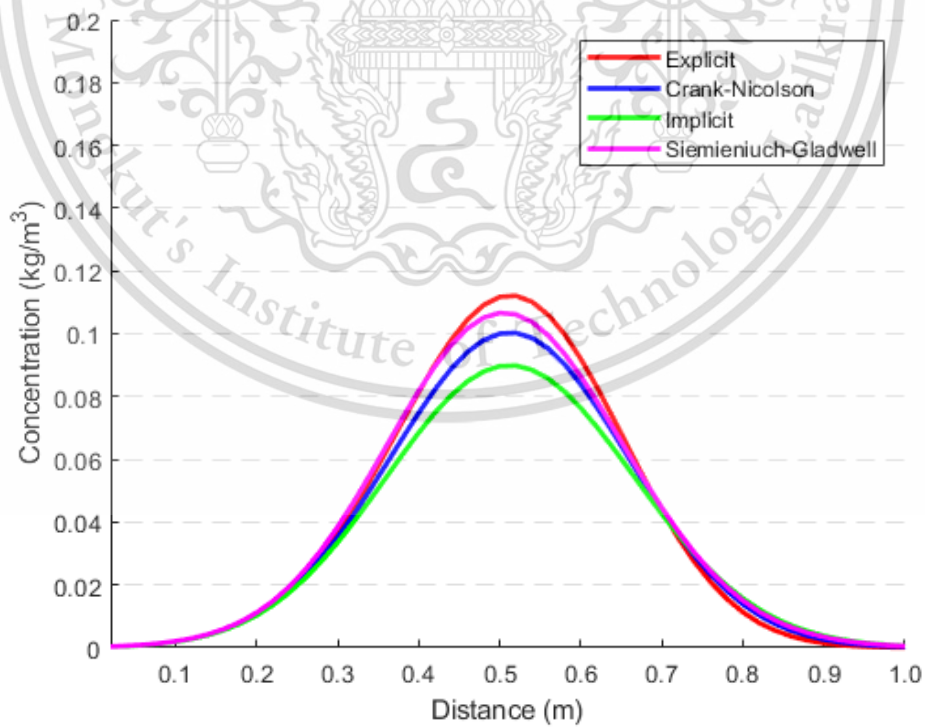


Figure 3.6 Comparison of numerical solutions techniques at $T=1$ for $K=1$

3.3.2 Simulation B

We approximate the pollutant concentration [11] centered at $x_0 = 1$,

$$c(x,0) = \exp\left[-\frac{(x-x_0)^2}{D}\right], \quad (3.28)$$

with boundary and initial condition following, the initial condition,

$$c(x,0) = \exp\left[-\frac{(x-x_0)^2}{D}\right], \quad (3.29)$$

the left boundary condition,

$$c(0,t) = c(0,t) = \frac{1}{\sqrt{4t+1}} \exp\left[-\frac{(-1-ut)^2}{D(4t+1)}\right], \quad (3.30)$$

and the right boundary condition,

$$c(9,t) = \frac{1}{\sqrt{4t+1}} \exp\left[-\frac{(8-ut)^2}{D(4t+1)}\right]. \quad (3.31)$$

In the analysis conducted in this simulation, the various parameters used are $D=0.005$ (m^2/s), $u=0.8$ (m/s). The stream is meshed into 450 elements with the space step and time step being $\Delta x=0.02$ and $\Delta t=0.002$, respectively.

The comparison of approximated solutions levels after 1 second has passed of the explicit methods, the Crank-Nicolson methods, the implicit methods and the modified Siemieniuch-Gladwell methods with an advection-diffusion-reaction equation is shown in tables 3.7 - 3.10 and figures 3.7 - 3.10. Figure 3.7 shows the water pollutant concentrations from various finite difference methods with $K=-0.05$. Figure 3.8 shows the water pollutant concentrations from various finite difference methods with $K=-0.1$. Figure 3.9 shows the water pollutant concentrations from various finite difference methods with $K=0.05$ and figure 3.10 shows the water pollutant concentrations from various finite difference methods with $K=0.1$.

Table 3.7 The water pollutant concentration at $T=1$ for $K=-0.05$

Solution technique	Concentration (kg / m^3)										
	4	4.2	4.4	4.6	4.8	5	5.2	5.4	5.6	5.8	6
Explicit	0.000000	0.000054	0.002060	0.024374	0.111734	0.214841	0.178885	0.064490	0.009704	0.000550	0.000009
Implicit	0.000001	0.000119	0.002982	0.028284	0.114272	0.207918	0.174831	0.068160	0.012051	0.000908	0.000025
Crank-Nicolson	0.000004	0.000216	0.004034	0.031996	0.116215	0.201696	0.171027	0.071265	0.014413	0.001361	0.000055
Siemieniuch-Gladwell	-0.000001	0.000130	0.009482	0.091693	0.287705	0.384570	0.253154	0.090124	0.018553	0.002324	0.000184

Table 3.8 The water pollutant concentration at $T=1$ for $K=-0.1$

Solution technique	Concentration (kg / m^3)										
	4	4.2	4.4	4.6	4.8	5	5.2	5.4	5.6	5.8	6
Explicit	0.000000	0.000070	0.002654	0.031370	0.143658	0.275942	0.229519	0.082651	0.012421	0.000703	0.000011
Implicit	0.000005	0.000277	0.005179	0.041079	0.149219	0.258984	0.219602	0.091501	0.018504	0.001747	0.000070
Crank-Nicolson	0.000002	0.000153	0.003834	0.036354	0.146815	0.267008	0.224408	0.087441	0.015451	0.001163	0.000032
Siemieniuch-Gladwell	-0.000001	0.000168	0.012197	0.117854	0.369570	0.493760	0.324900	0.115624	0.023795	0.002980	0.000236

Table 3.9 The water pollutant concentration at $T = 1$ for $K = 0.05$

Solution technique	Concentration (kg / m^3)										
	4	4.2	4.4	4.6	4.8	5	5.2	5.4	5.6	5.8	6
Explicit	0.000000	0.000033	0.001241	0.014714	0.067589	0.130225	0.108658	0.039260	0.005922	0.000337	0.000005
Implicit	0.000001	0.000072	0.001803	0.017119	0.069225	0.126068	0.106111	0.041413	0.007331	0.000553	0.000015
Crank-Nicolson	0.000002	0.000131	0.002448	0.019409	0.070488	0.122328	0.103729	0.043227	0.008744	0.000826	0.000033
Siemieniuch-Gladwell	-0.000001	0.000078	0.005729	0.055500	0.174353	0.233278	0.153687	0.054753	0.011279	0.001414	0.000112

Table 3.10 The water pollutant concentration at $T = 1$ for $K = 0.1$

Solution technique	Concentration (kg / m^3)										
	4	4.2	4.4	4.6	4.8	5	5.2	5.4	5.6	5.8	6
Explicit	0.000000	0.000025	0.000963	0.011431	0.052566	0.101385	0.084683	0.030631	0.004626	0.000263	0.000004
Implicit	0.000002	0.000102	0.001907	0.015117	0.054895	0.095264	0.080781	0.033665	0.006810	0.000643	0.000026
Crank-Nicolson	0.000001	0.000056	0.001402	0.013318	0.053878	0.098164	0.082664	0.032280	0.005718	0.000432	0.000012
Siemieniuch-Gladwell	0.000000	0.000061	0.004453	0.043178	0.135725	0.181682	0.119744	0.042676	0.008794	0.001103	0.000088

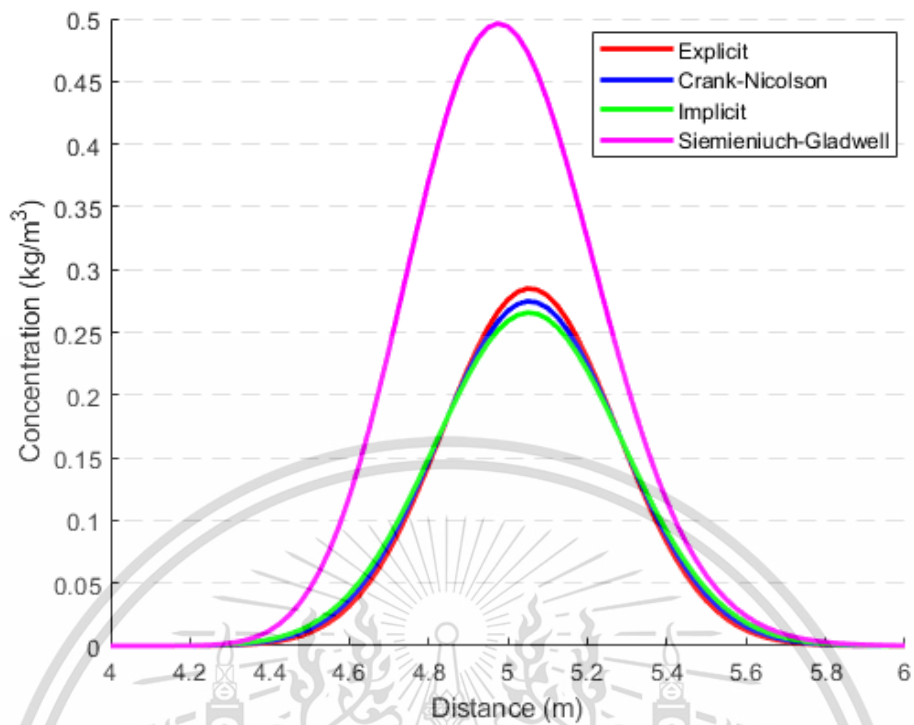


Figure 3.7 Comparison of numerical solutions techniques at $T=1$ for $K=-0.1$

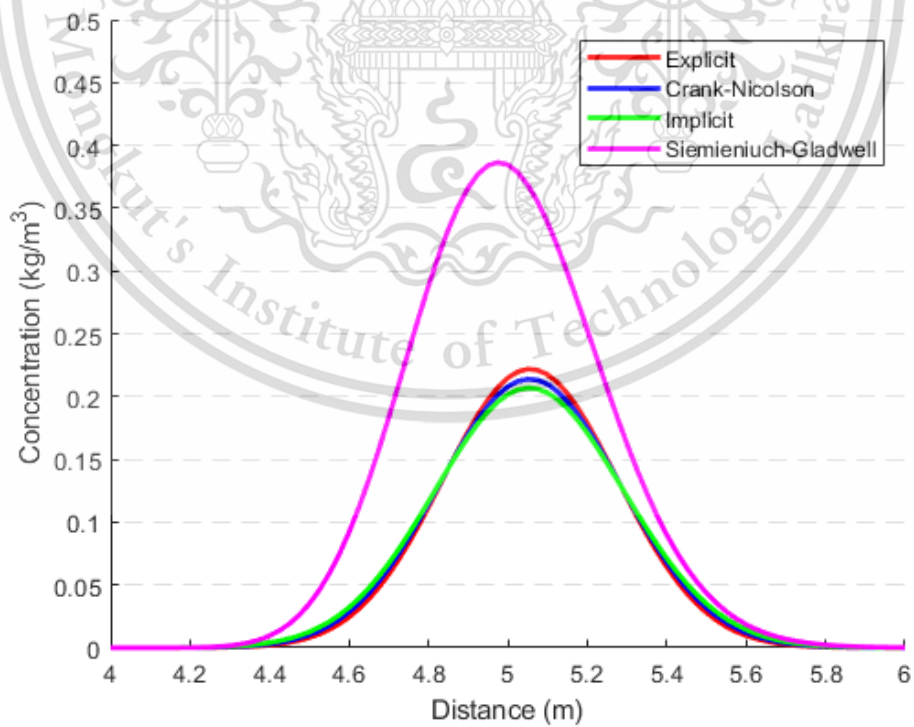


Figure 3.8 Comparison of numerical solutions techniques at $T=1$ for $K=-0.05$

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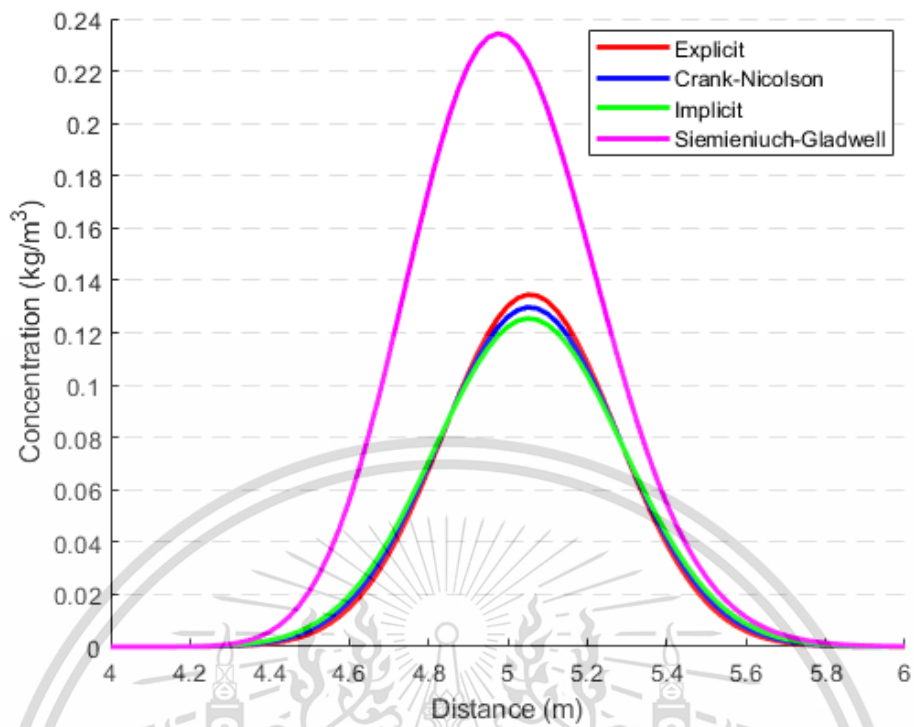


Figure 3.9 Comparison of numerical solutions techniques at $T=1$ for $K=0.05$

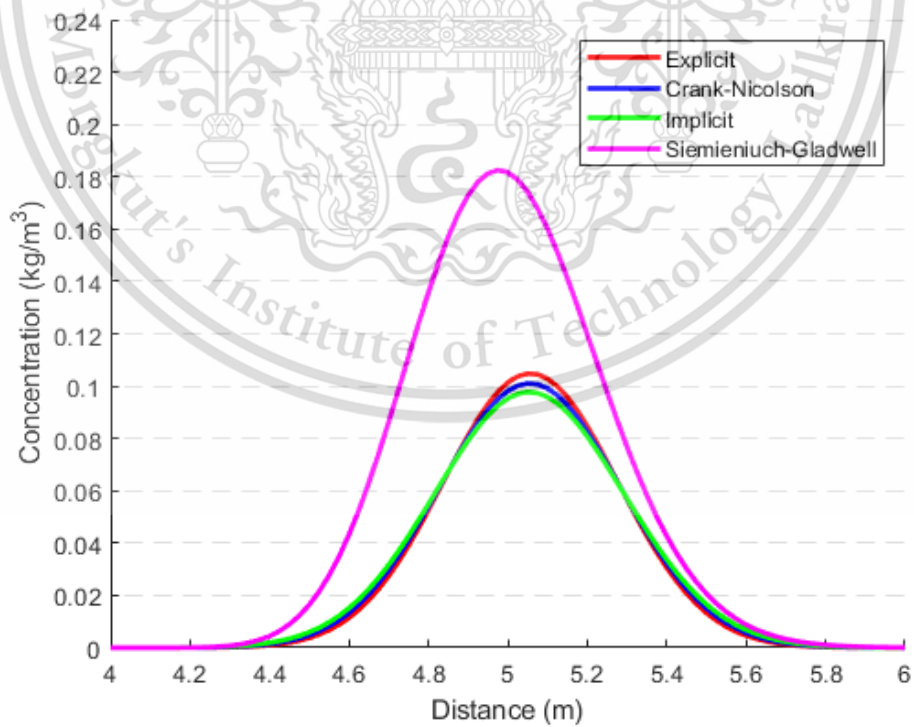


Figure 3.10 Comparison of numerical solutions techniques at $T=1$ for $K=0.1$

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Chapter 4

Water Quality Measurement Model in a Non-uniform Flow Stream

In this chapter, the hydrodynamic model and dispersion model are used to describe water flow and water pollutant concentration. A couple of mathematical models are used to simulate water quality in the problem. The stream has a simple one space dimension averaging the equation over the depth; discarding the term due to Coriolis force, it follows that the one-dimensional shallow water and advection-diffusion-reaction equations are applicable. The first model is the hydrodynamic model that provides the velocity fields and elevation of water. The Crank-Nicolson methods are used in the hydrodynamic model. At each step, the flow velocity fields calculated from the first model are input into the second model as the field data. The second model is the dispersion model that provides the pollutant concentration fields. We use the four points explicit upwind methods, the third order Crank-Nicolson methods, the four points implicit methods, the explicit upwind methods, and the Lax-Wendroff methods to approximate the concentration from the dispersion models.

4.1 Finite difference techniques for the hydrodynamic model

The hydrodynamic model provides the velocity field and elevation of the water. Then, the results are input from the hydrodynamic model into the dispersion model, which provides the pollutant concentration field.

4.1.1 The non-dimensional equation for the hydrodynamic model

For ease of calculation finite difference method, we transform equations (2.14 - 2.15) to the non-dimensional form of the hydrodynamic model by letting $U = u / \sqrt{gh}$, $X = x / l$, $Y = y / l$, $Z = \zeta / h$, and $T = t \sqrt{gh} / l$.

$$\text{Since } Z = \frac{\zeta}{h}, \zeta = Zh, \quad (4.1)$$

from equation (2.14) and equation (4.1) we consider $\frac{\partial \zeta}{\partial t} = \frac{\partial (Zh)}{\partial t} = h \frac{\partial Z}{\partial t}$,

$$\text{by using chain rules, then we have } \frac{\partial \zeta}{\partial t} = h \left(\frac{\partial Z}{\partial T} \frac{\partial T}{\partial t} \right),$$

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it can be obtained that

$$\frac{\partial \zeta}{\partial t} = h \frac{\partial Z}{\partial T} \left(\frac{\partial \left(\frac{\sqrt{gh}}{l} \right)}{\partial t} \right),$$

it follows that

$$\frac{\partial \zeta}{\partial t} = h \frac{\partial Z}{\partial T} \left(\frac{\sqrt{gh}}{l} \right),$$

that is

$$\frac{\partial \zeta}{\partial t} = \frac{h\sqrt{gh}}{l} \left(\frac{\partial Z}{\partial T} \right). \quad (4.2)$$

From equation (2.15) and equation (4.1) we consider $\frac{\partial \zeta}{\partial x} = \frac{\partial(Zh)}{\partial x} = h \frac{\partial Z}{\partial x}$,

by using chain rules, then we have $\frac{\partial \zeta}{\partial x} = h \left(\frac{\partial Z}{\partial X} \frac{\partial X}{\partial x} \right)$,

it can be obtained that

$$\frac{\partial \zeta}{\partial x} = h \frac{\partial Z}{\partial X} \left(\frac{\partial \left(\frac{x}{l} \right)}{\partial x} \right),$$

it follows that

$$\frac{\partial \zeta}{\partial x} = h \frac{\partial Z}{\partial X} \left(\frac{1}{l} \right),$$

that is

$$\frac{\partial \zeta}{\partial x} = \frac{h}{l} \left(\frac{\partial Z}{\partial X} \right). \quad (4.3)$$

Since $U = \frac{u}{\sqrt{gh}}$,

then, we get $u = U\sqrt{gh}$, (4.4)

from equation (2.14) and equation (4.4) we consider

$$\frac{\partial u}{\partial x} = \frac{\partial(U\sqrt{gh})}{\partial X} = \sqrt{gh} \frac{\partial U}{\partial X},$$

by using chain rules, then we have $\frac{\partial u}{\partial x} = \sqrt{gh} \left(\frac{\partial U}{\partial X} \frac{\partial X}{\partial x} \right)$,

it can be obtained that

$$\frac{\partial u}{\partial x} = \sqrt{gh} \left(\frac{\partial U}{\partial X} \frac{\partial \left(\frac{x}{l} \right)}{\partial x} \right),$$

it follows that

$$\frac{\partial u}{\partial x} = \sqrt{gh} \left(\frac{\partial U}{\partial X} \left(\frac{1}{l} \right) \right) = \frac{\sqrt{gh}}{l} \left(\frac{\partial U}{\partial X} \right),$$

that is

$$\frac{\partial u}{\partial x} = \frac{\sqrt{gh}}{l} \left(\frac{\partial U}{\partial X} \right), \quad (4.5)$$

from equation (2.15) and equation (4.4) we consider $\frac{\partial u}{\partial t} = \frac{\partial(U\sqrt{gh})}{\partial T} = \sqrt{gh} \frac{\partial U}{\partial T}$,

by using chain rules, then we have $\frac{\partial u}{\partial t} = \sqrt{gh} \left(\frac{\partial U}{\partial T} \frac{\partial T}{\partial t} \right)$,

it can be obtained that

$$\frac{\partial u}{\partial t} = \sqrt{gh} \left(\frac{\partial U}{\partial T} \frac{\partial \left(\frac{t\sqrt{gh}}{l} \right)}{\partial t} \right),$$

it follows that

$$\frac{\partial u}{\partial t} = \sqrt{gh} \left(\frac{\partial U}{\partial T} \left(\frac{\sqrt{gh}}{l} \right) \right) = \frac{gh}{l} \left(\frac{\partial U}{\partial T} \right),$$

that is

$$\frac{\partial u}{\partial t} = \frac{gh}{l} \left(\frac{\partial U}{\partial T} \right). \quad (4.6)$$

Substituting equation (4.2) and equation (4.5) into equation (2.14), we have

$$\begin{aligned} \frac{\partial \zeta}{\partial t} + h \frac{\partial u}{\partial x} &= 0, \\ h \frac{\sqrt{gh}}{l} \left(\frac{\partial Z}{\partial T} \right) + h \frac{\sqrt{gh}}{l} \left(\frac{\partial U}{\partial X} \right) &= 0, \\ \left(\frac{\partial Z}{\partial T} + \frac{\partial U}{\partial X} \right) &= 0. \end{aligned} \quad (4.7)$$

substituting equation (4.3) and equation (4.6) into equation (2.15), we have

$$\begin{aligned} \frac{\partial u}{\partial t} + g \frac{\partial \zeta}{\partial x} &= 0, \\ \frac{gh}{l} \left(\frac{\partial U}{\partial T} \right) + \frac{gh}{l} \left(\frac{\partial Z}{\partial X} \right) &= 0, \\ \left(\frac{\partial U}{\partial T} + \frac{\partial Z}{\partial X} \right) &= 0, \end{aligned} \quad (4.8)$$

equation (4.7) and equation (4.8) are called non-dimensional form of shallow water equation. By changing the variables U, Z to u and d , respectively, we obtain that

$$\frac{\partial d}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad (4.9)$$

$$\frac{\partial u}{\partial t} + \frac{\partial d}{\partial x} = 0. \quad (4.10)$$

[19, 30, 32], introduced a damping term into equation (4.8). We now introduce a damping term $-KU$ to represent frictional forces due to the drag of sides of the stream, thus equation (4.8) became;

$$\frac{\partial Z}{\partial T} + \frac{\partial U}{\partial X} = 0, \quad (4.11)$$

$$\frac{\partial U}{\partial T} + \frac{\partial Z}{\partial X} = -KU, \quad (4.12)$$

where $0 < K < 1$, with the initial conditions at $t=0$ and $0 \leq X \leq 1$ being specified: $Z=0$ and $U=0$. The boundary conditions for $t > 0$ are specified: $Z=f(x)$ at $X=0$

and $\frac{\partial Z}{\partial X} = 0$ at $X=1$. In order to solve damped equation in $[0,1] \times [0,T]$, for favorable using u, d for U and Z , respectively;

$$\frac{\partial u}{\partial t} + \frac{\partial d}{\partial x} = -ku, \quad (4.13)$$

$$\frac{\partial d}{\partial t} + \frac{\partial u}{\partial x} = 0. \quad (4.14)$$

with the initial conditions $u=0, d=0$ at $t=0$, and the boundary conditions $d(0,t)=f(t)$ and $\frac{\partial d}{\partial x} = 0$ at $x=1$.

Next, we will transform the initial conditions and the boundary conditions to dimensionless for equation (4.13) and equation (4.14) by change to variables $v = e^{kt}u$.

Consider $d(0,t) = f(t)$,
then, we get $\frac{\partial d}{\partial t} = \frac{\partial f}{\partial t}$, (4.15)

from equation (4.15) and equation (4.14), we have

$$\frac{\partial f}{\partial t} + \frac{\partial u}{\partial x} = 0,$$

that is $\frac{\partial u}{\partial x} = -\frac{\partial f}{\partial t}$, (4.16)

from equation (4.14), we get $\frac{\partial v}{\partial x} = e^{kt} \frac{\partial u}{\partial x}$,

thus $\frac{\partial u}{\partial x} = e^{-kt} \frac{\partial v}{\partial x}$, (4.17)

represent equations (4.17) into equation (4.16), we obtain that

$$e^{-kt} \frac{\partial v}{\partial x} = -\frac{\partial f}{\partial t},$$

$$\frac{\partial v}{\partial x} = e^{kt} \left(-\frac{\partial f}{\partial t} \right), \quad (4.18)$$

which $f(t)$ is the Wave Maker function. In this study, we choose $f(t) = \sin(t)$. Then equation (4.18) became,

$$\frac{\partial v}{\partial x} = -e^{kt} \left(\frac{\partial \sin(t)}{\partial t} \right),$$

$$\frac{\partial v}{\partial x} = -e^{kt} \cos(t), \quad (4.19)$$

can describe the initial conditions and boundary conditions as shown in figure 4.1.

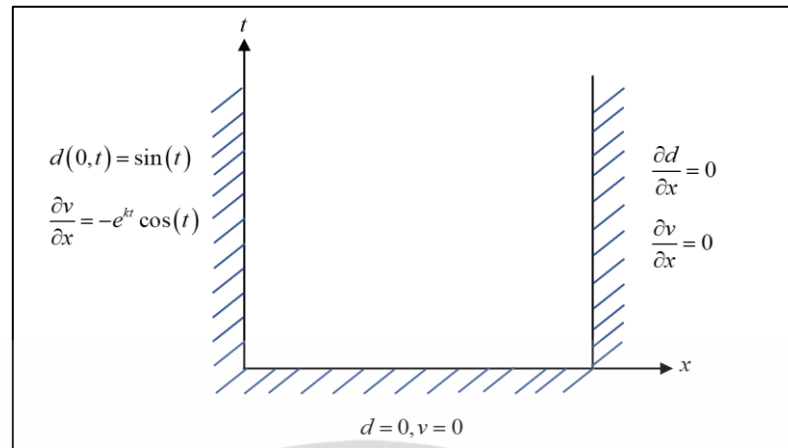


Figure 4.1 The initial conditions and the boundary conditions of dimensionless form

4.1.2 Crank-Nicolson method for the hydrodynamic model

To find the water velocity and water elevation from (4.13) and (4.14), we make the following change to variables $v = e^{kt}u$ and substitute them into equation (4.13) and equation (4.14).

Since $v = e^{kt}u$, (4.20)

then we have

$$\begin{aligned} \frac{\partial v}{\partial t} &= \frac{\partial(e^{kt}u)}{\partial t}, \\ \frac{\partial v}{\partial t} &= e^{kt} \frac{\partial u}{\partial t} + ku \frac{\partial e^{kt}}{\partial t}, \\ e^{kt} \frac{\partial u}{\partial t} &= \frac{\partial v}{\partial t} - ku \frac{\partial e^{kt}}{\partial t}, \\ \frac{\partial u}{\partial t} &= e^{-kt} \frac{\partial v}{\partial t} - ku, \end{aligned} \quad (4.21)$$

substituting equation (4.21) into equation (4.13), then we get

$$\begin{aligned} e^{-kt} \frac{\partial v}{\partial t} - ku + \frac{\partial d}{\partial x} &= -ku, \\ e^{-kt} \frac{\partial v}{\partial t} + \frac{\partial d}{\partial x} &= 0, \\ \frac{\partial v}{\partial t} + e^{kt} \frac{\partial d}{\partial x} &= 0, \end{aligned} \quad (4.22)$$

from (4.20) we consider, $\frac{\partial v}{\partial x} = \frac{\partial(e^{kt}u)}{\partial x}$,

therefore
$$\frac{\partial u}{\partial x} = e^{-kt} \frac{\partial v}{\partial x}, \quad (4.23)$$

substitute equation (4.23) into equation (4.14), then we get

$$\frac{\partial d}{\partial t} + e^{-kt} \frac{\partial v}{\partial x} = 0. \quad (4.24)$$

From equation (4.22) and equation (4.24) we can write in matrix follow as

$$\begin{pmatrix} v \\ d \end{pmatrix}_t + \begin{bmatrix} 0 & e^{kt} \\ e^{-kt} & 0 \end{bmatrix} \begin{pmatrix} v \\ d \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

that is $U_t + AU_x = \bar{0}$,

can be written as

$$\frac{\partial u}{\partial t} + A \frac{\partial u}{\partial x} = 0, \quad (4.25)$$

where $A = \begin{bmatrix} 0 & e^{kt} \\ e^{-kt} & 0 \end{bmatrix}$, $U = \begin{pmatrix} v \\ d \end{pmatrix}$, $\begin{pmatrix} v \\ d \end{pmatrix}_t = \begin{pmatrix} \frac{\partial v}{\partial t} \\ \frac{\partial d}{\partial t} \end{pmatrix}$, $\begin{pmatrix} v \\ d \end{pmatrix}_x = \begin{pmatrix} \frac{\partial v}{\partial x} \\ \frac{\partial d}{\partial x} \end{pmatrix}$.

We discretize equation (4.25) by dividing the interval $[0, 1]$ into M subintervals, such that $M\Delta x = 1$, and the interval $[0, T]$ into N subintervals, such that $N\Delta t = T$. We can then approximate $d(x, t_n)$ by d_i^n , value of the difference approximation of $d(x, t)$ at point $x = i\Delta x$ and $t = n\Delta t$, where $0 \leq i \leq M$ and $0 \leq n \leq N$, and similarly defined for v_i^n and U_i^n . The grid points (x_n, t_n) are defined by $x_i = i\Delta x$ for all $i = 0, 1, 2, \dots, M$ and $t_n = n\Delta t$ for all $n = 0, 1, 2, \dots, N$, in which M and N are positive integers. The Crank-Nicolson method [22] for solving equation (4.25) are as the following:

$$\frac{\partial U}{\partial t} \approx \frac{U_i^{n+1} - U_i^n}{\Delta t}, \quad (4.26)$$

$$\frac{\partial U}{\partial x} \approx \frac{U_{i-1}^n - U_{i+1}^n}{4(\Delta x)} + \frac{U_{i-1}^{n+1} - U_{i+1}^{n+1}}{4(\Delta x)}, \quad (4.27)$$

substituting equations (4.26 – 4.27) into equation (4.25), we have

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} + A \left[\frac{U_{i-1}^n - U_{i+1}^n}{4(\Delta x)} + \frac{U_{i-1}^{n+1} - U_{i+1}^{n+1}}{4(\Delta x)} \right] = 0,$$

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} + A \left[\frac{U_{i-1}^n - U_{i+1}^n}{4(\Delta x)} + \frac{U_{i-1}^{n+1} - U_{i+1}^{n+1}}{4(\Delta x)} \right] = 0,$$

$$\begin{aligned}
& (\Delta t) \frac{U_i^{n+1} - U_i^n}{\Delta t} + A(\Delta t) \left[\frac{U_{i-1}^n - U_{i+1}^n}{4(\Delta x)} + \frac{U_{i-1}^{n+1} - U_{i+1}^{n+1}}{4(\Delta x)} \right] = 0, \\
& U_i^{n+1} - U_i^n + \frac{1}{4} \frac{A(\Delta t)}{(\Delta x)} (U_{i-1}^n - U_{i+1}^n + U_{i-1}^{n+1} - U_{i+1}^{n+1}) = 0, \\
& U_i^{n+1} - U_i^n + \frac{1}{4} \lambda A U_{i-1}^n - \frac{1}{4} \lambda A U_{i+1}^n + \frac{1}{4} \lambda A U_{i-1}^{n+1} - \frac{1}{4} \lambda A U_{i+1}^{n+1} = 0, \\
& \frac{1}{4} \lambda A U_{i-1}^{n+1} + U_i^{n+1} - \frac{1}{4} \lambda A U_{i+1}^{n+1} = -\frac{1}{4} \lambda A U_{i-1}^n + U_i^n + \frac{1}{4} \lambda A U_{i+1}^n, \tag{4.28}
\end{aligned}$$

since $\Delta x U_i^n \approx U_{i+1}^n - U_i^n$, (4.29)

and $\nabla x U_i^n \approx U_i^n - U_{i-1}^n$, (4.30)

substituting equations (4.29 – 4.30) into equation (4.28), we obtain that

$$\begin{aligned}
& \left[I - \frac{1}{4} \lambda A (\Delta x - \nabla x) \right] U_i^{n+1} = \left[I + \frac{1}{4} \lambda A (\Delta x + \nabla x) \right] U_i^n, \\
& U_i^{n+1} - \frac{1}{4} \lambda A (\Delta x - \nabla x) U_i^{n+1} = U_i^n + \frac{1}{4} \lambda A (\Delta x + \nabla x) U_i^n, \\
& U_i^{n+1} - \frac{1}{4} \lambda A (\Delta x) U_i^{n+1} - \frac{1}{4} \lambda A (\nabla x) U_i^{n+1} \\
& \quad = U_i^n + \frac{1}{4} \lambda A (\Delta x) U_i^n + \frac{1}{4} \lambda A (\nabla x) U_i^n,
\end{aligned}$$

we get $U_i^{n+1} - \frac{1}{4} \lambda A (U_{i+1}^{n+1} - U_{i-1}^{n+1} - (U_i^{n+1} - U_{i-1}^{n+1}))$
 $= U_i^n + \frac{1}{4} \lambda A (U_{i+1}^n - U_i^n - (U_i^n + U_{i-1}^n))$,

then $U_i^{n+1} - \frac{1}{4} \lambda A (U_{i+1}^{n+1} + U_{i-1}^{n+1}) = U_i^n + \frac{1}{4} \lambda A (U_{i+1}^n - U_{i-1}^n)$,

$$U_i^{n+1} - \frac{1}{4} \lambda A U_{i+1}^{n+1} + \frac{1}{4} \lambda A U_{i-1}^{n+1} = U_i^n + \frac{1}{4} \lambda A U_{i+1}^n - \frac{1}{4} \lambda A U_{i-1}^n,$$

that is $\frac{1}{4} \lambda A U_{i-1}^{n+1} + U_i^{n+1} - \frac{1}{4} \lambda A U_{i+1}^{n+1} = -\frac{1}{4} \lambda A U_{i-1}^n + U_i^n + \frac{1}{4} \lambda A U_{i+1}^n$, (4.31)

where $\lambda = \frac{\Delta t}{\Delta x}$, $U = \begin{pmatrix} v \\ d \end{pmatrix}$, $A = \begin{bmatrix} 0 & e^{kt} \\ e^{-kt} & 0 \end{bmatrix}$ and I is the unit matrix. with the initial and boundary conditions given in equations (4.13 - 4.14), the general form can be obtained as the following;

At the left boundary condition for $i=0$, we approximate V_{i-1}^{n+1} by using forward time central space method in equations (4.19), and we have

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$$\begin{aligned}
\frac{V_i^{n+1} - V_{i-1}^{n+1}}{\Delta x} &= -e^{kt} \cos(t), \\
V_i^{n+1} - V_{i-1}^{n+1} &= -e^{kt} (\Delta x) \cos(t), \\
-V_{i-1}^{n+1} &= -e^{kt} (\Delta x) \cos(t) - V_i^{n+1}, \\
V_{i-1}^{n+1} &= -e^{kt} (\Delta x) \cos(t) + V_i^{n+1}, \\
V_{i-1}^{n+1} &= V_i^{n+1} - e^{kt} (\Delta x) \cos(t),
\end{aligned} \tag{4.32}$$

when $t_n = n\Delta t$,

$$\text{that is } V_0^{n+1} = V_1^{n+1} - e^{k(n+1)\Delta t} (\Delta x) \cos(t). \tag{4.33}$$

At the right boundary conditions for $i=M$, we approximate d_{i+1}^{n+1} by using backward time in space,

$$\text{since } \frac{\partial d}{\partial x} = 0 \text{ and } \frac{\partial u}{\partial x} = 0,$$

then we have

$$\begin{aligned}
\frac{d_{i+1}^{n+1} - d_i^{n+1}}{\Delta x} &= 0, \\
d_{i+1}^{n+1} &= d_i^{n+1},
\end{aligned} \tag{4.34}$$

$$\text{that is } d_M^{n+1} = d_{M-1}^{n+1}, \tag{4.35}$$

next, we approximate V_{i+1}^{n+1} at the right boundary conditions from equation (4.14),

where $\frac{\partial d}{\partial t} = 0$ then equation (4.13) became $\frac{\partial u}{\partial x} = 0$, which $u = ve^{-kt}$, we get

$$\begin{aligned}
\frac{\partial (ve^{-kt})}{\partial x} &= 0, \\
e^{-kt} \frac{\partial v}{\partial x} &= 0,
\end{aligned} \tag{4.36}$$

using the back ward in space in equation (4.36), then we have

$$V_{i+1}^{n+1} = V_i^{n+1}, \tag{4.37}$$

$$\text{that is } V_M^{n+1} = V_{M-1}^{n+1}. \tag{4.38}$$

Applying the initial conditions $u=0, d=0$ at $t=0$ and boundary conditions given in equation (4.33) at $x=0$, equation (4.35), and equation (4.38) at $x=1$, the general form can be obtained;

$$A^{n+1} \bar{U}^{n+1} = B^n \bar{U}^n + F^n. \tag{4.39}$$

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where

$$\begin{aligned}
 A^{n+1} &= \begin{bmatrix} 1 & 0 & 0 & -\frac{1}{4}\lambda e^{kt_{n+1}} & 0 & 0 \\ \frac{1}{4}\lambda e^{-kt_{n+1}} & 1 & -\frac{1}{4}\lambda e^{-kt_{n+1}} & 0 & 0 & 0 \\ 0 & \frac{1}{4}\lambda e^{kt_{n+1}} & 1 & 0 & 0 & -\frac{1}{4}\lambda e^{kt_{n+1}} \\ \frac{1}{4}\lambda e^{-kt_{n+1}} & 0 & 0 & 1 & -\frac{1}{4}\lambda e^{-kt_{n+1}} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \frac{1}{4}\lambda e^{kt_{n+1}} & 1 & -\frac{1}{4}\lambda e^{kt_{n+1}} \\ 0 & 0 & \frac{1}{4}\lambda e^{-kt_{n+1}} & 0 & -\frac{1}{4}\lambda e^{-kt_{n+1}} & 1 \end{bmatrix}, \\
 B^n &= \begin{bmatrix} 1 & 0 & 0 & -\frac{1}{4}\lambda e^{kt_n} & 0 & 0 \\ -\frac{1}{4}\lambda e^{-kt_n} & 1 & \frac{1}{4}\lambda e^{-kt_n} & 0 & 0 & 0 \\ 0 & -\frac{1}{4}\lambda e^{kt_n} & 1 & 0 & 0 & \frac{1}{4}\lambda e^{kt_n} \\ -\frac{1}{4}\lambda e^{-kt_n} & 0 & 0 & 1 & \frac{1}{4}\lambda e^{-kt_n} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & -\frac{1}{4}\lambda e^{kt_n} & 1 & \frac{1}{4}\lambda e^{kt_n} \\ 0 & 0 & -\frac{1}{4}\lambda e^{-kt_n} & 0 & \frac{1}{4}\lambda e^{-kt_n} & 1 \end{bmatrix}, \\
 \bar{U}^n &= \begin{pmatrix} U_1^{n+1} \\ U_2^{n+1} \\ \vdots \\ U_3^{n+1} \end{pmatrix}, \\
 F^n &= \begin{bmatrix} -\frac{1}{4}\lambda e^{kt_{n+1}} \sin(t_{n+1}) - \frac{1}{4}\lambda e^{kt_n} \sin(t_n) \\ -\frac{1}{4}\lambda e^{-kt_{n+1}} (\Delta x) e^{kt_{n+1}} \cos(t_{n+1}) - \frac{1}{4}\lambda e^{-kt_n} (\Delta x) e^{kt_n} \cos(t_n) \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix},
 \end{aligned}$$

which $t_n = n(\Delta t)$ for all $n = 0, 1, 2, 3, \dots, N$.

4.1.3 Numerical experiments and results for the hydrodynamic model

In this section, we use the Crank-Nicolson equation (4.39) for the hydrodynamic model to find the water velocity and water elevation. The water velocity at the discharge point can be described as a function $\sin(t)$ for all $t > 0$, and the elevation is not changed at $x = 1$ km, after 20 seconds have passed, with the initial conditions $u = 0, d = 0$ at $t = 0$, and the left boundary conditions $d(0, t) = \sin(t)$ and $\frac{\partial d}{\partial x} = -e^{kt} \cos(t)$ at $t > 0$, and the right boundary conditions $\frac{\partial d}{\partial x} = 0$ and $\frac{\partial v}{\partial x} = 0$ at $x = 1$. In the analysis conducted in this experiment, the stream is meshed, using $\Delta x = 0.04$, time increment with $\Delta t = 0.02$, and the physical parameter of the stream system is diffusion coefficient $D = 0.02$ m²/s. Using equation (4.39) for $k = -0.03$, we obtain the elevation and the velocity of water, as shown in table 4.1 and figure 4.2, respectively. The elevation and the velocity of water at $k = 0$ are shown in table 4.2 and figure 4.3, respectively. The elevation and the velocity of water at $k = 0.02$ are shown in table 4.3 and figure 4.4, respectively. In figure 4.8, we compare the elevation of water at $k = -0.03, 0, 0.02$, and in figure 4.9, we compare the velocity of water at $k = -0.03, 0, 0.02$; we can see that if we take the damping term into our system, the velocity and elevation of water levels decreases.

Table 4.1 The elevation of water flow at $k = -0.03$ when after passed 20 s

t (sec), x (km)	x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
4	0.611858	0.037478	-0.446197	-1.342895	-1.906452	-2.150119	0.611858	0.037478	-0.446197	-1.342895	-1.906452
8	0.998543	-0.096256	-0.414760	-0.975464	-0.984584	-0.846551	0.998543	-0.096256	-0.414760	-0.975464	-0.984584
12	0.693525	-0.125120	-0.597865	-0.936429	-1.188795	-1.135280	0.693525	-0.125120	-0.597865	-0.936429	-1.188795
16	0.091907	-0.103638	-0.371701	-0.474762	-0.488828	-0.679358	0.091907	-0.103638	-0.371701	-0.474762	-0.488828
20	0.813674	0.458255	-0.146138	-0.682372	-1.038682	-1.265647	0.813674	0.458255	-0.146138	-0.682372	-1.038682

Table 4.2 The velocity of water flow at $k = 0$ when after passed 20 s

t (sec), x (km)	x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
4	0.611858	0.069780	-0.399759	-1.262317	-1.802668	-2.036578	0.611858	0.069780	-0.399759	-1.262317	-1.802668
8	0.998543	-0.003519	-0.286033	-0.784644	-0.763727	-0.619346	0.998543	-0.003519	-0.286033	-0.784644	-0.763727
12	0.693525	0.023939	-0.370754	-0.668179	-0.898352	-0.850130	0.693525	0.023939	-0.370754	-0.668179	-0.898352
16	0.091907	0.032294	-0.126321	-0.133233	-0.112515	-0.253000	0.091907	0.032294	-0.126321	-0.133233	-0.112515
20	0.813674	0.553929	0.094939	-0.305544	-0.572990	-0.757749	0.813674	0.553929	0.094939	-0.305544	-0.572990

Table 4.3 The elevation of water flow at $k = 0.02$ when after passed 20 s

t (sec), x (km)	x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
4	0.611858	0.090496	-0.369888	-1.210499	-1.735996	-1.963668	0.611858	0.090496	-0.369888	-1.210499	-1.735996
8	0.998543	0.053618	-0.206849	-0.667735	-0.628946	-0.480901	0.998543	0.053618	-0.206849	-0.667735	-0.628946
12	0.693525	0.109890	-0.239834	-0.513468	-0.730758	-0.685905	0.693525	0.109890	-0.239834	-0.513468	-0.730758
16	0.091907	0.104850	0.005978	0.052524	0.093228	-0.018826	0.091907	0.104850	0.005978	0.052524	0.093228
20	0.813674	0.602512	0.219480	-0.114184	-0.336661	-0.498905	0.813674	0.602512	0.219480	-0.114184	-0.336661

Table 4.4 The velocity of water flow at $K = -0.03$ when after passed 20 s

t (sec), x (km)	x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
4	2.610971	2.583252	2.390045	2.227666	1.586067	0.998144	2.610971	2.583252	2.390045	2.227666	1.586067
8	1.042248	1.056271	1.121407	1.145663	0.984761	0.678741	1.042248	1.056271	1.121407	1.145663	0.984761
12	0.080940	0.068841	-0.078776	-0.154091	0.108119	0.225758	0.080940	0.068841	-0.078776	-0.154091	0.108119
16	2.153967	2.325972	2.034130	1.777823	1.357201	0.964549	2.153967	2.325972	2.034130	1.777823	1.357201
20	1.564799	1.426789	1.206481	1.006457	0.656912	0.454190	1.564799	1.426789	1.206481	1.006457	0.656912

Table 4.5 The velocity of water flow at $k = 0$ when after passed 20 s

t (sec), x (km)	x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
4	2.783345	2.758803	2.555691	2.383197	1.683867	1.040888	2.783345	2.758803	2.555691	2.383197	1.683867
8	1.027512	1.043821	1.131175	1.184130	1.043308	0.723322	1.027512	1.043821	1.131175	1.184130	1.043308
12	-0.303511	-0.334005	-0.507012	-0.573429	-0.145513	0.077422	-0.303511	-0.334005	-0.507012	-0.573429	-0.145513
16	2.860197	3.145580	2.767857	2.406631	1.797891	1.207349	2.860197	3.145580	2.767857	2.406631	1.797891
20	1.952418	1.766613	1.437037	1.124076	0.655525	0.378875	1.952418	1.766613	1.437037	1.124076	0.655525

Table 4.6 The velocity of water flow at $k = 0.02$ when after passed 20 s

t (sec), x (km)	x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
4	2.905499	2.883536	2.673649	2.494080	1.753150	1.070405	2.905499	2.883536	2.673649	2.494080	1.753150
8	1.005656	1.023729	1.129304	1.206807	1.086476	0.760053	1.005656	1.023729	1.129304	1.206807	1.086476
12	-0.660111	-0.708516	-0.900420	-0.955795	-0.378749	-0.059094	-0.660111	-0.708516	-0.900420	-0.955795	-0.378749
16	3.530340	3.926561	3.473736	3.013550	2.222936	1.440886	3.530340	3.926561	3.473736	3.013550	2.222936
20	2.297546	2.071018	1.632631	1.205647	0.636155	0.295197	2.297546	2.071018	1.632631	1.205647	0.636155

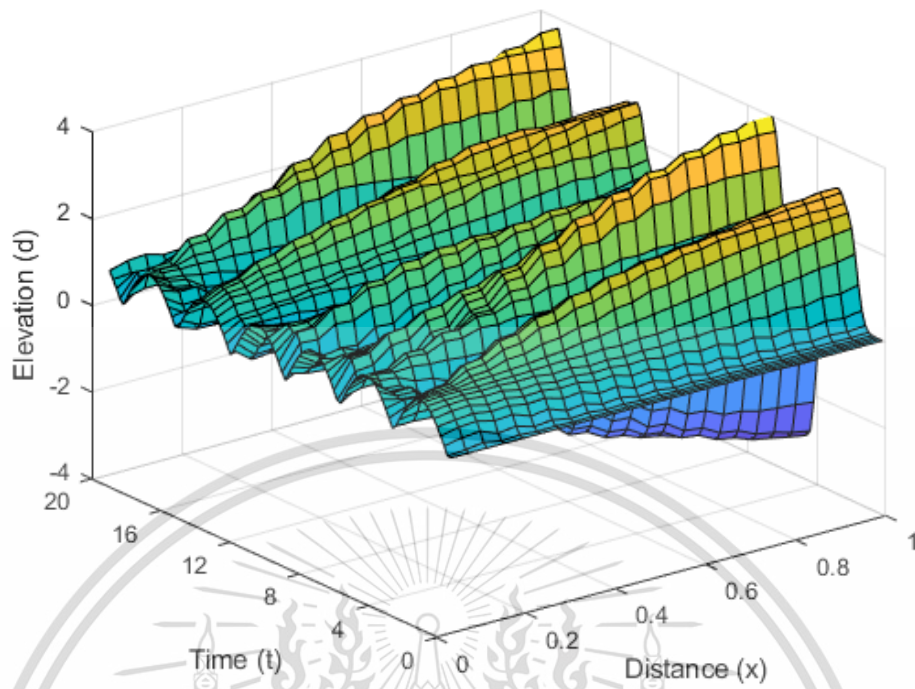


Figure 4.2 The elevation of water flow at $k = -0.03$ when after passed 20 s

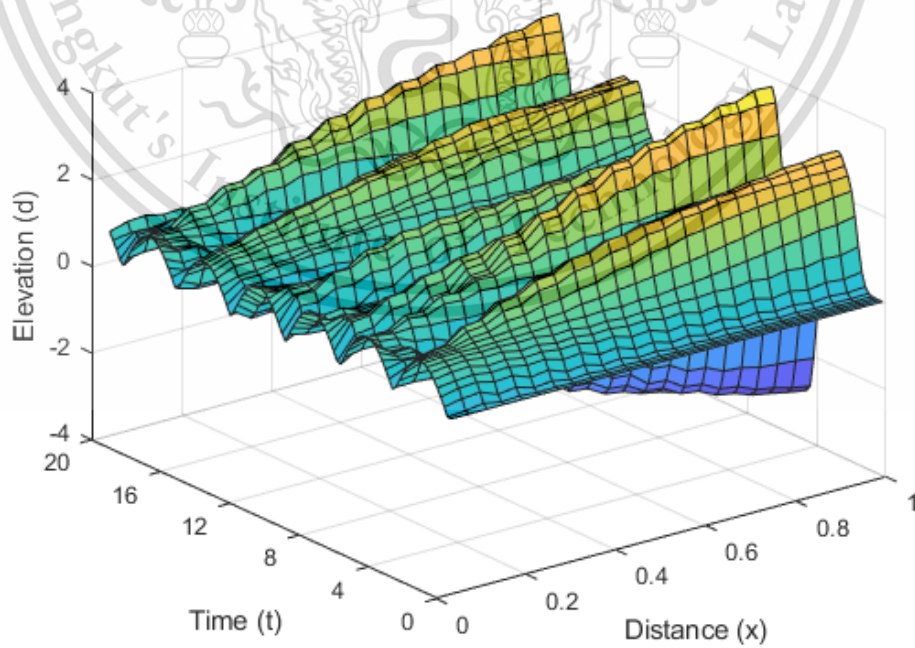


Figure 4.3 The elevation of water flow at $k = 0$ when after passed 20 s

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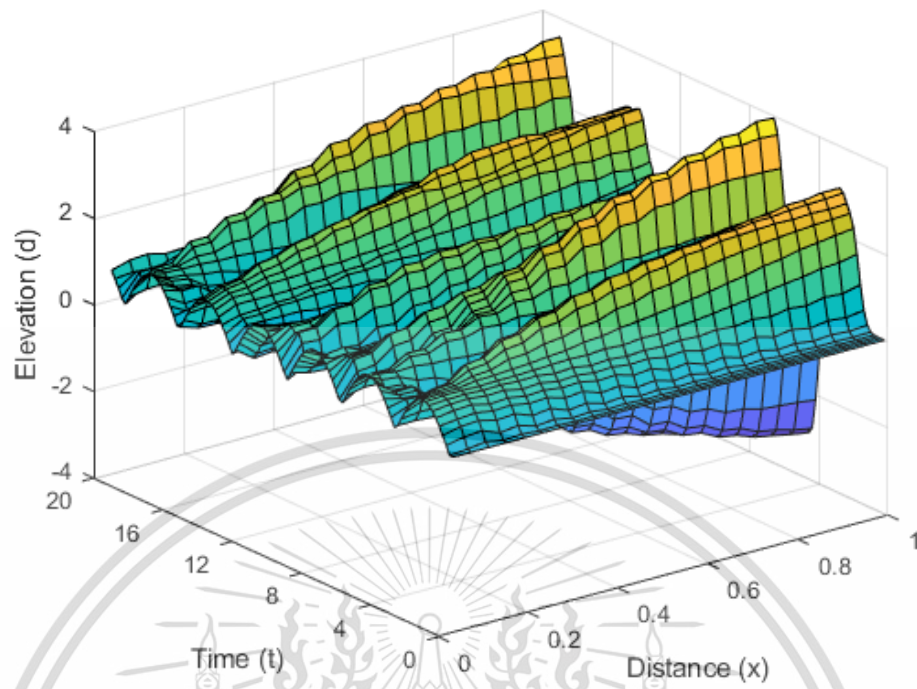


Figure 4.4 The elevation of water flow at $k = 0.02$ when after passed 20 s

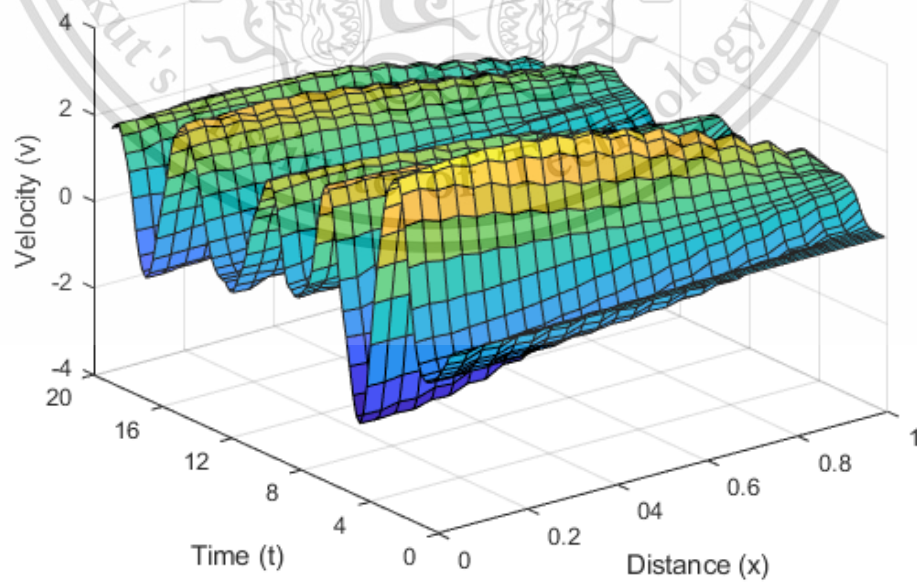


Figure 4.5 The velocity of water flow at $k = -0.03$ when after passed 20 s

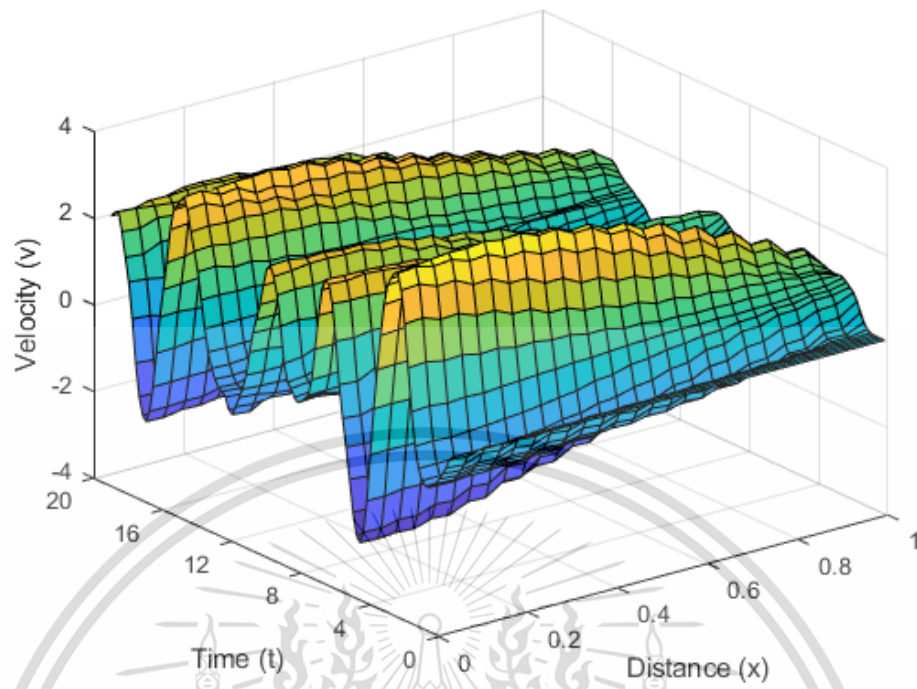


Figure 4.6 The velocity of water flow at $k=0$ when after passed 20 s

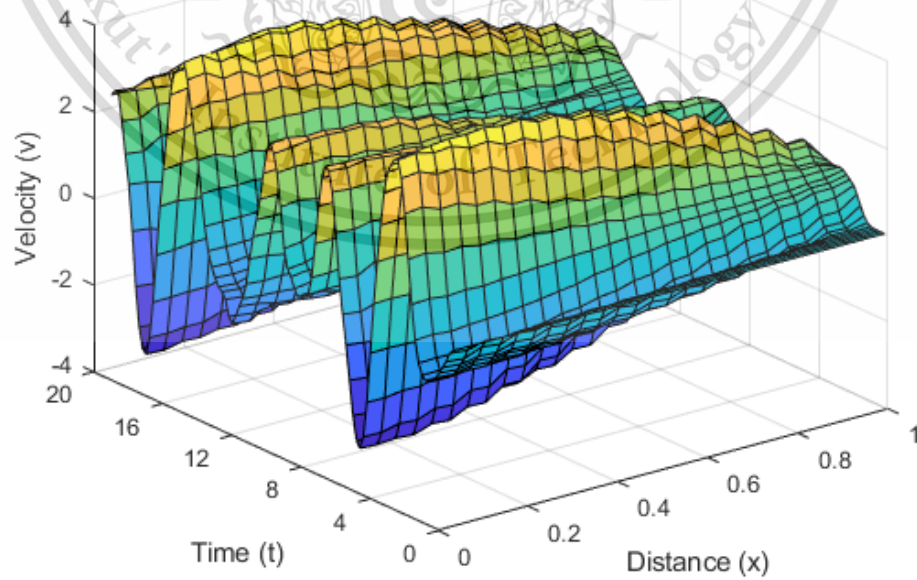


Figure 4.7 The velocity of water flow at $k=0.02$ when after passed 20 s

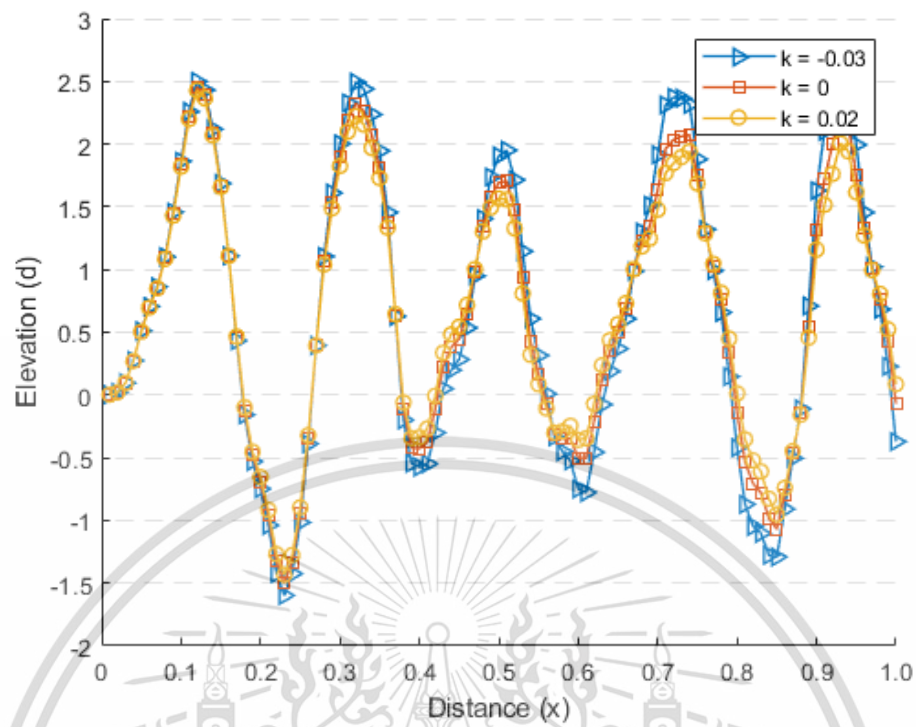


Figure 4.8 The comparison elevation of water flow at $k = -0.03, 0, 0.02$ when after passed 20 s

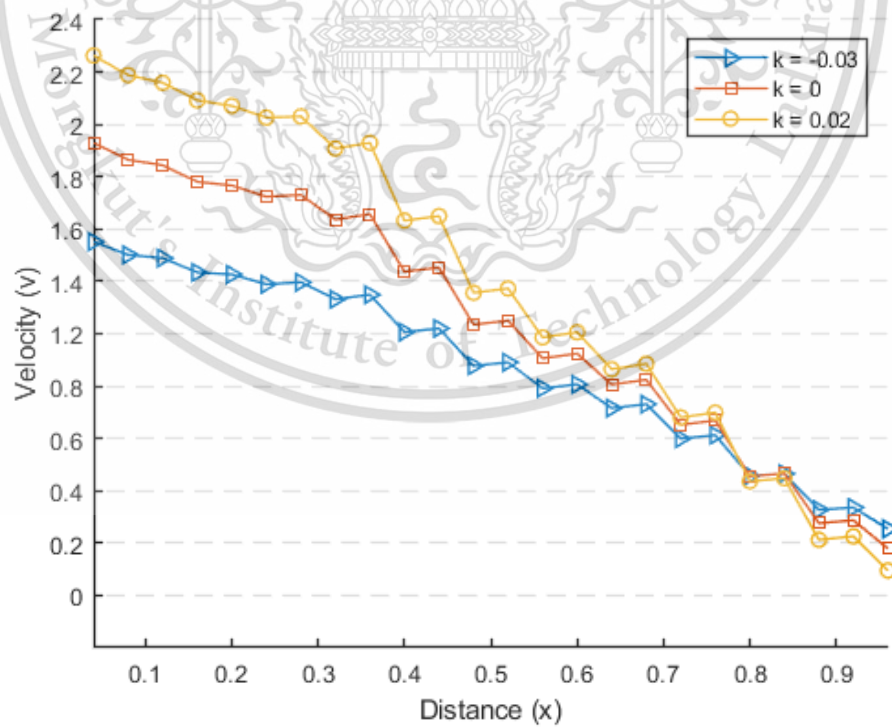


Figure 4.9 The comparison velocity of water flow at $k = -0.03, 0, 0.02$ when after passed 20 s

4.2 Finite difference techniques for the dispersion model by using third-order upwind schemes

We proposed the numerical techniques in [11], obtain the explicit schemes and implicit schemes for the advection-dispersion-reaction equation which provides the pollutant concentration field. We can approximate $C(x_i, t_n)$ by C_i^n , the value of the difference approximation of $C(x, t)$ at point $x = i\Delta x$ and $t = n\Delta t$, where $1 \leq i \leq M$, and $0 \leq n \leq N$. The grid point (x_i, t_n) is defined by $x_i = i\Delta x$ for all $i = 0, 1, 2, \dots, M$, and $t_n = n\Delta t$ for all $n = 0, 1, 2, \dots, N$ in which M and N are positive integers.

In this section, we consider the numerical techniques using the forward times central space scheme for the time derivatives and the central difference for the second times derivative, respectively, as follows;

$$\frac{\partial C}{\partial t} \approx \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad (4.40)$$

$$\frac{\partial^2 C}{\partial x^2} \approx \frac{1}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n], \quad (4.41)$$

4.2.1 The four points explicit upwind methods

Consider the explicit schemes for the advection-dispersion-reaction equation (2.19), we approximate the spatial derivative, following discretization: for near left boundary,

$$\frac{\partial C}{\partial x} \approx \frac{1}{6\Delta x} [-11C_i^n + 18C_{i+1}^n - 9C_{i+2}^n + 2C_{i+3}^n], \quad (4.42)$$

for interior node,

$$\frac{\partial C}{\partial x} \approx \frac{1}{6\Delta x} [C_{i-2}^n - 6C_{i-1}^n + 3C_i^n + 2C_{i+1}^n], \quad (4.43)$$

for near the right boundary,

$$\frac{\partial C}{\partial x} \approx \frac{1}{6\Delta x} [-2C_{i-3}^n + 9C_{i-2}^n - 18C_{i-1}^n + 11C_i^n]. \quad (4.44)$$

Near the left boundary, substituting equations (4.40 - 4.41) and equation (4.42) into equation (2.19), we then obtain

$$C_i^{n+1} = \beta C_{i-1}^n + [1 - 2\beta - (\Delta t)K + 11\gamma_i^n] C_i^n + [\beta - 18\gamma_i^n] C_{i+1}^n - 9\gamma_i^n C_{i+2}^n - 2\gamma_i^n C_{i+3}^n, \quad (4.45)$$

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for $i=0$, we plug the known value of the left boundary by arranging $C_{i-1}^n = C_i^n - (\Delta x)f$ in equation (4.45) on the right-hand side. We obtain;

$$C_i^{n+1} = \left[1 - \beta - (\Delta t)K + 11\gamma_i^n\right]C_i^n + \left[\beta - 18\gamma_i^n\right]C_{i+1}^n - 9\gamma_i^n C_{i+2}^n - 2\gamma_i^n C_{i+3}^n - \beta(\Delta x)f, \quad (4.46)$$

At interior, substituting equations (4.40 - 4.41) and equation (4.43) into equation (2.19). We obtain,

$$C_i^{n+1} = -\gamma_i^n C_{i-2}^n + \left[\beta + 6\gamma_i^n\right]C_{i-1}^n + \left[1 - 2\beta - 3\gamma_i^n - (\Delta t)K\right]C_i^n + \left[\beta - 2\gamma_i^n\right]C_{i+1}^n, \quad (4.47)$$

for all $1 \leq i \leq M-1$ and $0 \leq n \leq N$.

Near the right boundary substituting equations (4.40 - 4.41) and equation (4.44) into equation (2.19), we obtain

$$C_i^{n+1} = 2\beta C_{i-3}^n + \left[\beta - 9\gamma_i^n\right]C_{i-2}^n + 18\gamma_i^n C_{i-1}^n + \left[1 - 2\beta - (\Delta t)K - 11\gamma_i^n\right]C_i^n + \gamma_i^n C_{i+1}^n, \quad (4.48)$$

for $i=M$, the known value of the right boundary conditions is approximated as $C_{i+1}^n = C_i^n + (\Delta x)f$ in equation (4.48) and, by rearranging, we obtain;

$$C_M^{n+1} = 2\beta C_{M-3}^n + \left[\beta - 9\gamma_M^n\right]C_{M-2}^n + 18\gamma_M^n C_{M-1}^n + \left[1 - 2\beta - (\Delta t)K - 10\gamma_M^n\right]C_M^n + \gamma_M^n (\Delta x), \quad (4.49)$$

where $\beta = D \frac{\Delta t}{(\Delta x)^2}$, $\gamma_i^n = u_i^n \frac{\Delta t}{6\Delta x}$, and $u \approx \tilde{u}_i^n$ which \tilde{u}_i^n are obtained by the Crank-Nicolson method with the hydrodynamic model.

4.2.2 The third-order Crank-Nicolson methods

Consider the Crank-Nicolson schemes [11], for the advection-dispersion-reaction equations (2.19), we approximate the spatial derivative, following discretization:

for near the left boundary,

$$\frac{\partial C}{\partial x} \approx \frac{1}{12\Delta x} \left[-11C_i^{n+1} + 18C_{i+1}^{n+1} - 9C_{i+2}^{n+1} + 2C_{i+3}^{n+1} - 11C_i^n + 18C_{i+1}^n - 9C_{i+2}^n + 2C_{i+3}^n \right], \quad (4.50)$$

for interior node,

$$\frac{\partial C}{\partial x} \approx \frac{1}{12\Delta x} \left[C_{i-2}^{n+1} - 6C_{i-1}^{n+1} + 3C_i^{n+1} + 2C_{i+1}^{n+1} + C_{i-2}^n - 6C_{i-1}^n + 3C_i^n + 2C_{i+1}^n \right], \quad (4.51)$$

for near the right boundary,

$$\frac{\partial C}{\partial x} \approx \frac{1}{12\Delta x} \left[-2C_{i-3}^{n+1} + 9C_{i-2}^{n+1} - 18C_{i-1}^{n+1} + 11C_i^{n+1} - 2C_{i-3}^n + 9C_{i-2}^n - 18C_{i-1}^n + 11C_i^n \right]. \quad (4.52)$$

Near the left boundary, substituting equations (4.40 - 4.41) and equation (4.50) into equation (2.19), we then obtain;

$$\begin{aligned} & [1 - 11\gamma_i^n] C_i^{n+1} + 18\gamma_i^n C_{i+1}^{n+1} - 9\gamma_i^n C_{i+2}^{n+1} + 2\gamma_i^n C_{i+3}^{n+1} \\ & = \beta C_{i-1}^n + [1 - 2\beta - (\Delta t)K + 11\gamma_i^n] C_i^n \\ & + [\beta - 18\gamma_i^n] C_{i+1}^n + 9\gamma_i^n C_{i+2}^n - 2\gamma_i^n C_{i+3}^n. \end{aligned} \quad (4.53)$$

For $i=0$, we plug the known value of the left boundary by arranging $C_{i-1}^n = C_i^n - (\Delta x)f$ in equation (4.53) on the right-hand side. We obtain;

$$\begin{aligned} & [1 - 11\gamma_i^n] C_i^{n+1} + 18\gamma_i^n C_{i+1}^{n+1} - 9\gamma_i^n C_{i+2}^{n+1} + 2\gamma_i^n C_{i+3}^{n+1} \\ & = + [1 - \beta - (\Delta t)K + 11\gamma_i^n] C_i^n \\ & + [\beta - 18\gamma_i^n] C_{i+1}^n + 9\gamma_i^n C_{i+2}^n - 2\gamma_i^n C_{i+3}^n - (\Delta x)f. \end{aligned} \quad (4.54)$$

At interior, for all $1 \leq i \leq M-1$ substituting equations (4.40 - 4.41) and equation (4.51) into equation (2.19), then we obtain;

$$\begin{aligned} & \gamma_i^n C_{i-2}^{n+1} - 6\gamma_i^n C_{i-1}^{n+1} + [1 - 3\gamma_i^n] C_i^{n+1} + 2\gamma_i^n C_{i+1}^{n+1} \\ & = [\beta - \gamma_i^n] C_{i-2}^n + 6\gamma_i^n C_{i-1}^n \\ & + [1 - 2\beta - (\Delta t)K - 3\gamma_i^n] C_i^n + [\beta - 2\gamma_i^n] C_{i+1}^n. \end{aligned} \quad (4.55)$$

Near right boundary substituting equations (4.40 - 4.41) and equation (4.52) into equation (2.19), we obtain

$$\begin{aligned} & -2\gamma_i^n C_{i-3}^{n+1} + 9\gamma_i^n C_{i-2}^{n+1} - 18\gamma_i^n C_{i-1}^{n+1} + [1 + 11\gamma_i^n] C_i^{n+1} \\ & = 2\gamma_i^n C_{i-3}^n - 9\gamma_i^n C_{i-2}^n + \beta C_{i-1}^{n+1} \\ & + [1 - 2\beta - (\Delta t)K - 11\gamma_i^n] C_i^n + [\beta + 18\gamma_i^n] C_{i+1}^n, \end{aligned} \quad (4.56)$$

for $i=M$, the known value of the right boundary conditions is approximated as

$C_{M+1}^n = C_M^n + (\Delta x)f$ in equation (4.56), and by rearranging, we obtain;

$$\begin{aligned} & -2\gamma_M^n C_{M-3}^{n+1} + 9\gamma_M^n C_{M-2}^{n+1} - 18\gamma_M^n C_{M-1}^{n+1} + [1 + 11\gamma_M^n] C_M^{n+1} \\ & = 2\gamma_M^n C_{M-3}^n - 9\gamma_M^n C_{M-2}^n + \beta C_{M-1}^{n+1} \\ & + [1 - \beta - (\Delta t)K + 7\gamma_M^n] C_M^n + (\Delta x)f, \end{aligned} \quad (4.57)$$

where $\beta = D \frac{\Delta t}{(\Delta x)^2}$, $\gamma_i^n = u_i^n \frac{\Delta t}{6\Delta x}$, and $u \approx \tilde{u}_i^n$ which \tilde{u}_i^n are obtained by the Crank-Nicolson method with the hydrodynamic model.

4.2.3 The four points implicit upwind methods

Consider the implicit schemes from [11] for the advection-dispersion-reaction equations. we approximate the spatial derivative, following discretization: for near the left boundary,

$$\frac{\partial C}{\partial x} \approx \frac{1}{6\Delta x} [-11C_i^{n+1} + 18C_{i+1}^{n+1} - 9C_{i+2}^{n+1} + 2C_{i+3}^{n+1}], \quad (4.58)$$

for interior node,

$$\frac{\partial C}{\partial x} \cong \frac{1}{6\Delta x} [C_{i-2}^{n+1} - 6C_{i-1}^{n+1} + 3C_i^{n+1} + 2C_{i+1}^{n+1}], \quad (4.59)$$

for near the right boundary,

$$\frac{\partial C}{\partial x} \cong \frac{1}{6\Delta x} [-2C_{i-3}^{n+1} + 9C_{i-2}^{n+1} - 18C_{i-1}^{n+1} + 11C_i^{n+1}], \quad (4.60)$$

Near the left boundary, substituting equations (4.40 - 4.41) and equation (4.58) into equation (2.19), we then obtain;

$$C_i^{n+1} = \beta C_{i-1}^n + [1 - 2\beta - (\Delta t)K + 11\gamma_i^n] C_i^n + [\beta - 18\gamma_i^n] C_{i+1}^n - 9\gamma_i^n C_{i+2}^n - 2\gamma_i^n C_{i+3}^n, \quad (4.61)$$

for $i=0$, we plug the known value of the left boundary by arranging $C_{i-1}^n = C_i^n - (\Delta x)f$ in equation (4.61) on the right-hand side. We obtain;

$$C_i^{n+1} = [1 - \beta - (\Delta t)K + 11\gamma_i^n] C_i^n + [\beta - 18\gamma_i^n] C_{i+1}^n - 9\gamma_i^n C_{i+2}^n - 2\gamma_i^n C_{i+3}^n - \beta(\Delta x)f. \quad (4.62)$$

At interior, for all $1 \leq i \leq M-1$ substituting equations (4.40-4.41) and equation (4.59) into equation (2.19), we obtain,

$$\begin{aligned} \gamma_i^n C_{i-2}^{n+1} - 6\gamma_i^n C_{i-1}^{n+1} + [1 - 3\gamma_i^n] C_i^{n+1} + 2\gamma_i^n C_{i+1}^{n+1} \\ = \beta C_{i-1}^n + [1 - 2\beta - (\Delta t)K] C_i^n + \beta C_{i+1}^n. \end{aligned} \quad (4.63)$$

Near the right boundary substituting equations (4.40-4.41) and equation (4.60) into equation (2.19), we obtain

$$\begin{aligned} -2\gamma_i^n C_{i-3}^{n+1} + 9\gamma_i^n C_{i-2}^{n+1} - 18\gamma_i^n C_{i-1}^{n+1} + [1 + 11\gamma_i^n] C_i^{n+1} \\ = \beta C_{i-1}^n + [1 - 2\beta - (\Delta t)K] C_i^n + \beta C_{i+1}^n, \end{aligned} \quad (4.64)$$

for $i=M$, the known value of the right boundary conditions is approximated as $C_{M+1}^n = (\Delta x)f + C_M^n$ in equation (4.64) and, by rearranging, we obtain,

$$\begin{aligned} & -2\gamma_M^n C_{M-3}^{n+1} + 9\gamma_M^n C_{M-2}^{n+1} - 18\gamma_M^n C_{M-1}^{n+1} + [1 + 11\gamma_M^n] C_M^{n+1} \\ & = \beta C_{M-1}^{n+1} + [1 - \beta - (\Delta t)K] C_M^n + \beta(\Delta x)f, \end{aligned} \quad (4.65)$$

where $\beta = D \frac{\Delta t}{(\Delta x)^2}$, $\gamma_i^n = u_i^n \frac{\Delta t}{6\Delta x}$, and $u \approx \tilde{u}_i^n$ which \tilde{u}_i^n are obtained by the Crank-Nicolson method with the hydrodynamic model.

4.2.4 Numerical experiments and results

Suppose that the measurement of pollutant concentration $C(x,t)$ (km/m^3) in a uniform stream at time t (sec) is considered. A stream is aligned with longitudinal distance, 1.0 km total length. There is a plant which discharges waste-water into the stream, and the pollutant concentration at the end of the river is assumed in 3 cases; **case 1**; $C(0,t) = 0.4 + \sin(t)$ km/m^3 at $x=0$ for all $t > 0$, and $\frac{\partial C}{\partial x}(1,t) = -0.5$ km/m^3 at $x=1$ for all $t > 0$, and $C(x,0) = 0$ km/m^3 at $t=0$.

case 2; $C(0,t) = 0.4 + \sin(t)$ km/m^3 at $x=0$ for all $t > 0$, and $\frac{\partial C}{\partial x}(1,t) = 0$ km/m^3 at $x=1$ for all $t > 0$, and $C(x,0) = 0$ km/m^3 at $t=0$.

case 3; $C(0,t) = 0.4 + \sin(t)$ km/m^3 at $x=0$ for all $t > 0$, and $\frac{\partial C}{\partial x}(1,t) = 1$ km/m^3 at $x=1$ for all $t > 0$, and $C(x,0) = 0$ km/m^3 at $t=0$.

In the analysis conducted in this experiment, meshes the stream, using $\Delta x = 0.02$, and time increment with $\Delta t = 0.002$, the physical parameter of the stream system is diffusion coefficient $D = 0.02$ m^2/s for above 3 case. The approximate water velocity from the hypodermic model in section 4.1 can be plugged into the dispersion model to obtain the four points explicit upwind methods in equations (4.46), (4.47) and, (4.50); the third order Crank-Nicolson methods in equations (4.54), (4.55) and, (4.57), and the four points implicit methods in equations (4.62), (4.63), and (4.65). The approximation of pollutant concentration at $K = -1$ of the four points explicit methods, the third order Crank-Nicolson methods, and the four points implicit methods in the above 3 cases are shown in table 4.7, table 4.8, and table 4.9, respectively. The approximation of pollutant concentration at $K = -0.05$ of the four points explicit methods, the third order Crank-Nicolson methods, and the four points

implicit methods in the above 3 cases are shown in table 4.10, table 4.11, and table 4.12, respectively. The approximation of pollutant concentration at $K = 0$ of the four points explicit methods, the third order Crank-Nicolson methods, and the four points implicit methods in the above 3 cases are shown in table 4.13, table 4.14, and table 4.15, respectively. The approximation of pollutant concentration at $K = 0.05$ of the four points explicit methods, the third order Crank-Nicolson methods, and the four points implicit methods in the above 3 cases are shown in table 4.16, table 4.17, and table 4.18, respectively. The approximation of pollutant concentration at $K = 1$ of the four points explicit methods, the third order Crank-Nicolson methods, and the four points implicit methods in the above 3 cases are shown in table 4.19, table 4.20, and table 4.21, respectively.

The comparison of the approximated pollutant concentrations, for the above 3 cases at $K = -1$ of the four points explicit upwind methods, the third order Crank-Nicolson methods, and the four points implicit methods are shown in figure 4.10, figure 4.11, and figure 4.12, respectively. Similarly, comparison $K = -0.05$ is shown in figures 4.13 - 4.15, for $K = 0$ is shown in figures 4.16 - 4.18, for $K = 0.05$ is shown in figures 4.19 - 4.21 and, for $K = 1$ is shown in figures 4.22 - 4.24.

Table 4.7 The pollutant concentration at $K = -1$ of the four points explicit methods when after passed 20 s

t (sec) x (km)		Concentration $C(x,t)$ Kg / m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13388683	0.01275161	0.00042256	0.00000480	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27603853	0.06635899	0.01027764	0.00095667	0.00004886	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41556165	0.13773746	0.03450134	0.00635247	0.00081604	-0.00024938	-0.00211319	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.56290780	0.22489454	0.07217117	0.01843115	0.00351607	-0.00070911	-0.00549082	-0.01828731	-0.04636889	-0.09096688
	20	1.24147098	0.71802159	0.33000427	0.12473063	0.03892169	0.00933274	-0.00122330	-0.01073596	-0.02939539	-0.06373023	-0.11170083
case 2	4	0.59866933	0.13388683	0.01275161	0.00042256	0.00000480	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27603853	0.06635899	0.01027764	0.00095670	0.00005012	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41556165	0.13773746	0.03450149	0.00635520	0.00085173	0.00007932	0.00000493	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.56290782	0.22489484	0.07217476	0.01846441	0.00375356	0.00059688	0.00007412	0.00000691	0.00000047	0.00000004
	20	1.24147098	0.71802199	0.33000804	0.12475905	0.03909469	0.01018633	0.00219268	0.00038945	0.00005640	0.00000669	0.00000099
case 3	4	0.59866933	0.10707942	0.00947651	0.00030656	0.00000347	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18531137	0.03701062	0.00534897	0.00048741	0.00002651	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.23419964	0.05693291	0.01231541	0.00213883	0.00031219	0.00027075	0.00167183	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.26628388	0.06810515	0.01717734	0.00391074	0.00089314	0.00084964	0.00337644	0.01262528	0.03904641	0.10273526
	20	1.24147098	0.28749832	0.07327205	0.01951271	0.00508813	0.00156861	0.00176434	0.00538854	0.01635231	0.04474852	0.10992325

Table 4.8 The pollutant concentration at $K = -1$ of the third-order Crank-Nicolson methods when after passed 20 s

t (sec) / x (km)		Concentration $C(x,t)$ Kg/m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13360251	0.01274288	0.00042270	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27492798	0.06615308	0.01025488	0.00095551	0.00004883	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41368256	0.13716398	0.03437414	0.00633224	0.00081396	-0.00024950	-0.00211319	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.56051384	0.22388996	0.07185689	0.01835477	0.00350166	-0.00071116	-0.00549097	-0.01828728	-0.04636889	-0.09096688
	20	1.24147098	0.71541185	0.32858690	0.12416455	0.03874295	0.00928675	-0.00123312	-0.01073767	-0.02939522	-0.06372994	-0.11170082
case 2	4	0.59866933	0.13360251	0.01274288	0.00042270	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27492798	0.06615308	0.01025488	0.00095554	0.00005010	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41368256	0.13716398	0.03437429	0.00633497	0.00084965	0.00007920	0.00000493	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.56051386	0.22389026	0.07186049	0.01838805	0.00373919	0.00059485	0.00007392	0.00000689	0.00000047	0.00000004
	20	1.24147098	0.71541225	0.32859068	0.12419301	0.03891606	0.01014058	0.00218317	0.00038787	0.00005620	0.00000667	0.00000099
case 3	4	0.59866933	0.10677687	0.00946791	0.00030664	0.00000347	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18389995	0.03683186	0.00533240	0.00048659	0.00002649	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.23125814	0.05643951	0.01223858	0.00212867	0.00031120	0.00027069	0.00167182	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.26164172	0.06723897	0.01701652	0.00388245	0.00088863	0.00084904	0.00337634	0.01262523	0.03904641	0.10273526
	20	1.24147098	0.28123266	0.07204122	0.01926582	0.00503916	0.00155921	0.00176283	0.00538834	0.01635193	0.04474830	0.10992325

Table 4.9 The pollutant concentration at $k = -1$ the four points implicit methods when after passed 20 s

t (sec) x (km)		Concentration $C(x,t)$ Kg/m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13331809	0.01273417	0.00042284	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27381193	0.06594694	0.01023213	0.00095434	0.00004881	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41178680	0.13658788	0.03424678	0.00631203	0.00081188	-0.00024962	-0.00211320	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.55809229	0.22287787	0.07154139	0.01827832	0.00348726	-0.00071320	-0.00549113	-0.01828725	-0.04636889	-0.09096688
	20	1.24147098	0.71276793	0.32715595	0.12359495	0.03856364	0.00924072	-0.00124293	-0.01073937	-0.02939506	-0.06372964	-0.11170082
case 2	4	0.59866933	0.13331809	0.01273417	0.00042284	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27381193	0.06594694	0.01023213	0.00095437	0.00005008	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41178680	0.13658789	0.03424693	0.00631476	0.00084757	0.00007907	0.00000492	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.55809231	0.22287817	0.07154499	0.01831162	0.00372483	0.00059283	0.00007373	0.00000688	0.00000047	0.00000004
	20	1.24147098	0.71276834	0.32715975	0.12362345	0.03873687	0.01009481	0.00217368	0.00038631	0.00005599	0.00000665	0.00000099
case 3	4	0.59866933	0.10647424	0.00945931	0.00030672	0.00000348	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18248000	0.03665294	0.00531586	0.00048577	0.00002647	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.22827903	0.05594316	0.01216167	0.00211853	0.00031021	0.00027063	0.00167182	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.25690984	0.06636256	0.01685482	0.00385414	0.00088412	0.00084845	0.00337624	0.01262519	0.03904641	0.10273526
	20	1.24147098	0.27480950	0.07078863	0.01901629	0.00498995	0.00154982	0.00176132	0.00538814	0.01635156	0.04474808	0.10992326

Table 4.10 The pollutant concentration at $K = -0.05$ of the four points explicit methods when after passed 20 s

t(sec) x (km)		Concentration $C(x,t)$ Kg / m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13388683	0.01275161	0.00042256	0.00000480	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27603853	0.06635899	0.01027764	0.00095667	0.00004886	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41556165	0.13773746	0.03450134	0.00635247	0.00081604	-0.00024938	-0.00211319	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.56290780	0.22489454	0.07217117	0.01843115	0.00351607	-0.00070911	-0.00549082	-0.01828731	-0.04636889	-0.09096688
	20	1.24147098	0.71802159	0.33000427	0.12473063	0.03892169	0.00933274	-0.00122330	-0.01073596	-0.02939539	-0.06373023	-0.11170083
case 2	4	0.59866933	0.13388683	0.01275161	0.00042256	0.00000480	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27603853	0.06635899	0.01027764	0.00095670	0.00005012	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41556165	0.13773746	0.03450149	0.00635520	0.00085173	0.00007932	0.00000493	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.56290782	0.22489484	0.07217476	0.01846441	0.00375356	0.00059688	0.00007412	0.00000691	0.00000047	0.00000004
	20	1.24147098	0.71802199	0.33000804	0.12475905	0.03909469	0.01018633	0.00219268	0.00038945	0.00005640	0.00000669	0.00000099
case 3	4	0.59866933	0.10647424	0.00945931	0.00030672	0.00000348	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18248000	0.03665294	0.00531586	0.00048577	0.00002647	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.22827903	0.05594316	0.01216167	0.00211853	0.00031021	0.00027063	0.00167182	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.25690984	0.06636256	0.01685482	0.00385414	0.00088412	0.00084845	0.00337624	0.01262519	0.03904641	0.10273526
	20	1.24147098	0.27480950	0.07078863	0.01901629	0.00498995	0.00154982	0.00176132	0.00538814	0.01635156	0.04474808	0.10992326

Table 4.11 The pollutant concentration at $K = -0.05$ of the third-order Crank-Nicolson methods when after passed 20 s

t (sec) x (km)		Concentration $C(x,t)$ Kg / m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13360251	0.01274288	0.00042270	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27492798	0.06615308	0.01025488	0.00095551	0.00004883	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41368256	0.13716398	0.03437414	0.00633224	0.00081396	-0.00024950	-0.00211319	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.56051384	0.22388996	0.07185689	0.01835477	0.00350166	-0.00071116	-0.00549097	-0.01828728	-0.04636889	-0.09096688
	20	1.24147098	0.71541185	0.32858690	0.12416455	0.03874295	0.00928675	-0.00123312	-0.01073767	-0.02939522	-0.06372994	-0.11170082
case 2	4	0.59866933	0.13360251	0.01274288	0.00042270	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27492798	0.06615308	0.01025488	0.00095554	0.00005010	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41368256	0.13716398	0.03437429	0.00633497	0.00084965	0.00007920	0.00000493	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.56051386	0.22389026	0.07186049	0.01838805	0.00373919	0.00059485	0.00007392	0.00000689	0.00000047	0.00000004
	20	1.24147098	0.71541225	0.32859068	0.12419301	0.03891606	0.01014058	0.00218317	0.00038787	0.00005620	0.00000667	0.00000099
case 3	4	0.59866933	0.10677687	0.00946791	0.00030664	0.00000347	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18389995	0.03683186	0.00533240	0.00048659	0.00002649	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.23125814	0.05643951	0.01223858	0.00212867	0.00031120	0.00027069	0.00167182	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.26164172	0.06723897	0.01701652	0.00388245	0.00088863	0.00084904	0.00337634	0.01262523	0.03904641	0.10273526
	20	1.24147098	0.28123266	0.07204122	0.01926582	0.00503916	0.00155921	0.00176283	0.00538834	0.01635193	0.04474830	0.10992325

Table 4.12 The pollutant concentration at $K = -0.05$ of the four points implicit methods when after passed 20 s

t (sec) x (km)		Concentration $C(x,t)$ Kg / m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13331809	0.01273417	0.00042284	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27381193	0.06594694	0.01023213	0.00095434	0.00004881	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41178680	0.13658788	0.03424678	0.00631203	0.00081188	-0.00024962	-0.00211320	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.55809229	0.22287787	0.07154139	0.01827832	0.00348726	-0.00071320	-0.00549113	-0.01828725	-0.04636889	-0.09096688
	20	1.24147098	0.71276793	0.32715595	0.12359495	0.03856364	0.00924072	-0.00124293	-0.01073937	-0.02939506	-0.06372964	-0.11170082
case 2	4	0.59866933	0.13331809	0.01273417	0.00042284	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27381193	0.06594694	0.01023213	0.00095437	0.00005008	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41178680	0.13658789	0.03424693	0.00631476	0.00084757	0.00007907	0.00000492	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.55809231	0.22287817	0.07154499	0.01831162	0.00372483	0.00059283	0.00007373	0.00000688	0.00000047	0.00000004
	20	1.24147098	0.71276834	0.32715975	0.12362345	0.03873687	0.01009481	0.00217368	0.00038631	0.00005599	0.00000665	0.00000099
case 3	4	0.59866933	0.10647424	0.00945931	0.00030672	0.00000348	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18248000	0.03665294	0.00531586	0.00048577	0.00002647	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.22827903	0.05594316	0.01216167	0.00211853	0.00031021	0.00027063	0.00167182	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.25690984	0.06636256	0.01685482	0.00385414	0.00088412	0.00084845	0.00337624	0.01262519	0.03904641	0.10273526
	20	1.24147098	0.27480950	0.07078863	0.01901629	0.00498995	0.00154982	0.00176132	0.00538814	0.01635156	0.04474808	0.10992326

Table 4.13 The pollutant concentration at $K = 0$ of the four points explicit methods when after passed 20 s

t (sec) x (km)		Concentration $C(x,t)$ Kg / m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59867000	0.13389000	0.01275200	0.00042256	0.00000480	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543970	-0.03342100
	8	0.78942000	0.27604000	0.06635900	0.01027800	0.00095667	0.00004886	-0.00002855	-0.00041859	-0.00345410	-0.01718900	-0.05318100
	12	0.96464000	0.41556000	0.13774000	0.03450100	0.00635250	0.00081604	-0.00024938	-0.00211320	-0.00959470	-0.03091000	-0.07178200
	16	1.11740000	0.56291000	0.22489000	0.07217100	0.01843100	0.00351610	-0.00070911	-0.00549080	-0.01828700	-0.04636900	-0.09096700
	20	1.24150000	0.71802000	0.33000000	0.12473000	0.03892200	0.00933270	-0.00122330	-0.01073600	-0.02939500	-0.06373000	-0.11170000
case 2	4	0.59866933	0.13388683	0.01275161	0.00042256	0.00000480	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27603853	0.06635899	0.01027764	0.00095670	0.00005012	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41556165	0.13773746	0.03450149	0.00635520	0.00085173	0.00007932	0.00000493	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.56290782	0.22489484	0.07217476	0.01846441	0.00375356	0.00059688	0.00007412	0.00000691	0.00000047	0.00000004
	20	1.24147098	0.71802199	0.33000804	0.12475905	0.03909469	0.01018633	0.00219268	0.00038945	0.00005640	0.00000669	0.00000099
case 3	4	0.59866933	0.10707942	0.00947651	0.00030656	0.00000347	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18531137	0.03701062	0.00534897	0.00048741	0.00002651	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.23419964	0.05693291	0.01231541	0.00213883	0.00031219	0.00027075	0.00167183	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.26628388	0.06810515	0.01717734	0.00391074	0.00089314	0.00084964	0.00337644	0.01262528	0.03904641	0.10273526
	20	1.24147098	0.28749832	0.07327205	0.01951271	0.00508813	0.00156861	0.00176434	0.00538854	0.01635231	0.04474852	0.10992325

Table 4.14 The pollutant concentration at $K = 0$ of the third-order Crank-Nicolson methods when after passed 20 s

t (sec) x (km)		Concentration $C(x,t)$ Kg / m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13360251	0.01274288	0.00042270	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27492798	0.06615308	0.01025488	0.00095551	0.00004883	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41368256	0.13716398	0.03437414	0.00633224	0.00081396	-0.00024950	-0.00211319	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.56051384	0.22388996	0.07185689	0.01835477	0.00350166	-0.00071116	-0.00549097	-0.01828728	-0.04636889	-0.09096688
	20	1.24147098	0.71541185	0.32858690	0.12416455	0.03874295	0.00928675	-0.00123312	-0.01073767	-0.02939522	-0.06372994	-0.11170082
case 2	4	0.59866933	0.13360251	0.01274288	0.00042270	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27492798	0.06615308	0.01025488	0.00095554	0.00005010	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41368256	0.13716398	0.03437429	0.00633497	0.00084965	0.00007920	0.00000493	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.56051386	0.22389026	0.07186049	0.01838805	0.00373919	0.00059485	0.00007392	0.00000689	0.00000047	0.00000004
	20	1.24147098	0.71541225	0.32859068	0.12419301	0.03891606	0.01014058	0.00218317	0.00038787	0.00005620	0.00000667	0.00000099
case 3	4	0.59866933	0.10677687	0.00946791	0.00030664	0.00000347	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18389995	0.03683186	0.00533240	0.00048659	0.00002649	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.23125814	0.05643951	0.01223858	0.00212867	0.00031120	0.00027069	0.00167182	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.26164172	0.06723897	0.01701652	0.00388245	0.00088863	0.00084904	0.00337634	0.01262523	0.03904641	0.10273526
	20	1.24147098	0.28123266	0.07204122	0.01926582	0.00503916	0.00155921	0.00176283	0.00538834	0.01635193	0.04474830	0.10992325

Table 4.15 The pollutant concentration at $K = 0$ of the four points implicit methods when after passed 20 s

t (sec) x (km)		Concentration $C(x,t)$ Kg / m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13331809	0.01273417	0.00042284	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27381193	0.06594694	0.01023213	0.00095434	0.00004881	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41178680	0.13658788	0.03424678	0.00631203	0.00081188	-0.00024962	-0.00211320	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.55809229	0.22287787	0.07154139	0.01827832	0.00348726	-0.00071320	-0.00549113	-0.01828725	-0.04636889	-0.09096688
	20	1.24147098	0.71276793	0.32715595	0.12359495	0.03856364	0.00924072	-0.00124293	-0.01073937	-0.02939506	-0.06372964	-0.11170082
case 2	4	0.59866933	0.13331809	0.01273417	0.00042284	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27381193	0.06594694	0.01023213	0.00095437	0.00005008	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41178680	0.13658789	0.03424693	0.00631476	0.00084757	0.00007907	0.00000492	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.55809231	0.22287817	0.07154499	0.01831162	0.00372483	0.00059283	0.00007373	0.00000688	0.00000047	0.00000004
	20	1.24147098	0.71276834	0.32715975	0.12362345	0.03873687	0.01009481	0.00217368	0.00038631	0.00005599	0.00000665	0.00000099
case 3	4	0.59866933	0.10647424	0.00945931	0.00030672	0.00000348	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18248000	0.03665294	0.00531586	0.00048577	0.00002647	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.22827903	0.05594316	0.01216167	0.00211853	0.00031021	0.00027063	0.00167182	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.25690984	0.06636256	0.01685482	0.00385414	0.00088412	0.00084845	0.00337624	0.01262519	0.03904641	0.10273526
	20	1.24147098	0.27480950	0.07078863	0.01901629	0.00498995	0.00154982	0.00176132	0.00538814	0.01635156	0.04474808	0.10992326

Table 4.16 The pollutant concentration at $K = 0.05$ of the four points explicit methods when after passed 20 s

t(sec) x (km)		Concentration $C(x,t)$ Kg / m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13388683	0.01275161	0.00042256	0.00000480	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27603853	0.06635899	0.01027764	0.00095667	0.00004886	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41556165	0.13773746	0.03450134	0.00635247	0.00081604	-0.00024938	-0.00211319	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.56290780	0.22489454	0.07217117	0.01843115	0.00351607	-0.00070911	-0.00549082	-0.01828731	-0.04636889	-0.09096688
	20	1.24147098	0.71802159	0.33000427	0.12473063	0.03892169	0.00933274	-0.00122330	-0.01073596	-0.02939539	-0.06373023	-0.11170083
case 2	4	0.59866933	0.13388683	0.01275161	0.00042256	0.00000480	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27603853	0.06635899	0.01027764	0.00095670	0.00005012	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41556165	0.13773746	0.03450149	0.00635520	0.00085173	0.00007932	0.00000493	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.56290782	0.22489484	0.07217476	0.01846441	0.00375356	0.00059688	0.00007412	0.00000691	0.00000047	0.00000004
	20	1.24147098	0.71802199	0.33000804	0.12475905	0.03909469	0.01018633	0.00219268	0.00038945	0.00005640	0.00000669	0.00000099
case 3	4	0.59866933	0.10707942	0.00947651	0.00030656	0.00000347	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18531137	0.03701062	0.00534897	0.00048741	0.00002651	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.23419964	0.05693291	0.01231541	0.00213883	0.00031219	0.00027075	0.00167183	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.26628388	0.06810515	0.01717734	0.00391074	0.00089314	0.00084964	0.00337644	0.01262528	0.03904641	0.10273526
	20	1.24147098	0.28749832	0.07327205	0.01951271	0.00508813	0.00156861	0.00176434	0.00538854	0.01635231	0.04474852	0.10992325

Table 4.17 The pollutant concentration at $K = 0.05$ of the third-order Crank-Nicolson methods when after passed 20 s

t(sec) x (km)		Concentration $C(x,t)$ Kg / m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13360251	0.01274288	0.00042270	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27492798	0.06615308	0.01025488	0.00095551	0.00004883	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41368256	0.13716398	0.03437414	0.00633224	0.00081396	-0.00024950	-0.00211319	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.56051384	0.22388996	0.07185689	0.01835477	0.00350166	-0.00071116	-0.00549097	-0.01828728	-0.04636889	-0.09096688
	20	1.24147098	0.71541185	0.32858690	0.12416455	0.03874295	0.00928675	-0.00123312	-0.01073767	-0.02939522	-0.06372994	-0.11170082
case 2	4	0.59866933	0.13360251	0.01274288	0.00042270	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27492798	0.06615308	0.01025488	0.00095554	0.00005010	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41368256	0.13716398	0.03437429	0.00633497	0.00084965	0.00007920	0.00000493	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.56051386	0.22389026	0.07186049	0.01838805	0.00373919	0.00059485	0.00007392	0.00000689	0.00000047	0.00000004
	20	1.24147098	0.71541225	0.32859068	0.12419301	0.03891606	0.01014058	0.00218317	0.00038787	0.00005620	0.00000667	0.00000099
case 3	4	0.59866933	0.10677687	0.00946791	0.00030664	0.00000347	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18389995	0.03683186	0.00533240	0.00048659	0.00002649	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.23125814	0.05643951	0.01223858	0.00212867	0.00031120	0.00027069	0.00167182	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.26164172	0.06723897	0.01701652	0.00388245	0.00088863	0.00084904	0.00337634	0.01262523	0.03904641	0.10273526
	20	1.24147098	0.28123266	0.07204122	0.01926582	0.00503916	0.00155921	0.00176283	0.00538834	0.01635193	0.04474830	0.10992325

Table 4.18 The pollutant concentration at $K = 0.05$ of the four points implicit methods when after passed 20 s

t (sec) x (km)		Concentration $C(x,t)$ Kg / m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13331809	0.01273417	0.00042284	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27381193	0.06594694	0.01023213	0.00095434	0.00004881	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41178680	0.13658788	0.03424678	0.00631203	0.00081188	-0.00024962	-0.00211320	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.55809229	0.22287787	0.07154139	0.01827832	0.00348726	-0.00071320	-0.00549113	-0.01828725	-0.04636889	-0.09096688
	20	1.24147098	0.71276793	0.32715595	0.12359495	0.03856364	0.00924072	-0.00124293	-0.01073937	-0.02939506	-0.06372964	-0.11170082
case 2	4	0.59866933	0.13331809	0.01273417	0.00042284	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27381193	0.06594694	0.01023213	0.00095437	0.00005008	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41178680	0.13658789	0.03424693	0.00631476	0.00084757	0.00007907	0.00000492	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.55809231	0.22287817	0.07154499	0.01831162	0.00372483	0.00059283	0.00007373	0.00000688	0.00000047	0.00000004
	20	1.24147098	0.71276834	0.32715975	0.12362345	0.03873687	0.01009481	0.00217368	0.00038631	0.00005599	0.00000665	0.00000099
case 3	4	0.59866933	0.10647424	0.00945931	0.00030672	0.00000348	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18248000	0.03665294	0.00531586	0.00048577	0.00002647	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.22827903	0.05594316	0.01216167	0.00211853	0.00031021	0.00027063	0.00167182	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.25690984	0.06636256	0.01685482	0.00385414	0.00088412	0.00084845	0.00337624	0.01262519	0.03904641	0.10273526
	20	1.24147098	0.27480950	0.07078863	0.01901629	0.00498995	0.00154982	0.00176132	0.00538814	0.01635156	0.04474808	0.10992326

Table 4.19 The pollutant concentration at $K=1$ of the four points explicit methods when after passed 20 s

t (sec) x (km)		Concentration $C(x,t)$ Kg / m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13388683	0.01275161	0.00042256	0.00000480	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27603853	0.06635899	0.01027764	0.00095667	0.00004886	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41556165	0.13773746	0.03450134	0.00635247	0.00081604	-0.00024938	-0.00211319	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.56290780	0.22489454	0.07217117	0.01843115	0.00351607	-0.00070911	-0.00549082	-0.01828731	-0.04636889	-0.09096688
	20	1.24147098	0.71802159	0.33000427	0.12473063	0.03892169	0.00933274	-0.00122330	-0.01073596	-0.02939539	-0.06373023	-0.11170083
case 2	4	0.59866933	0.13388683	0.01275161	0.00042256	0.00000480	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27603853	0.06635899	0.01027764	0.00095670	0.00005012	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41556165	0.13773746	0.03450149	0.00635520	0.00085173	0.00007932	0.00000493	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.56290782	0.22489484	0.07217476	0.01846441	0.00375356	0.00059688	0.00007412	0.00000691	0.00000047	0.00000004
	20	1.24147098	0.71802199	0.33000804	0.12475905	0.03909469	0.01018633	0.00219268	0.00038945	0.00005640	0.00000669	0.00000099
case 3	4	0.59866933	0.10707942	0.00947651	0.00030656	0.00000347	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18531137	0.03701062	0.00534897	0.00048741	0.00002651	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.23419964	0.05693291	0.01231541	0.00213883	0.00031219	0.00027075	0.00167183	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.26628388	0.06810515	0.01717734	0.00391074	0.00089314	0.00084964	0.00337644	0.01262528	0.03904641	0.10273526
	20	1.24147098	0.28749832	0.07327205	0.01951271	0.00508813	0.00156861	0.00176434	0.00538854	0.01635231	0.04474852	0.10992325

Table 4.20 The pollutant concentration at $K=1$ of the third-order Crank-Nicolson methods when after passed 20 s

t (sec) x (km)		Concentration $C(x,t)$ Kg / m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13360251	0.01274288	0.00042270	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27492798	0.06615308	0.01025488	0.00095551	0.00004883	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41368256	0.13716398	0.03437414	0.00633224	0.00081396	-0.00024950	-0.00211319	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.56051384	0.22388996	0.07185689	0.01835477	0.00350166	-0.00071116	-0.00549097	-0.01828728	-0.04636889	-0.09096688
	20	1.24147098	0.71541185	0.32858690	0.12416455	0.03874295	0.00928675	-0.00123312	-0.01073767	-0.02939522	-0.06372994	-0.11170082
case 2	4	0.59866933	0.13360251	0.01274288	0.00042270	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27492798	0.06615308	0.01025488	0.00095554	0.00005010	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41368256	0.13716398	0.03437429	0.00633497	0.00084965	0.00007920	0.00000493	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.56051386	0.22389026	0.07186049	0.01838805	0.00373919	0.00059485	0.00007392	0.00000689	0.00000047	0.00000004
	20	1.24147098	0.71541225	0.32859068	0.12419301	0.03891606	0.01014058	0.00218317	0.00038787	0.00005620	0.00000667	0.00000099
case 3	4	0.59866933	0.10677687	0.00946791	0.00030664	0.00000347	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18389995	0.03683186	0.00533240	0.00048659	0.00002649	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.23125814	0.05643951	0.01223858	0.00212867	0.00031120	0.00027069	0.00167182	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.26164172	0.06723897	0.01701652	0.00388245	0.00088863	0.00084904	0.00337634	0.01262523	0.03904641	0.10273526
	20	1.24147098	0.28123266	0.07204122	0.01926582	0.00503916	0.00155921	0.00176283	0.00538834	0.01635193	0.04474830	0.10992325

Table 4.21 The pollutant concentration at $K=1$ of the four points implicit methods when after passed 20 s

t (sec) x (km)		Concentration $C(x,t)$ Kg / m ³										
		x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1
Case 1	4	0.59866933	0.13331809	0.01273417	0.00042284	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089
	8	0.78941834	0.27381193	0.06594694	0.01023213	0.00095434	0.00004881	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134
	12	0.96464247	0.41178680	0.13658788	0.03424678	0.00631203	0.00081188	-0.00024962	-0.00211320	-0.00959469	-0.03090974	-0.07178201
	16	1.11735609	0.55809229	0.22287787	0.07154139	0.01827832	0.00348726	-0.00071320	-0.00549113	-0.01828725	-0.04636889	-0.09096688
	20	1.24147098	0.71276793	0.32715595	0.12359495	0.03856364	0.00924072	-0.00124293	-0.01073937	-0.02939506	-0.06372964	-0.11170082
case 2	4	0.59866933	0.13331809	0.01273417	0.00042284	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	8	0.78941834	0.27381193	0.06594694	0.01023213	0.00095437	0.00005008	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
	12	0.96464247	0.41178680	0.13658789	0.03424693	0.00631476	0.00084757	0.00007907	0.00000492	0.00000021	0.00000001	0.00000000
	16	1.11735609	0.55809231	0.22287817	0.07154499	0.01831162	0.00372483	0.00059283	0.00007373	0.00000688	0.00000047	0.00000004
	20	1.24147098	0.71276834	0.32715975	0.12362345	0.03873687	0.01009481	0.00217368	0.00038631	0.00005599	0.00000665	0.00000099
case 3	4	0.59866933	0.10647424	0.00945931	0.00030672	0.00000348	0.00000001	0.00000010	0.00001182	0.00050910	0.00834603	0.05751333
	8	0.78941834	0.18248000	0.03665294	0.00531586	0.00048577	0.00002647	0.00003126	0.00043902	0.00384194	0.02126083	0.07945003
	12	0.96464247	0.22827903	0.05594316	0.01216167	0.00211853	0.00031021	0.00027063	0.00167182	0.00834309	0.03139476	0.09322770
	16	1.11735609	0.25690984	0.06636256	0.01685482	0.00385414	0.00088412	0.00084845	0.00337624	0.01262519	0.03904641	0.10273526
	20	1.24147098	0.27480950	0.07078863	0.01901629	0.00498995	0.00154982	0.00176132	0.00538814	0.01635156	0.04474808	0.10992326

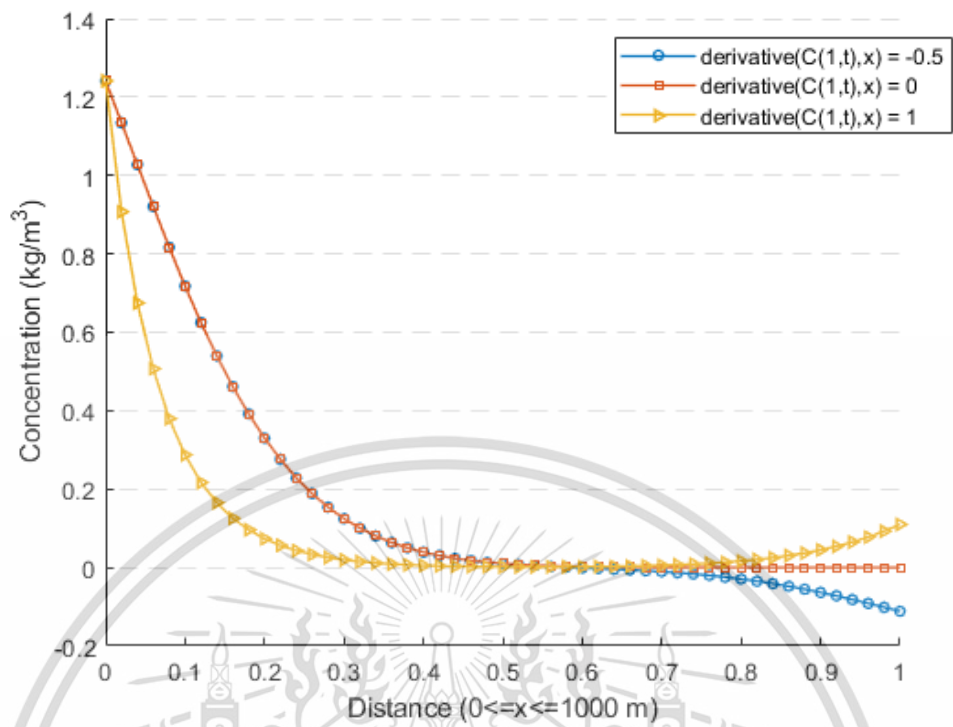


Figure 4.10 The comparison of pollutant concentrations for 3 cases at $K = -1$ of the four points explicit upwind methods when after passed 20 s

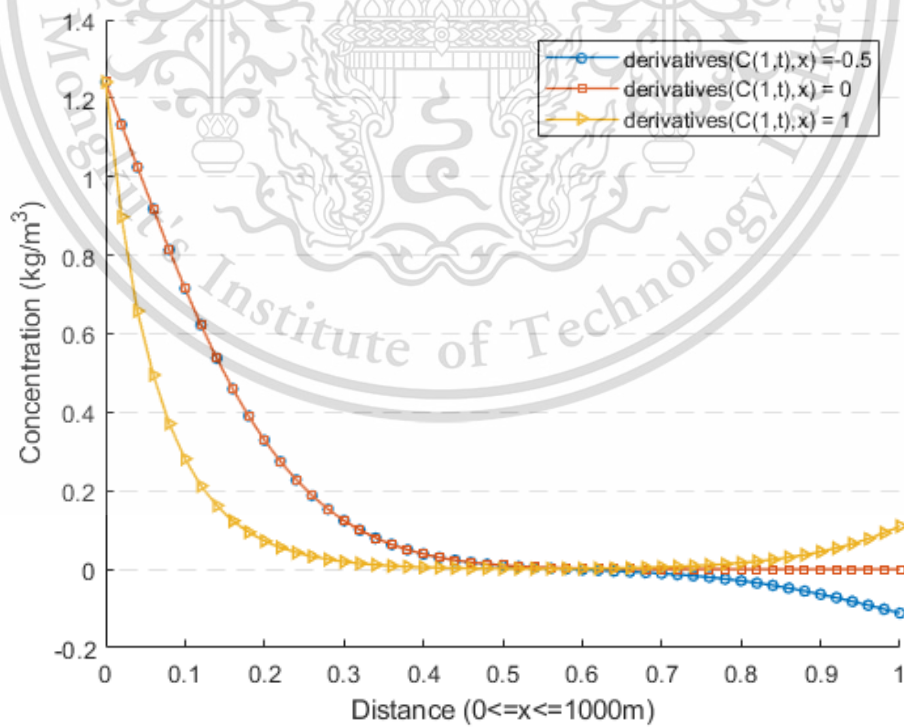


Figure 4.11 The comparison of pollutant concentrations for 3 cases at $K = -1$ of the third-order Crank-Nicolson methods when after passed 20 s

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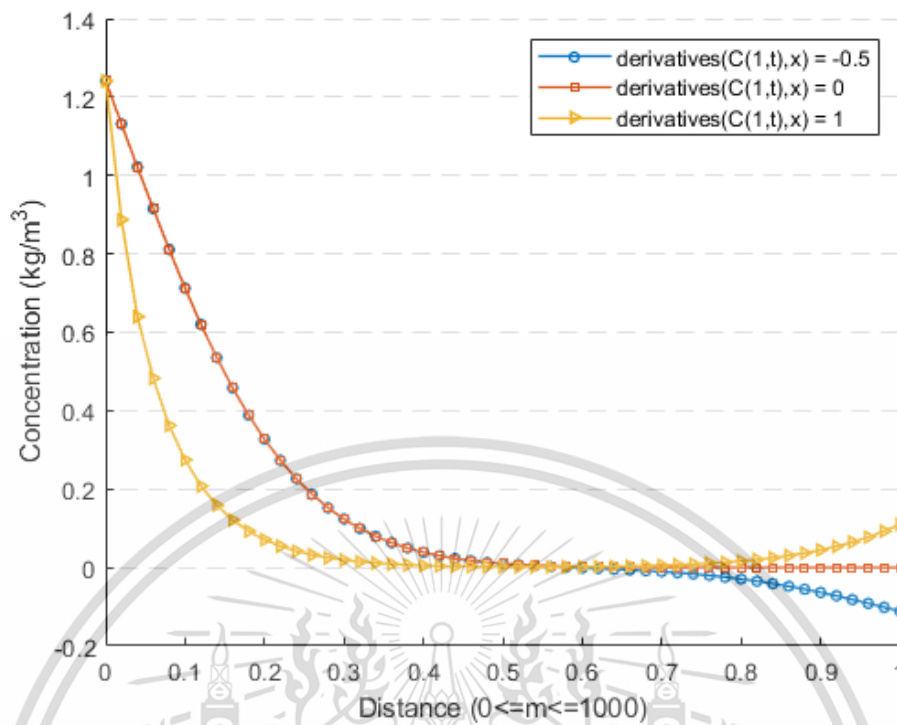


Figure 4.12 The comparison of pollutant concentrations for 3 cases at $K = -1$ of the four points implicit upwind methods when after passed 20 s

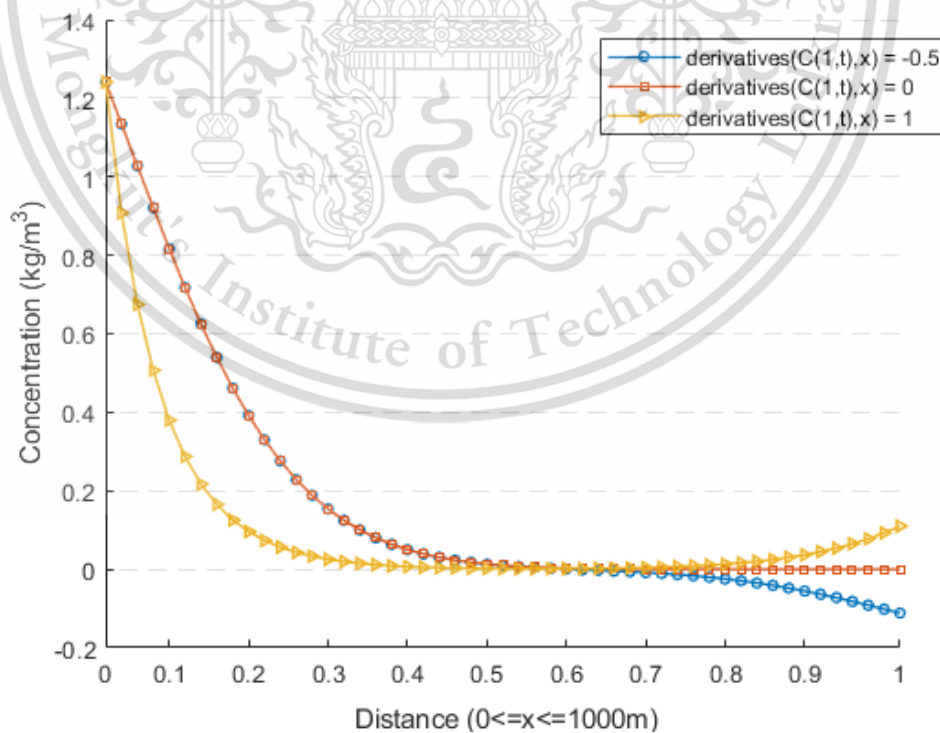


Figure 4.13 The comparison of pollutant concentrations for 3 cases at $K = -0.05$ of the four points explicit upwind methods when after passed 20 s

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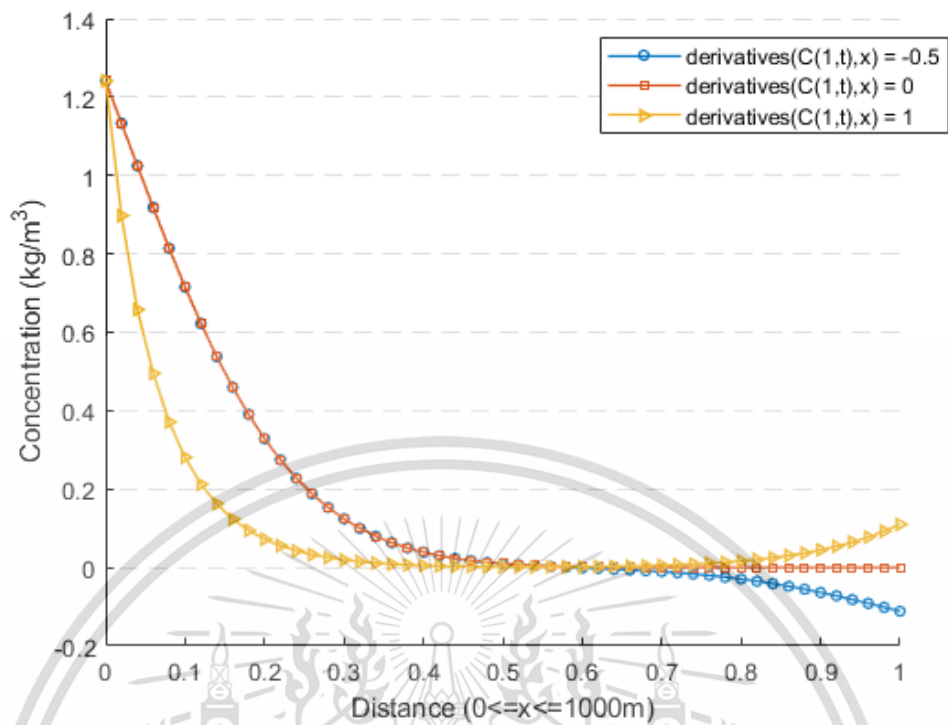


Figure 4.14 The comparison of pollutant concentrations for 3 cases at $K = -0.05$ of the third-order Crank-Nicolson methods when after passed 20 s

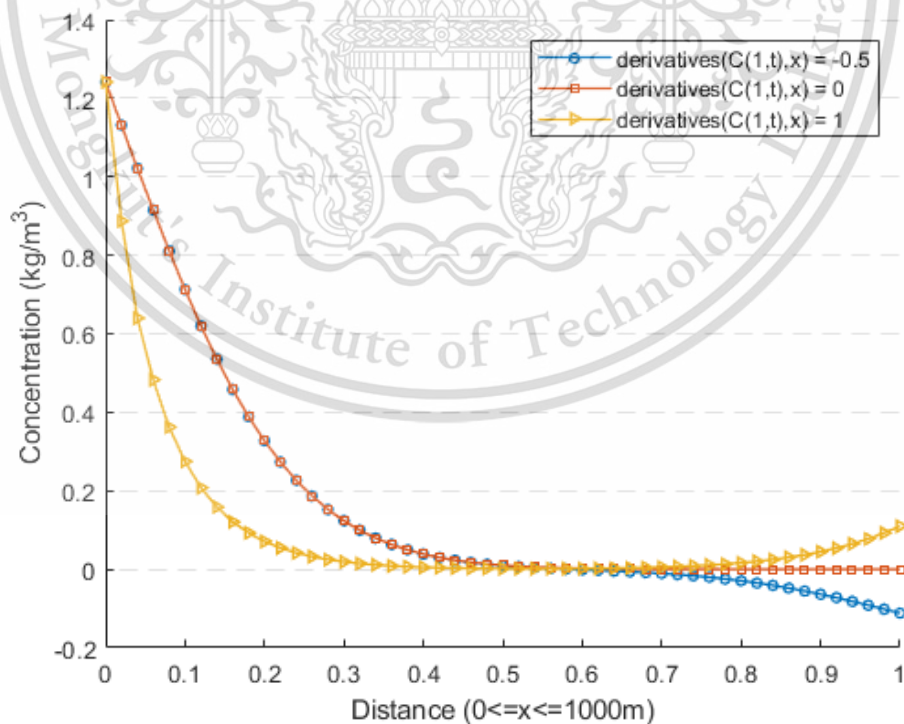


Figure 4.15 The comparison of pollutant concentrations for 3 cases at $K = -0.05$ of the four points implicit upwind methods when after passed 20 s

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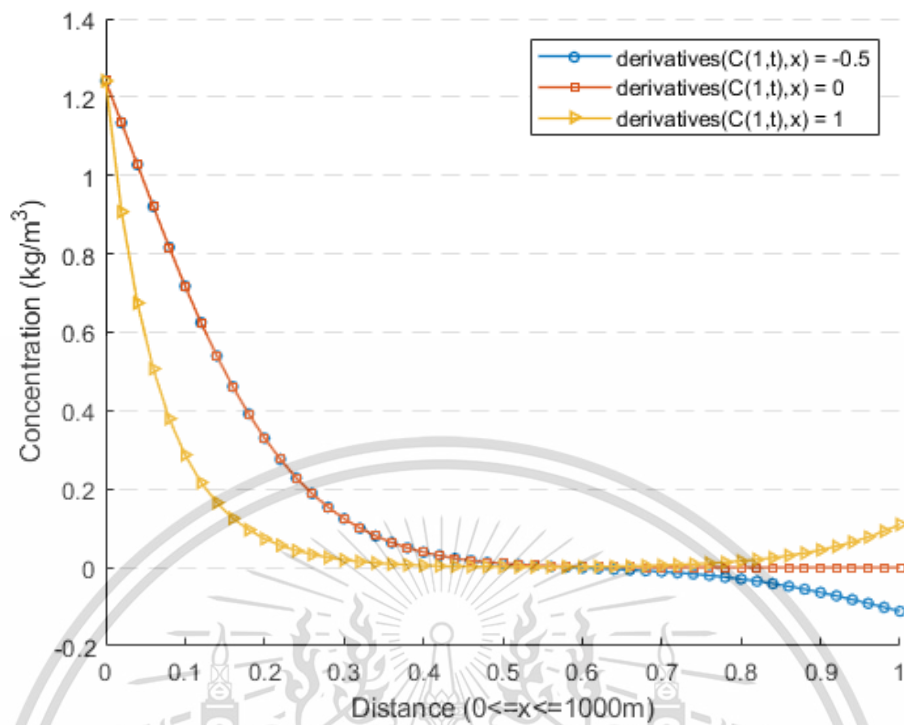


Figure 4.16 The comparison of pollutant concentrations for 3 cases at $K = 0$ of the four points explicit upwind methods when after passed 20 s

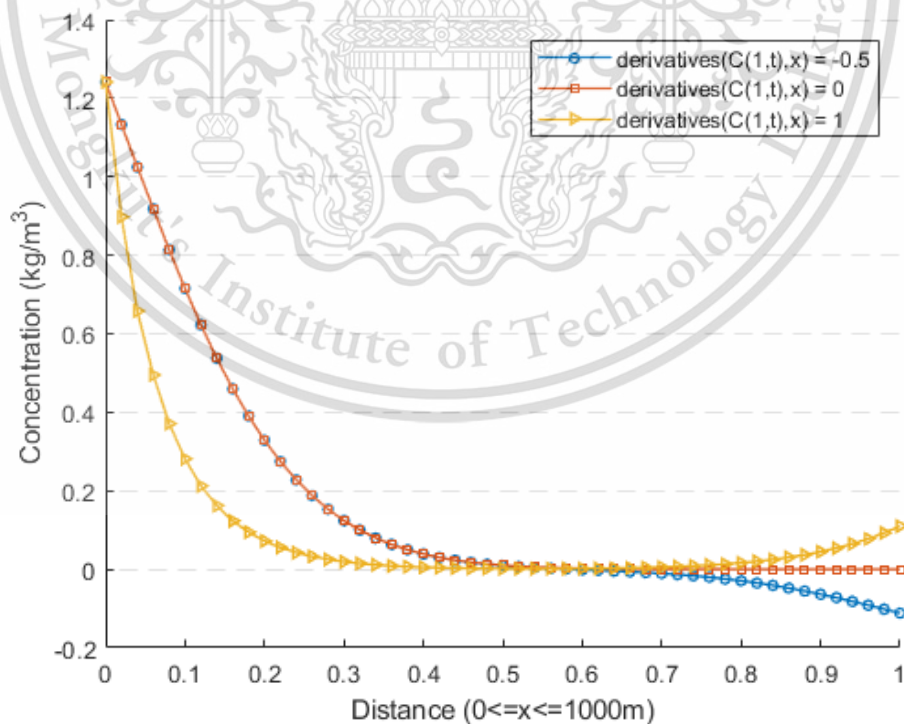


Figure 4.17 The comparison of pollutant concentrations for 3 cases at $K = 0$ of the third-order Crank-Nicolson methods when after passed 20 s

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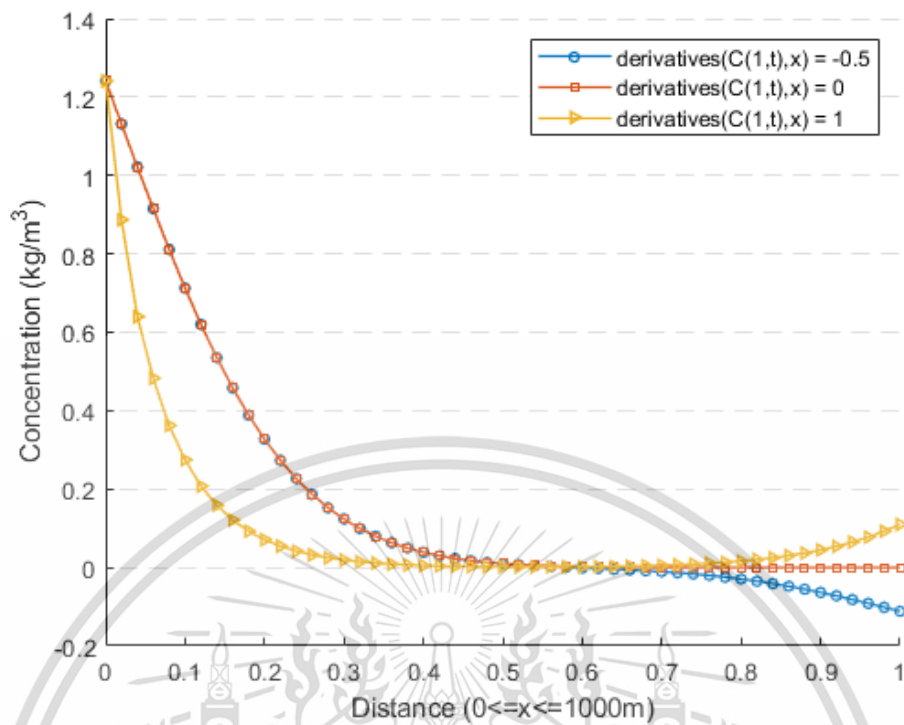


Figure 4.18 The comparison of pollutant concentrations for 3 cases at $K = 0$ of the four points implicit upwind methods when after passed 20 s

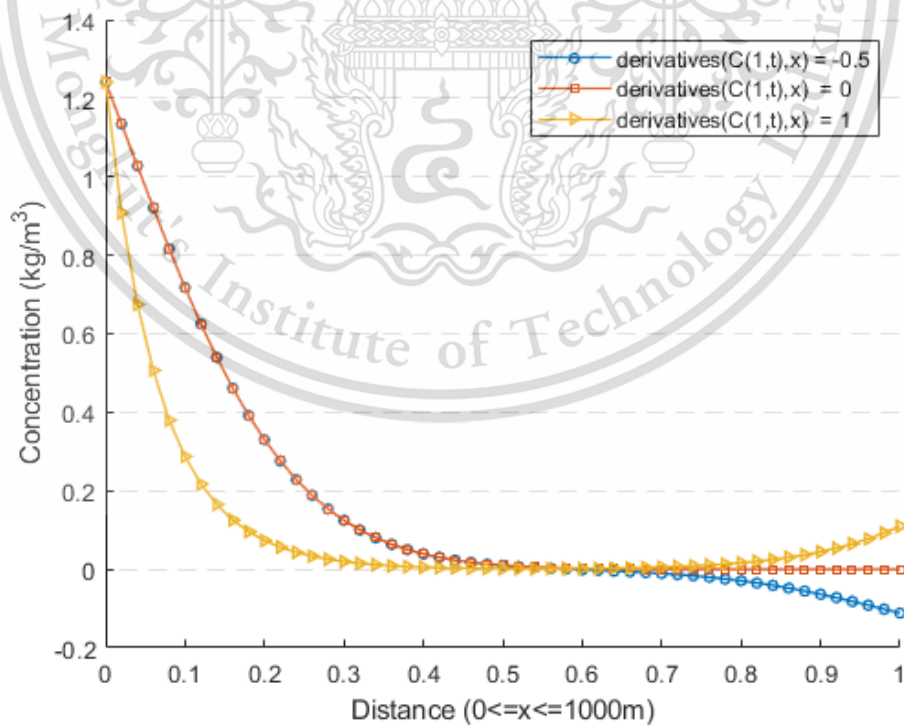


Figure 4.19 The comparison of pollutant concentrations for 3 cases at $K = 0.05$ of the four points explicit upwind methods when after passed 20 s

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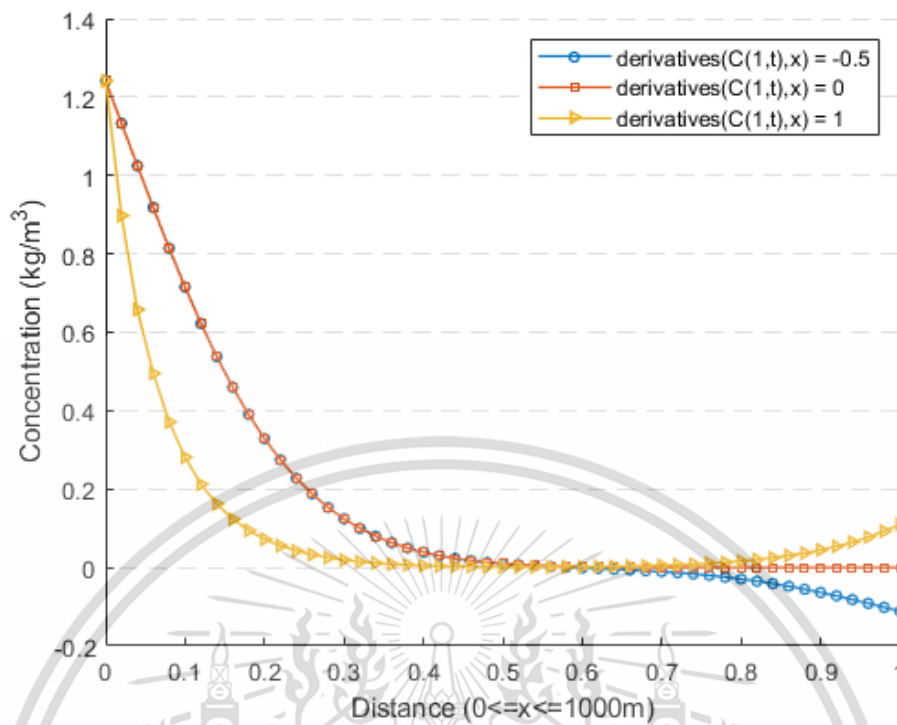


Figure 4.19 The comparison of pollutant concentrations for 3 cases at $K = 0.05$ of the third-order Crank-Nicolson methods when after passed 20 s

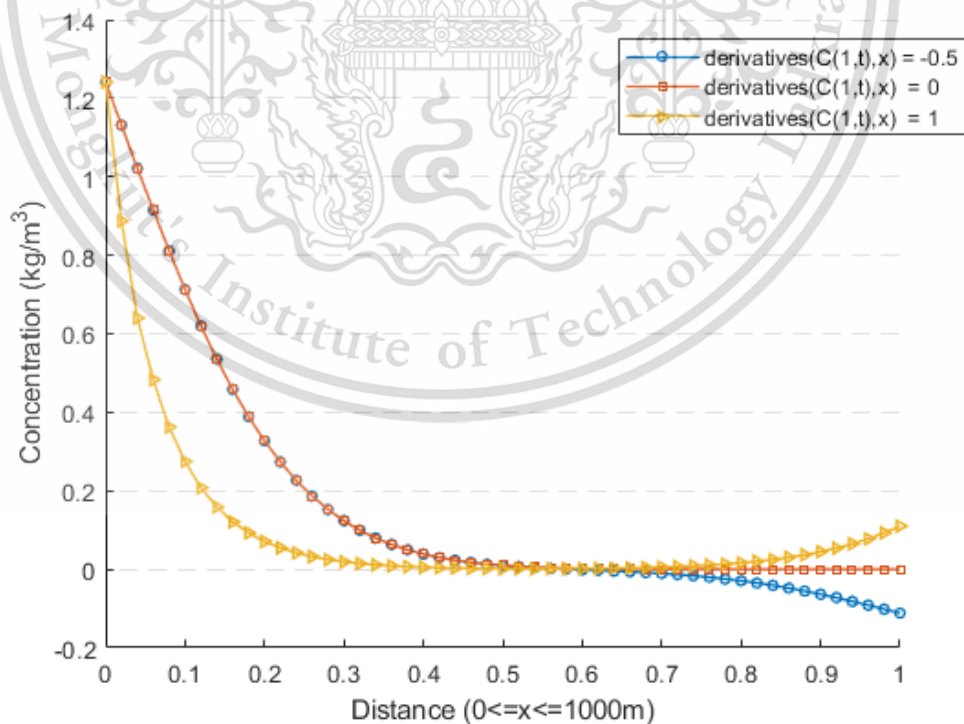


Figure 4.20 The comparison of pollutant concentrations for 3 cases at $K = 0.5$ of the four points implicit upwind methods when after passed 20 s

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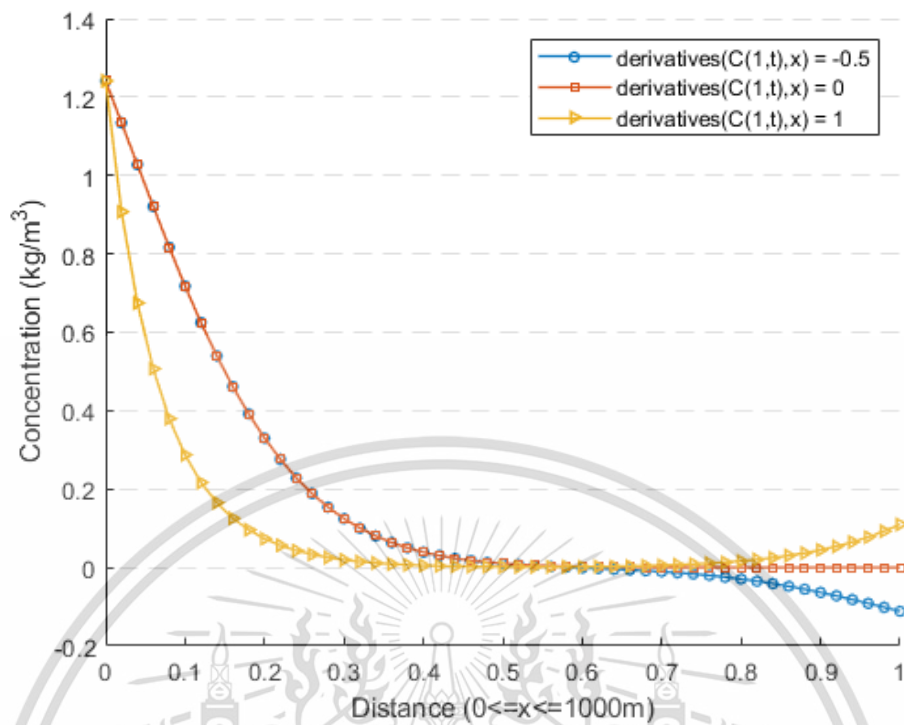


Figure 4.21 The comparison of pollutant concentrations for 3 cases at $K = 1$ of the four points explicit upwind methods when after passed 20 s

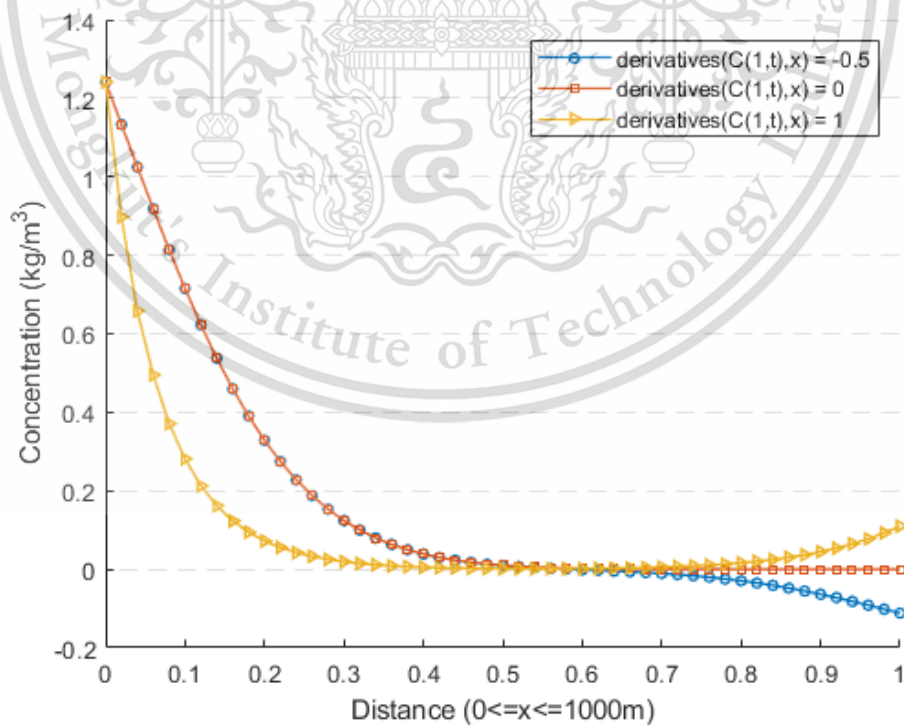


Figure 4.22 The comparison of pollutant concentrations for 3 cases at $K = 1$ of the third-order Crank-Nicolson methods when after passed 20 s

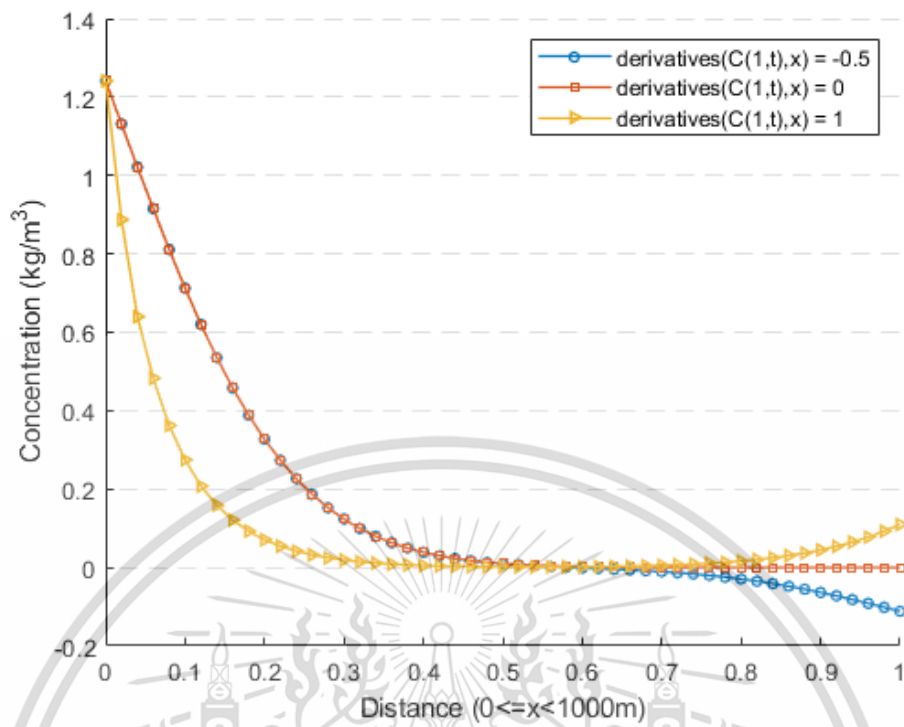


Figure 4.23 The comparison of pollutant concentrations for 3 cases at $K = 1$ of the four points implicit upwind methods when after passed 20 s

4.3 Finite difference techniques for the dispersion model by using explicit methods

We propose the numerical techniques in [9] and [11] and obtain the explicit schemes for the advection-dispersion-reaction equation which provides the pollutant concentration field. The explicit methods can be obtained so that the technique is not required to generate any systems of linear equations. We can see that the application of the technique is an example of economical computer implementation. We can approximate $C(x_i, t_n)$ by C_i^n , the value of the difference approximation of $C(x, t)$ at point $x = i\Delta x$ and $t = n\Delta t$, where $1 \leq i \leq M$, and $0 \leq n \leq N$. The grid point (x_i, t_n) is defined by $x_i = i\Delta x$ for all $i = 0, 1, 2, \dots, M$, and $t_n = n\Delta t$ for all $n = 0, 1, 2, \dots, N$ in which M and N are positive integers.

4.3.1 The four points explicit upwind methods

Consider the numerical techniques from [11] for the advection-dispersion-reaction equation using the forward times central space scheme for the times derivatives and the central difference for the second times derivatives, respectively, approximate the spatial derivative, following discretization:

$$\frac{\partial C}{\partial t} \approx \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad (4.66)$$

$$\frac{\partial^2 C}{\partial x^2} \approx \frac{1}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n], \quad (4.67)$$

for near the left boundary,

$$\frac{\partial C}{\partial x} \approx \frac{1}{6\Delta x} [-11C_i^n + 18C_{i+1}^n - 9C_{i+2}^n + 2C_{i+3}^n], \quad (4.68)$$

for interior node,

$$\frac{\partial C}{\partial x} \approx \frac{1}{6\Delta x} [C_{i-2}^n - 6C_{i-1}^n + 3C_i^n + 2C_{i+1}^n], \quad (4.69)$$

for near the right boundary,

$$\frac{\partial C}{\partial x} \approx \frac{1}{6\Delta x} [-2C_{i-3}^n + 9C_{i-2}^n - 18C_{i-1}^n + 11C_i^n]. \quad (4.70)$$

Near the left boundary, substituting equations (4.66 - 4.67) and equation (4.68) into equation (2.19), we then obtain;

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$$C_i^{n+1} = \beta C_{i-1}^n + [1 - 2\beta - (\Delta t)K + 11\alpha_i^n] C_i^n + [\beta - 18\alpha_i^n] C_{i+1}^n - 9\alpha_i^n C_{i+2}^n - 2\alpha_i^n C_{i+3}^n, \quad (4.71)$$

for $i=0$, we plug the known value of the left boundary by arranging $C_{i-1}^n = C_i^n - (\Delta x)f$ in equation (4.71) on the right-hand side. We obtain;

$$C_i^{n+1} = [1 - \beta - (\Delta t)K + 11\alpha_i^n] C_i^n + [\beta - 18\alpha_i^n] C_{i+1}^n - 9\alpha_i^n C_{i+2}^n - 2\alpha_i^n C_{i+3}^n - \beta(\Delta x)f. \quad (4.72)$$

At interior, substituting equations (4.66 - 4.67) and equation (4.69) into equation (2.19), we obtain,

$$C_i^{n+1} = -\alpha_i^n C_{i-2}^n + [\beta + 6\alpha_i^n] C_{i-1}^n + [1 - 2\beta - 3\alpha_i^n - (\Delta t)K] C_i^n + [\beta - 2\alpha_i^n] C_{i+1}^n, \quad (4.73)$$

for all $1 \leq i \leq M-1$ and $0 \leq n \leq N$.

Near the left boundary substituting equations (4.66 - 4.67) and equation (4.70) into equation (2.19), we obtain

$$C_i^{n+1} = 2\beta C_{i-3}^n + [\beta - 9\alpha_i^n] C_{i-2}^n + 18\alpha_i^n C_{i-1}^n + [1 - 2\beta - (\Delta t)K - 11\alpha_i^n] C_i^n + \alpha_i^n C_{i+1}^n, \quad (4.74)$$

for $i=M$, the known value of the right boundary conditions is approximated as $C_{i+1}^n = C_i^n + (\Delta x)f$ in equation (4.74) and, by rearranging, we obtain,

$$C_M^{n+1} = 2\beta C_{M-3}^n + [\beta - 9\alpha_M^n] C_{M-2}^n + 18\alpha_M^n C_{M-1}^n + [1 - 2\beta - (\Delta t)K - 10\alpha_M^n] C_M^n + \alpha_M^n (\Delta x), \quad (4.75)$$

where $\beta = D \frac{\Delta t}{(\Delta x)^2}$, $\alpha_i^n = u_i^n \frac{\Delta t}{6\Delta x}$, and $u \approx \tilde{u}_i^n$ which \tilde{u}_i^n are obtained by the Crank-

Nicolson method with the hydrodynamic model.

4.3.2 The upwind explicit methods

Consider the numerical techniques form [9] for the advection-dispersion-reaction equation; the upwind explicit scheme is considered by the following discretization;

$$\frac{\partial C}{\partial t} \approx \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad (4.76)$$

$$\frac{\partial C}{\partial x} \approx \frac{C_i^n - C_{i-1}^n}{\Delta x}, \quad (4.77)$$

$$\frac{\partial^2 C}{\partial x^2} \approx \frac{1}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n], \quad (4.78)$$

substituting equations (4.76 - 4.78) into equation (2.19), we then obtain;

$$C_i^{n+1} = (\alpha_i^n + \beta)C_{i-1}^n + (1 - \alpha_i^n - 2\beta - (\Delta t)K)C_i^n + \beta C_{i+1}^n, \quad (4.79)$$

for all $1 \leq i \leq M-1$.

For $i=0$, we plug the known value of the left boundary by arranging $C_{i-1}^n = C_i^n - (\Delta x)f$ in equation (4.79) on the right-hand side. We obtain;

$$C_i^{n+1} = [1 - \alpha_i^n - 2\beta - (\Delta t)K]C_i^n + [3\beta + \alpha_i^n]C_{i+1}^n - [2\beta + \alpha_i^n](\Delta x)f. \quad (4.80)$$

Similarly, for the right boundary condition, for $i=M$, the known value of the right boundary conditions is approximated as $C_{M+1}^n = C_M^n + (\Delta x)f$ in equation (4.79) and, by rearranging, we obtain;

$$C_M^{n+1} = (\alpha_M^n + 2\beta)C_{M-1}^n + [1 - \alpha_M^n - 2\beta - (\Delta t)K]C_M^n + \beta(\Delta x)f, \quad (4.81)$$

where $\beta = D \frac{\Delta t}{(\Delta x)^2}$, $\lambda_i^n = u_i^n \frac{\Delta t}{\Delta x}$, and $u \approx \tilde{u}_i^n$ which \tilde{u}_i^n are obtained by the Crank-Nicolson method with the hydrodynamic model.

4.3.3 The Lax-Wendroff methods

Consider the numerical techniques form [9] for the advection-dispersion-reaction equation; the Lax-Wendroff scheme is considered by the following discretization;

$$\frac{\partial C}{\partial t} \approx \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad (4.82)$$

$$\frac{\partial C}{\partial x} \approx \lambda_i^n \frac{(C_i^n - C_{i-1}^n)}{\Delta x} + (1 - \lambda_i^n) \frac{(C_{i+1}^n - C_{i-1}^n)}{2\Delta x}, \quad (4.83)$$

$$\frac{\partial^2 C}{\partial x^2} \approx \frac{1}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n], \quad (4.84)$$

substituting equations (4.82 - 4.84) into equation (2.19), we then obtain;

$$C_i^{n+1} = \frac{1}{2} \left[\alpha_i^n + (\alpha_i^n)^2 + 2\beta \right] C_{i-1}^n + \left[1 - \alpha_i^n - 2\beta - (\Delta t)K \right] C_i^n + \frac{1}{2} \left[2\beta - \alpha_i^n - (\alpha_i^n)^2 \right] C_{i+1}^n, \quad (4.85)$$

for all $1 \leq i \leq M-1$.

For $i=0$, we plug the known value of the left boundary by arranging $C_{-1}^n = C_{i+1}^n - (\Delta x)f$ in equation (4.85) on the right-hand side. We obtain;

$$C_i^{n+1} = \left[1 - (\alpha_i^n)^2 - 2\beta - (\Delta t)K \right] C_i^n + [2\beta] C_{i+1}^n - \frac{1}{2} \left[\alpha_i^n - (\alpha_i^n)^2 + 2\beta \right] (\Delta x)f. \quad (4.86)$$

Similarly, for the right boundary condition, for $i=M$, the known value of the right boundary conditions is approximated as $C_{M+1}^n = C_{M-1}^n + (\Delta x)f$ in equation (4.85) and, by rearranging, we obtain;

$$C_i^{n+1} = [2\beta] C_{i-1}^n + \left[1 - (\alpha_i^n)^2 - 2\beta - (\Delta t)K \right] C_i^n + \frac{1}{2} \left[2\beta - \alpha_i^n - (\alpha_i^n)^2 \right] C_{i+1}^n, \quad (4.87)$$

where $\beta = D \frac{\Delta t}{(\Delta x)^2}$, $\lambda_i^n = u_i^n \frac{\Delta t}{\Delta x}$, and $u \approx \tilde{u}_i^n$ which \tilde{u}_i^n are obtained by the Crank-Nicolson method with the hydrodynamic model.

4.3.4 Numerical experiments and results

We use the velocity of water from the hypodermic model in section 4.1 as input for the dispersion model to approximate the pollutant concentration, and obtain the four points explicit upwind methods in equations (4.72), (4.73), (4.75), the upwind explicit methods in equations (4.79 - 4.81), and the Lax-Wendroff methods in equations (4.85 - 4.87). We suppose that the measurement of pollutant concentration (km / m^3) in a non-uniform stream at time (sec) is considered. A stream is aligned with longitudinal distance, 1.0 km total length. There is a plant which discharges waste water into the stream, and the pollutant concentration at discharge point with the initial condition and the boundary conditions are agreeable as $C(0,t) = 0.4 + \sin(t)$ km / m^3 at $x=0$ for all $t > 0$, and $\frac{\partial C}{\partial x}(1,t) = 1$ km / m^3 at $x=1$ for all $t > 0$, and $C(x,0) = 0$ km / m^3 at $t=0$. In the analysis conducted in this experiment, we use the physical parameter of the stream system as being diffusion coefficient $D = 0.02$ (m^2 / s). The approximation of pollutant concentrations of all methods, where

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$\Delta x = 0.2$, $\Delta x = 0.1$ and $\Delta x = 0.05$, are shown in figure 4.25, figure 4.26, and figure 4.27, respectively. It can be seen that the trend of results from the three methods are similar; when we choose a small Δx , the graph will gradually smooth upwards. Table 4.22 shows the stable of the four points explicit upwind methods, the upwind explicit methods, and the Lax-Wendroff methods. We can see that, if we choose $\Delta t = 0.2$ and $\Delta x = 0.06$, then the solution of the four points explicit upwind methods and upwind explicit methods are unstable but the Lax-Wendroff methods is stable. Consequently, the Lax-Wendroff methods gives better results than the four points explicit upwind methods and upwind explicit methods.

Table 4.1 stability of the three methods approximate solutions

Δt	Δx	four points explicit	upwind explicit	Lax-Wendroff
0.005	0.2	stable	stable	stable
	0.1	stable	stable	stable
	0.05	stable	stable	stable
	0.02	stable	stable	stable
0.05	0.2	stable	stable	stable
	0.1	stable	stable	stable
	0.05	unstable	stable	stable
	0.04	unstable	unstable	stable
0.2	0.2	stable	stable	stable
	0.1	unstable	stable	stable
	0.06	unstable	unstable	stable

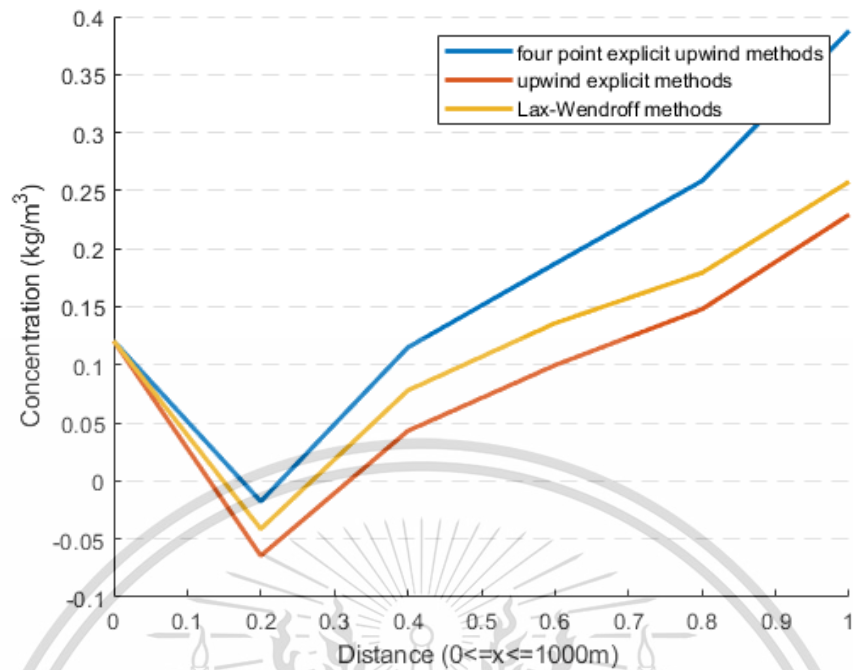


Figure 4.24 Comparison of water pollutant concentration with the four points explicit upwind methods, the upwind explicit methods, and the Lax-Wendroff methods, where $\Delta x = 0.2$

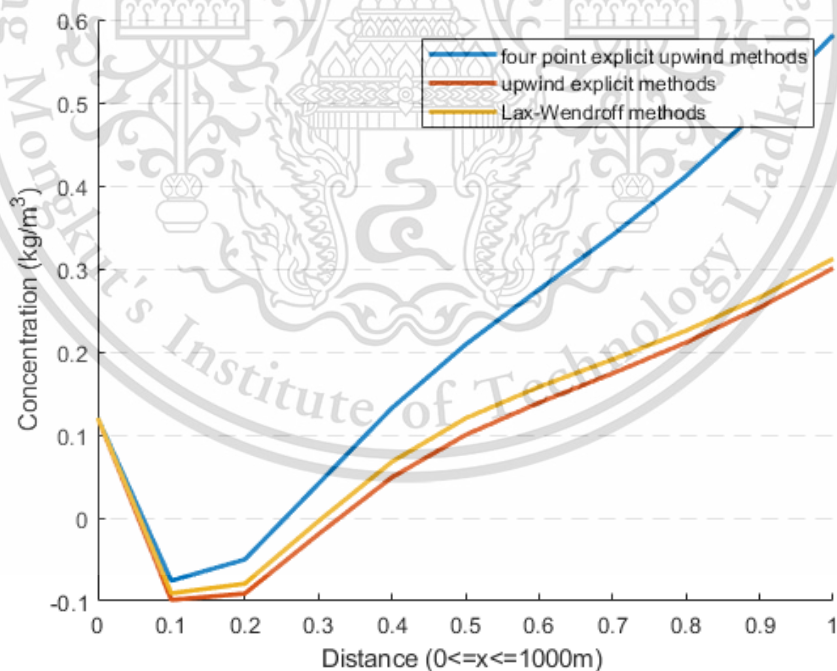


Figure 4.25 Comparison of water pollutant concentration with the four points explicit upwind methods, the upwind explicit methods, and the Lax-Wendroff methods where $\Delta x = 0.1$

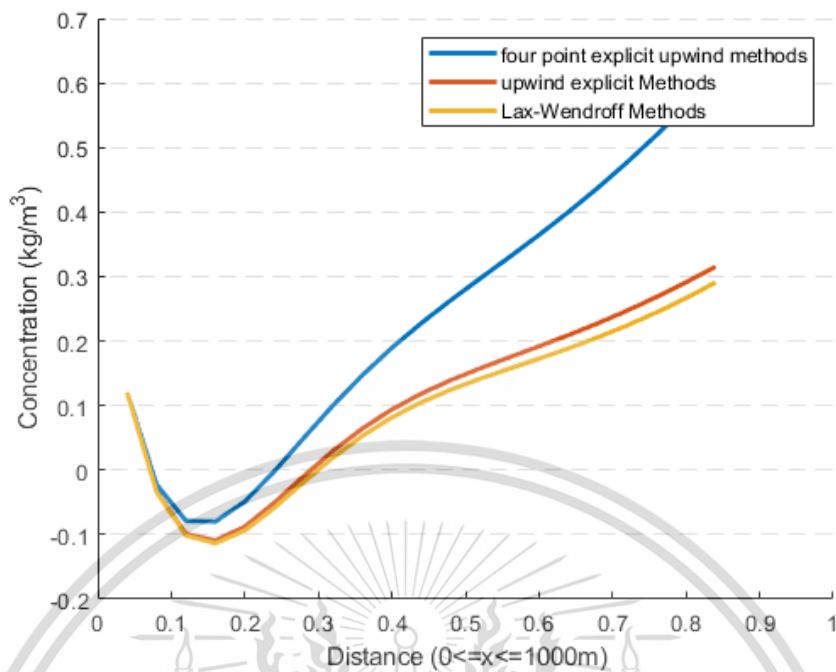


Figure 4.26 Comparison of water pollutant concentration with the four points explicit upwind methods, the upwind explicit methods, and the Lax-Wendroff methods where $\Delta x = 0.05$

Chapter 5

Discussion and Conclusion

5.1 Discussion

For the water quality measurement model in a uniform flow stream, there were two simulations of released water pollutant concentration. [11] had a numerical solution of the advection-diffusion equation with a third-order upwind scheme, which is different from our work. In this study, to simulate the one-dimensional water quality model, we assume that there is a mass decaying rate (K) for the absorber of the pollution concentration. We consider water pollutant concentration that decreased the mass decaying rate in our system problem, increased the mass decaying rate in our system problem, or did not change the mass decaying rate in our system problem. The comparison of approximated solutions of the explicit methods, the Crank-Nicolson methods, the implicit methods, and the modified Siemieniuch-Gladwell methods with advection-diffusion-reaction show that the explicit methods and the modified Siemieniuch-Gladwell methods are in good agreement with the analytical solutions, as shown in table 3.3 and figure 3.1 for simulation A. In simulation B, the explicit methods are in good agreement with the analytical solutions. The approximate solution and the exact solution for the ideal problem are compared. It turns out that the numerical computations give good agreement solutions by the illustrated examples. In simulation A, from figure 3.4 -3.6 for $K=1$, the concentration is lower than $K=0.05$, $K=0.06$. In simulation B, from figure 3.9 - 3.10 for $K=0.1$, the concentration is lower than $K=0.05$.

For the water quality measurement model in a non-uniform flow stream, finite difference techniques for the hydrodynamic model, we use the speed from the hydrodynamic model due to the hydrodynamic model describing water current and elevation by using the system of shallow water equations as the conservation of mass and conservation of momentum, which corresponds to real-world problems. We input velocity of water from the hydrodynamic model into the dispersion model. For the numerical simulation of the hydrodynamic model, we used the Crank-Nicolson methods and assume the mass decaying rate in our system problem corresponds to real-world problems. The comparison of the elevation of water and the velocity of

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water with various mass decaying rates are shown in figure 4.8 and figure 4.9; we can see that the velocity of water levels decreases when 20 seconds have passed. Real-world problems require small amounts of time intervals in order to obtain accurate solutions. Unfavorably, the analytical solutions of the hydrodynamic model can not be found over every domain. This also implies that the analytical solutions of the dispersion model can not work out at any point in the entire domain in either [20] and [22].

Finite difference techniques for the dispersion model are conducted by using third-order upwind schemes; the water pollutant concentration model is presented and the velocity of water from the hydrodynamic model is used. We divide the water pollutant concentration data into three cases. In Case I, we assume that at the end of the river there is a decrease in the rate of change of pollution concentration, such as may be caused by a septic tank at the end of the river. In Case II, we assume that at the end of the river there is no rate of change of pollution concentration (rate of change = 0). In Case III, we assume that at the end of the river there is an increase in the rate of change of pollution concentration, such as may be caused by factories releasing waste water at the end of the river, causing increased pollution concentration. In the three Cases, for a more realistic problem, the mass decaying rate is added in to the domain. The finite difference methods, such as the four points explicit upwind methods, the third order Crank-Nicolson methods, and the four points implicit upwind methods are used so, by figure 4.12 - 4.24, we can see that the mass decay rate of pollutant matter can reduce the concentration in a non-uniform stream.

Finite difference techniques for the dispersion model are conducted by using explicit methods; the water pollutant concentration model is presented. We input the velocity of water from the hydrodynamic model into the dispersion model. The finite difference methods, such as the four points explicit upwind methods, the upwind explicit methods, and the Lax-Wendroff methods, can be used to estimate the water pollutant concentration. Also, it is appealing that the grid spacing is different, so the Lax-Wendroff methods are chosen because, when making comparisons with the four points explicit upwind methods and the upwind explicit methods, in some cases, the solutions for the four points explicit upwind methods and the upwind explicit methods are unstable, while the solutions for the Lax-Wendroff methods are stable. Hence,

the Lax-Wendroff methods provide a better result than the four points explicit upwind methods or the upwind explicit methods.

5.2 Conclusion

The finite difference techniques for the one-dimensional water quality model are proposed. The approximate solutions and the analytical solutions for the problem are compared. It turns out that the numerical computations are in reasonable agreement with the solutions obtained using illustrated simulations. Figures 3.1 - 3.10, show that, when the mass decay rate increases, the concentration in a uniform flow stream can reduce.

We then combine the hydrodynamic model and the convection-diffusion-reaction equation for an approximation of the pollutant concentration in a stream when the velocity of the current is non-uniform. With the technique in this thesis, the solution at each point in the stream when using the velocity of water and the pollutant concentration at the discharge point can be computed. The technique constructed in this study can respond to the aspects of the stream in two varied external inputs, which are the level of water and the pollutant concentration at the end of the river. All of the four points explicit upwind methods, third order Crank-Nicolson methods, and four points implicit methods can be used in the dispersion model; we consider that the proposed technique is applicable and economical due to its simplicity to program and the straightforwardness of the implementation. It is also possible to find tentative better locations and better periods of time for the different discharge points in the stream.

We have employed explicit finite difference methods to the dispersion model in a stream while there are two different external factors, the velocity of water and the discharged pollutant. Three explicit finite difference techniques are economical. It is shown that the Lax-Wendroff methods are more stable than the upwind explicit methods and the four points explicit methods.

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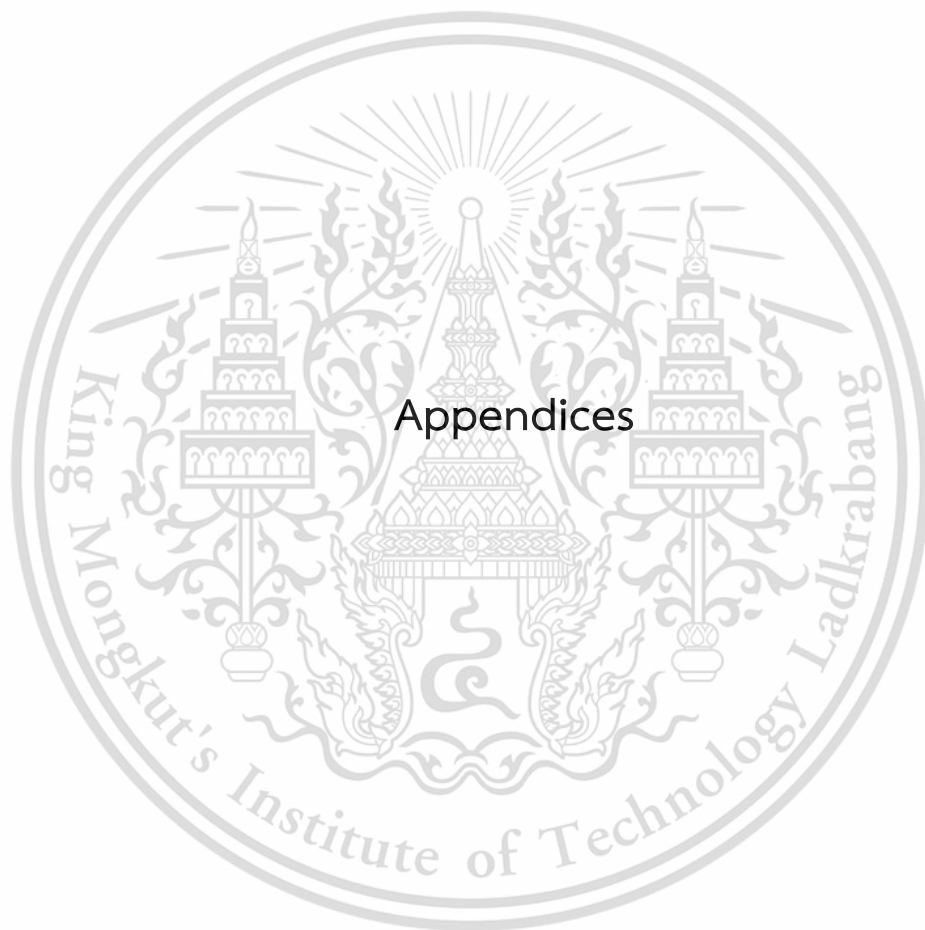
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Numerical Computation of a Water-Quality Model with Advection-Diffusion-Reaction Equation Using an Upwind Implicit Scheme

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Abstract : In this research, numerical computations of water-quality model in a uniform flow stream are proposed. The governing equation, which is an advection-diffusion-reaction equation, is approximated by using a finite difference technique. The upwind implicit scheme is used to approximate the pollutant concentration in each point at all times on a uniform flow stream. The accurate of the proposed computation technique is compared with the analytical and approximated solutions show in the examples.

Keywords : advection-diffusion-reaction equation; water-quality model; uniform flow stream; upwind implicit scheme

2000 Mathematics Subject Classification : 35K57; 65M06; 76R99;
(2000 MSC)

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1 Introduction

The mathematical simulation is an important method to detect the water quality assumption in consideration area. There are many people using the numerical scheme for approximating direction advection diffusion reaction equation by using the finite difference method [1], [2], [3], [4], [5] and [6]. The numerical techniques for solving the uniform flow of stream water quality model, especially the one-dimensional advection diffusion reaction equation, are presented in [7]-[11]. In the recent year, the water quality model in a nonuniform flow of stream, one-dimensional hydrodynamic advection diffusion reaction equations is presented in [12] by using the fully implicit schemes are propose. In this research, we used the finite difference technique to approximate the pollutant concentration in a uniform flow stream using an upwind implicit scheme.

2 The governing equation

A one-dimensional water quality model is described the mass transport and diffusion processes. It can be modeled in the advection-diffusion-reaction equations (ADREs).

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} - Kc, \quad 0 < x < L, \quad 0 < t \leq T. \quad (2.1)$$

where $c(x, t)$ is the pollutant concentration (kg/m^3) of water at the displacement x (m) and time t (s) for all $(x, t) \in (0, L) \times (0, T)$, $u(x, t)$ is the velocity in x direction (m/s), D is the diffusion coefficient (m^2/s) and K is the mass decaying rate (s^{-1}) with the potential pollutant concentration as the initial condition,

$$c(x, 0) = f(x), \quad 0 \leq x \leq L, \quad (2.2)$$

and the released pollutant concentration on the left boundary and the right boundary

$$(0, t) = g(t), \quad 0 < t \leq T, \quad (2.3)$$

$$(L, t) = h(t), \quad 0 < t \leq T, \quad (2.4)$$

the initial condition and the boundary conditions are illustrated in Fig. 1.

3 Numerical Techniques

We consider both implicit and explicit methods to approximate the solution of the advection-diffusion-reaction equations (ADREs).

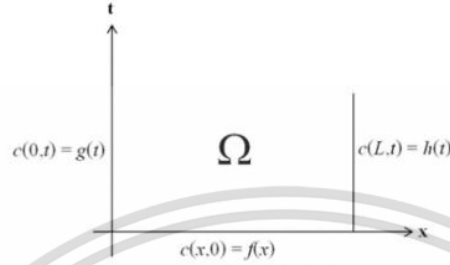


Figure 1: The initial condition and boundary conditions.

3.1 A third-order finite difference schemes

The solution domain of the problem is covered by a mesh of grid point x (x_i, t_n) by $x_i = i\Delta x$, $i = 0, 1, 2, \dots, M$, and $t_n = n\Delta t$, $n = 0, 1, 2, \dots, N$, where x_i and t_n are parallel to the space and time coordinate axes. We can approximate $c(x_i, t_n)$ by c_i^n , value of the difference approximation of $c(x, t)$. The constant spatial and time increment grid-spacing are $\Delta x = L/M$ and $\Delta t = T/N$. From [13], we get the following discretization, the time derivative $t = n\Delta t$ by using forward-difference,

$$\frac{\partial c}{\partial t} \approx \frac{c_i^{n+1} - c_i^n}{\Delta t}, \quad (3.1)$$

to approximate the advective term in the advection diffusion reaction equation which incorporate temporal weight parameter (ϕ), near the left boundary, for $i = 2$,

$$u \frac{\partial c}{\partial x} \approx \frac{u}{6\Delta t} [\phi(-11c_i^{n+1} + 18c_{i+1}^{n+1} - 9c_{i+2}^{n+1} + 2c_{i+3}^{n+1}) + (1-\phi)(-11c_i^n + 18c_{i+1}^n - 9c_{i+2}^n + 2c_{i+3}^n)], \quad (3.2)$$

interior nodes of the solution domain, for $i = 3, \dots, M-2$,

$$u \frac{\partial c}{\partial x} \approx \frac{u}{6\Delta t} [\phi(c_{i-2}^{n+1} - 6c_{i-1}^{n+1} + 3c_i^{n+1} + 2c_{i+1}^{n+1}) + (1-\phi)(c_{i-2}^n - 6c_{i-1}^n + 3c_i^n + 2c_{i+1}^n)], \quad (3.3)$$

near right boundary, for $i = M-1$

$$u \frac{\partial c}{\partial x} \approx \frac{u}{6\Delta t} [\phi(-2c_{i-3}^{n+1} + 9c_{i-2}^{n+1} - 18c_{i-1}^{n+1} + 11c_i^{n+1}) + (1-\phi)(-2c_{i-3}^n + 9c_{i-2}^n - 18c_{i-1}^n + 11c_i^n)], \quad (3.4)$$

the diffusive term by using central-difference scheme,

$$\frac{\partial^2 c}{\partial x^2} \approx \frac{D}{\Delta x^2} [c_{i-1}^n - 2c_i^n + c_{i+1}^n]. \quad (3.5)$$

We can assume each term by substituting Eqs. (3.1)-(3.5) into Eq.(2.1), we obtain the computed solution near left boundary, for $i = 2$,

$$\begin{aligned} c_i^{n+1} = & ((1 - K\Delta t)c_i^n - \frac{1}{6}Cr[\phi(18c_{i+1}^{n+1} - 9c_{i+2}^{n+1} + 2c_{i+3}^{n+1}) \\ & + (1 - \phi)(-11c_i^n + 18c_{i+1}^n - 9c_{i+2}^n + 2c_{i+3}^n)] \\ & + \frac{Cr}{Pe}[c_{i-1}^n - 2c_i^n + c_{i+1}^n]) / (1 - \frac{11}{6}Cr\phi). \end{aligned} \quad (3.6)$$

Interior nodes of the solution domain, for $i = 3, \dots, M - 2$,

$$\begin{aligned} c_i^{n+1} = & ((1 - K\Delta t)c_i^n - \frac{1}{6}Cr[\phi(c_{i-2}^{n+1} - 6c_{i-1}^{n+1} + 2c_{i+1}^{n+1}) \\ & + (1 - \phi)(c_{i-2}^n - 6c_{i-1}^n + 3c_i^n + 2c_{i+1}^n)] \\ & + \frac{Cr}{Pe}[c_{i-1}^n - 2c_i^n + c_{i+1}^n]) / (1 + \frac{1}{2}Cr\phi). \end{aligned} \quad (3.7)$$

Near the right boundary, for $i = M - 1$,

$$\begin{aligned} c_i^{n+1} = & ((1 - K\Delta t)c_i^n - \frac{1}{6}Cr[\phi(-2c_{i-3}^{n+1} + 9c_{i-2}^{n+1} - 18c_{i-1}^{n+1}) \\ & + (1 - \phi)(-2c_{i-3}^n + 9c_{i-2}^n - 18c_{i-1}^n + 11c_i^n)] \\ & + \frac{Cr}{Pe}[c_{i-1}^n - 2c_i^n + c_{i+1}^n]) / (1 + \frac{11}{6}Cr\phi). \end{aligned} \quad (3.8)$$

where $Cr = \frac{u\Delta t}{\Delta x}$ is Courant number (dimensionless), $Pe = \frac{u\Delta x}{D}$ is Peclet number (dimensionless) and $\phi \in \{0, 0.5, 1\}$.

3.2 The modified Siemieniuch-Gladwell implicit scheme

The modified Siemieniuch-Gladwell technique for solving the one-dimensional advection diffusion reaction Eq. (2.1) following:

$$\begin{aligned} \frac{\partial c}{\partial t} \approx & \left(\frac{2\frac{Cr}{Pe} - Cr}{4} \right) \left(\frac{c_{i-1}^{n+1} - c_{i-1}^n}{\Delta t} \right) + \left(\frac{2 - 2\frac{Cr}{Pe} + Cr}{2} \right) \left(\frac{c_i^{n+1} - c_i^n}{\Delta t} \right) \\ & + \left(\frac{2\frac{Cr}{Pe} - Cr}{4} \right) \left(\frac{c_{i+1}^{n+1} - c_{i+1}^n}{\Delta t} \right), \end{aligned} \quad (3.9)$$

$$\frac{\partial c}{\partial x} \approx \left(\frac{c_{i+1}^n - c_{i-1}^n}{4\Delta x} \right) + \left(\frac{c_{i+1}^{n+1} - c_{i-1}^{n+1}}{4\Delta x} \right), \quad (3.10)$$

$$\frac{\partial^2 c}{\partial x^2} \approx \frac{1}{2} \left(\frac{c_{i+1}^{n+1} - 2c_i^{n+1} + c_{i-1}^{n+1}}{(\Delta x)^2} \right) + \frac{1}{2} \left(\frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta x)^2} \right), \quad (3.11)$$

substituting Eqs. (3.9-3.11) into Eq.(2.1), we have

$$\begin{aligned} -Crc_{i-1}^{n+1} + (2 + Pe)c_i^{n+1} &= \left(2\frac{Cr}{Pe}\right)c_{i-1}^n + \left(2 - 4\frac{Cr}{Pe} + Pe - 2K\Delta\right)c_i^n \\ &+ \left(2\frac{Cr}{Pe} - Pe\right)c_{i+1}^n, \end{aligned} \quad (3.12)$$

for $i = 1, 2, \dots, M - 1$.

4 Numerical Experiments

Example 1. The analytical solution to the one-dimensional advection-diffusion in a region bounded $0 \leq x \leq 1$ is taken from [13] and given,

$$c(x, t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}} \exp\left[-\frac{(x + 0.5 - t)^2}{(0.00125 + 0.004t)}\right], \quad (4.1)$$

the initial condition

$$c(x, 0) = \exp\left[-\frac{(x + 0.5)^2}{0.00125}\right], \quad (4.2)$$

and the boundary conditions

$$c(0, t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}} \exp\left[-\frac{(0.5 - t)^2}{(0.00125 + 0.004t)}\right], \quad (4.3)$$

$$c(1, t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}} \exp\left[-\frac{(1.5 - t)^2}{(0.00125 + 0.004t)}\right]. \quad (4.4)$$

In the analysis conducted in this study the various parameters used are $D = 0.01 \text{ m}^2/\text{s}$, $u = 1 \text{ m/s}$, meshes the stream into 50 elements with the space step and time step are $\Delta x = 0.02 \text{ m}$ and $\Delta t = 0.002 \text{ s}$, respectively. Using a third order finite difference scheme Eqs. (3.6-3.8) and the modified Siemieniuch-Gladwell method Eq. (3.12) to obtain the pollutant concentration $c(x, t)$ in each point at all time on a uniform flow stream. As can see from Eqs. (3.6-3.8), $\phi = 0$ the formula corresponding to the explicit expansion of the advective term, $\phi = 1$ the formula corresponding to the explicit expansion and $\phi = 0.5$ the formula corresponding to the Crank-Nicolson scheme. The approximation of pollutant concentrations c of all schemes are shown in Table 1- Table 4. The comparison of approximated solutions of an explicit, an implicit, the Crank-Nicolson schemes, the modified Siemieniuch-Gladwell with advection diffusion reaction are shown in Fig. 2.

Table 1: The computed pollutant concentrations $c(x, t)$ (kg/m^3) when $K = 0.01$ (s^{-1}).

The concentrations at $T=1$ s							
Solution technique	0.00	0.20	0.40	0.50	0.60	0.80	1.00
Explicit	0.0004	0.0184	0.1392	0.1827	0.1410	0.0143	0.0004
Implicit	0.0004	0.0179	0.1151	0.1459	0.1193	0.0222	0.0004
Crank-Nicolson	0.0004	0.0182	0.1267	0.1632	0.1300	0.0188	0.0004
Siemieniuch-Gladwell	0.0004	0.0194	0.1387	0.1733	0.1335	0.0207	0.0004

Table 2: The computed pollutant concentrations $c(x, t)$ (kg/m^3) when $K = 0.1$ (s^{-1}).

The concentrations at $T=1$ s							
Solution technique	0.00	0.20	0.40	0.50	0.60	0.80	1.00
Explicit	0.0004	0.0194	0.1386	0.1733	0.1334	0.0207	0.0004
Implicit	0.0004	0.0194	0.1386	0.1733	0.1334	0.0207	0.0004
Crank-Nicolson	0.0004	0.0194	0.1386	0.1733	0.1334	0.0207	0.0004
Siemieniuch-Gladwell	0.0004	0.0189	0.1327	0.1650	0.1265	0.0195	0.0004

Table 3: The computed pollutant concentrations $c(x, t)$ (kg/m^3) when $K = 0.5$ (s^{-1}).

The concentrations at $T=1$ s							
Solution technique	0.00	0.20	0.40	0.50	0.60	0.80	1.00
Explicit	0.0004	0.0161	0.1119	0.1430	0.1081	0.0107	0.0004
Implicit	0.0004	0.0156	0.0928	0.1144	0.0915	0.0165	0.0004
Crank-Nicolson	0.0004	0.0159	0.1020	0.1279	0.0997	0.0140	0.0004
Siemieniuch-Gladwell	0.0004	0.0170	0.1114	0.1356	0.1023	0.0154	0.0004

Table 4: The computed pollutant concentrations $c(x, t)$ (kg/m^3) when $K = 1$ (s^{-1}).

The concentrations at $T=1$ s							
Solution technique	0.00	0.20	0.40	0.50	0.60	0.80	1.00
Explicit	0.0004	0.0140	0.0902	0.1121	0.0830	0.0080	0.0004
Implicit	0.0004	0.0136	0.0748	0.0898	0.0703	0.0122	0.0004
Crank-Nicolson	0.0004	0.0138	0.0822	0.1003	0.0765	0.0104	0.0004
Siemieniuch-Gladwell	0.0004	0.0148	0.0896	0.1062	0.0785	0.0115	0.0004

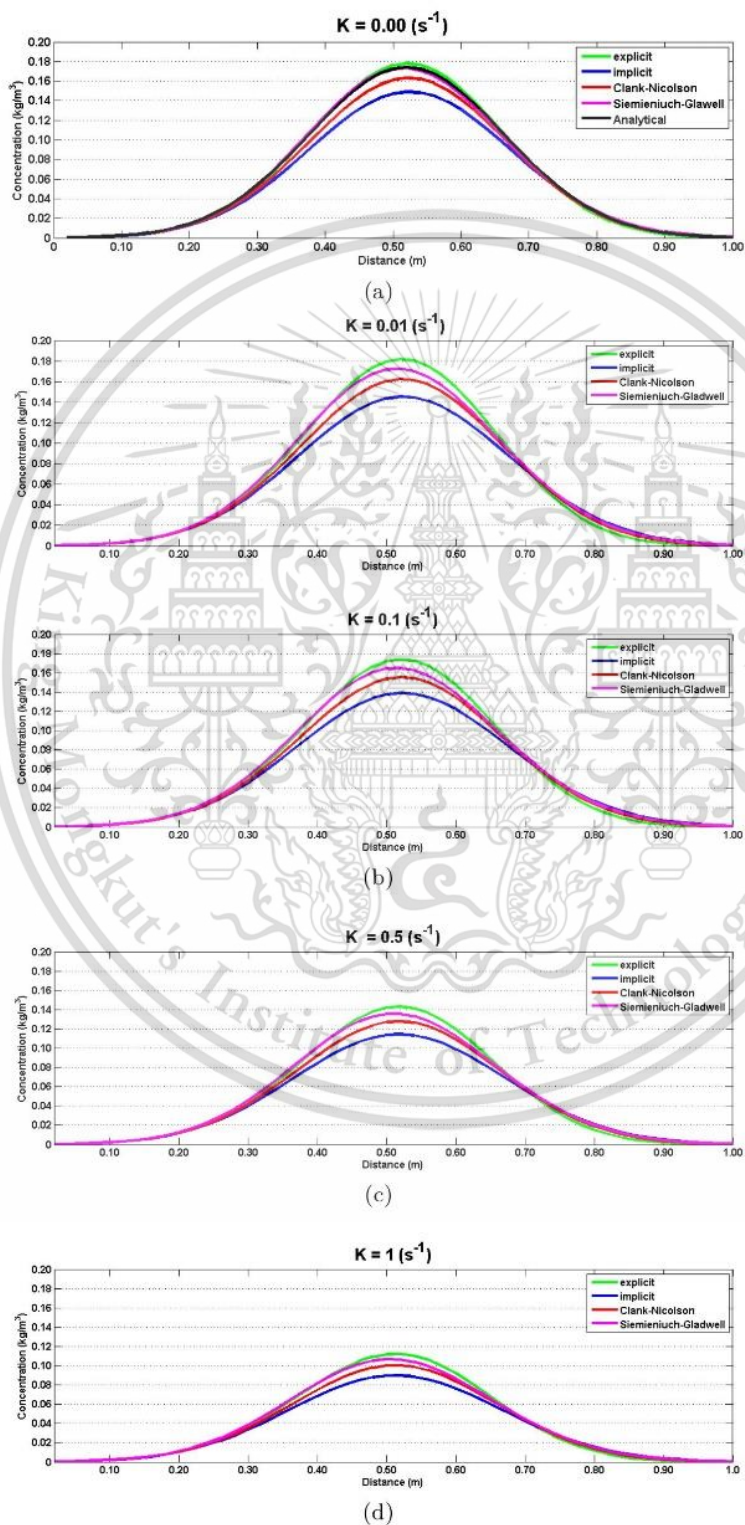


Figure 2: Comparison of numerical solutions techniques at $T = 1$ s for all $0 \leq x \leq 1$ which K are varied 0.00, 0.01, 0.1, 0.5 and 1, respectively. Forbidden to modify the content, and cite the document when use.

Example 2. The analytical solution to the one-dimensional advection-diffusion equation of a Gaussian pulse of unit height, centred at $x_0 = 1$ in a region bounded $0 \leq x \leq 9$ is taken from [14] and given,

$$c(x, t) = \frac{1}{\sqrt{4t+1}} \exp \left[-\frac{(x - x_0 - ut)^2}{D(4t+1)} \right], \quad (4.5)$$

the initial condition

$$c(x, 0) = \exp \left[-\frac{(x - x_0)^2}{D} \right], \quad (4.6)$$

and the boundary conditions

$$c(0, t) = \frac{1}{\sqrt{4t+1}} \exp \left[-\frac{(-1 - ut)^2}{D(4t+1)} \right], \quad (4.7)$$

$$c(1, t) = \frac{1}{\sqrt{4t+1}} \exp \left[-\frac{(8 - ut)^2}{D(4t+1)} \right]. \quad (4.8)$$

The values of the various parameters used $D = 0.005 \text{ m}^2/\text{s}$, $u = 0.8 \text{ m/s}$, meshes the stream into 450 elements with the space step and time step are $\Delta x = 0.02 \text{ m}$ and $\Delta t = 0.002 \text{ s}$, respectively. The approximation of pollutant concentrations c of all schemes are comparison, the solution are obtain an explicit, an implicit, the Crank-Nicolson schemes and the modified Siemieniuch-Gladwell with advection diffusion reaction are shown in Fig. 3.

5 Discussion and Conclusion

The one-dimensional advection-diffusion-reaction equation can be used to describes the pollutant concentration in a uniform water channel. The cross sectional average of pollutant concentration for each point in the flat bottom is considered in this research. Finite difference techniques for the one-dimensional water-quality model are propose. The approximate solution and the exact solution on the ideal problem are compared. It turn out that, the numerical computations give good agreement solutions by illustrated examples.

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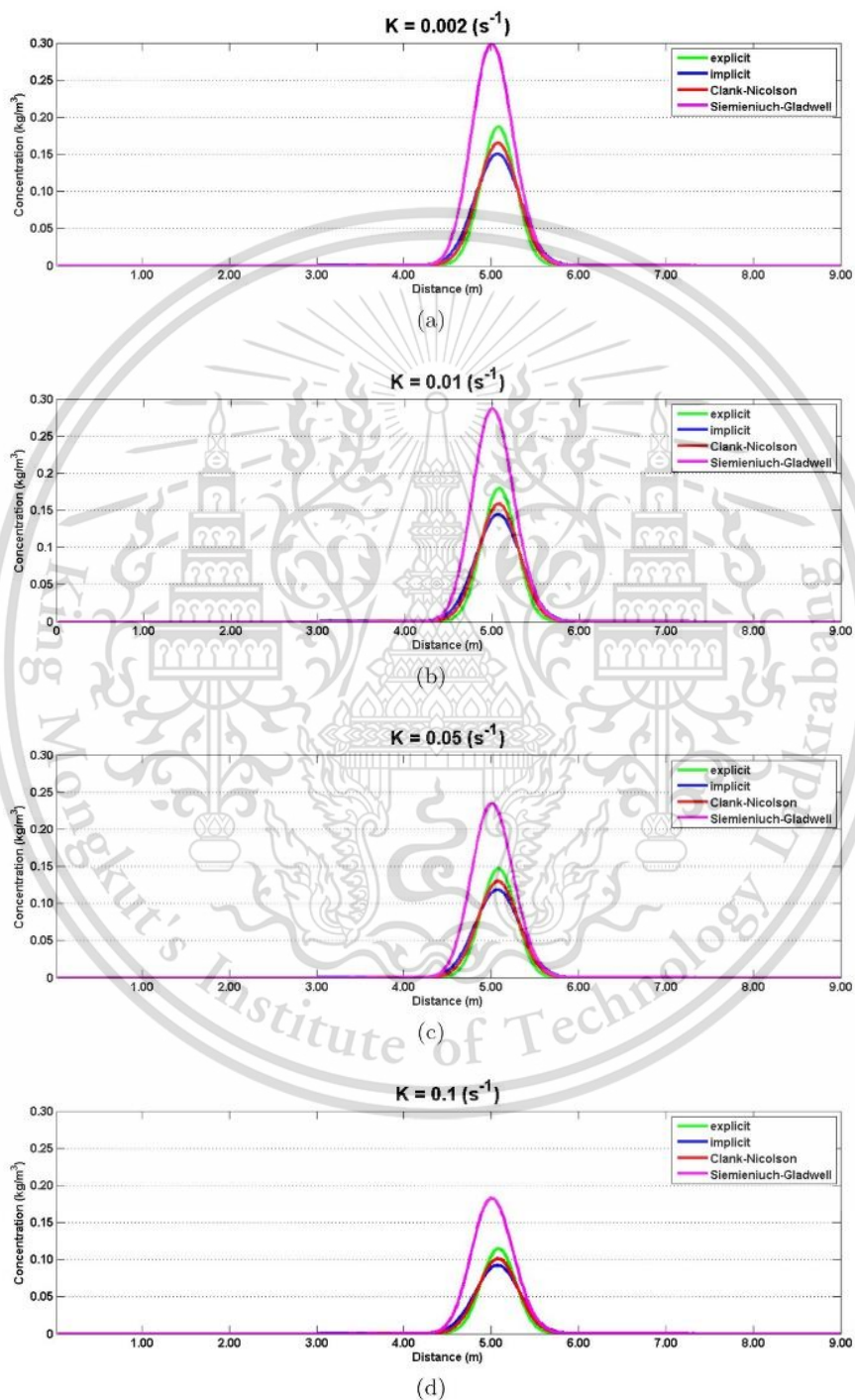


Figure 3: Comparison of numerical solutions techniques at $T = 1 \text{ s}$ for all $0 \leq x \leq 1$ which K are varied 0.002, 0.01, 0.05 and 0.1, respectively.

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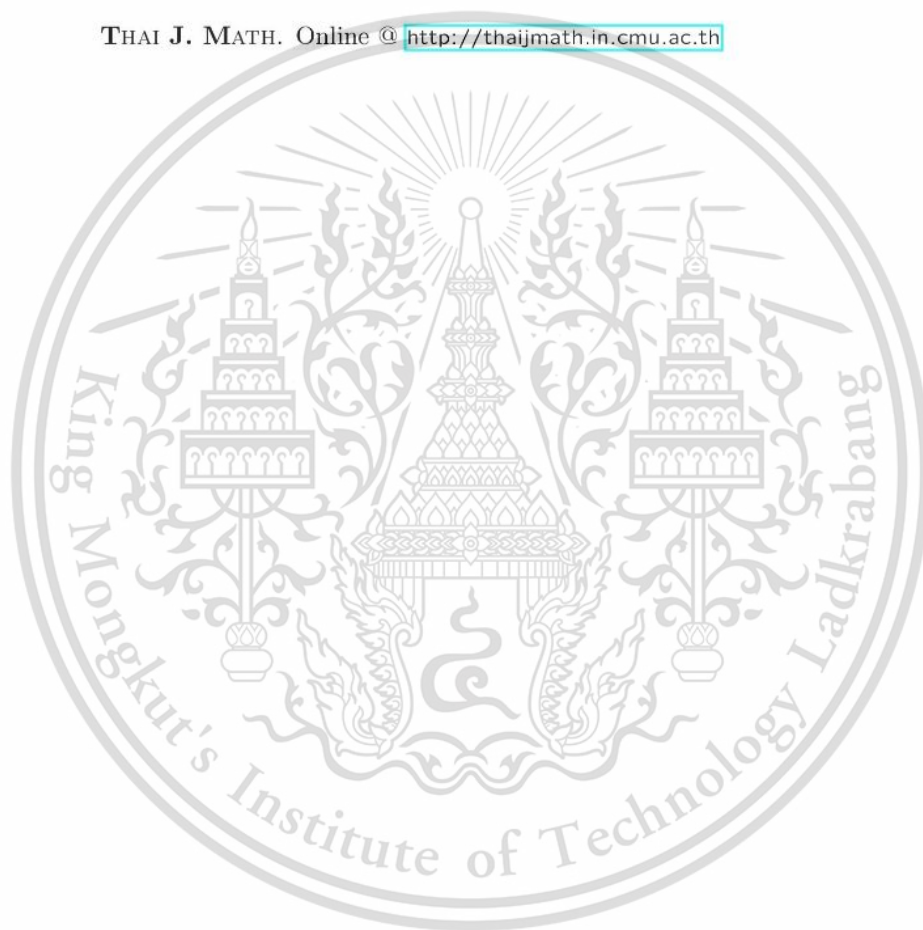
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A Couple Mathematical Models of the Water Quality Measurement in a Stream using Upwind Implicit Methods

Piyada Phosri, Nopparat Pochai

Abstract— Two mathematical models are used to simulate water quality in a non-uniform flow stream. The first model is a hydrodynamic model, which provides the velocity fields and elevation of water by using the Crank-Nicolson method. The second model is a dispersion model, where the governing factor uses advection-dispersion-reaction equations to provide the pollutant concentrations. The first model and second model are formulated as one-dimensional equations. At each step, the first calculated flow velocity fields of the hydrodynamic model are the input into the dispersion model. The finite difference methods are proposed to solve the dispersion model a four points explicit upwind schemes, a third order Crank-Nicolson schemes, and a four points implicit methods, which give the approximated pollutant concentrations. Finally, we present a numerical simulation of all schemes, so as to illustrate their applicability to real-world problems. The proposed technique is applicable and economical to be used in real-world problems due to its simplicity to program and the straight-forwardness of the implementation. It is also possible to find tentative better locations and better periods of time for the different discharge points of a stream.

Index Terms— Finite differences, water quality, one-dimensional, hydrodynamic model, advection-dispersion-reaction.

I. INTRODUCTION

WATER pollution is a major problem; everyone should be aware of this problem. Monitoring water quality can be achieved by field measurement and calculation of data of water current in each position and time. Another way is a mathematical simulation. A water quality model in a non-uniform flow stream must include velocities and elevations. The modeling used in a non-uniform flow stream is hydrodynamic model in a one-dimensional shallow water equation, and a dispersion model in an advection-dispersion equation.

There are many numerical techniques available for solving such models. [1] presented a hydrodynamic model and a dispersion model with the finite element method to solve a steady water pollution control to achieve minimum cost. [2], finite element methods were used in a hydrodynamic model and a dispersion model to simulate pollution in the Bay of Santander. In 2009, [26] presented

a three-dimensional numerical model with the turbulent Reynolds Stress Model (RSM) and a non-uniform grid system was used to examine the effects of a double tandem obstacle cubic on the development of the incoming flow. The results obtained configuration make possible the description of the dynamic and masses features and the determination of the velocity ratio effect on the pollutant distribution. In 2010, [27] studied Padé schemes for the numerical solution of two-dimensional diffusion equations with nonlocal boundary conditions. The numerical results show that these Padé schemes are efficient and provide very accurate results. In 2015, [28] mathematical model is used to air flow and pollutant dispersion in an Urban Street Canyon with Steady Wind Boundary Conditions (SWBC) and developed the Fluctuating Wind Boundary Conditions (FWBC). Three dimensional (3D) numerical simulations are performed using Large Eddy Simulation (LES), the results of FWBC produces more realistic results when compared to the frequently employed SWBC. In 2018, [29] proposed numerical developments on the coal combustion and gasification by using CFD (Computational Fluid Dynamics) techniques with an Eddy Break Up (EBU) model. The results of the simulation show that the H₂ and CH₄ products from the gasification are significantly higher than those from the combustion. This particle model can thus be considered for further investigation for various coal combustion and gasification applications. [3-7], proposed numerical techniques to solve a uniform flow of stream water quality model, especially the one-dimensional advection-dispersion-reaction equation.

Most non-uniform flow models require data concerned with the velocity of a current at any point and any time in a domain. The hydrodynamics model provides flow velocity fields and elevation of the water. In [1, 9-13], the hydrodynamics model was used to approximate the velocity of water currents, and the advection-dispersion equation to simulate pollutant concentration in bays, uniform reservoirs, and streams. In all the numerical techniques, the explicit finite difference methods and implicit finite difference methods are mostly used for one-dimensional domains such as in longitudinal stream systems [14, 15].

Mathematical models are used to simulate water quality in a non-uniform water flow systems. The first is a hydrodynamic model that provides velocity field and elevation of water, and the second is a dispersion model that gives the pollutant concentration. Twin models are formulated in one-dimensional equations. The traditional

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Crank-Nicolson method is also used in the hydrodynamic model. At each step, the flow velocity fields calculated from the first model are the input into the second model as the field data, presented by [10-13, 16-17]

In [11], numerical techniques were used to solve the non-uniform flow of stream water quality model with one-dimensional advection-dispersion-reaction equation by using the fully implicit scheme: Crank-Nicolson method for the hydrodynamic model, and backward time central space (BTCS) for the dispersion model. [16], used the Crank-Nicolson method to solve the hydrodynamic model, and the explicit Saul'yev scheme used to solve the dispersion model. In [17], the Crank-Nicolson method was used in the hydrodynamic model and a modified MacCormack method used in the dispersion model for one-dimensional advection-dispersion-reaction equation.

Most researches on finite difference method have considered numerical accuracy and stability. There are several high-quality numerical schemes; [18] proposed a numerical dispersion by introducing an up-stream interpolation method, namely, QUICK (Quadratic Upstream Interpolation Convective Kinematics), for one-dimensional unsteady flow. [4] proposed simple revisions to these schemes that make them more accurate without significant loss of computation efficiency. [19] presented a third-order upwind difference that is used for the convection terms of the convection-diffusion equation. [20], proposed a third-order upwind scheme for the convective terms of shallow water momentum equations. [21] used a third-order upwind scheme for the advection-diffusion equation using a simple spreadsheets simulation.

The data of the water flow velocity derived from the hydrodynamic model are used for the dispersion model with advection-dispersion-reaction equation, which provides the pollutant concentration field. The term of friction forces, due to the drag of sides of the stream, is considered. The theoretical solution of the model at the end point of the domain, which guarantees the accuracy of the approximate solution, is presented in [10-11, 16-17].

In this research, the hydrodynamic model and dispersion model are used to describe water flow and water pollutant concentration. A couple of mathematical models are used to simulate water-quality in the problem. The stream has a simple one space dimension, as shown in Fig. 1; averaging the equation over the depth, discarding the term due to Coriolis force, it follows that the one-dimensional shallow water and advection-diffusion-reaction equations are applicable. The first model is the hydrodynamic model that provides the velocity fields and elevation of water. The Crank-Nicolson method is used in the hydrodynamic model. At each step, the flow velocity fields calculated from the first model are the input into the second model as the field data. The second model is the dispersion model that provides the pollutant concentration fields. We use a four points explicit upwind schemes, a third order Crank-Nicolson schemes, and a four points implicit schemes to approximate the concentration from the dispersion models.

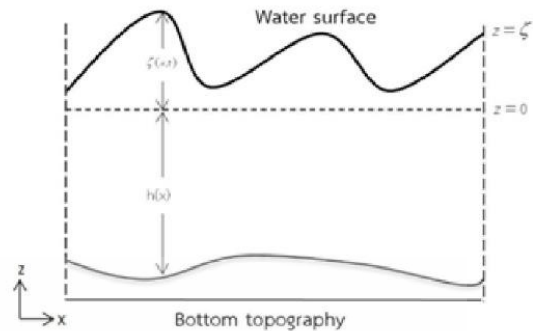


Fig. 1. The shallow water system

II. MODEL FORMULATION

A. The Hydrodynamic Model

The continuity and momentum equations are governed by the hydrodynamic behavior of the stream, which are described by one-dimensional shallow water equations obtained by integrating the Navier-Stokes equations over the flow depth; under the assumptions discarding diffusion of momentum due to turbulence and discarding the terms due to friction and wind [1, 10-14, 22], we obtain the one-dimensional shallow water equations;

$$\frac{\partial \zeta}{\partial t} + \frac{\partial}{\partial x} [(h + \zeta)u] = 0, \quad (1)$$

$$\frac{\partial u}{\partial t} + g \frac{\partial \zeta}{\partial x} = 0, \quad (2)$$

where x is the longitudinal distance along a stream (m), time t (s^{-1}), $h(x)$ is the depth measured from the mean water to the bed of reservoir (m), $\zeta(x, t)$ is the elevation from the mean water level to the temporary water surface (m/s), and $u(x, t)$ are the velocity components (m/s), for all $x \in [0, L]$. We assume that h is a constant and $\zeta \ll h$.

Then (1) and (2) become;

$$\frac{\partial \zeta}{\partial t} + h \frac{\partial u}{\partial x} = 0, \quad (3)$$

$$\frac{\partial u}{\partial t} + g \frac{\partial \zeta}{\partial x} = 0. \quad (4)$$

We will transform (3) and (4) into non-dimensional [23], by letting $U = u / \sqrt{gh}$, $Y = y/l$, $X = x/l$, $Z = \zeta/h$ and $T = t\sqrt{gh}/l$. Substituting into (3) and (4) leads to;

$$\frac{\partial Z}{\partial T} + \frac{\partial U}{\partial X} = 0, \quad (5)$$

$$\frac{\partial U}{\partial T} + \frac{\partial Z}{\partial X} = 0. \quad (6)$$

[10 – 11, 16], introduced a damping term $-U$ into (6). We now introduce a damping term $-KU$ (6) to represent frictional forces due to the drag of sides of the stream, thus;

$$\frac{\partial Z}{\partial T} + \frac{\partial U}{\partial X} = 0, \quad (7)$$

$$\frac{\partial U}{\partial T} + \frac{\partial Z}{\partial X} = -KU, \quad (8)$$

where $0 < K < 1$, with the initial conditions at $t=0$ and $0 \leq X \leq 1$ being specified: $Z=0$ and $U=0$. The boundary conditions for $t > 0$ are specified: $Z=e^t$ at $X=0$ and $\frac{\partial Z}{\partial X}=0$ at $X=1$. The system of (7) and (8) is called the damped hydrodynamic equations.

B. A Non-dimensional form of the Damped Hydrodynamic Model

In order to solve damped equation in $[0,1] \times [0,T]$, for favorable using u,d for U and Z , respectively;

$$\frac{\partial u}{\partial t} + \frac{\partial d}{\partial x} = -ku, \quad (9)$$

$$\frac{\partial d}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad (10)$$

with the initial conditions $u=0, d=0$ at $t=0$, and the boundary conditions $d(0,t)=f(t)$, and $\frac{\partial d}{\partial x}=0$ at $x=1$.

C. Dispersion Model

The stream water quality model can be described by one-dimensional advection-dispersion-reaction equations (ADRE). A simplified representation by averaging the equation over the depth is shown in [3-5, 7, 11-13] as:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2} - KC, \quad (11)$$

where $C(x,t)$ is the concentration averaged in depth at the point x and at time t , D is the diffusion coefficient, K is the mass decay rate, and $u(x,t)$ is the velocity component, for all $x \in [0,L]$. We will consider conditions in this model following. The initial condition $C(x,0)=0$ at $t=0$ for all $x > 0$. The boundary conditions $C(0,t)=C_0$ at $x=0$, and $\frac{\partial C}{\partial X}=C_0$ at $x=1$ where C_0 is a constant.

III. CRANK-NICOLSON METHOD FOR THE HYDRODYNAMIC MODEL

The hydrodynamic model provides the velocity field and elevation of the water. Then, input the results from the hydrodynamic model into the dispersion model, which provides the pollutant concentration field. In this section, we will follow the numerical techniques of [10]. To find the water velocity and water elevation from (9) and (10), we make the following change to variables $v=e^{kt}u$ and represent into (9) and (10). Then we have,

$$\frac{\partial v}{\partial t} + e^{kt} \frac{\partial d}{\partial x} = 0, \quad (12)$$

$$\frac{\partial d}{\partial t} + e^{-kt} \frac{\partial v}{\partial x} = 0. \quad (13)$$

From (12) and (13) can be written in the matrix form

$$\begin{pmatrix} v \\ d \end{pmatrix}_t + \begin{bmatrix} 0 & e^{kt} \\ e^{-kt} & 0 \end{bmatrix} \begin{pmatrix} v \\ d \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (14)$$

That is

$$U_t + AU_x = \bar{0}, \quad (15)$$

where

$$A = \begin{bmatrix} 0 & e^{kt} \\ e^{-kt} & 0 \end{bmatrix}, \quad (16)$$

$$U = \begin{pmatrix} v \\ d \end{pmatrix}_t, \begin{pmatrix} v \\ d \end{pmatrix}_x = \begin{pmatrix} \frac{\partial v}{\partial t} \\ \frac{\partial d}{\partial t} \end{pmatrix}, \begin{pmatrix} v \\ d \end{pmatrix}_x = \begin{pmatrix} \frac{\partial v}{\partial x} \\ \frac{\partial d}{\partial x} \end{pmatrix}, \quad (17)$$

with initial condition $d,v=0$ at $t=0$. The left boundary conditions for $x=0, t > 0$ is specified: $d(0,t)=\text{sint}$ and $\frac{\partial v}{\partial x} = -e^{kt} \text{cost}$, and the right boundary conditions for

$x=1, t > 0$ is specified: $\frac{\partial d}{\partial x}=0$ and $v(0,t)=0$. We now

discretize (15) by dividing the interval $[0,1]$ into M subintervals, such that $M\Delta x=1$, and the interval $[0,T]$ into N subintervals, such that $N\Delta t=T$. We can then approximate $d(x,t_n)$ by d_i^n , value of the difference approximation of $d(x,t)$ at point $x=i\Delta x$ and $t=n\Delta t$, where $0 \leq i \leq M$ and $0 \leq n \leq N$, and similarly defined for v_i^n and U_i^n . The grid points (x_n, t_n) are defined by $x_i = i\Delta x$ for all $i=0,1,2,\dots,M$ and $t_n = n\Delta t$ for all $n=0,1,2,\dots,N$, in which M and N are positive integers. Using the Crank-Nicolson method [23] with (15), the following finite difference equation can be obtained;

$$\left[I - \frac{1}{4} \kappa A [(\Lambda_x + \nabla_x)] U_i^{n+1} \right] = \left[I + \frac{1}{4} \kappa A [(\Lambda_x + \nabla_x)] U_i^n \right], \quad (18)$$

where

$$U_i^n = \begin{pmatrix} v_i^n \\ d_i^n \end{pmatrix}, \Lambda_x U_i^n = U_{i+1}^n - U_i^n, \nabla_x U_i^n = U_i^n - U_{i-1}^n, \quad (19)$$

and I is the unit matrix of order 2, and $\kappa = \frac{\Delta t}{\Delta x}$. Applying the initial and boundary conditions given in (12) - (13), the general form can be obtained;

$$G^{n+1} \bar{U}^{n+1} = E^n \bar{U}^n + F^n, \quad (20)$$

where

$$G^{n+1} = \begin{bmatrix} 1 & 0 & 0 & -\frac{\kappa}{4} a_1^{n+1} & 0 & 0 \\ \frac{\kappa}{4} a_2^{n+1} & 1 & -\frac{\kappa}{4} a_2^{n+1} & 0 & 0 & 0 \\ 0 & \frac{\kappa}{4} a_1^{n+1} & 1 & 0 & 0 & -\frac{\kappa}{4} a_1^{n+1} \\ \frac{\kappa}{4} a_2^{n+1} & 0 & 0 & 1 & -\frac{\kappa}{4} a_2^{n+1} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \frac{\kappa}{4} a_1^{n+1} & 1 & -\frac{\kappa}{4} a_1^{n+1} \\ 0 & 0 & \frac{\kappa}{4} a_2^{n+1} & 0 & 0 & 1 \end{bmatrix}, \quad (21)$$

$$E^n = \begin{bmatrix} 1 & 0 & 0 & -\frac{\kappa}{4}a_1^n & 0 & 0 \\ -\frac{\kappa}{4}a_2^n & 1 & \frac{\kappa}{4}a_2^n & 0 & 0 & 0 \\ 0 & -\frac{\kappa}{4}a_1^n & 1 & 0 & 0 & \frac{\kappa}{4}a_1^n \\ -\frac{\kappa}{4}a_2^n & 0 & 0 & 1 & \frac{\kappa}{4}a_2^n & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & -\frac{\kappa}{4}a_1^n & 1 & \frac{\kappa}{4}a_1^n \\ 0 & 0 & -\frac{\kappa}{4}a_2^n & 0 & 0 & 1 \end{bmatrix},$$

$$\bar{U}^n = \begin{pmatrix} U_1^{n+1} \\ U_2^{n+1} \\ \vdots \\ U_3^{n+1} \end{pmatrix},$$

$$I^n = \begin{bmatrix} -\frac{\kappa}{4}a_1^{n+1}\sin(t_{n+1}) - \frac{\kappa}{4}a_1^n\sin(t_n) \\ -\frac{\kappa}{4}a_2^{n+1}\Delta x e^{-t_{n+1}}\cos(t_{n+1}) - \frac{\kappa}{4}a_2^n\Delta x e^{-t_n}\cos(t_n) \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix},$$

where $a_1^n = e^{kx_n}$, $a_2^n = e^{-kx_n}$ and $t_n = n\Delta t$ for all $n=0,1,2,\dots,N$.

IV. FINITE DIFFERENCE TECHNIQUES FOR THE DISPERSION MODEL

In this section, we consider the numerical techniques in [21] for the advection-dispersion-reaction equation which provides the pollutant concentration field. We can approximate $C(x_i, t_n)$ by C_i^n , the value of the difference approximation of $C(x, t)$ at point $x=i\Delta x$ and $t=n\Delta t$, where $1 \leq i \leq M$, and $0 \leq n \leq N$. The grid point (x_i, t_n) is defined by $x_i = i\Delta x$ for all $i=0,1,2,\dots,M$, and $t_i = n\Delta t$ for all $n=0,1,2,\dots,N$ in which M and N are positive integers.

A Third-Order Upwind Schemes

We consider the numerical techniques [21], using the forward times central space scheme for the times derivatives and the central difference for the second times derivatives, respectively, as follows;

$$\frac{\partial C}{\partial t} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad (24)$$

$$\frac{\partial^2 C}{\partial x^2} \cong \frac{1}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n], \quad (25)$$

using a third-order scheme for the spatial derivative of advection-dispersion-reaction equations, as given in [15]. For the boundary points, a four-point upwind formula may be written, such that either point to the left or to the right is considered in the finite difference approximation. Next, we approximate the spatial derivative for a four points explicit upwind schemes, a third order Crank-Nicolson schemes, and

a four points implicit schemes at left boundary conditions, respectively, as follows;

$$\frac{\partial C}{\partial x} \cong \frac{1}{6\Delta x} [-11C_i^n + 18C_{i+1}^n - 9C_{i+2}^n + 2C_{i+3}^n], \quad (26)$$

$$\frac{\partial C}{\partial x} \cong \frac{1}{12\Delta x} [-11C_i^{n+1} + 18C_{i+1}^{n+1} - 9C_{i+2}^{n+1} + 2C_{i+3}^{n+1}], \quad (27)$$

$$\frac{\partial C}{\partial x} \cong \frac{1}{6\Delta x} [-11C_i^{n+1} + 18C_{i+1}^{n+1} - 9C_{i+2}^{n+1} + 2C_{i+3}^{n+1}]. \quad (28)$$

At the interior nodes, as follows, respectively,

$$\frac{\partial C}{\partial x} \cong \frac{1}{6\Delta x} [C_{i-2}^n - 6C_{i-1}^n + 3C_i^n + 2C_{i+1}^n], \quad (29)$$

$$\frac{\partial C}{\partial x} \cong \frac{1}{12\Delta x} [C_{i-2}^{n+1} - 6C_{i-1}^{n+1} + 3C_i^{n+1} + 2C_{i+1}^{n+1}], \quad (30)$$

$$\frac{\partial C}{\partial x} \cong \frac{1}{6\Delta x} [C_{i-2}^{n+1} - 6C_{i-1}^{n+1} + 3C_i^{n+1} + 2C_{i+1}^{n+1}]. \quad (31)$$

At right boundary conditions, as follows, respectively,

$$\frac{\partial C}{\partial x} \cong \frac{1}{6\Delta x} [-2C_{i-3}^n + 9C_{i-2}^n - 18C_{i-1}^n + 11C_i^n], \quad (32)$$

$$\frac{\partial C}{\partial x} \cong \frac{1}{12\Delta x} [-2C_{i-3}^{n+1} + 9C_{i-2}^{n+1} - 18C_{i-1}^{n+1} + 11C_i^{n+1}], \quad (33)$$

$$\frac{\partial C}{\partial x} \cong \frac{1}{6\Delta x} [-2C_{i-3}^{n+1} + 9C_{i-2}^{n+1} - 18C_{i-1}^{n+1} + 11C_i^{n+1}]. \quad (34)$$

A. A Four points Explicit Upwind Method

A four points explicit upwind schemes can be obtained so that the technique does not require the systems of linear equations. This technique is economical computer implementation. Now, we take the explicit finite difference technique [21] into (11).

At the left boundary, substituting (24) – (25) into (11), then we obtain that;

$$\begin{aligned} & \frac{C_i^{n+1} - C_i^n}{\Delta t} + \frac{u_i^n}{6\Delta x} [-11C_i^n + 18C_{i+1}^n - 9C_{i+2}^n + 2C_{i+3}^n] \\ & = \frac{D}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n] - kC_i^n, \end{aligned} \quad (35)$$

where $C \cong C_i^n$, $u \cong \tilde{u}_i^n$ and \tilde{u}_i^n are obtained by the Crank-Nicolson method with the hydrodynamic model of (9), for all $1 \leq i \leq M$ and $0 \leq n \leq N$. Let $\beta = D \frac{\Delta t}{(\Delta x)^2}$ and

$\beta_i^n = u_i^n \frac{\Delta t}{6\Delta x}$, so (35) becomes;

$$\begin{aligned} C_i^{n+1} = & \beta C_{i-1}^n + [1 - 2\beta - (\Delta t)k + 11\beta_i^n] C_i^n \\ & + [\beta - 18\beta_i^n] C_{i+1}^n - 9\beta_i^n C_{i+2}^n - 2\beta_i^n C_{i+3}^n. \end{aligned} \quad (36)$$

For $i=0$, plug the known value of the left boundary by arranging $C_{i-1}^n = C_0^n$ in (36) on the right-hand side. We obtain;

$$\begin{aligned} C_0^{n+1} = & [1 - \beta - (\Delta t)k + 11\beta_0^n] C_0^n + [\beta - 18\beta_0^n] C_1^n \\ & - 9\beta_0^n C_2^n - 2\beta_0^n C_3^n. \end{aligned} \quad (37)$$

At interior, substituting (24) – (25) and (29) into (11). Then, we obtain;

$$\begin{aligned} C_i^{n+1} = & -\beta_i^n C_{i-2}^n + [\beta + 6\beta_i^n] C_{i-1}^n \\ & + [1 - 2\beta - 3\beta_i^n - (\Delta t)k] C_i^n + [\beta - 2\beta_i^n] C_{i+1}^n. \end{aligned} \quad (38)$$

At the right boundary, substituting (24) – (25) and (32) into (11). Then we obtain;

$$C_i^{n+1} = 2\beta C_{i-3}^n + [\beta - 9\beta_i^n] C_{i-2}^n + 18\beta_i^n C_{i-1}^n + [1 - 2\beta - (\Delta t)k - 11\beta_i^n] C_i^n + \beta_i^n C_{i+1}^n. \quad (39)$$

For $i=M$, unknown value of the right boundary by boundary conditions, we can let $C_{M+1}^n = C_M^n$ in (39) and, by rearranging, we obtain;

$$C_M^{n+1} = 2\beta_M^n C_{M-3}^n + [\beta - 9\beta_M^n] C_{M-2}^n + 18\beta_M^n C_{M-1}^n + [1 - \beta - (\Delta t)k + 11\beta_M^n] C_M^n. \quad (40)$$

B. A Third Order Crank-Nicolson Method

Consider the Crank-Nicolson method for the advection-dispersion-reaction equations. Take the Crank-Nicolson scheme in [21] in (11).

At the left boundary, substituting (24) – (25) and (27) into (11), then we have

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} + \frac{u_i^n}{12\Delta x} \left[\frac{-11C_i^{n+1} + 18C_{i+1}^{n+1} - 9C_{i+2}^{n+1} + 2C_{i+3}^{n+1}}{-11C_i^n + 18C_{i+1}^n - 9C_{i+2}^n + 2C_{i+3}^n} \right] = \frac{D}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n] - kC_i^n. \quad (41)$$

where $C \equiv C_i^n$, $u \equiv \tilde{u}_i^n$ and \tilde{u}_i^n are obtained by the Crank-Nicolson method with the hydrodynamic model of (9), for all $1 \leq i \leq M$ and $0 \leq n \leq N$. Let $\beta = D \frac{\Delta t}{(\Delta x)^2}$ and

$$\alpha_i^n = u_i^n \frac{\Delta t}{12\Delta x}, \text{ so (41) becomes,} \\ [1 - 11\alpha_i^n] C_i^{n+1} + 18\alpha_i^n C_{i+1}^{n+1} - 9\alpha_i^n C_{i+2}^{n+1} + 2\alpha_i^n C_{i+3}^{n+1} = \beta C_{i-1}^n + [1 - 2\beta - (\Delta t)k + 11\alpha_i^n] C_i^n + [\beta - 18\alpha_i^n] C_{i+1}^n + 9\alpha_i^n C_{i+2}^n - 2\alpha_i^n C_{i+3}^n. \quad (42)$$

For the left boundary condition, $i=0$, the known value on the left boundary are approximated $C_{i-1}^n = C_0^n$ in (42), we can see that;

$$[1 - 11\alpha_0^n] C_0^{n+1} + 18\alpha_0^n C_1^{n+1} - 9\alpha_0^n C_2^{n+1} + 2\alpha_0^n C_3^{n+1} = \beta C_{-1}^n + [1 - 2\beta - (\Delta t)k + 11\alpha_0^n] C_0^n + [\beta - 18\alpha_0^n] C_1^n + 9\alpha_0^n C_2^n - 2\alpha_0^n C_3^n. \quad (43)$$

At interior, substituting (24) – (25) and (30) into (11). Then we obtain;

$$\alpha_i^n C_{i-2}^{n+1} - 6\alpha_i^n C_{i-1}^{n+1} + [1 - 3\alpha_i^n] C_i^{n+1} + 2\alpha_i^n C_{i+1}^{n+1} = [\beta - \alpha_i^n] C_{i-2}^n + 6\alpha_i^n C_{i-1}^n + [1 - 2\beta - (\Delta t)k - 3\alpha_i^n] C_i^n + [\beta - 2\alpha_i^n] C_{i+1}^n. \quad (44)$$

Similarly, the right boundary condition, substituting (24) – (25) and (33) into (11). Then, we get;

$$-2\alpha_i^n C_{i-3}^{n+1} + 9\alpha_i^n C_{i-2}^{n+1} - 18\alpha_i^n C_{i-1}^{n+1} + [1 + 11\alpha_i^n] C_i^{n+1} = 2\alpha_i^n C_{i-3}^n - 9\alpha_i^n C_{i-2}^n + \beta C_{i-1}^n + [1 - 2\beta - (\Delta t)k - 11\alpha_i^n] C_i^n + [\beta + 18\alpha_i^n] C_{i+1}^n. \quad (45)$$

For $i=M$, the known value on the right boundary condition are approximated $C_{M+1}^n = C_M^n$ in (45), and by rearranging, we obtain;

$$-2\alpha_M^n C_{M-3}^{n+1} + 9\alpha_M^n C_{M-2}^{n+1} - 18\alpha_M^n C_{M-1}^{n+1} + [1 + 11\alpha_M^n] C_M^{n+1} = 2\alpha_M^n C_{M-3}^n - 9\alpha_M^n C_{M-2}^n + \beta C_{M-1}^n + [1 - \beta - (\Delta t)k + 7\alpha_M^n] C_M^n. \quad (46)$$

C. A Four points Implicit Upwind Method

Consider the implicit method for the advection-dispersion-reaction equations. Take the implicit scheme in [21] in (11).

For the left boundary, substituting (24) – (25) and (28) into (11). Then, we have;

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} + \frac{u_i^n}{6\Delta x} [-11C_i^{n+1} + 18C_{i+1}^{n+1} - 9C_{i+2}^{n+1} + 2C_{i+3}^{n+1}] = \frac{D}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n] - kC_i^n. \quad (47)$$

where $C \equiv C_i^n$, $u \equiv \tilde{u}_i^n$ and \tilde{u}_i^n are obtained by the Crank-Nicolson method with the hydrodynamic model of (9), for all $1 \leq i \leq M$, and $0 \leq n \leq N$. Let $\beta = D \frac{\Delta t}{(\Delta x)^2}$, and

$$\beta_i^n = u_i^n \frac{\Delta t}{12\Delta x}, \text{ so (47) becomes;} \\ [1 - 11\beta_i^n] C_i^{n+1} + 18\beta_i^n C_{i+1}^{n+1} - 9\beta_i^n C_{i+2}^{n+1} + 2\beta_i^n C_{i+3}^{n+1} = \beta C_{i-1}^n + [1 - 2\beta - (\Delta t)k] C_i^n + \beta C_{i+1}^n. \quad (48)$$

For $i=0$, substituting the approximate unknown value of the left boundary, we can let $C_{i-1}^n = C_0^n$ in (48), and by rearranging, we obtain;

$$[1 - 11\beta_0^n] C_0^{n+1} + 18\beta_0^n C_1^{n+1} - 9\beta_0^n C_2^{n+1} + 2\beta_0^n C_3^{n+1} = [1 - \beta - (\Delta t)k] C_0^n + \beta C_1^n. \quad (49)$$

At interior, substituting (24-25) and (31) into (11). Then we obtain;

$$\beta_i^n C_{i-2}^{n+1} - 6\beta_i^n C_{i-1}^{n+1} + [1 + 3\beta_i^n] C_i^{n+1} + 2\beta_i^n C_{i+1}^{n+1} = \beta C_{i-1}^n + [1 - 2\beta - (\Delta t)k] C_i^n + \beta C_{i+1}^n. \quad (50)$$

Similarly, the right boundary condition, substituting (24) – (25) and (34) into (11). Then we get;

$$-2\beta_i^n C_{i-3}^{n+1} + 9\beta_i^n C_{i-2}^{n+1} - 18\beta_i^n C_{i-1}^{n+1} + [1 + 11\beta_i^n] C_i^{n+1} = \beta C_{i-1}^n + [1 - 2\beta - (\Delta t)k] C_i^n + \beta C_{i+1}^n. \quad (51)$$

For $i=M$, the known value on the right boundary condition are approximated $C_{M+1}^n = C_M^n$ in (51), and by rearranging, we obtain;

$$-2\beta_M^n C_{M-3}^{n+1} + 9\beta_M^n C_{M-2}^{n+1} - 18\beta_M^n C_{M-1}^{n+1} + [1 + 11\beta_M^n] C_M^{n+1} = \beta C_{M-1}^n + [1 - \beta - (\Delta t)k] C_M^n. \quad (52)$$

V. NUMERICAL EXPERIMENTS

Suppose that the measurement of pollutant concentration C (Kg/m³) in a uniform stream at time t (sec) is considered. A stream is aligned with longitudinal distance, 1.0 km total length. There is a plant which discharges waste water into the stream, and the pollutant concentration at discharge point is assumed in to 3 case;

case 1; $C(0,t) = 0.4 + \sin(t)$ Kg/m³ at $x=0$ for all $t > 0$, and

$\frac{\partial C}{\partial x}(1,t) = -0.5$ Kg/m³ at $x=1$ for all $t > 0$, and $C(x,0) = 0$ Kg/m³ at $t = 0$.

case 2; $C(0,t)=0.4+\sin(t)$ Kg/m³ at $x=0$ for all $t > 0$, and $\frac{\partial C}{\partial x}(1,t)=0$ Kg/m³ at $x=1$ for all $t > 0$, and $C(x,0)=0$ Kg/m³ at $t=0$

case 3; $C(0,t)=0.4+\sin(t)$ Kg/m³ at $x=0$ for all $t > 0$, and $\frac{\partial C}{\partial x}(1,t)=1$ Kg/m³ at $x=1$ for all $t > 0$, and $C(x,0)=0$ Kg/m³ at $t=0$.

The velocity of water at the discharge point can be described as a function $d(0,t)=f(t)=0.4+|\sin(t)|$ for all $t > 0$, and the elevation is not changed at $x=1$ km. In the analysis conducted in this study, meshes the stream, using $\Delta x=0.02$, and time increment with $\Delta t=0.002$. Using (20); for $k=0$, we obtained the elevation of water $d(x,t)$ in Table 1 and Fig. 2. For $k=-0.03, k=0$, and $k=0.02$, can be obtained the velocity of water $u(x,t)$ in Table 2-4, and Fig. 3-5. The

comparison of elevation and velocity at $k=-0.03, k=0$, and $k=0.02$ are show in Fig. 6-7, respectively. The physical parameter of the stream system is diffusion coefficient $D=0.02$ m²/s.

Next the approximate water velocity can be plugged into implicit and explicit methods such as four points explicit upwind methods, third order Crank-Nicolson methods, and four points implicit methods in (37, 38, 40), (43, 44, 46), and (49, 50, 52), respectively. The approximation of pollutant concentration C of all schemes at $k=-1, k=0$, and $k=0.02$ are shown in tables 5-7, respectively. The comparison of approximated pollutant concentrations, for the above 3 cases at $k=-1$ of a four points explicit upwind methods, a third order Crank-Nicolson methods, and a four points implicit methods are show in Fig. 8-10, respectively. Similar, for $k=0, k=1$ are shown in Figs. 11-13, and 14-16, respectively, for the above 3 cases.

Table I. The elevation of water flow $d(x,t)$ m/s where $\Delta x=0.02, \Delta t=0.002$ and $k=0$

t(sec), x (km)	x=0	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
4	0.611858	0.069780	-0.399759	-1.262317	-1.802668	-2.036578	0.611858	0.069780	-0.399759	-1.262317	-1.802668
8	0.998543	-0.003519	-0.286033	-0.784644	-0.763727	-0.619346	0.998543	-0.003519	-0.286033	-0.784644	-0.763727
12	0.693525	0.023939	-0.370754	-0.668179	-0.898352	-0.850130	0.693525	0.023939	-0.370754	-0.668179	-0.898352
16	0.091907	0.032294	-0.126321	-0.133233	-0.112515	-0.253000	0.091907	0.032294	-0.126321	-0.133233	-0.112515
20	0.813674	0.553929	0.094939	-0.305544	-0.572990	-0.757749	0.813674	0.553929	0.094939	-0.305544	-0.572990

Table II. The water of velocity flow $u(x,t)$ m/s where $\Delta x=0.02, \Delta t=0.002$ and $k=-0.03$

t(sec), x (km)	x=0	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
4	2.610971	2.583252	2.390045	2.227666	1.586067	0.998144	2.610971	2.583252	2.390045	2.227666	1.586067
8	1.042248	1.056271	1.121407	1.145663	0.984761	0.678741	1.042248	1.056271	1.121407	1.145663	0.984761
12	0.080940	0.068841	-0.078776	-0.154091	0.108119	0.225758	0.080940	0.068841	-0.078776	-0.154091	0.108119
16	2.153967	2.325972	2.034130	1.777823	1.357201	0.964549	2.153967	2.325972	2.034130	1.777823	1.357201
20	1.564799	1.426789	1.206481	1.006457	0.656912	0.454190	1.564799	1.426789	1.206481	1.006457	0.656912

Table III. The water of velocity flow $u(x,t)$ m/s where $\Delta x=0.02, \Delta t=0.002$ and $k=0$

t(sec), x (km)	x=0	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
4	2.783345	2.758803	2.555691	2.383197	1.683867	1.040888	2.783345	2.758803	2.555691	2.383197	1.683867
8	1.027512	1.043821	1.131175	1.184130	1.043308	0.723322	1.027512	1.043821	1.131175	1.184130	1.043308
12	-0.303511	-0.334005	-0.507012	-0.573429	-0.145513	0.077422	-0.303511	-0.334005	-0.507012	-0.573429	-0.145513
16	2.860197	3.145580	2.767857	2.406631	1.797891	1.207349	2.860197	3.145580	2.767857	2.406631	1.797891
20	1.952418	1.766613	1.437037	1.124076	0.655525	0.378875	1.952418	1.766613	1.437037	1.124076	0.655525

Table IV. The water of velocity flow $u(x,t)$ m/s where $\Delta x=0.02, \Delta t=0.002$ and $k=0.02$

t(sec), x (km)	x=0	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
4	2.905499	2.883536	2.673649	2.494080	1.753150	1.070405	2.905499	2.883536	2.673649	2.494080	1.753150
8	1.005656	1.023729	1.129304	1.206807	1.086476	0.760053	1.005656	1.023729	1.129304	1.206807	1.086476
12	-0.660111	-0.708516	-0.900420	-0.955795	-0.378749	-0.059094	-0.660111	-0.708516	-0.900420	-0.955795	-0.378749
16	3.530340	3.926561	3.473736	3.013550	2.222936	1.440886	3.530340	3.926561	3.473736	3.013550	2.222936
20	2.297546	2.071018	1.632631	1.205647	0.636155	0.295197	2.297546	2.071018	1.632631	1.205647	0.636155

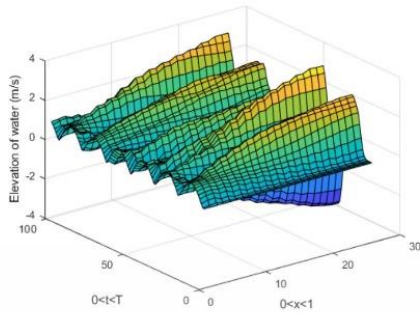


Fig. 2. The elevation of water flow $d(x,t)$ m/s at $k = 0$ when after pass 20 s

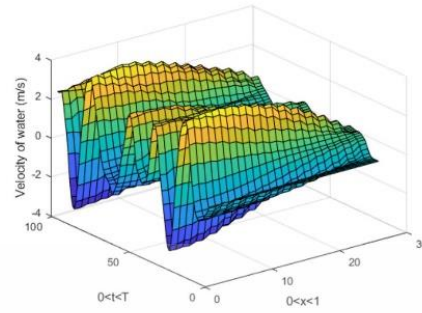


Fig. 5. The velocity of water flow $u(x,t)$ m/s at $k = 0.02$ when after pass 20 s

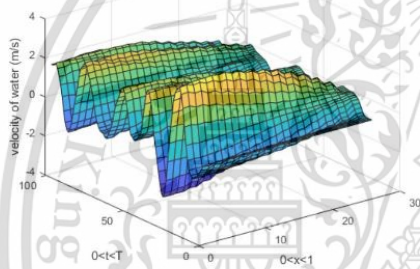


Fig. 3. The velocity of water flow $u(x,t)$ m/s at $k = -0.3$ when after pass 20 s

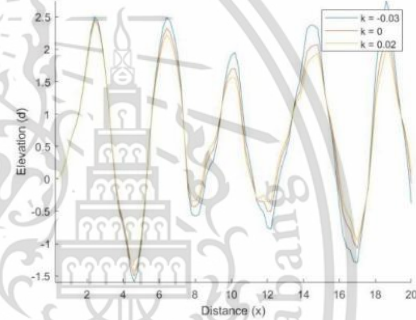


Fig. 6. The comparison elevation of water flow $u(x,t)$ m/s at $k = -0.03$, $k = 0$, and $k = 0.02$ when after pass 20 s

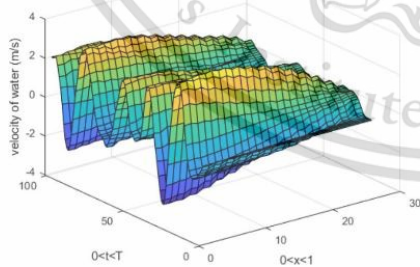


Fig. 4. The velocity of water flow $u(x,t)$ m/s at $k = 0$ when after pass 20 s

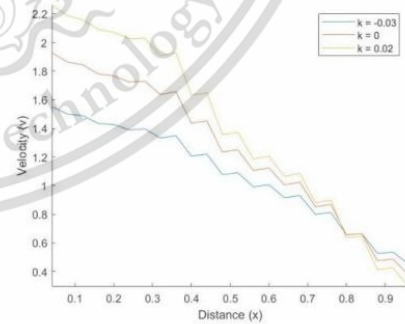


Fig. 7. The comparison velocity of water flow $u(x,t)$ m/s at $k = -0.03$, $k = 0$, and $k = 0.02$ when after pass 20 s

Table 5. The pollutant concentration $C(x,t)$ Kg / m³ where $\Delta x = 0.04$, $\Delta t = 0.2$ and $k = -1$ of all methods for the above 3 cases.

t(sec), x (km)			x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1.0	
four points explicit upwind methods	case 1	4	0.59866933	0.13388683	0.01275161	0.00042256	0.00000480	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543974	-0.03342089	
		8	0.78941834	0.27603853	0.06635899	0.01027764	0.00095667	0.00004886	-0.00002855	-0.00041859	-0.00345410	-0.01718876	-0.05318134	
		12	0.96464247	0.41556165	0.13773746	0.03450134	0.00635247	0.00081604	-0.00024938	-0.00211319	-0.00959469	-0.03090974	-0.07178201	
		16	1.11735609	0.56290780	0.22489454	0.07217117	0.01843115	0.00351607	-0.00070911	-0.00549082	-0.01828731	-0.04636889	-0.09096688	
		20	1.24147098	0.71802159	0.33000427	0.12473063	0.03892169	0.00933274	-0.00122330	-0.01073596	-0.02939539	-0.06373023	-0.11170083	
	case 2	4	0.59900000	0.13400000	0.01280000	0.00042300	0.00000480	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
		8	0.78941800	0.27603900	0.06640000	0.01030000	0.00095700	0.00005010	-0.00000148	0.00000003	0.00000000	0.00000000	0.00000000	0.00000000
		12	0.96464200	0.41556200	0.13773700	0.03450000	0.00636000	0.00085200	0.00007930	0.00000493	0.00000021	0.00000001	0.00000001	0.00000000
		16	1.11735600	0.56290800	0.22489500	0.07217500	0.01850000	0.00375000	0.00059700	0.00007410	0.00000691	0.00000047	0.00000004	0.00000004
		20	1.24147100	0.71802200	0.33000800	0.12475900	0.03910000	0.01020000	0.00219000	0.00038900	0.00005640	0.00000669	0.00000099	0.00000099
	case 3	4	0.59900000	0.13400000	0.01280000	0.00042300	0.00000480	0.00000002	0.00000014	0.00001640	0.00069600	0.01090000	0.06680000	0.06680000
		8	0.78941800	0.27603900	0.06640000	0.01030000	0.00095700	0.00005260	0.00006160	0.00083700	0.00691000	0.03440000	0.10600000	0.10600000
		12	0.96464200	0.41556200	0.13773700	0.03450000	0.00636000	0.00092300	0.00073700	0.00424000	0.01920000	0.06180000	0.14400000	0.14400000
		16	1.11735600	0.56290800	0.22489500	0.07218200	0.01850000	0.00423000	0.00321000	0.01120000	0.03660000	0.09270000	0.18200000	0.18200000
		20	1.24147100	0.71802300	0.33001600	0.12481600	0.03940000	0.01190000	0.00902000	0.02260000	0.05900000	0.12700000	0.22340500	0.22340500
third order Crank-Nicolson methods	case 1	4	0.59900000	0.13300000	0.01270000	0.00042300	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034800	-0.00544000	-0.03340000	
		8	0.78941800	0.27408500	0.06610000	0.01020000	0.00095500	0.00004880	-0.00002850	-0.00041900	-0.00345000	-0.01720000	-0.05320000	
		12	0.96464200	0.41168500	0.13672800	0.03430000	0.00632000	0.00081300	-0.00025000	-0.00211000	-0.00959000	-0.03090000	-0.07180000	
		16	1.11735600	0.55727900	0.22289700	0.07162600	0.01830000	0.00350000	-0.00071200	-0.00549000	-0.01830000	-0.04640000	-0.09100000	
		20	1.24147100	0.71107600	0.32687400	0.12364400	0.03860000	0.00926000	-0.00124000	-0.01070000	-0.02940000	-0.06370000	-0.11170000	
	case 2	4	0.59867000	0.13350000	0.01274100	0.00042268	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	
		8	0.78942000	0.27408000	0.06605000	0.01024700	0.00095519	0.00005009	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000	
		12	0.96464000	0.41169000	0.13673000	0.03430600	0.00632720	0.00084902	0.00007916	0.00000493	0.00000021	0.00000001	0.00000000	
		16	1.11740000	0.55728000	0.22290000	0.07162900	0.01834700	0.00373340	0.00059422	0.00007387	0.00000689	0.00000047	0.00000004	
		20	1.24150000	0.71108000	0.32688000	0.12367000	0.03879000	0.01011600	0.00217930	0.00038736	0.00005614	0.00000666	0.00000099	
	case 3	4	0.59867000	0.13350000	0.01274100	0.00042268	0.00000481	0.00000002	0.00000014	0.00001641	0.00069575	0.01087900	0.06684200	
		8	0.78942000	0.27408000	0.06605000	0.01024700	0.00095525	0.00005262	0.00006155	0.00083725	0.00690820	0.03437800	0.10636000	
		12	0.96464000	0.41169000	0.13673000	0.03430600	0.00633270	0.00092040	0.00073656	0.00424120	0.01919000	0.06182000	0.14356000	
		16	1.11740000	0.55728000	0.22290000	0.07163700	0.01841300	0.00420850	0.00320620	0.01120400	0.03659500	0.09273900	0.18193000	
		20	1.24150000	0.71108000	0.32689000	0.12373000	0.03913700	0.01182400	0.00901190	0.02263800	0.05895900	0.12748000	0.22340000	
four points implicit methods	case 1	4	0.59866900	0.13311200	0.01272900	0.00042300	0.00000500	0.00000000	0.00000000	-0.00000800	-0.00034800	-0.00544000	-0.03342100	
		8	0.78941800	0.27213300	0.06574200	0.01021700	0.00095400	0.00004900	-0.00002900	-0.00041900	-0.00345400	-0.01718900	-0.05318100	
		12	0.96464200	0.40781100	0.13572100	0.03411100	0.00629700	0.00081100	-0.00025000	-0.00211300	-0.00959500	-0.03091000	-0.07178200	
		16	1.11735600	0.55165200	0.22090200	0.07108200	0.01819600	0.00347600	-0.00071400	-0.00549100	-0.01828700	-0.04636900	-0.09096700	
		20	1.24147100	0.70413100	0.32374700	0.12256000	0.03851400	0.00919200	-0.00125100	-0.01074000	-0.02939500	-0.06373000	-0.11170100	
	case 2	4	0.59867000	0.13311000	0.01272900	0.00042280	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	
		8	0.78942000	0.27213000	0.06574200	0.01021700	0.00095368	0.00005006	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000	
		12	0.96464000	0.40781000	0.13572000	0.03411100	0.00629940	0.00084632	0.00007900	0.00000492	0.00000021	0.00000001	0.00000000	
		16	1.11740000	0.55165000	0.22090000	0.07108500	0.01822900	0.00371330	0.00059158	0.00007362	0.00000687	0.00000047	0.00000004	
		20	1.24150000	0.70413000	0.32375000	0.12259000	0.03848700	0.01004600	0.00216590	0.00038529	0.00005589	0.00000664	0.00000099	
	case 3	4	0.59867000	0.13311000	0.01272900	0.00042280	0.00000481	0.00000002	0.00000014	0.00001641	0.00069575	0.01087900	0.06684200	
		8	0.78942000	0.27213000	0.06574200	0.01021700	0.00095374	0.00005259	0.00006155	0.00083725	0.00690820	0.03437800	0.10636000	
		12	0.96464000	0.40781000	0.13572000	0.03411100	0.00630490	0.00091770	0.00073640	0.00424120	0.01919000	0.06182000	0.14356000	
		16	1.11740000	0.55165000	0.22090000	0.07109300	0.01829600	0.00418850	0.00320360	0.01120300	0.03659500	0.09273900	0.18193000	
		20	1.24150000	0.70413000	0.32376000	0.12265000	0.03883400	0.01175400	0.00899910	0.02263700	0.05895800	0.12748000	0.22340000	

Table 6. The pollutant concentration $C(x,t)$ Kg/m³ where $\Delta x = 0.04$, $\Delta t = 0.2$ and $k = 0$ of all methods for the above 3 cases.

t(sec), x (km)			x=0	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
four points explicit upwind methods	case 1	4	0.59867000	0.13389000	0.01275200	0.00042256	0.00000480	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543970	-0.03342100
		8	0.78942000	0.27604000	0.06635900	0.01027800	0.00095667	0.00004886	-0.00002855	-0.00041859	-0.00345410	-0.01718900	-0.05318100
		12	0.96464000	0.41556000	0.13774000	0.03450100	0.00635250	0.00081604	-0.00024938	-0.00211320	-0.00959470	-0.03091000	-0.07178200
		16	1.11740000	0.56291000	0.22489000	0.07217100	0.01843100	0.00351610	-0.00070911	-0.00549080	-0.01828700	-0.04636900	-0.09096700
	20	1.24150000	0.71802000	0.33000000	0.12473000	0.03892200	0.00933270	-0.00122330	-0.01073600	-0.02939500	-0.06373000	-0.11170000	
	case 2	4	0.59867000	0.13389000	0.01275200	0.00042256	0.00000480	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
		8	0.78942000	0.27604000	0.06635900	0.01027800	0.00095670	0.00005012	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
		12	0.96464000	0.41556000	0.13774000	0.03450100	0.00635520	0.00085173	0.00007932	0.00000493	0.00000021	0.00000001	0.00000000
		16	1.11740000	0.56291000	0.22489000	0.07217500	0.01846400	0.00375360	0.00059688	0.00007412	0.00000691	0.00000047	0.00000004
	20	1.24150000	0.71802000	0.33001000	0.12476000	0.03890500	0.01018600	0.00219270	0.00038945	0.00005640	0.00000669	0.00000099	
	case 3	4	0.59867000	0.13389000	0.01275200	0.00042256	0.00000480	0.00000002	0.00000014	0.00001641	0.00069575	0.01087900	0.06684200
		8	0.78942000	0.27604000	0.06635900	0.01027800	0.00095676	0.00005265	0.00006155	0.00083725	0.00690820	0.03437800	0.10636000
12		0.96464000	0.41556000	0.13774000	0.03450200	0.00636070	0.00092311	0.00073672	0.00424120	0.01919000	0.06182000	0.14356000	
16		1.11740000	0.56291000	0.22490000	0.07218200	0.01853100	0.00422850	0.00320880	0.01120400	0.03659500	0.09273900	0.18193000	
20	1.24150000	0.71802000	0.33002000	0.12482000	0.03944100	0.01189400	0.00902460	0.02264000	0.05896000	0.12748000	0.22340000		
third order Crank-Nicolson methods	case 1	4	0.59867000	0.13350000	0.01274100	0.00042268	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543970	-0.03342100
		8	0.78942000	0.27408000	0.06605000	0.01024700	0.00095516	0.00004883	-0.00002855	-0.00041859	-0.00345410	-0.01718900	-0.05318100
		12	0.96464000	0.41169000	0.13673000	0.03430600	0.00632450	0.00081333	-0.00024954	-0.00211320	-0.00959470	-0.03091000	-0.07178200
		16	1.11740000	0.55728000	0.22290000	0.07162600	0.01831300	0.00349590	-0.00071179	-0.00549100	-0.01828700	-0.04636900	-0.09096700
	20	1.24150000	0.71108000	0.32687000	0.12364000	0.03861700	0.00926220	-0.00123700	-0.01073800	-0.02939500	-0.06373000	-0.11170000	
	case 2	4	0.59867000	0.13350000	0.01274100	0.00042268	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
		8	0.78942000	0.27408000	0.06605000	0.01024700	0.00095519	0.00005009	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
		12	0.96464000	0.41169000	0.13673000	0.03430600	0.00632720	0.00084902	0.00007916	0.00000493	0.00000021	0.00000001	0.00000000
		16	1.11740000	0.55728000	0.22290000	0.07162900	0.01834700	0.00373340	0.00059422	0.00007387	0.00000689	0.00000047	0.00000004
	20	1.24150000	0.71108000	0.32688000	0.12367000	0.03879000	0.01011600	0.00217930	0.00038736	0.00005614	0.00000666	0.00000099	
	case 3	4	0.59867000	0.13350000	0.01274100	0.00042268	0.00000481	0.00000002	0.00000014	0.00001641	0.00069575	0.01087900	0.06684200
		8	0.78942000	0.27408000	0.06605000	0.01024700	0.00095525	0.00005262	0.00006155	0.00083725	0.00690820	0.03437800	0.10636000
12		0.96464000	0.41169000	0.13673000	0.03430600	0.00633270	0.00092040	0.00073656	0.00424120	0.01919000	0.06182000	0.14356000	
16		1.11740000	0.55728000	0.22290000	0.07163700	0.01841300	0.00420850	0.00320620	0.01120400	0.03659500	0.09273900	0.18193000	
20	1.24150000	0.71108000	0.32689000	0.12373000	0.03913700	0.01182400	0.00901190	0.02263800	0.05895900	0.12748000	0.22340000		
four points implicit methods	case 1	4	0.59867000	0.13311000	0.01272900	0.00042280	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543970	-0.03342100
		8	0.78942000	0.27213000	0.06574200	0.01021700	0.00095364	0.00004880	-0.00002855	-0.00041859	-0.00345410	-0.01718900	-0.05318100
		12	0.96464000	0.40781000	0.13572000	0.03411100	0.00629670	0.00081063	-0.00024969	-0.00211320	-0.00959470	-0.03091000	-0.07178200
		16	1.11740000	0.55165000	0.22090000	0.07108200	0.01819600	0.00347570	-0.00071445	-0.00549120	-0.01828700	-0.04636900	-0.09096700
	20	1.24150000	0.70413000	0.32375000	0.12256000	0.03831400	0.00919190	-0.00125070	-0.01074000	-0.02939500	-0.06373000	-0.11170000	
	case 2	4	0.59867000	0.13311000	0.01272900	0.00042280	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
		8	0.78942000	0.27213000	0.06574200	0.01021700	0.00095368	0.00005006	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000
		12	0.96464000	0.40781000	0.13572000	0.03411100	0.00629940	0.00084632	0.00007900	0.00000492	0.00000021	0.00000001	0.00000000
		16	1.11740000	0.55165000	0.22090000	0.07108500	0.01822900	0.00371330	0.00059158	0.00007362	0.00000687	0.00000047	0.00000004
	20	1.24150000	0.70413000	0.32375000	0.12259000	0.03848700	0.01004600	0.00216590	0.00038529	0.00005589	0.00000664	0.00000099	
	case 3	4	0.59867000	0.13311000	0.01272900	0.00042280	0.00000481	0.00000002	0.00000014	0.00001641	0.00069575	0.01087900	0.06684200
		8	0.78942000	0.27213000	0.06574200	0.01021700	0.00095374	0.00005259	0.00006155	0.00083725	0.00690820	0.03437800	0.10636000
12		0.96464000	0.40781000	0.13572000	0.03411100	0.00630490	0.00091770	0.00073640	0.00424120	0.01919000	0.06182000	0.14356000	
16		1.11740000	0.55165000	0.22090000	0.07109300	0.01829600	0.00418850	0.00320360	0.01120300	0.03659500	0.09273900	0.18193000	
20	1.24150000	0.70413000	0.32376000	0.12265000	0.03883400	0.01175400	0.00899910	0.02263700	0.05895800	0.12748000	0.22340000		

Table 7. The pollutant concentration $C(x,t)$ Kg/m^3 where $\Delta x = 0.04$, $\Delta t = 0.2$ and $k = 1$ of all methods for the above 3 cases.

t(sec), x (km)			x = 0	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8	x = 0.9	x = 1.0	
four points explicit upwind methods	case 1	4	0.59867000	0.13389000	0.01275200	0.00042256	0.00000480	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543970	-0.03342100	
		8	0.78942000	0.27604000	0.06635900	0.01027800	0.00095667	0.00004886	0.00004886	-0.00002855	-0.00041859	-0.00345410	-0.01718900	-0.05318100
		12	0.96464000	0.41556000	0.13774000	0.03450100	0.00635250	0.00081604	0.00081604	-0.00024938	-0.00211320	-0.00959470	-0.03091000	-0.07178200
		16	1.11740000	0.56291000	0.22489000	0.07217100	0.01843100	0.00351610	0.00351610	-0.00070911	-0.00549080	-0.01828700	-0.04636900	-0.09096700
		20	1.24150000	0.71802000	0.33000000	0.12473000	0.03892200	0.00933270	0.00933270	-0.00122330	-0.01073600	-0.02939500	-0.06373000	-0.11170000
	case 2	4	0.59867000	0.13389000	0.01275200	0.00042256	0.00000480	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
		8	0.78942000	0.27604000	0.06635900	0.01027800	0.00095670	0.00005012	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000	0.00000000
		12	0.96464000	0.41556000	0.13774000	0.03450100	0.00635520	0.00085173	0.00007932	0.00000493	0.00000021	0.00000001	0.00000001	0.00000000
		16	1.11740000	0.56291000	0.22489000	0.07217500	0.01846400	0.00375360	0.00059688	0.00007412	0.00000691	0.00000047	0.00000004	0.00000004
		20	1.24150000	0.71802000	0.33001000	0.12476000	0.03909500	0.01018600	0.00219270	0.00038945	0.00005640	0.00000669	0.00000000	0.00000099
	case 3	4	0.59867000	0.13389000	0.01275200	0.00042256	0.00000480	0.00000002	0.00000014	0.00001641	0.00069575	0.01087900	0.06684200	0.06684200
		8	0.78942000	0.27604000	0.06635900	0.01027800	0.00095676	0.00005265	0.00006155	0.000083725	0.00690820	0.03437800	0.10636000	0.10636000
12		0.96464000	0.41556000	0.13774000	0.03450200	0.00636070	0.00092311	0.00073672	0.00424120	0.01919000	0.06182000	0.14356000	0.14356000	
16		1.11740000	0.56291000	0.22490000	0.07218200	0.01853100	0.00422850	0.00320880	0.01120400	0.03659500	0.09273900	0.18193000	0.18193000	
20		1.24150000	0.71802000	0.33002000	0.12482000	0.03944100	0.01189400	0.00902460	0.02264000	0.05896000	0.12748000	0.22340000	0.22340000	
third order Crank-Nicolson methods	case 1	4	0.59867000	0.13350000	0.01274100	0.00042268	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543970	-0.03342100	
		8	0.78942000	0.27408000	0.06605000	0.01024700	0.00095516	0.00004883	-0.00002855	-0.00041859	-0.00345410	-0.01718900	-0.05318100	
		12	0.96464000	0.41169000	0.13673000	0.03430600	0.00632450	0.00081333	-0.00024954	-0.00211320	-0.00959470	-0.03091000	-0.07178200	
		16	1.11740000	0.55728000	0.22290000	0.07162600	0.01831300	0.00349590	-0.00071179	-0.00549100	-0.01828700	-0.04636900	-0.09096700	
		20	1.24150000	0.71108000	0.32687000	0.12364000	0.03861700	0.00926220	-0.00123700	-0.01073800	-0.02939500	-0.06373000	-0.11170000	
	case 2	4	0.59867000	0.13350000	0.01274100	0.00042268	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
		8	0.78942000	0.27408000	0.06605000	0.01024700	0.00095519	0.00005009	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000	0.00000000
		12	0.96464000	0.41169000	0.13673000	0.03430600	0.00632720	0.00084902	0.00007916	0.00000493	0.00000021	0.00000001	0.00000000	0.00000000
		16	1.11740000	0.55728000	0.22290000	0.07162900	0.01834700	0.00373340	0.00059422	0.00007387	0.00000689	0.00000047	0.00000004	0.00000004
		20	1.24150000	0.71108000	0.32688000	0.12367000	0.03879000	0.01011600	0.00217930	0.00038736	0.00005614	0.00000666	0.00000099	0.00000099
	case 3	4	0.59867000	0.13350000	0.01274100	0.00042268	0.00000481	0.00000002	0.00000014	0.00001641	0.00069575	0.01087900	0.06684200	0.06684200
		8	0.78942000	0.27408000	0.06605000	0.01024700	0.00095525	0.00005262	0.00006155	0.000083725	0.00690820	0.03437800	0.10636000	0.10636000
12		0.96464000	0.41169000	0.13673000	0.03430600	0.00633270	0.00092040	0.00073656	0.00424120	0.01919000	0.06182000	0.14356000	0.14356000	
16		1.11740000	0.55728000	0.22290000	0.07163700	0.01841800	0.00420850	0.00320620	0.01120400	0.03659500	0.09273900	0.18193000	0.18193000	
20		1.24150000	0.71108000	0.32689000	0.12373000	0.03913700	0.01182400	0.00901190	0.02263800	0.05895900	0.12748000	0.22340000	0.22340000	
four points implicit methods	case 1	4	0.59867000	0.13311000	0.01272900	0.00042280	0.00000481	0.00000002	-0.00000007	-0.00000821	-0.00034787	-0.00543970	-0.03342100	
		8	0.78942000	0.27213000	0.06574200	0.01021700	0.00095364	0.00004880	-0.00002855	-0.00041859	-0.00345410	-0.01718900	-0.05318100	
		12	0.96464000	0.40781000	0.13572000	0.03411100	0.00629670	0.00081063	-0.00024969	-0.00211320	-0.00959470	-0.03091000	-0.07178200	
		16	1.11740000	0.55165000	0.22090000	0.07108200	0.01819600	0.00347570	-0.00071445	-0.00549120	-0.01828700	-0.04636900	-0.09096700	
		20	1.24150000	0.70413000	0.32375000	0.12256000	0.03831400	0.00919190	-0.00125070	-0.01074000	-0.02939500	-0.06373000	-0.11170000	
	case 2	4	0.59867000	0.13311000	0.01272900	0.00042280	0.00000481	0.00000002	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
		8	0.78942000	0.27213000	0.06574200	0.01021700	0.00095368	0.00005006	0.00000148	0.00000003	0.00000000	0.00000000	0.00000000	0.00000000
		12	0.96464000	0.40781000	0.13572000	0.03411100	0.00629940	0.00084632	0.00007900	0.00000492	0.00000021	0.00000001	0.00000001	0.00000000
		16	1.11740000	0.55165000	0.22090000	0.07108500	0.01822900	0.00371330	0.00059158	0.00007362	0.00000687	0.00000047	0.00000004	0.00000004
		20	1.24150000	0.70413000	0.32375000	0.12259000	0.03848700	0.01004600	0.00216590	0.00038529	0.00005589	0.00000664	0.00000099	0.00000099
	case 3	4	0.59867000	0.13311000	0.01272900	0.00042280	0.00000481	0.00000002	0.00000014	0.00001641	0.00069575	0.01087900	0.06684200	0.06684200
		8	0.78942000	0.27213000	0.06574200	0.01021700	0.00095374	0.00005259	0.00006155	0.000083725	0.00690820	0.03437800	0.10636000	0.10636000
12		0.96464000	0.40781000	0.13572000	0.03411100	0.00630490	0.00091770	0.00073640	0.00424120	0.01919000	0.06182000	0.14356000	0.14356000	
16		1.11740000	0.55165000	0.22090000	0.07109300	0.01829600	0.00418850	0.00320360	0.01120300	0.03659500	0.09273900	0.18193000	0.18193000	
20		1.24150000	0.70413000	0.32376000	0.12265000	0.03883400	0.01175400	0.00899910	0.02263700	0.05895800	0.12748000	0.22340000	0.22340000	

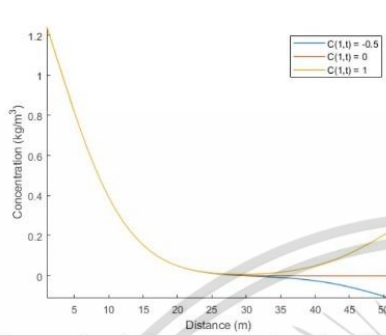


Fig. 8. The comparison of pollutant concentration at three difference $C(1,t)$ instants of four points explicit upwind method for $k = -1$ when after pass 60s.

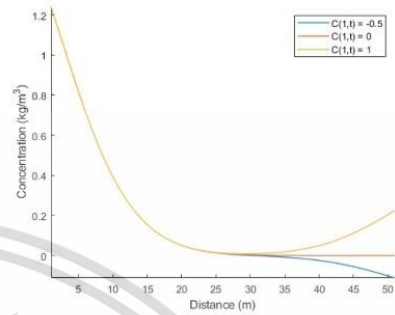


Fig. 11. The comparison of pollutant concentration at three difference $C(1,t)$ instants of four points explicit upwind method for $k = 0$ when after pass 60s.

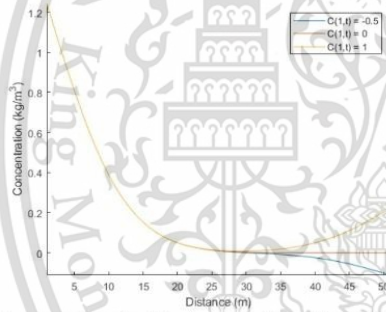


Fig. 9. The comparison of pollutant concentration at three difference $C(1,t)$ instants of third order Crank-Nicolson method for $k = -1$ when after pass 60s.

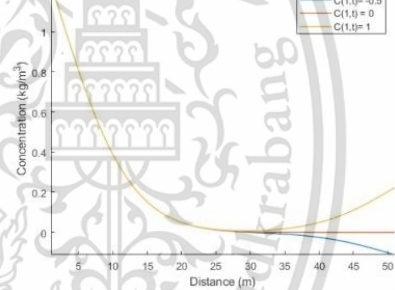


Fig. 12. The comparison of pollutant concentration at three difference $C(1,t)$ instants of third order Crank-Nicolson method for $k = 0$ when after pass 60s.

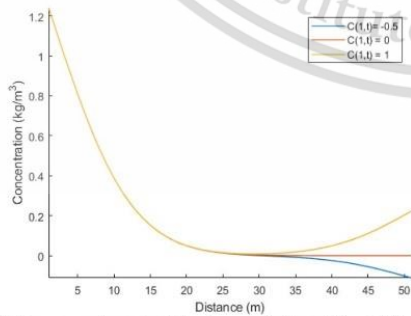


Fig. 10. The comparison of pollutant concentration at three difference $C(1,t)$ instants of four points implicit method for $k = -1$ when after pass 60s.

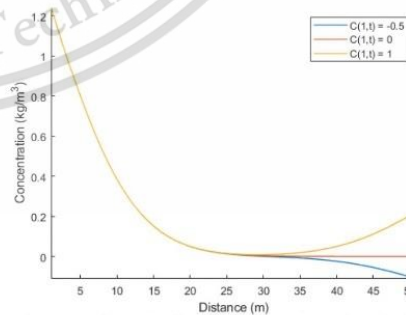


Fig. 13. The comparison of pollutant concentration at three difference $C(1,t)$ instants of four points implicit method for $k = 0$ when after pass 60s.

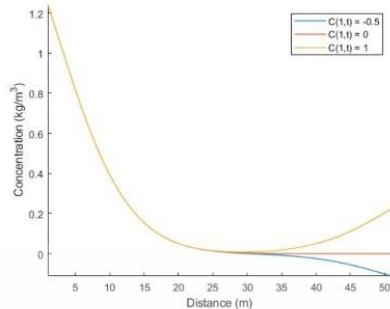


Fig. 14. The comparison of pollutant concentration at three difference $C(t, t)$ instants of four points explicit upwind method for $k=1$ when after pass 60s.

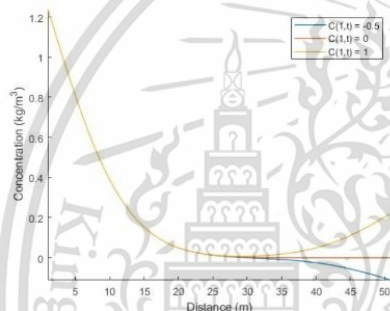


Fig. 15. The comparison of pollutant concentration at three difference $C(t, t)$ instants of third order Crank-Nicolson method for $k=1$ when after pass 60s.

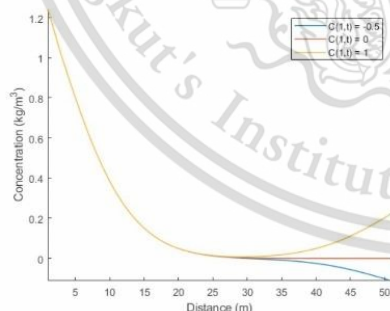


Fig. 16. The comparison of pollutant concentration at three difference $C(t, t)$ instants of four points implicit method for $k=1$ when after pass 60s.

VI. DISCUSSION

The approximation of the pollutant concentrations of finite difference methods, a four points explicit upwind methods, third order Crank-Nicolson methods, and four points implicit methods at $k=-1$ are shown in Table 5 and, at $k=0$ are shown in Table 6, at $k=1$ are shown in Table 7,

of the above 3 cases, respectively. For the comparison of the approximated pollutant concentrations of all schemes where $k=-1$, $k=0$, $k=1$, of the above 3 cases are shown in Fig. 8-10, Fig. 11-13, and Fig. 14-16, respectively. The implicit schemes show excessive dispersion effects for large time and space step lengths, significantly decreasing the efficiency of the implicit schemes. In addition, implicit methods still generate a lot of large systems of linear equations. The four points explicit upwind scheme is economical to use. The proposed method shows a good agreement in accuracy, the implicit schemes becomes less efficient than the explicit schemes. Real-world problems require a small amount of time interval in obtaining accurate solutions. Unfavorably, the analytical solutions of the hydrodynamic model cannot be found over every domain. This also implies that the analytical solutions of dispersion model could not work out at any point on the entire domain either [16] and [17].

By Fig. 6-8, 9-11 and 12-14, we can see that the mass decay rate of pollutant matter can reduce the concentration in a non-uniform stream. If sewage effluent with a low mass decay rate has discharged into a non-uniform flow stream, then the water quality will be lower than the discharging of mass decay rate of other pollutant matters.

VII. CONCLUSIONS

In this paper, we combine the hydrodynamic model and the convection-diffusion-reaction equation for an approximation of the pollutant concentration in a stream when the velocity of the current is not uniform. With the technique in this paper, the response of the stream to the different external inputs; the velocity of water and the pollutant concentration at the discharge point can be obtained. The technique constructed in this study is to respond the aspects of the stream in two varied external inputs, which are the level of water and the pollutant concentration at the discharge point. In terms of the explicit finite difference formulations, it is believed that the implemented technique is practical and applicable. All of four points explicit upwind methods, third order Crank-Nicolson methods, and four points implicit methods can be used in the dispersion model; we consider that the proposed technique is applicable and economical to be used in real-world problems due to its simplicity to program and the straight-forwardness of the implementation. It is also possible to find tentative better locations and better periods of time for the different discharge points of a stream.

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Explicit Finite Difference Techniques for a One-Dimensional Water Pollutant Dispersion Model in a Stream

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Abstract— Currently, water pollution is one of the most important environmental problems in Thailand. Pollution makes it impossible to make full use of the water source, which affects the quality of life and economic and social development. Therefore, if we know the value of the concentration of pollution that is from sources of emissions, such as from littering down the river, we might be able to control the concentration of water pollution in that area and prevent it from exceeding the standard. The mathematical simulation is an important method to detect the water quality assumption in consideration area. In this research, the hydrodynamic model and dispersion model are used to describe water flow and water pollutant concentration. A couple of mathematical models are used to simulate water-quality in the problem. The first model is the hydrodynamic model that provides the velocity fields and elevation of water. The Crank-Nicolson method is used in the hydrodynamic model. At each step, the flow velocity fields calculated from the first model are the input into the second model as the field data. The second model is the one-dimensional dispersion model that provides the pollutant concentration fields. We use the four points explicit upwind methods, the upwind explicit method and the Lax-Wendroff methods to approximate the concentration from the dispersion models. The comparison three methods and the simulations of pollutant concentration are proposed. The results obtained indicate that the Lax-Wendroff method provides a better result than four points explicit upwind methods and upwind explicit method.

Keywords- Finite differences; water quality; one-dimensional; hydrodynamic model; advection-dispersion-reaction

I. INTRODUCTION

A water quality model in a non-uniform flow stream must include velocities and elevations. The modeling used in a non-uniform flow stream is the hydrodynamics model in a one-dimensional shallow water equation and a dispersion model in an Advection-Dispersion Equation (ADE).

There are many numerical techniques available for solving such models. [1] presented a hydrodynamic model and a dispersion model with the finite element method to solve a steady water pollution control to achieve minimum cost. [2], finite element methods were used in a hydrodynamic model and a dispersion model to simulate pollution in the Bay of Santander. [3-7], proposed numerical techniques to solve a uniform flow of stream water quality model, especially the one-dimensional Advection-Dispersion-Reaction Equation (ADREs).

Mathematical models are used to simulate water quality in a non-uniform water flow system. The first is a hydrodynamic model that provides velocity field and elevation of water, and the second is a dispersion model that gives the pollutant concentration. Twin models are formulated in one-dimensional equations. The traditional Crank-Nicolson method is also used in the hydrodynamic model. At each step, the flow velocity fields calculated from

the first model are the input into the second model as the field data, presented by [8-13]

In [9], numerical techniques were used to solve the non-uniform flow of stream water quality model with one-dimensional Advection-Dispersion-Reaction equation by using the fully implicit scheme: Crank-Nicolson method for the hydrodynamic model, and Backward Time Central Space (BTCS) for the dispersion model. In [12] they used the Crank-Nicolson method to solve the hydrodynamic model, and the explicit Saulyev scheme used to solve the dispersion model. In [13], the Crank-Nicolson method was used in the hydrodynamic model and a modified MacCormack method used in the dispersion model for one-dimensional advection-dispersion-reaction equation. In [14] they presented a third-order upwind difference that is used for the convection terms of the convection-diffusion equation. In [15] they proposed a third-order upwind scheme for the convective terms of shallow water momentum equations. [16] used a third-order upwind scheme for the Advection-Diffusion Equation (ADE) using a simple spreadsheets simulation.

In this research, the hydrodynamic model and dispersion model are used to describe water flow and water pollutant

concentration. A couple of mathematical models are used to simulate water-quality in the problem. The first model is the hydrodynamic model that provides the velocity fields and elevation of water. The Crank-Nicolson method is used in the hydrodynamic model. At each step, the flow velocity fields calculated from the first model are the input into the second model as the field data. The second model is the dispersion model that provides the pollutant concentration fields. We use the four points explicit upwind methods, the upwind explicit method and, the Lax-Wendroff methods to approximate the concentration from the dispersion models.

II. MODEL FORMULATION

The modeling used in a non-uniform flow stream is the hydrodynamics model in a one-dimensional shallow water equation, that provides the velocity fields and elevation of water, and a dispersion model in an Advection-Dispersion-Reaction Equation (ADREs), that provides the pollutant concentration.

A. The Hydrodynamic Model

The continuity and momentum equations are governed by the hydrodynamic behavior of the stream which describes by one-dimensional shallow water equations obtained by integrating the Navier-Stokes equations over the flow depth under the assumptions discarding diffusion of momentum due to turbulence and discarding the terms due to friction and wind [1, 8-11, 17], we obtain the one-dimensional shallow water equations:

$$\frac{\partial \zeta}{\partial t} + \frac{\partial}{\partial x} [(h + \zeta)u] = 0, \quad (1)$$

$$\frac{\partial u}{\partial t} + g \frac{\partial \zeta}{\partial x} = 0, \quad (2)$$

where x is the longitudinal distance along a stream (m), time t (s^{-1}), $h(x)$ is the depth measured from the mean water to the bed of reservoir (m), $\zeta(x,t)$ is the elevation from the mean water level to the temporary water surface (m/s), and $u(x,t)$ are the velocity components (m/s), for all $x \in [0, L]$. We assume that h is a constant and $\zeta \ll h$.

Then Eq. (1) and Eq. (2) become

$$\frac{\partial \zeta}{\partial t} + h \frac{\partial}{\partial x} = 0, \quad (3)$$

$$\frac{\partial u}{\partial t} + g \frac{\partial \zeta}{\partial x} = 0. \quad (4)$$

We will transform Eq. (3) and Eq. (4) into non-dimensional [18], by letting $U = u / \sqrt{gh}$, $Y = y/l$, $X = x/l$, $Z = \zeta/h$ and $T = t\sqrt{gh}/l$. Substituting into Eq. (3) and Eq. (4) leads to

$$\frac{\partial Z}{\partial t} + \frac{\partial U}{\partial X} = 0, \quad (5)$$

$$\frac{\partial U}{\partial T} + \frac{\partial Z}{\partial X} = 0. \quad (6)$$

In [8 -9, 12], they introduce a damping term $-U$ into Eq. (6). We now introduce a damping term $-KU$ Eq. (6) to represent frictional forces due to the drag of sides of the stream, thus

$$\frac{\partial Z}{\partial T} + \frac{\partial U}{\partial X} = 0, \quad (7)$$

$$\frac{\partial U}{\partial T} + \frac{\partial Z}{\partial X} = -KU, \quad (8)$$

where $0 < K < 1$, with the initial conditions at $t=0$ and $0 \leq X \leq 1$ being specified: $Z=0$ and $U=0$. The boundary conditions for $t > 0$ are specified: $Z=e^t$ at $X=0$ and $\frac{\partial Z}{\partial X}=0$ at $X=1$. The system of Eq. (7) and Eq. (8) is called the damped hydrodynamic equations.

B. A Non-dimensional form of the Damped Hydrodynamic Model

In order to solve damped equation in $[0,1] \times [0,T]$, for favorable using u,d for U and Z , respectively;

$$\frac{\partial u}{\partial t} + \frac{\partial d}{\partial x} = -ku, \quad (9)$$

$$\frac{\partial d}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad (10)$$

with the initial conditions $u=0, d=0$ at $t=0$, and the boundary conditions $d(0,t)=f(t)$, and $\frac{\partial d}{\partial x}=0$ at $x=1$.

C. Dispersion Model

The stream water quality model can be described by one-dimensional Advection-Dispersion-Reaction Equations (ADREs). A simplified representation by averaging the equation over the depth is shown in [3 -5, 7, 9 - 11] as:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2} - KC, \quad (11)$$

where $C(x,t)$ is the concentration averaged in depth at the point x and at time t , D is the diffusion coefficient, K is the mass decay rate, and $u(x,t)$ is the velocity component, for all $x \in [0, L]$. We will consider conditions in this model following. The initial condition $C(x,0)=0$ at $t=0$ for all $x > 0$. The boundary conditions $C(0,t)=C_0$ at $x=0$, and $\frac{\partial C}{\partial X}=C_0$ at $x=1$ where C_0 is a constant.

III. MODEL FORMULATION CRANK-NICOLSON METHOD FOR THE HYDRODYNAMIC MODEL

The hydrodynamic model provides the velocity field and elevation of the water. Then, input the results from the hydrodynamic model into the dispersion model, which

provides the pollutant concentration field. In this section, we will follow the numerical techniques of [8]. To find the water velocity and water elevation from Eq. (9) and Eq. (10), we make the following change to variables $v = e^{kt}u$ and represent them into Eq. (9) and Eq. (10). Then we have,

$$\frac{\partial v}{\partial t} + e^{kt} \frac{\partial d}{\partial x} = 0, \quad (12)$$

$$\frac{\partial d}{\partial t} + e^{-kt} \frac{\partial v}{\partial x} = 0. \quad (13)$$

From Eq. (12) and Eq. (13) can be written in the matrix form

$$\begin{pmatrix} v \\ d \end{pmatrix}_t + \begin{bmatrix} 0 & e^{kt} \\ e^{-kt} & 0 \end{bmatrix} \begin{pmatrix} v \\ d \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (14)$$

That is

$$U_t + AU_x = \bar{0}, \quad (15)$$

where

$$A = \begin{bmatrix} 0 & e^{kt} \\ e^{-kt} & 0 \end{bmatrix}, \quad (16)$$

$$U = \begin{pmatrix} v \\ d \end{pmatrix}, \quad \begin{pmatrix} v \\ d \end{pmatrix}_t = \begin{pmatrix} \frac{\partial v}{\partial t} \\ \frac{\partial d}{\partial t} \end{pmatrix}, \quad \begin{pmatrix} v \\ d \end{pmatrix}_x = \begin{pmatrix} \frac{\partial v}{\partial x} \\ \frac{\partial d}{\partial x} \end{pmatrix}, \quad (17)$$

with initial condition $d, v = 0$ at $t = 0$. The left boundary conditions for $x = 0, t > 0$ are specified: $d(0, t) = \sin t$ and $\frac{\partial v}{\partial x} = -e^{kt} \cos t$, and the right boundary conditions for $x = 1, t > 0$ are specified: $\frac{\partial d}{\partial x} = 0$ and $v(0, t) = 0$. We now discretize Eq. (15) by dividing the interval $[0, 1]$ into M subintervals, such that $M\Delta x = 1$, and the interval $[0, T]$ into N subintervals, such that $N\Delta t = T$. We can then approximate $d(x_i, t_n)$ by d_i^n , value of the difference approximation of $d(x, t)$ at point $x = i\Delta x$ and $t = n\Delta t$, where $0 \leq i \leq M$ and $0 \leq n \leq N$, and similarly defined for v_i^n and U_i^n . The grid points (x_n, t_n) are defined by $x_i = i\Delta x$ for all $i = 0, 1, 2, \dots, M$ and $t_n = n\Delta t$ for all $n = 0, 1, 2, \dots, N$, in which M and N are positive integers. Using the Crank-Nicolson method [18] with Eq. (15), the following finite difference equation can be obtained;

$$\left[I - \frac{1}{4} \kappa A [(\Delta_x + \nabla_x)] U_i^{n+1} \right] = \left[I + \frac{1}{4} \kappa A [(\Delta_x + \nabla_x)] U_i^n \right], \quad (18)$$

where

$$U_i^n = \begin{pmatrix} v_i^n \\ d_i^n \end{pmatrix}, \quad \Delta_x U_i^n = U_{i+1}^n - U_i^n, \quad \nabla_x U_i^n = U_i^n - U_{i-1}^n, \quad (19)$$

and I is the unit matrix of order 2, and $\kappa = \frac{\Delta t}{\Delta x}$. Applying the initial and boundary conditions given in Eqs. (12) - (13),

the general form can be obtained;

$$G^{n+1} \bar{U}^{n+1} = E^n \bar{U}^n + F^n, \quad (20)$$

where

$$G^{n+1} = \begin{bmatrix} 1 & 0 & 0 & -\frac{\kappa}{4} a_1^{n+1} & 0 & 0 \\ \frac{\kappa}{4} a_2^{n+1} & 1 & -\frac{\kappa}{4} a_2^{n+1} & 0 & 0 & 0 \\ 0 & \frac{\kappa}{4} a_1^{n+1} & 1 & 0 & 0 & -\frac{\kappa}{4} a_1^{n+1} \\ \frac{\kappa}{4} a_2^{n+1} & 0 & 0 & 1 & -\frac{\kappa}{4} a_2^{n+1} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \frac{\kappa}{4} a_1^{n-1} & 1 \\ 0 & 0 & \frac{\kappa}{4} a_2^{n+1} & 0 & 0 & 1 \end{bmatrix}, \quad (21)$$

$$E^n = \begin{bmatrix} 1 & 0 & 0 & -\frac{\kappa}{4} a_1^n & 0 & 0 \\ -\frac{\kappa}{4} a_2^n & 1 & -\frac{\kappa}{4} a_2^n & 0 & 0 & 0 \\ 0 & \frac{\kappa}{4} a_1^n & 1 & 0 & 0 & -\frac{\kappa}{4} a_1^n \\ -\frac{\kappa}{4} a_2^n & 0 & 0 & 1 & -\frac{\kappa}{4} a_2^n & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \frac{\kappa}{4} a_1^n & 1 \\ 0 & 0 & -\frac{\kappa}{4} a_2^n & 0 & 0 & 1 \end{bmatrix}, \quad (22)$$

$$F^n = \begin{bmatrix} U_1^{n+1} \\ U_2^{n+1} \\ \vdots \\ U_M^{n+1} \\ -\frac{\kappa}{4} a_1^{n+1} \sin(t_{n+1}) - \frac{\kappa}{4} a_1^n \sin(t_n) \\ -\frac{\kappa}{4} a_2^{n+1} \Delta x e^{-t_{n+1}} \cos(t_{n+1}) - \frac{\kappa}{4} a_2^n \Delta x e^{-t_n} \cos(t_n) \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}, \quad (23)$$

where $a_1^n = e^{kt_n}$, $a_2^n = e^{-kt_n}$ and $t_n = n\Delta t$ for all $n = 0, 1, 2, \dots, N$.

IV. FINITE DIFFERENCE TECHNIQUES FOR THE DISPERSION MODEL

In this section, we consider the numerical techniques in [16] for the Advection-Dispersion-Reaction Equation (ADREs) which provides the pollutant concentration field.

We can approximate $C(x, t_n)$ by C_i^n , the value of the difference approximation of $C(x, t)$ at point $x = i\Delta x$ and $t = n\Delta t$, where $1 \leq i \leq M$, and $0 \leq n \leq N$. The grid point (x_i, t_n) is defined by $x_i = i\Delta x$ for all $i = 0, 1, 2, \dots, M$, and $t_i = n\Delta t$ for all $n = 0, 1, 2, \dots, N$ in which M and N are positive integers.

A. Four Points Explicit Upwind Method

We consider the numerical techniques [16], using the forward time central space scheme for the time derivatives and the central difference for the second time derivatives, respectively, as follows:

$$\frac{\partial C}{\partial t} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad (24)$$

$$\frac{\partial^2 C}{\partial x^2} \cong \frac{1}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n], \quad (25)$$

using a third-order scheme for the spatial derivative of Advection-Dispersion-Reaction Equations (ADREs), as given in [19]. For the boundary points, a four-point upwind formula may be written, such that either point to the left or to the right is considered in the finite difference approximation. Next, we approximate the spatial derivative for four points explicit as follows:

$$\frac{\partial C}{\partial x} \cong \frac{1}{6\Delta x} [-11C_i^n + 18C_{i+1}^n - 9C_{i+2}^n + 2C_{i+3}^n], \quad (26)$$

At the interior nodes, as follows,

$$\frac{\partial C}{\partial x} \cong \frac{1}{6\Delta x} [C_{i+2}^n - 6C_{i+1}^n + 3C_i^n + 2C_{i+4}^n]. \quad (27)$$

At right boundary conditions, as follows

$$\frac{\partial C}{\partial x} \cong \frac{1}{6\Delta x} [-2C_{i-3}^n + 9C_{i-2}^n - 18C_{i-1}^n + 11C_i^n], \quad (28)$$

A four points explicit upwind schemes can be obtained so that the technique does not require the systems of linear equations. This technique is an economical computer implementation. Now, we take the explicit finite difference technique [16] into Eq. (11).

At the left boundary, substituting Eqs. (24) – (26) into Eq. (11), then we obtain that;

$$\begin{aligned} \frac{C_i^{n+1} - C_i^n}{\Delta t} + \frac{u_i^n}{6\Delta x} [-11C_i^n + 18C_{i+1}^n - 9C_{i+2}^n + 2C_{i+3}^n] \\ = \frac{D}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n] - kC_i^n, \end{aligned} \quad (29)$$

where $C \cong C_i^n$, $u \cong \tilde{u}_i^n$ and \tilde{u}_i^n are obtained by the Crank-Nicolson method with the hydrodynamic model of Eq. (9),

for all $1 \leq i \leq M$ and $0 \leq n \leq N$. Let $\beta = D \frac{\Delta t}{(\Delta x)^2}$ and

$\beta_i^n = u_i^n \frac{\Delta t}{6\Delta x}$, so Eq. (29) becomes:

$$\begin{aligned} C_i^{n+1} = \beta C_{i-1}^n + [1 - 2\beta - (\Delta t)k + 11\beta_i^n] C_i^n \\ + [\beta - 18\beta_i^n] C_{i+1}^n - 9\beta_i^n C_{i+2}^n - 2\beta_i^n C_{i+3}^n. \end{aligned} \quad (30)$$

For $i = 0$, plug the known value of the left boundary by arranging $C_{i-1}^n = C_0^n$ in Eq. (30) on the right-hand side. We obtain;

$$\begin{aligned} C_0^{n+1} = [1 - \beta - (\Delta t)k + 11\beta_0^n] C_0^n + [\beta - 18\beta_0^n] C_1^n \\ - 9\beta_0^n C_2^n - 2\beta_0^n C_3^n. \end{aligned} \quad (31)$$

At interior, substituting Eqs. (24) – (25) and Eq. (27) into Eq. (11). Then, we obtain;

$$\begin{aligned} C_i^{n+1} = -\beta_i^n C_{i-2}^n + [\beta + 6\beta_i^n] C_{i-1}^n \\ + [1 - 2\beta - 3\beta_i^n - (\Delta t)k] C_i^n + [\beta - 2\beta_i^n] C_{i+1}^n. \end{aligned} \quad (32)$$

At the right boundary, substituting Eqs. (24) – (25) and Eq. (28) into Eq. (11). Then we obtain;

$$\begin{aligned} C_i^{n+1} = 2\beta C_{i-3}^n + [\beta - 9\beta_i^n] C_{i-2}^n + 18\beta_i^n C_{i-1}^n \\ + [1 - 2\beta - (\Delta t)k - 11\beta_i^n] C_i^n + \beta_i^n C_{i+1}^n. \end{aligned} \quad (33)$$

For $i = M$, unknown value of the right boundary by boundary conditions, we can let $C_{M+1}^n = f\Delta x + C_M^n$ in Eq. (33) and, by rearranging, we obtain;

$$\begin{aligned} C_M^{n+1} = 2\beta C_M^n C_{M+1}^n + [\beta - 9\beta_M^n] C_{M+2}^n \\ + 18\beta_M^n C_{M+1}^n + [1 - \beta - (\Delta t)k + 11\beta_M^n] C_M^n + \beta_M^n f\Delta x. \end{aligned} \quad (34)$$

B. The Upwind Explicit Method

The upwind explicit scheme is considered by the following discretization;

$$\frac{\partial C}{\partial t} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad (35)$$

$$\frac{\partial C}{\partial x} \cong \frac{C_i^n - C_{i-1}^n}{\Delta x}, \quad (36)$$

$$\frac{\partial^2 C}{\partial x^2} \cong \frac{1}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n]. \quad (37)$$

Substituting Eqs. (35) – (37) into Eq. (11), then we obtain that;

$$C_i^{n+1} = (\lambda + \beta) C_{i-1}^n + (1 - \lambda - 2\beta - \kappa\Delta t) C_i^n + \beta C_{i+1}^n. \quad (38)$$

For $i = 0$, plug the known value of the left boundary by arranging $C_{i-1}^n = C_0^n - (f\Delta x)$ in Eq. (38) on the right-hand side. We obtain;

$$\begin{aligned} C_0^{n+1} = [1 - \lambda - 2\beta - \kappa\Delta t] C_0^n + [3\beta + \lambda] C_{i-1}^n \\ - [2\beta + \lambda] (f\Delta x). \end{aligned} \quad (39)$$

Similarly, the right boundary condition, for $i = M$, the known value of the right boundary conditions are approximated $C_{M+1}^n = C_M^n + f(\Delta x)$ in Eq. (38) and, by rearranging, we obtain;

$$\begin{aligned} C_M^{n+1} = (\lambda + 2\beta) C_{M-1}^n + [1 - \lambda - 2\beta - \kappa(\Delta t)] C_M^n \\ + \beta (f\Delta x). \end{aligned} \quad (40)$$

The stability of upwind explicit scheme is [20]

$$\frac{\lambda^2 - \lambda}{2} \leq \beta \leq \frac{1 - \lambda}{2}. \quad (41)$$

C. The Lax-Wendroff Method

The Lax-Wendroff scheme is considered by the following discretization;

$$\frac{\partial C}{\partial t} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad (42)$$

$$\frac{\partial C}{\partial x} \cong \lambda \frac{(C_i^n - C_{i-1}^n)}{\Delta x} + (1-\lambda) \frac{(C_{i+1}^n - C_{i-1}^n)}{2\Delta x} \quad (43)$$

$$\frac{\partial^2 C}{\partial x^2} \cong \frac{1}{(\Delta x)^2} [C_{i-1}^n - 2C_i^n + C_{i+1}^n]. \quad (44)$$

Substituting Eqs. (42) – (44) into Eq. (11), then we obtain that;

$$C_i^{n+1} = \frac{1}{2} [\lambda + \lambda^2 + 2\beta] C_{i-1}^n + [1 - \lambda^2 - 2\beta - \kappa(\Delta t)] C_i^n + \frac{1}{2} [2\beta - \lambda - \lambda^2] C_{i+1}^n. \quad (45)$$

For $i=0$, plug the known value of the left boundary by arranging $C_{i-1}^n = C_{i+1}^n - f\Delta x$ in Eq. (45) on the right-hand side. We obtain;

$$C_i^{n+1} = [1 - \lambda^2 - 2\beta - \kappa(\Delta t)] C_i^n + [2\beta] C_{i+1}^n - \frac{1}{2} [\lambda - \lambda^2 + 2\beta] (f\Delta x). \quad (46)$$

Similarly, the right boundary condition, for $i=M$, the known value of the right boundary conditions are approximated $C_{M+1}^n = C_{M-1}^n + f(\Delta x)$ in Eq. (46) and, by rearranging, we obtain;

$$C_i^{n+1} = [2\beta] C_{i-1}^n + [1 - \lambda^2 - 2\beta - \kappa(\Delta t)] C_i^n + \frac{1}{2} [2\beta - \lambda - \lambda^2] C_{i+1}^n. \quad (47)$$

The stability of upwind explicit scheme is [20]

$$0 < \beta < \frac{1 - \lambda^2}{2}. \quad (48)$$

V. NUMERICAL EXPERIMENTS

Suppose that the measurement of pollutant concentration C (Kg/m^3) in a uniform stream at time t (sec) is considered. A stream is aligned with longitudinal distance, 1.0 km total length. There is a plant which discharges waste water into the stream, and the pollutant concentration at discharge point is assumed as; $C(0,t) = 4.0 + \sin(t) - \text{Kg}/\text{m}^3$

at $x=0$ for all $t > 0$, and $C(1,t) = \frac{\partial C}{\partial x} = 0 \text{ Kg}/\text{m}^3$ at $x=1$ for all $t > 0$, and $C(x,0) = 0 \text{ Kg}/\text{m}^3$ at $t=0$.

The velocity of water at the discharge point can be described as a function $d(0,t) = f(t) = 0.4 + |\sin(t)|$ for all $t > 0$, and the elevation is not changed at $x=1$ km. In the analysis conducted in this study, meshes the stream, using $\Delta x = 0.02$, and time increment with $\Delta t = 0.002$. Using Eq. (20); for $k=0$, we obtained the elevation of water $d(x,t)$ as show in Figure1 when after pass 20, and velocity of water

flow $u(x,t)$ as show in Figure 2 when after pass 20. The physical parameter of the stream system is diffusion coefficient $D = 0.02 \text{ m}^2/\text{s}$.

Next the approximate water velocity can be plugged into explicit methods such as four points explicit upwind methods, upwind explicit method and, Lax-Wendroff methods in Eqs. (31, 32, 34), Eqs. (38-40), and Eqs. (45-47), respectively. The approximation of pollutant concentration C of all schemes at $k=0$ where $\Delta x = 0.2$, $\Delta x = 0.05$ and $\Delta x = 0.028591$ are shown in Figure 3-5, respectively. It can see that the trend of results from three methods in the same way. Table I show the stable of four points explicit method, upwind explicit method and, Lax-Wendroff method. We can see that, if we choose $\Delta t = 0.2$ and $\Delta x = 0.06$ then the solution of the four points explicit upwind methods and upwind explicit method are unstable but the Lax-Wendroff method is stable. Consequently, Lax-Wendroff method gives better than the four points explicit upwind methods and upwind explicit method.

TABLE I. THE STABLE OF THREE METHOD APPROXIMATE SOLUTIONS

Δt	Δx	four points explicit	upwind explicit	Lax-Wendroff
0.005	0.2	stable	stable	stable
	0.1	stable	stable	stable
	0.05	stable	stable	stable
	0.02	stable	stable	stable
0.05	0.2	stable	stable	stable
	0.1	stable	stable	stable
	0.05	unstable	stable	stable
	0.04	unstable	unstable	stable
0.2	0.2	stable	stable	stable
	0.1	unstable	stable	stable
	0.06	unstable	unstable	stable

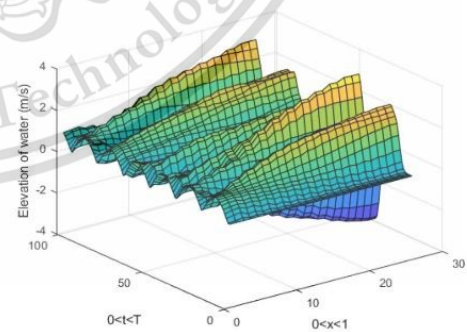


Figure 1. The elevation of water flow $d(x,t) \text{ m/s}$ at $k=0$ when after pass 20

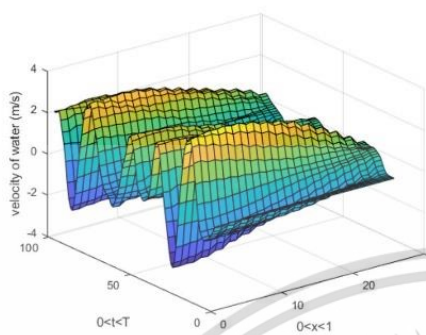


Figure 2. The velocity of water flow $u(x,t)$ m/s at $k=0$ when after pass 20

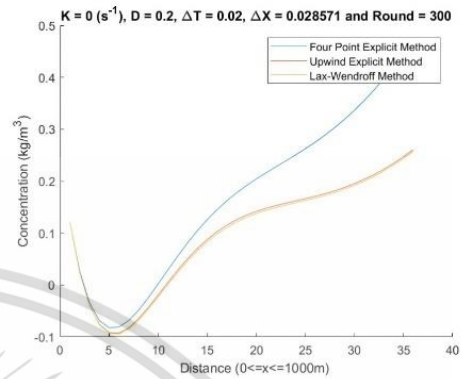


Figure 5. Comparison of water pollutant concentration of the four points explicit upwind methods, the upwind explicit method and, the Lax-Wendroff methods $\Delta x = 0.028591$

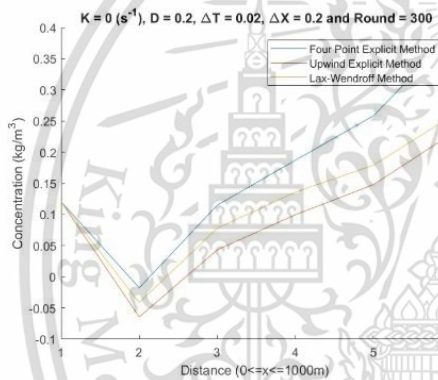


Figure 3. Comparison of water pollutant concentration of the four points explicit upwind methods, the upwind explicit method and, the Lax-Wendroff methods $\Delta x = 0.2$

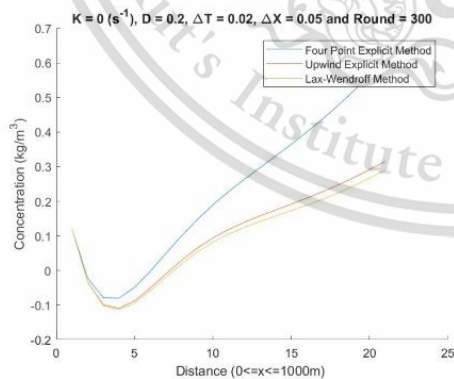


Figure 4. Comparison of water pollutant concentration of the four points explicit upwind methods, the upwind explicit method and, the Lax-Wendroff methods $\Delta x = 0.05$

VI. DISCUSSION

In this research, the water pollutant concentration model is presented. The finite difference methods such as four points explicit upwind methods, upwind explicit method and, Lax-Wendroff methods can be used to estimate the water pollutant concentration. Also, it is appealing that the grid spacing is different so Lax-Wendroff method has been chosen because when making comparisons four points explicit upwind methods, the upwind explicit method in some cases, the solution for four points explicit upwind methods and the upwind explicit method are unstable while the solution for Lax-Wendroff method is stable. Hence, Lax-Wendroff method provides a better result than four points explicit upwind methods and the upwind explicit method.

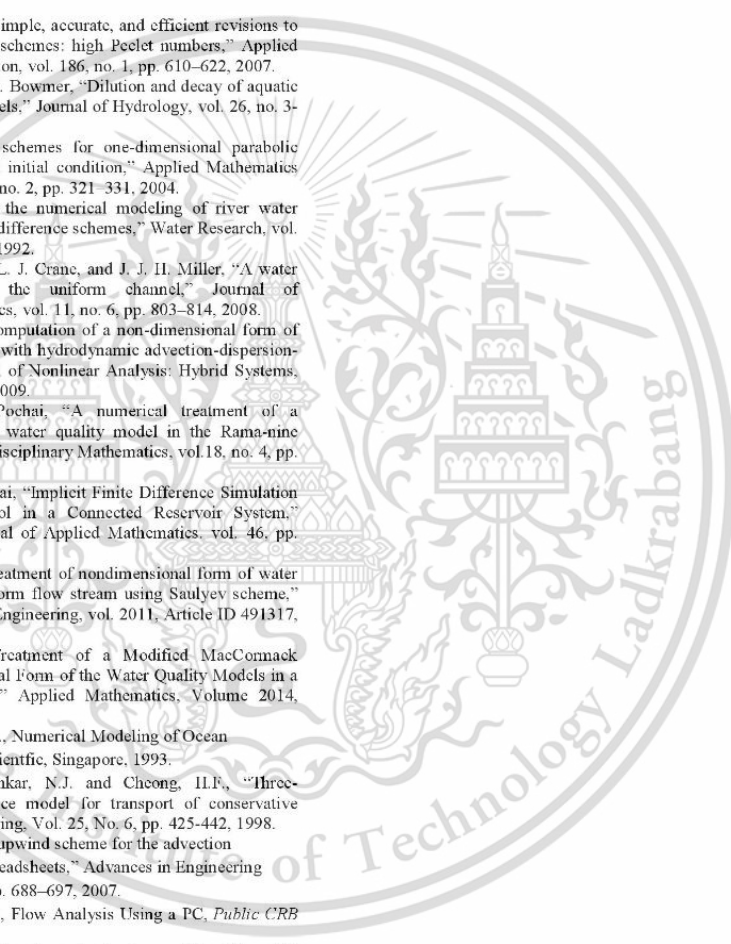
VII. CONCLUSIONS

We have employed explicit finite difference methods to the dispersion model in a stream while there are two different external factors such as the elevation of water and the discharged pollutant. Three explicit finite difference techniques are economical to be used in the real-world problem due to its simplicity to program and the straightforwardness of the implementation. We can see that the Lax-Wendroff explicit method and the upwind explicit method provides better stability conditions than the condition of the four points explicit method.

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