Final Report

Project Title

Numerical Computation of Nondimensional Form of Water Quality Model in a Nonuniform Flow Stream Using Revised Saulyev Scheme

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Month/ Year (30 May 2016)

Contract No. TRF5780016

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This project granted by the Thailand Research Fund

Abstract

The stream water quality model of water quality assessment problems often involves numerical methods to solve the equations. The governing equation of the uniform flow model is one-dimensional advection-dispersion-reaction equations (ADRE). In this project, a better finite difference scheme for solving ADRE is focused and the effect of non-uniform water flows in a stream is considered. Two mathematical models are used to simulate pollution due to sewage effluent. The first is a hydrodynamic model that provides the velocity field and elevation of the water flow. The second is a advection-dispersion-reaction model that gives the pollutant concentration fields after input the velocity data from the hydrodynamic model. For numerical techniques, we used the Crank-Nicolson method for system of a hydrodynamic model and the explicit schemes to the dispersion model. The revised Saulyev schemes are modified from two computation techniques of uniform flow stream problems: forward time central space (FTCS) and modified Saulyev schemes for dispersion model. A comparison of both schemes regarding stability aspect is provided so as to illustrate their applicability to the real-world problem.

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Project Period : May 2014-May2016

Keywords : Finite differences, Crank-Nicolson scheme, New Fourth-orderscheme, Saulyev scheme, One-dimensional/ Hydrodynamic model, Shallow water equation, Dispersion model, Advection-dispersion-reaction equations.

Executive summary

Two mathematical models are used to simulate water quality in a non-uniform flow stream. The first model is the hydrodynamic model that provides the velocity field and the elevation of water. The second model is the advection-diffusion-reaction model that provides the pollutant concentration field. Both 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. A new fourth-order scheme and a Saulyev scheme are simultaneously employed in the second model. This paper proposes a simply remarkable alteration to the fourth-order method so as to make it more accurate without any significant loss of computational efficiency. The results obtained indicate that the proposed new couple fourth-order scheme with Saulyev method do improve the prediction accuracy compared to that of their traditional methods.

Objective

The approximation of the pollutant concentrations from the FTCS technique that stability requirement is one of the disadvantages of the technique. The real-world problems are requiring a small amount of time interval in obtaining accurate solutions. We can see that the FTCS scheme is not good agreement for real application. From many researches can be obtained that the Saulyev technique has an advantage over compared to FTCS. It is unconditionally stable, easy, and economical to implement. In this project, the topic is looking for an improvement method that simple finite difference schemes become more inviting for general model use. The simple explicit schemes include Forward-Time/Centered-Space (FTCS) scheme, the Traditional Saulyev scheme and the Revised Saulyev scheme. These schemes are either first-order or second-order accurate (Li, 2007) and (Pochai, 2011) and have the advantages of simplicity in coding and time effectiveness in computing without losing too much accuracy and thus are preceding for several model applications.

Research methodology

1. To combined the hydrodynamic model and the convection-diffusion-reaction equation to approximate the pollutant concentration in a stream.
2. To develop a numerical technique for the model of the stream of the two different external inputs: the elevation of water and the pollutant concentration at the discharged point can be obtained.
3. To use the Crank-Nicolson Method to find the numerical solution of the hydrodynamic model.
4. To modified the Saulyev technique that can be used in the dispersion model.
5. The collection of all numerical results for writing manuscript to submit in international publication and complete research report.

Result

CHAPTER I

A Non-dimensional Form of Water Quality Model in a Non-Uniform Flow Stream

In this study, two mathematical models are used to simulate water quality in a non-uniform flow stream. The first is the hydrodynamic model that provides the velocity field and elevation of water level. The second is the dispersion model that provides the pollutant concentration field. Both models are formulated in one-dimensional flows 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 input into the second model as the field data. A modified Saulyev method is subsequently employed in the second model. This research propose a simply remarkable alteration to the Saulyev method so as to make it more accurate without any significant loss of computational efficiency. We proposed modified Saulyev scheme to improve the prediction accuracy compared to that of the traditional Saulyev method.

1 Introduction

In general, the amount of pollution levels in the a stream are can be measured via in data collection at the real of field data site. It is somehow often rather difficult complex, and the results deviation obtained tentatively deviate from one in the measurement of each point of time/place to another and each time when the water flow in the stream is not uniform. In water quality modelling in non-uniform flow stream studies, the general used governing equation are the hydrodynamic model and the dispersion model. The one-dimensional shallow water equation and advection-dispersion-reaction equation are govern the first and the second model respectively.

Numerous numerical techniques for solving such models are available. In [18], the finite element method for solving a steady water pollution control to achieve a minimum cost is presented. The numerical techniques for solving the uniform flow of stream water quality model, especially the one-dimensional advection-dispersion-reaction equation are presented in [5], [12], [17], [6] and [23].

The most of non-uniform flow model require data concerned with velocity of the current at any point and any time in the domain. The hydrodynamics model provides the velocity field and tidal elevation of the water. In [25, 21], [19] and [20], they used the hydrodynamics model and convection-dispersion equation to approximate the velocity of the water current in bay, uniform reservoir and stream, respectively. Among these numerical techniques, the finite difference methods, including both explicit and implicit schemes, are mostly used for one-dimensional domain such as in longitudinal stream systems [2], [4].

There are two mathematical models used to simulate water quality in a non-uniform water flow systems. The first is the hydrodynamic model that provides the velocity field and elevation of water. The second is the dispersion model that gives the pollutant concentration field. A couple models is formulated in one-dimensional equations. The traditional Crank-Nicolson method is used for the hydrodynamic model. At each time step the calculated flow velocity fields of the first model are input to the second model as field data [19], [20], [22].

The numerical techniques to solves the non-uniform flow of stream water quality model, one-dimensional advection-dispersion-reaction equation have been presented in [20] by using the fully implicit schemes: Crank-Nicolson method is used to solve the hydrodynamic model and backward time central space (BTCS) for dispersion model in respectively. In [22], the Crank-Nicolson method is also used to solve the hydrodynamic model and the explicit Saulyev scheme is used to solve the dispersion model.

Their research on finite difference techniques for the dispersion model have concentrated on computation accuracy and numerical stability. There are many complicate numerical techniques, such as QUICK scheme, Lax-Wendroff scheme, Crandall scheme and etc. have been studied to increase performances. These techniques have focused on advantages in terms of stability and higher order accuracy[12].

The simple finite difference schemes become more attractive for model use. The simple explicit methods include the Forward Time-Central Space (FTCS) scheme, the MacCormack scheme, and the Saulyev scheme, and the implicit schemes include the Backward Time-Central Space (BTCS) scheme and Crank-Nicolson scheme [4]. These scheme are either first-order or second order accurate and have the advantages in programming and computing without losing much accuracy and thus are used for many model applications [12].

In this research, we will proposes simple revisions to MacCormack scheme that improve its accuracy for problem of water quality measurement in a non-uniform water flow in a stream. In the following sections, the formulation of the traditional MacCormack scheme is reviewed; the proposed revision of modified MacCormack scheme is then described.

The results from hydrodynamic model are data of the water flow velocity for 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 that guaranteed the accurate of the approximate solution is presented in [19], [20] and [22].

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-dispersion-reaction equations are applicable. We use the Crank-Nicolson scheme, the traditional MacCormack scheme and the Modified MacCormack scheme to approximate the velocity, the elevation, and the pollutant concentration from the first model and second model, respectively.

1 Model Formulation

1.1 The Hydrodynamic Model

In this section, we derive a simple hydrodynamic model for describing water current and elevation by one-dimensional shallow water equation. We make the usual assumption in the continuity and momentum balance, i.e., we assume that the Coriolis, shearing stresses and surface wind are small [16], [25], [19] and [20], we obtain the one-dimensional shallow water equations

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

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

where x is longitudinal distance along the stream (m), t is time (s), $h(x)$ be the depth measured from the mean water level to the stream bed (m), $\zeta(x,t)$ is the

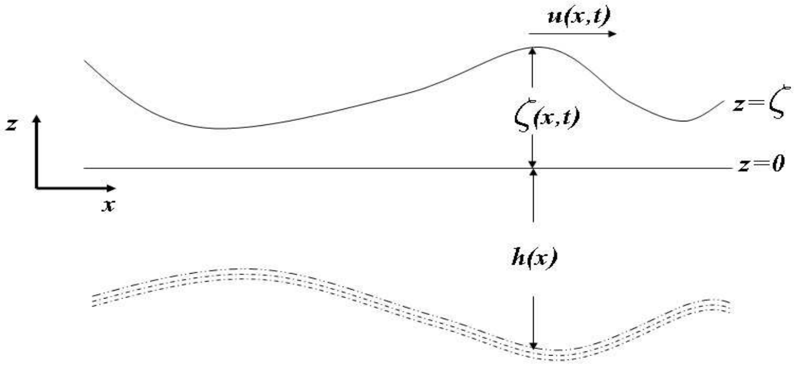

Figure 1: The shallow water system.

elevation from the mean water level to the temporary water surface or the tidal elevation (m/s), and $u(x,t)$ is the velocity components (m/s), for all $x \in [0,l]$.

Assume that h is a constant and $\zeta \ll h$. Then the equations (1)-(2) leads to

$$\frac{\partial \zeta}{\partial t} + h\frac{\partial u}{\partial x} \doteq 0, \quad (3)$$
$$\frac{\partial u}{\partial t} + g\frac{\partial \zeta}{\partial x} = 0. \quad (4)$$

We will consider the equation in dimensionless problem by letting $U = u/\sqrt{gh}, X = x/l, Z = \zeta/h$ and $T = t\sqrt{gh}/l$. Substituting them into the equations(3)-(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 [19], [20] and [22], they introduce a damping term into Eqs.(5)-(6) to represent frictional forces due to the drag of sides of the stream,

$$\frac{\partial Z}{\partial T} + \frac{\partial U}{\partial X} = 0, \quad (7)$$
$$\frac{\partial U}{\partial T} + \frac{\partial Z}{\partial X} = -U, \quad (8)$$

with the initial conditions at $t = 0$ and $0 \le X \le 1$ are specified: $Z = 0$ and $U = 0$. The boundary conditions for $t > 0$ are specified: $Z = e^{it}$ at $X = 0$ and $\frac{\partial Z}{\partial X} = 0$ at $X = 1$. The system of Eqs.(7-8) is called the damped equation. We solve the damped equation by using the finite difference method. In order to solve the equations (7-8) in $[0,1] \times [0,T]$, for convenient using u, d for U and Z respectively,

$$\frac{\partial u}{\partial t} + \frac{\partial d}{\partial x} = -u, \tag{9}$$

$$\frac{\partial d}{\partial t} + \frac{\partial u}{\partial x} = 0, \tag{10}$$

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 $x = 1$.

1.2 Dispersion Model

In a stream water quality model, the governing equations are the dynamic one-dimensional advection-dispersion-reaction equations (ADRE). A simplified representation by averaging the equation over the depth is shown in [5], [12], [17], [20] and [23] as

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

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 $x \in [0,1]$. We will consider the model with following conditions. 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 $\frac{\partial C}{\partial x} = 0$ at $x = 1$ where C_0 is a constant.

CHAPTER II

Numerical Methods for the Hydrodynamic Model

The hydrodynamic model provides the velocity field and elevation of the water. Then the calculated results of the model will be input into the dispersion model which provides the pollutant concentration field. We will follow the numerical techniques of [19]. To find the water velocity and water elevation from equations (9)-(10), we make the following change of variable, $v = e^t u$ and substituting them into Eqs.(9)-(10), we have

$$\frac{\partial v}{\partial t} + e^{-t}\frac{\partial d}{\partial x} = 0, \tag{12}$$
$$\frac{\partial d}{\partial t} + e^{-t}\frac{\partial v}{\partial x} = 0. \tag{13}$$

The equations (12)-(13) can be written in the matrix form

$$\begin{pmatrix} v \\ d \end{pmatrix}_t + \begin{bmatrix} 0 & e^t \\ e^{-t} & 0 \end{bmatrix} \begin{pmatrix} v \\ d \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{14}$$

That is

$$U_t + AU_x = \bar{0}, \tag{15}$$

where

$$A = \begin{bmatrix} 0 & e^t \\ e^{-t} & 0 \end{bmatrix}, \tag{16}$$
$$U = \begin{pmatrix} v \\ d \end{pmatrix} \text{ and } \begin{pmatrix} v \\ d \end{pmatrix}_t = \begin{pmatrix} \partial v/\partial t \\ \partial d/\partial t \end{pmatrix}, \tag{17}$$

with the initial condition $d = v = 0$ at $t = 0$. The left boundary condition for $x = 0, t > 0$ are specified: $d(0,t) = \sin t$ and $\frac{\partial v}{\partial x} = -e^t \cos t$, and the right boundary condition 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 point (x_n, t_n) are defined by $x_i = i\Delta x$

for all $i = 0, 1, 2, \ldots, M$ and $t_n = n\Delta t$ for all $n = 0, 1, 2, \ldots, N$ in which M and N are positive integers. Using the Crank-Nicolson method [15] to Eq.(15), it can be obtained following finite difference equation:

$$[I - \frac{1}{4}\lambda A(\Delta_x + \nabla_x)]U_i^{n+1} = [I + \frac{1}{4}\lambda A(\Delta_x + \nabla_x)]U_i^n, \tag{18}$$

where

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

I is the unit matrix of order 2 and $\lambda = \Delta t/\Delta x$. Applying the initial and boundary conditions given for Eqs.(12)-(13), it can be obtained the general form

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

where

$$G^{n+1} = \begin{bmatrix} 1 & 0 & 0 & -\frac{\lambda}{4}a_1^{n+1} & 0 & 0 & \\ \frac{\lambda}{4}a_2^{n+1} & 1 & -\frac{\lambda}{4}a_2^{n+1} & 0 & 0 & 0 & \\ 0 & \frac{\lambda}{4}a_1^{n+1} & 1 & 0 & 0 & -\frac{\lambda}{4}a_1^{n+1} & \\ \frac{\lambda}{4}a_2^{n+1} & 0 & 0 & 1 & -\frac{\lambda}{4}a_2^{n+1} & 0 & \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & 0 & 0 & 0 & \frac{\lambda}{4}a_1^{n+1} & 1 & -\frac{\lambda}{4}a_1^{n+1} \\ & 0 & 0 & \frac{\lambda}{4}a_2^{n+1} & 0 & 0 & 1 \end{bmatrix},$$

$$E^{n} = \begin{bmatrix} 1 & 0 & 0 & -\frac{\lambda}{4}a_1^{n} & 0 & 0 & \\ -\frac{\lambda}{4}a_2^{n} & 1 & \frac{\lambda}{4}a_2^{n} & 0 & 0 & 0 & \\ 0 & -\frac{\lambda}{4}a_1^{n} & 1 & 0 & 0 & \frac{\lambda}{4}a_1^{n} & \\ -\frac{\lambda}{4}a_2^{n} & 0 & 0 & 1 & \frac{\lambda}{4}a_2^{n} & 0 & \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & 0 & 0 & 0 & -\frac{\lambda}{4}a_1^{n} & 1 & \frac{\lambda}{4}a_1^{n} \\ & 0 & 0 & -\frac{\lambda}{4}a_2^{n} & 0 & 0 & 1 \end{bmatrix}, \bar{U}^n = \begin{pmatrix} U_1^{n+1} \\ U_2^{n+1} \\ \vdots \\ U_{M-1}^{n+1} \end{pmatrix},$$

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

where $a_1^n = e^{t_n}, a_2^n = e^{-t_n}$ and $t_n = n\Delta t$ for all $n = 0, 1, 2, \ldots, N$. The Crank-Nicolson scheme is unconditionally stable [15, 4].

CHAPTER III

The Traditional MacCormack Scheme for the Advection-Dispersion-Reaction Equation

Traditional MacCormack scheme

First of all, we will consider the forward time central space scheme. The scheme is an explicit finite difference scheme with one-step method. The scheme is a forward time central space (FTCS) by changing the central space evaluation at time n to a forward space evaluation. This step is a forward time forward space (FTFS) scheme. The FTFS scheme approximates the temporal and spacial derivatives and the decay in Eq.(11) with the following discretization.

We can then 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 $0 \le i \le M$ and $0 \le n \le N$. The grid point (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.

1.2.1 Forward time central space explicit finite difference scheme

Taking the forward time central space technique [15] into Eq.(11), we get the following discretization:

$$C \cong C_i^n, \tag{21}$$

$$\frac{\partial C}{\partial t} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \tag{22}$$

$$\frac{\partial C}{\partial x} \cong \frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}, \tag{23}$$

$$\frac{\partial^2 C}{\partial x^2} \cong \frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2}, \tag{24}$$

$$u \cong \widehat{U}_i^n. \tag{25}$$

Substitute Eqs.(32)-(36) into Eq.(11), we get

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} + \widehat{U}_i^n\left(\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}\right) = D\left(\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2}\right) - KC_i^n, \tag{26}$$

for $1 \le i \le M$ and $0 \le n \le N-1$. Let $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma_i^{n+1} = \frac{\Delta t}{\Delta x}\widehat{U}_i^{n+1}$, Eq.(37) becomes

$$C_i^{n+1} = \left(\frac{1}{2}\gamma_i^n + \lambda\right)C_{i-1}^n + (1 - 2\lambda - K\Delta t)C_i^n + \left(\lambda - \frac{1}{2}\gamma_i^n\right)C_{i+1}^n. \tag{27}$$

For $i = 1$, plug the known value of the left boundary $C_0^n = C_0$ to Eq.(27) in the right hand side, we obtain

$$C_1^{n+1} = (\frac{1}{2}\gamma_1^n + \lambda)C_0 + (1 - 2\lambda - K\Delta t)C_1^n + (\lambda - \frac{1}{2}\gamma_1^n)C_2^n. \tag{28}$$

For $i = M$, substitute the approximate unknown value of the right boundary by [12], we can let $C_{M+1}^n = 2C_M^n - C_{M-1}^n$ and rearrange, we obtain

$$C_M^{n+1} = (2\lambda)C_{M-1}^n + (1 - 4\lambda - K\Delta t - \gamma_m^n)C_M^n. \tag{29}$$

The forward time central space scheme is conditionally stable subject to constraints in Eq.(37). The stability requirement for the scheme are [2, 12]

$$\lambda = \frac{D\Delta t}{(\Delta x)^2} < \frac{1}{2}, \tag{30}$$

$$\gamma_i^n = \frac{U_i^n \Delta t}{\Delta t} < 1, \tag{31}$$

where λ is the diffusion number (dimensionless) and γ_i^n is the advection number or Courant number (dimensionless). It can be obtained that the strictly stability requirements are the main disadvantage of this scheme.

2 A Modified MacCormack scheme for the advection-dispersion-reaction equation

2.1 The traditional MacCormack scheme

First of all, we consider the traditional MacCormack scheme. The scheme is an explicit finite difference scheme with predictor-corrector two-step method. The first step is a modification of forward time central space (FTCS) by changing the central space evaluation at time n to a forward space evaluation. This step is a forward time forward space (FTFS) scheme. The FTFS scheme approximates the temporal and spacial derivatives and the decay in Eq.(11) with the following discretization.

We can then 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 $0 \le i \le M$ and $0 \le n \le N$. The grid point (x_n, t_n) is defined by $x_i = i\Delta x$ for all $i = 0, 1, 2, \ldots, M$

and $t_n = n\Delta t$ for all $n = 0, 1, 2, \ldots, N$ in which M and N are positive integers. Taking the forward time forward space technique [15] and [12] into Eq.(11), we get the following discretization:

$$\begin{aligned} C &\cong C_i^n, && (32)\\ \frac{\partial C}{\partial t} &\cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, && (33)\\ \frac{\partial C}{\partial x} &\cong \frac{C_{i+1}^n - C_i^n}{\Delta x}, && (34)\\ \frac{\partial^2 C}{\partial x^2} &\cong \frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2}, && (35)\\ u &\cong \widehat{U}_i^n. && (36) \end{aligned}$$

Note that $\widehat{U}_i^n$ are obtained by the Crank-Nicolson method with the hydrodynamic model of Eqs.(9)-(10) that are presented in [19], [20] and [22].

Substitute Eqs.(32)-(36) into Eq.(11), we get

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} + \widehat{U}_i^n\left(\frac{C_{i+1}^n - C_i^n}{\Delta x}\right) = D\left(\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2}\right) - KC_i^n, \quad (37)$$

for $1 \leq i \leq M$ and $0 \leq n \leq N-1$. Substitute the difference equation into Eq.(37), and then define slope S_{i_1} as,

$$S_{i_1} = -\widehat{U}_i^n\left(\frac{C_{i+1}^n - C_i^n}{\Delta x}\right) + D\left(\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2}\right) - KC_i^n, \quad (38)$$

Let $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma_i^{n+1} = \frac{\Delta t}{\Delta x}\widehat{U}_i^{n+1}$, and then define $\acute{\gamma}_i^n = \frac{\gamma_i^n}{\Delta t} = \frac{\widehat{U}_i^n}{\Delta x}$ and $\acute{\lambda} = \frac{D}{(\Delta x)^2} = \frac{\lambda}{\Delta t}$. Eq.(38) takes a simplified form:

$$S_{i_1} = -\acute{\gamma}_i^n(C_{i+1}^n - C_i^n) + \acute{\lambda}(C_{i+1}^n - 2C_i^n + C_{i-1}^n) - KC_i^n, \quad (39)$$

or

$$S_{i_1} = (\acute{\lambda} - \acute{\gamma}_i^n)C_{i+1}^n - (2\acute{\lambda} - \acute{\gamma}_i^n + K)C_i^n + \acute{\lambda}C_{i-1}^n. \quad (40)$$

For upper boundary, where $i = 1$, plug the known value of the left boundary $C_0^n = C_0$ to Eq.(40) in the right hand side, we obtain

$$S_{1_1} = (\acute{\lambda} - \acute{\gamma}_1^n)C_2^n - (2\acute{\lambda} - \acute{\gamma}_1^n + K)C_1^n + \acute{\lambda}C_0. \quad (41)$$

For the lower boundary, where $i = M$, substitute the approximate unknown value of the right boundary by the forward difference approximation to $\frac{\partial C}{\partial x} = 0$, we can let $C_M = C_{M-1}$ and rearrange, we obtain

$$S_{M_1} = -(\acute{\lambda} + K)C_{M-1}^n + \acute{\lambda}C_{M-2}^n. \quad (42)$$

Take the Euler formula, we obtain the MacCormack predictor step formulation,

$$C_i^{n+1} = C_i^n + S_{i_1}\Delta t. \tag{43}$$

The second step is a modified backward time central space (BTCS) scheme by changing the central space evaluation time n with a backward space evaluation. It is essentially a backward time backward space (BTBS) scheme. The BTBS scheme approximates the temporal and spacial derivatives and the decay in Eq.(11) with the following discretization:

$$C \cong \frac{1}{2}(C_i^n + C_i^{n+1}), \tag{44}$$

$$\frac{\partial C}{\partial t} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \tag{45}$$

$$\frac{\partial C}{\partial x} \cong \frac{C_i^{n+1} - C_{i-1}^{n+1}}{\Delta x}, \tag{46}$$

$$\frac{\partial^2 C}{\partial x^2} \cong \frac{1}{2}(\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} + \frac{C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}). \tag{47}$$

Because the values at time level $n+1$ have calculated in predictor step, the second step is also explicit. It follows that the slope base on their predictor points can be calculated as:

$$S_{i_2} = \acute{\lambda} C_{i+1}^{n+1} - (2\acute{\lambda} + \acute{\gamma}_i^{n+1} + K)C_i^{n+1} + (\acute{\lambda} + \acute{\gamma}_i^{n+1})C_{i-1}^{n+1}. \tag{48}$$

For upper boundary, where $i = 1$, plug the known value of the left boundary $C_0^{n+1} = C_0$ to Eq.(48) in the right hand side. We obtain

$$S_{1_2} = \acute{\lambda} C_2^{n+1} - (2\acute{\lambda} + \acute{\gamma}_1^{n+1} + K)C_1^{n+1} + (\acute{\lambda} + \acute{\gamma}_1^{n+1})C_0. \tag{49}$$

For the lower boundary, where $i = M$, substitute the approximate unknown value of the right boundary by the backward difference approximation to $\frac{\partial C}{\partial x} = 0$, we can let $C_{M+1} = C_M$ and rearrange, then we obtain

$$S_{M_2} = \acute{\lambda} C_M^{n+1} - (2\acute{\lambda} + \acute{\gamma}_M^{n+1} + K)C_M^{n+1} + (\acute{\lambda} + \acute{\gamma}_M^{n+1})C_{M-1}^{n+1}. \tag{50}$$

From the both steps, the MacCormack scheme takes the following form.

$$C_i^{n+1} = C_i^n + \frac{\Delta t}{2}(S_{i_1} + S_{i_2}). \tag{51}$$

The MacCormack scheme is conditionally stable subject to constraints in Eq.(37). The stability requirements for the scheme are [3]

$$\lambda = \frac{D\Delta t}{(\Delta x)^2} < \frac{1}{2}, \tag{52}$$

$$\gamma_i^n = \frac{\widehat{U}_i^n \Delta t}{\Delta x} < 0.9, \tag{53}$$

where λ is the diffusion number (dimensionless) and γ_i^n is the advection number or Courant number (dimensionless).

2.2 The Modified MacCormack scheme

Since the derivative approximation during discretization is not centered, numerical dispersion will be introduced. The dispersion coefficients used in the dispersion model would take the value obtained by subtracting the numerical dispersion from the real data of the stream. The amounts of the numerical dispersion introduced by backward space denoted by Dn_1, and forward time denoted by Dn_2 schemes as follow [4], [12],

$$Dn_{1i}^{\,n} = \frac{\Delta x}{2}\widehat{U}_i^n, \tag{54}$$

$$Dn_{2i}^{\,n} = -\frac{\Delta x}{2}(\widehat{U}_i^n)^2. \tag{55}$$

There are temporal and spacial numerical dispersion in both predictor and corrector steps since the scheme uses forward time forward space difference for prediction and backward time backward space difference for correction. From Eqs.(54)-(55), the numerical dispersion for forward time forward space prediction step and backward time backward space correction step are

$$D_{n_{prd}}{}_i^n = -\frac{\Delta x}{2}\widehat{U}_i^n - \frac{\Delta t}{2}(\widehat{U}_i^n)^2, \tag{56}$$

$$D_{n_{crc}}{}_i^n = \frac{\Delta x}{2}\widehat{U}_i^n + \frac{\Delta t}{2}(\widehat{U}_i^n)^2. \tag{57}$$

The modified MacCormack scheme uses the following corrected dispersion, rather than the real dispersion coefficients for calculation in both prediction and correction steps,

$$D_{1i}^{\,n} = D_{real} - D_{n_{prd}}{}_i^n, \tag{58}$$

$$D_{2i}^{\,n} = D_{real} - D_{n_{crc}}{}_i^n, \tag{59}$$

where ${D_1}_i^n$ is the dispersion coefficient used in the prediction step, and ${D_2}_i^n$ is the dispersion coefficient used in the correction step.

The Modified MacCormack scheme is conditionally stable subject to the constraint in Eq.(37). The stability requirements for the scheme

$$\lambda = \frac{D_{max}\Delta t}{(\Delta x)^2} < \frac{1}{2}, \tag{60}$$

$$\gamma_i^n = \frac{\widehat{U}_i^n \Delta t}{\Delta x} < 0.9, \tag{61}$$

where the maximum of numerical dispersion coefficients is $D_{max} = \max\{{D_1}_i^n, {D_2}_i^n : 0 \leq i \leq M, 0 \leq n \leq N\}$.

CHAPTER IV

Two-Level Explicit Methods for the Advection-Dispersion-Reaction Equation

Two-Level Explicit Methods

We can then 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 $0 \leq i \leq M$ and $0 \leq n \leq N$. The grid point (x_n, t_n) are defined by $x_i = i\Delta x$ for all $i = 0, 1, 2, \ldots, M$ and $t_n = n\Delta t$ for all $n = 0, 1, 2, \ldots, N$ in which M and N are positive integers.

2.2.1 Forward time central space explicit finite difference scheme

Taking the approximations of the derivatives with a weight ϕ into Eq.(11), we get the following discretization:

$$C \cong C_i^n, \tag{62}$$

$$\frac{\partial C}{\partial t} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \tag{63}$$

$$\frac{\partial C}{\partial x} \cong \phi \frac{C_i^n - C_{i-1}^n}{\Delta x} + (1-\phi)\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}, \tag{64}$$

$$\frac{\partial^2 C}{\partial x^2} \cong \frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2}, \tag{65}$$

$$u \cong \widehat{U}_i^n. \tag{66}$$

Then the weighted explicit finite difference equation becomes

$$C_i^{n+1} = ((\frac{1+\phi}{2})\gamma_i^n + \lambda)C_{i-1}^n + (1 - 2\lambda - k\Delta t - \gamma_i^n \phi)C_i^n + (\lambda - (\frac{1-\phi}{2})\gamma_i^n)C_{i+1}^n, \tag{67}$$

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

$$\gamma_i^n = \widehat{U}_i^n(\frac{\Delta t}{\Delta x}), \tag{68}$$

$$\mu = \frac{\Delta t}{(\Delta x)^2}, \tag{69}$$

$$\lambda = D\mu. \tag{70}$$

If we putting $\phi = 0$ in Eq.(67), we can obtain

$$C_i^{n+1} = (\frac{1}{2}\gamma_i^n + \lambda)C_{i-1}^n + (1 - 2\lambda - k\Delta t)C_i^n + (\lambda - \frac{1}{2}\gamma_i^n)C_{i+1}^n, \tag{71}$$

for $1 \leq i \leq M$ and $0 \leq n \leq N-1$. For $i=1$, we can plug the constant know value of the left boundary condition that $C_0^n = C_0$ to Eq.(71) on the right hand side, we get

$$C_1^{n+1} = (\frac{1}{2}\gamma_1^n + \lambda)C_0 + (1 - 2\lambda - k\Delta t)C_1^n + (\lambda - \frac{1}{2}\gamma_1^n)C_2^n. \quad (72)$$

For $i = M$, we will substituting the approximation unknown point on the right boundary condition by [12], letting $C_{M+1}^n = 2C_M^n - C_{M-1}^n$, we can obtain that

$$C_M^{n+1} = \gamma_M^n C_{M-1}^n + (1 - 4\lambda - k\Delta t + \gamma_M^n)C_M^n. \quad (73)$$

A von Neumann stability condition of Eq.(71) [] is

$$\gamma_i^n \;<\; 1, \quad (74)$$

$$\frac{(\gamma_i^n)^2}{2} \leq \lambda \;\leq\; \frac{1}{2}. \quad (75)$$

where λ is the diffusion number (dimensionless) and γ_i^n is the advection number or Courant number (dimensionless). It can be obtained that the strictly stability requirements are the main disadvantage of this scheme.

The finite difference formula Eq.(27) has been derived in [**?**] that the truncation error for this method is $O\{(\Delta x^2), \Delta t\}$.

2.2.2 The Lax-Wenfroff method

If we putting $\phi = \gamma_i^n$ in Eq.(67), we can obtain

$$\begin{aligned} C_i^{n+1} &= \frac{1}{2}(2\lambda + \gamma_i^n + (\gamma_i^n)^2)C_{i-1}^n + (1 - 2\lambda - (\gamma_i^n)^2 - k\Delta t)C_i^n \\ &\quad + \frac{1}{2}(2\lambda - \gamma_i^n + (\gamma_i^n)^2)C_{i+1}^n, \end{aligned} \quad (76)$$

for $1 \leq i \leq M$ and $0 \leq n \leq N-1$. For $i=1$, we can plug the constant know value of the left boundary condition that $C_0^n = C_0$ to Eq.(76) on the right hand side, we get

$$\begin{aligned} C_1^{n+1} &= \frac{1}{2}(2\lambda + \gamma_1^n + (\gamma_1^n)^2)C_0 + (1 - 2\lambda - (\gamma_1^n)^2 - k\Delta t)C_1^n \\ &\quad + \frac{1}{2}(2\lambda - \gamma_1^n + (\gamma_1^n)^2)C_2^n. \end{aligned} \quad (77)$$

For $i = M$, we will substituting the approximation unknown point on the right boundary condition by [12], letting $C_{M+1}^n = 2C_M^n - C_{M-1}^n$, we can obtain that

$$C_M^{n+1} = \gamma_i^n C_{M-1}^n + (1 - 4\lambda - k\Delta t - \gamma_i^n)C_M^n. \quad (78)$$

A von Neumann stability condition of Eq.(71) [] is

$$\gamma_i^n < 1, \tag{79}$$

$$\frac{(\gamma_i^n)^2}{2} \leq \lambda \leq \frac{1}{2}. \tag{80}$$

where λ is the diffusion number (dimensionless) and γ_i^n is the advection number or Courant number (dimensionless). It can be obtained that the strictly stability requirements are the main disadvantage of this scheme.

The finite difference formula Eq.(27) has been derived in [**?**] that the truncation error for this method is $O\{(\Delta x^2), \Delta t\}$.

2.2.3 Saulyev explicit finite difference scheme

The Saulyev scheme is unconditionally stable [6]. It is clear that the non-strictly stability requirement of Saulyev scheme is the main of advantage and economical to use. Taking Saulyev technique [6] into Eq.(11), it can be obtained the following discretization:

$$C \cong C_i^n, \tag{81}$$

$$\frac{\partial C}{\partial t} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \tag{82}$$

$$\frac{\partial C}{\partial x} \cong \frac{C_{i+1}^n - C_{i-1}^{n+1}}{2\Delta x}, \tag{83}$$

$$\frac{\partial^2 C}{\partial x^2} \cong \frac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}, \tag{84}$$

$$u \cong \widehat{U}_i^n. \tag{85}$$

Substitute Eqs.(97)-(101) into Eq.(11), we get

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} + \widehat{U}_i^n(\frac{C_{i+1}^n - C_{i-1}^{n+1}}{2\Delta x}) = D(\frac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}) - kC_i^n, \tag{86}$$

for $1 \leq i \leq M$ and $0 \leq n \leq N-1$. Let $\lambda = \frac{D\Delta t}{(\Delta x)^2}$ and $\gamma_i^{n+1} = \frac{\Delta t}{\Delta x}\widehat{U}_i^{n+1}$, Eq.(102) becomes

$$C_i^{n+1} = (\frac{1}{1+\lambda})((\frac{1}{2}\gamma_i^n + \lambda)C_{i-1}^{n+1} + (1 - \lambda - K\Delta t)C_i^n + (\lambda - \frac{1}{2}\gamma_i^n)C_{i+1}^n). \tag{87}$$

For $i = 1$, plug the known value of the left boundary $C_0^{n+1} = C_0$ to Eq.(104) in the right hand side, we obtain

$$C_1^{n+1} = (\frac{1}{1+\lambda})((\frac{1}{2}\gamma_1^n + \lambda)C_0 + (1 - \lambda - K\Delta t)C_1^n + (\lambda - \frac{1}{2}\gamma_1^n)C_2^n). \tag{88}$$

For $i = M$, substitute the approximate unknown value of the right boundary by [26], we can let $C_{M+1}^n = C_M^n + C_M^{n+1} - C_{M-1}^{n+1}$ and rearrange, we obtain

$$C_M^{n+1} = (\frac{1}{1+\frac{1}{2}\gamma_M^n})(\gamma_M^n C_{M-1}^{n+1} + (1 - K\Delta t - \frac{1}{2}\gamma_M^n)C_M^n). \tag{89}$$

Using Taylor series expansions on the approximation, [?] has shown the truncation error is $O\{(\Delta x)^2 + (\Delta t)^2 + (\frac{\Delta t}{\Delta x})^2\}$ or $O\{2, 2, (1/1)^2\}$.

From Eqs.(102-106), it can be obtained that the technique does not generate the system of linear equations. It follows that the application of the technique is economical computer implementation.

3 A new fouth-order scheme with a Saulyev method for the advection-dispersion equation

Taking a new fourth-order technique [7] into Eq.(11), the discretization for each terms are obtained as follows,

$$C \cong C_i^n, \tag{90}$$

$$\frac{\partial C}{\partial t} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \tag{91}$$

$$\frac{\partial C}{\partial x} \cong F_i^n \frac{C_{i+2}^n - C_i^n}{2\Delta x} + G_i^n \frac{C_i^n - C_{i-2}^n}{2\Delta x} - H_i^n \frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}, \tag{92}$$

$$\frac{\partial^2 C}{\partial x^2} \cong P_i^n \frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} + Q_i^n \frac{C_{i+2}^n - 2C_i^n + C_{i-2}^n}{(\Delta x)^2} \tag{93}$$

$$u \cong \widehat{U}_i^n, \tag{94}$$

where

$$\begin{aligned}
\lambda &= \frac{D\Delta t}{(\Delta x)^2}, \\
\gamma_i^n &= \frac{\Delta t}{\Delta x}\widehat{U}_i^n, \\
F_i^n &= \frac{(12\lambda + 2(\gamma_i^n)^2 - 3\gamma_i^n - 2)}{12}, \\
G_i^n &= \frac{(12\lambda + 2(\gamma_i^n)^2 + 3\gamma_i^n - 2)}{12}, \\
H_i^n &= \frac{((\gamma_i^n)^2 + 6\lambda - 4)}{3}, \\
P_i^n &= \frac{(-(\gamma_i^n)^4 + 4(\gamma_i^n)^2 - 12\lambda^2 - 12\lambda(\gamma_i^n)^2 + 8\lambda)}{6\lambda}, \\
Q_i^n &= \frac{((\gamma_i^n)^4 - 4(\gamma_i^n)^2 + 12\lambda^2 + 12\lambda(\gamma_i^n)^2 - 2\lambda)}{6\lambda}.
\end{aligned}$$

Substitute Eqs.(90)-(94) into Eq.(11), we get

$$\begin{aligned}
&\frac{C_i^{n+1} - C_i^n}{\Delta t} + \widehat{U}_i^n\left(F_i^n\frac{C_{i+2}^n - C_i^n}{2\Delta x} + G_i^n\frac{C_i^n - C_{i-2}^n}{2\Delta x} - H_i^n\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}\right) \\
&\qquad = D\left(P_i^n\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} + Q_i^n\frac{C_{i+2}^n - 2C_i^n + C_{i-2}^n}{(\Delta x)^2}\right), \qquad (95)
\end{aligned}$$

for $2 \le i \le M-2$ and $0 \le n \le N-1$. The Eq.(95) can be written in an explicit form of finite difference equation as follows,

$$\begin{aligned}
C_i^{n+1} &= \left(\frac{1}{2}\gamma_i^n G_i^n + \lambda Q_i^n\right)C_{i-2}^n + \left(-\frac{1}{2}\gamma_i^n H_i^n + \lambda P_i^n\right)C_{i-1}^n \\
&\quad + \left(1 + \frac{1}{2}\gamma_i^n F_i^n - \frac{1}{2}\gamma_i^n G_i^n - 2\lambda P_i^n - \lambda Q_i^n\right)C_i^n + \left(\frac{1}{2}\gamma_i^n H_i^n + \lambda P_i^n\right)C_{i+1}^n \\
&\quad + \left(-\frac{1}{2}\gamma_i^n F_i^n + \lambda Q_i^n\right)C_{i+2}^n, \qquad (96)
\end{aligned}$$

for $2 \le i \le M-2$ and $0 \le n \le N-1$. For $i = 1, M-1$ and M, the new fourth-order finite difference equation Eq.(96) cannot be employed to calculate the value C_i^n on the grid point next to left and right boundaries of the domain of solution. The alternate appropriate finite difference method such as the Saulyev method will be employed to approximate them as the following section.

3.0.4 The employment of a Saulyev method to the left and the right boundary conditions

The Saulyev scheme is unconditionally stable [6] and [7]. It is clear that the non-strictly stability requirement of Saulyev scheme is the main of advantage and economical to use. Taking Saulyev technique [6] into Eq.(11), it can be obtained the following discretization:

$$
\begin{aligned}
C &\cong C_i^n, && (97)\\
\frac{\partial C}{\partial t} &\cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, && (98)\\
\frac{\partial C}{\partial x} &\cong \frac{C_{i+1}^n - C_{i-1}^{n+1}}{2\Delta x}, && (99)\\
\frac{\partial^2 C}{\partial x^2} &\cong \frac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}, && (100)\\
u &\cong \widehat{U}_i^n. && (101)
\end{aligned}
$$

Substitute Eqs.(97)-(101) into Eq.(11), we get

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} + \widehat{U}_i^n\left(\frac{C_{i+1}^n - C_{i-1}^{n+1}}{2\Delta x}\right) = D\left(\frac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}\right), \quad (102)$$

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

For $i = 1$, plug the known value of the left boundary $C_0^{n+1} = r_0^{n+1}$ to Eq.(102) in the right hand side, we obtain

$$C_1^{n+1} = \left(\frac{1}{1+\lambda}\right)\left(\left(\frac{1}{2}\gamma_1^n + \lambda\right)r_0^{n+1}\right) + (1-\lambda)C_1^n + \left(\lambda - \frac{1}{2}\gamma_1^n\right)C_2^n). \quad (103)$$

For $i = M-1$, we can obtain an explicit form of Eq.(102),

$$C_{M-1}^{n+1} = \left(\frac{1}{1+\lambda}\right)\left(\left(\frac{1}{2}\gamma_{M-1}^n + \lambda\right)C_{M-2}^{n+1} + (1-\lambda)C_{M-1}^n + \left(\lambda - \frac{1}{2}\gamma_{M-1}^n\right)C_M^n\right). \quad (104)$$

For $i = M$, substitute the approximate unknown value of the right boundary by a traditional central difference method [3] with the known derivative right boundary condition,

$$C_{M+1}^n = C_{M-1}^n + 2\Delta x S_0. \quad (105)$$

Substituting Eq.(105) into Eq.(102), we can obtain

$$C_{M+1}^{n+1} = \left(\frac{1}{1+\lambda}\right)\left(2\lambda C_{i-1}^n + (1-\lambda)C_i^n + \left(\lambda - \frac{1}{2}\gamma_i^n\right)(2\Delta x S_0)\right). \quad (106)$$

From Eqs.(103-106), it can be obtained that the technique does not generate their fictitious points along the both side of the solution domain. It follows that the new fourth-order finite difference equation Eq.(96) with the employed Saulyev finite difference equations Eqs.(103-104, 106) can be used to calculate the value C_i^n entire their grid points of the solution domain.

4 Numerical Experiment

The uniform flow of an advection-diffusion is considered in a uniform stream of constant cross-section and bottom slope. Flow velocity and diffusion coefficient are taken to be $U = 0.01$ m/s and $D = 0.002$ m^2/s. Assume that the length of the considered stream is $L = 100$ m. Let the pollutant concentration level that released at the left-end is

$$C(0,1) = 1. \tag{107}$$

There is no rate of change of pollutant on the right-end as follows

$$\frac{\partial C}{\partial x}(L,t) = 0. \tag{108}$$

The theoretical solution of the problem is [9], [24]

$$C(x,t) = \frac{1}{2}\text{erfc}(\frac{x-Ut}{\sqrt{4Dt}}) + \frac{1}{2}e^{\frac{Ux}{D}}\text{erfc}(\frac{x+Ut}{\sqrt{4Dt}}). \tag{109}$$

The accuracy of the proposed new fourth-order scheme with employed Saulyev method to the boundary and the theoretical methods are compared in Fig.2.

5 Application to a nonuniform flow stream water quality assessment problem

Suppose that the measurement of pollutant concentration C in a non-uniform flow stream is considered. A stream is aligned with longitudinal distance, 1.0 (km.) total length and 1.0 (m.) depth. There is a plant which discharges waste water into the stream and the pollutant concentration at the discharge point is $C(0,t) = C_0 = 1$ (mg/L) at $x = 0$ for all $t > 0$, there is no rate of change of pollutant level $\frac{\partial C}{\partial x} = 0$ at $x = 1.0$ for all $t > 0$, and there is no initial pollutant $C(x,0) = 0$ (mg/L) at $t = 0$. The elevation of water at the discharge point can be described as a function $d(0,t) = f(t) = \sin t$ (m.) for all $t > 0$, and the elevation does not change at $x = 1.0$ (km.) The physical parameters of the stream system is a diffusion coefficient $D = 0.1$ (m^2/s). In the analysis conducted in this study, meshing the stream into 40 elements with $\Delta x = 0.05$, and the time increment is 0.4 (s) with $\Delta t = 0.00125$, characterizing a one-dimensional flow. Using the

Crank-Nicolson method of [19], [20] and [22], it can be obtained the water velocity $u(x,t)$ in Table 1 and Fig 6. Next, the approximate water velocity can be plugged new fourth-order scheme and employing the Saulyev method to the left boundary near the discharge point and the right boundary in Eq.(96). The approximation of pollutant concentrations C of the proposed scheme is shown in Table **??** and Fig.4.

Table 1: The velocity of water flow $u(x,t)$

t	$x=0$	$x=0.1$	$x=0.2$	$x=0.3$	$x=0.4$	$x=0.5$	$x=0.6$	$x=0.7$	$x=0.8$	$x=0.9$	$x=1.0$
10	0.5421	0.5505	0.5421	0.5202	0.4859	0.4362	0.3701	0.2901	0.1998	0.1029	0.0000
20	1.3284	1.2315	1.1228	1.0041	0.8766	0.7416	0.6001	0.4538	0.3042	0.1526	0.0000
30	0.3291	0.2628	0.2058	0.1578	0.1182	0.0861	0.0606	0.0405	0.0246	0.0116	0.0000
40	-1.1343	-1.0752	-0.9995	-0.9086	-0.8044	-0.6884	-0.5627	-0.4290	-0.2894	-0.1457	0.0000

Table 2: The pollutant concentration $C(x,t)$ using the new fourth-order scheme and employing Saulyev scheme, $\Delta x = 0.05$, $\Delta t = 0.00125$

t	$x=0$	$x=0.1$	$x=0.2$	$x=0.3$	$x=0.4$	$x=0.5$	$x=0.6$	$x=0.7$	$x=0.8$	$x=0.9$	$x=1.0$
10	1.00000	0.98707	0.96381	0.92269	0.85430	0.75311	0.62458	0.48989	0.38012	0.31931	0.30376
20	1.00000	0.99226	0.97058	0.92379	0.84269	0.72904	0.60095	0.48632	0.40726	0.36902	0.35910
30	1.00000	0.81678	0.67155	0.60392	0.58238	0.57723	0.57518	0.57294	0.57033	0.56750	0.56423
40	1.00000	0.73266	0.71148	0.71812	0.71721	0.71552	0.71391	0.71215	0.71013	0.70778	0.70470

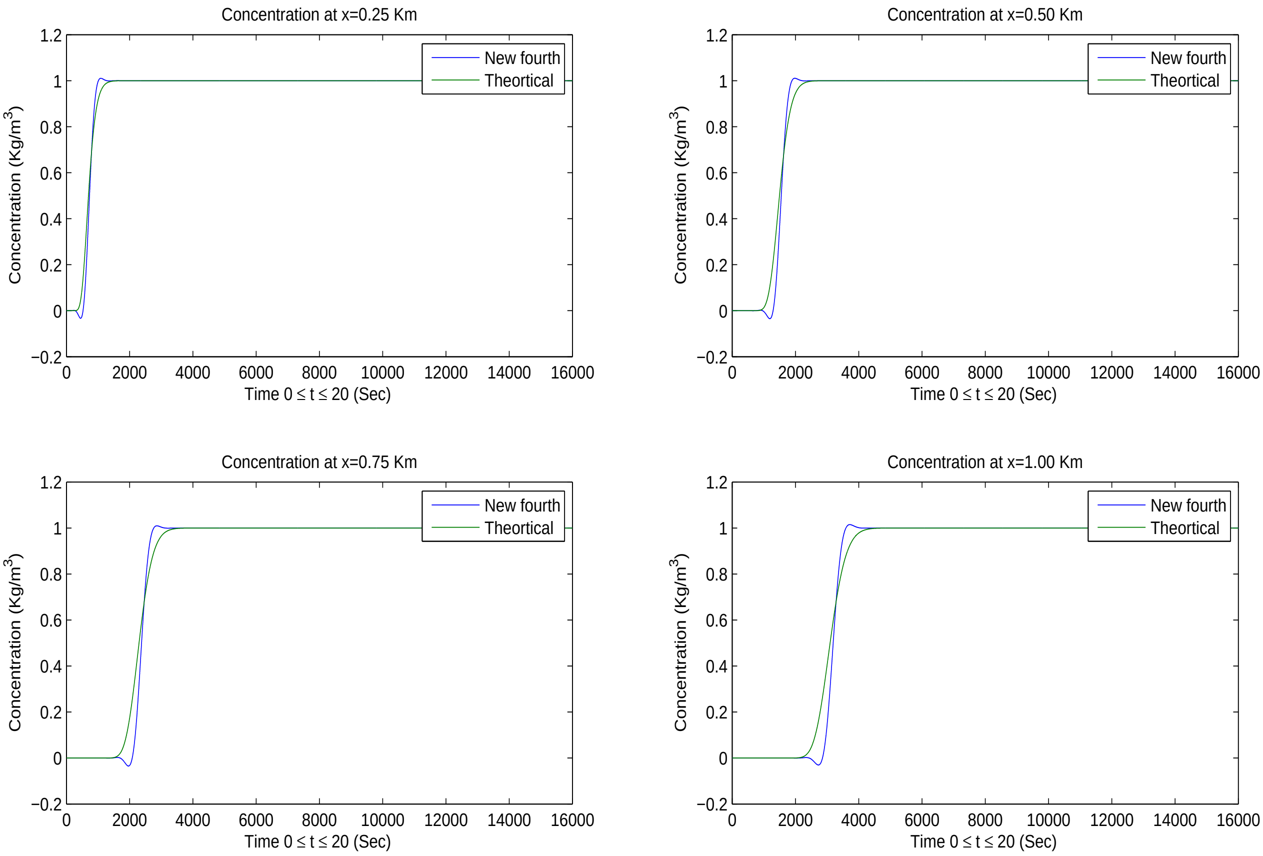

Figure 2: The comparison of exact solution and new fourth-order scheme

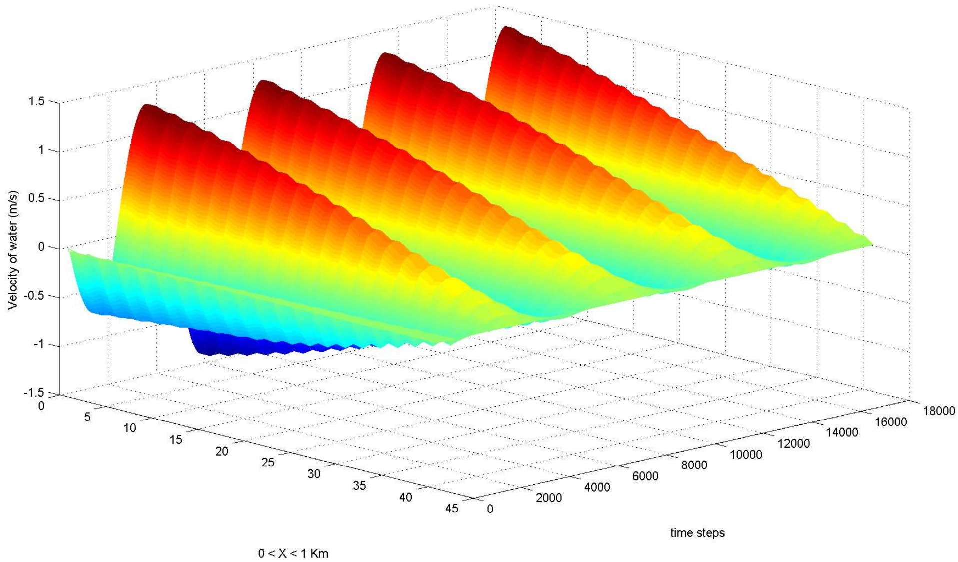

Figure 3: The water velocity $u(x,t)$ m/s

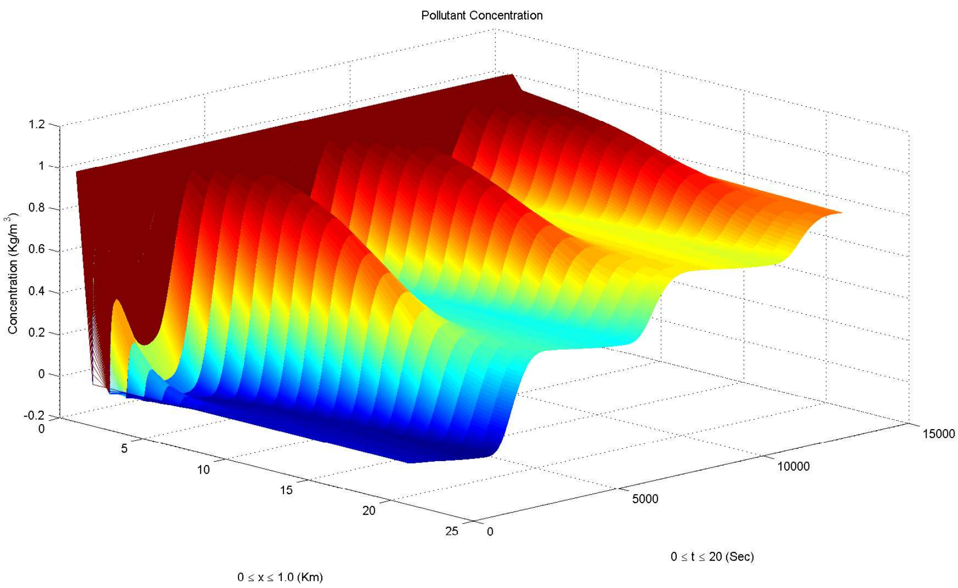

Figure 4: The pollutant concentration $C(x,t)$ (mg/L) using new fourth-order scheme and employing Saulyev scheme

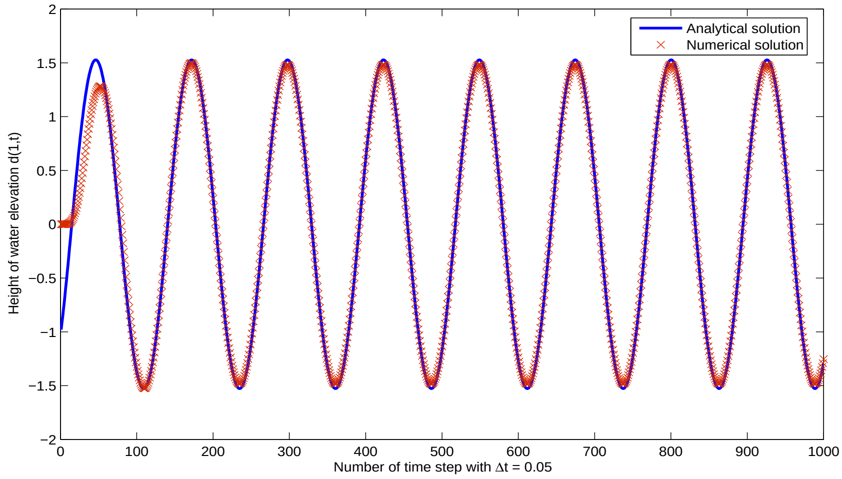

Figure 5: Comparison of analytical solution for height of water elevation with results obtained by numerical technique at the end point of the domain.

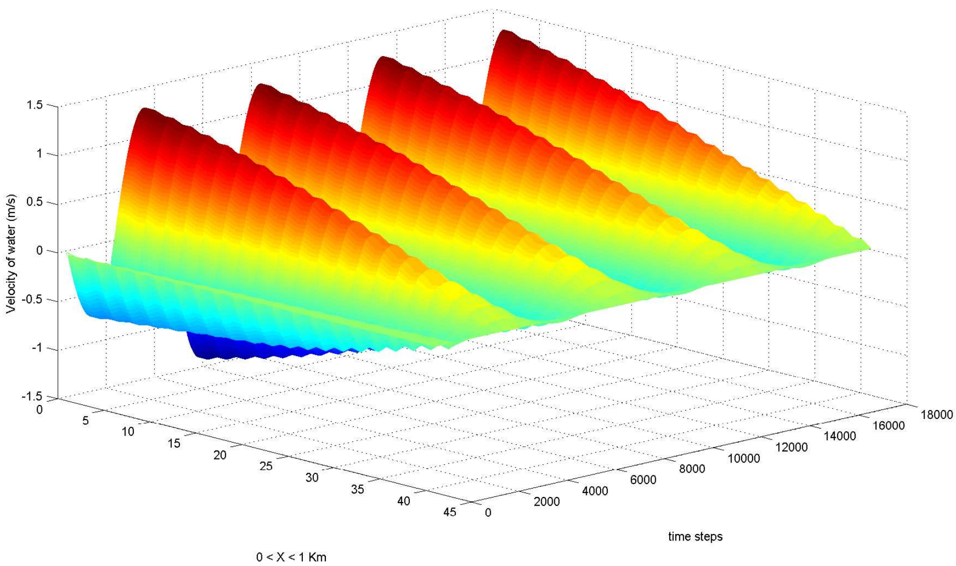

Figure 6: The water velocity $u(x,t)$ m/s

CHAPTER VI
Discussion and Conclusions

The approximation of the pollutant concentrations of the FTCS schemes are shown in Tables **??**. The real-world problems are require a small amount of time interval in obtaining accurate solutions. Unfortunately, the analytical solutions of hydrodynamic model could not found over entire domain. This implies that the analytical solutions of dispersion model could not carry out at any point on the domain as well [22].

In [22], we can obtain that the diffusion coefficients of pollutant matter can be reduce the concentration in a non-uniform stream. If sewage effluent with a low diffusion coefficient has discharged into a non-uniform flow stream, then the water quality will be lower than a discharging of high diffusion coefficients of other pollutant matters.

In this report, it can be combined the hydrodynamic model and the convection-diffusion-reaction equation to approximate the pollutant concentration in a stream when the current reflects water in the stream is not uniform. The technique developed in this research the response of the stream to the two different external inputs: the elevation of water and the pollutant concentration at the discharged point can be obtained. The FTCS scheme can be used in the dispersion model since the scheme is very simple to implement. We obtain that the proposed technique is applicable and economical to be used in a simple problem since the simplicity of programming and the straight forwardness of the implementation. It is also possible to find tentative better locations and the periods of time of the different discharged points to a stream.

In this paper, the traditional Crank-Nicolson has bee used to solved a one-dimensional hydrodynamic model with damped force due to the drag of side of a stream. The one-dimensional advection-diffusion equation in a non-uniform flow in the stream are solved by using the new fourth-order scheme and employing the Saulyev method to their near left and right boundary conditions.

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Output (Acknowledge the Thailand Research Fund)

International Journal Publication

Numerical Treatment of a New Fourth-Order Scheme for a Non-dimensional Form of the Water Quality Models in a Non-Uniform Flow Stream Employing Saulyev Method to the Boundary Conditions

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Abstract

Two mathematical models are used to simulate water quality in a non-uniform flow stream. The first model is the hydrodynamic model that provides the velocity field and the elevation of water. The second model is the advection-diffusion-reaction model that provides the pollutant concentration field. Both 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. A new fourth-order scheme and a Saulyev scheme are simultaneously employed in the second model. This paper proposes a simply remarkable alteration to the fourth-order method so as to make it more accurate without any significant loss of computational efficiency. The results obtained indicate that the proposed new couple fourth-order scheme with Saulyev method do improve the prediction accuracy compared to that of their traditional methods.

Key words: Finite differences/ Crank-Nicolson scheme/ New Fourth-order scheme/ Saulyev scheme/ One-dimensional/ Hydrodynamic model/ Shallow water equation/ Dispersion model/ Advection-dispersion-reaction equations

Mathematics Subject Classification: 65M06, 62P12

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1. Introduction

In general, the amount of pollution levels in the a stream can be measured via data collection from a real of field data site. It is somehow rather difficult and complex, and the results obtained tentatively deviate in the measurement from one point in each time/place to another when the water flow in the stream is not uniform. In water quality modelling for non-uniform flow stream, the general governing equation used are the hydrodynamic model and the dispersion model. The one-dimensional shallow water equation and advection-dispersion-reaction equation are govern the first and the second models respectively.

Numerous numerical techniques for solving such models are available. In [18], the finite element method for solving a steady water pollution control to achieve a minimum cost is presented. The numerical techniques for solving the uniform flow of stream water quality model, especially the one-dimensional advection-dispersion-reaction equation are presented in [5], [12], [17], [6] and [23].

The non-uniform flow model requires data concerned with the velocity of the current at any point and any time in the domain. The hydrodynamics model provides the velocity field and tidal elevation of the water. In [25, 21], [19] and [20], they used the hydrodynamics model and the advection-dispersion equation to approximate the velocity of the water current in bay, uniform reservoir and stream, respectively. Among these numerical techniques, the finite difference methods, including both explicit and implicit schemes, are mostly used for one-dimensional domain such as in longitudinal stream systems [2], [4].

There are two mathematical models used to simulate water quality in a non-uniform water flow systems. The first is the hydrodynamic model that provides the velocity field and the elevation of water. The second is the dispersion model that gives the pollutant concentration field. A couple of models are formulated in one-dimensional equations. The traditional Crank-Nicolson method is used in the hydrodynamic model. At each step, the calculated flow velocity fields of the first model are input into the second model as the field data [19], [20], [22].

The numerical techniques to solving the non-uniform flow of stream water quality model containing one-dimensional advection-dispersion-reaction equation have been presented in [20] using the fully implicit scheme: Crank-Nicolson method is used to solve the hydrodynamic model and backward time central space (BTCS) for dispersion model respectively. In [22], the Crank-Nicolson method is also used to solve the hydrodynamic model while the explicit Saulyev scheme is used to solve the dispersion model.

Their research on finite difference techniques for the dispersion model have concentrated on computation accuracy and numerical stability. Many complicate numerical techniques, such as the QUICK scheme, the Lax-Wendroff scheme, the Crandall scheme, have been studied to increase performances. These techniques have focused on advantages in terms of stability and higher order accuracy[12].

The simple finite difference schemes become more attractive for model use. The simple explicit methods include the Forward Time-Central Space (FTCS) scheme, the MacCormack scheme, and the Saulyev scheme, and the implicit schemes include the Backward Time-Central Space (BTCS) scheme and the Crank-Nicolson scheme [4]. These scheme are either first-order or second order accurate and have the advantages in programming and computing without losing much accuracy and thus are used for many model applications [12].

A third-order upwind scheme for the advectiondiffusion equation using a simple spreadsheets simulation is proposed in [11]. In [13], a new flux splitting scheme is proposed. The scheme is robust and converges as fast as the Roe Splitting. The Godunov Mixed Methods for AdvectionDispersion Equations is introduced in [14]. A time-splitting approach for advectiondispersion equations is also considered. In addition, [8] proposes the time-split methods for multidimensional advection-diffusion equations that advection is approximated by a Godunov-type procedure, and diffusion is approximated by a low-order mixed finite element method. In [1], the flux-limiting solution techniques for simulation of reactiondiffusionconvection system is proposed. A composite scheme to solve the scalar transport equation in a two-dimensional space that accurately resolve sharp profiles in the flow is introduced. The total variation diminishing implicit RungeKutta methods for dissipative advectiondiffusion problems in astrophysics is proposed in [10]. They derive dissipative space discretizations and demonstrate that together with specially adapted total-variation-diminishing (TVD) or strongly stable Runge-Kutta time discretizations with adaptive step-size control this yields reliable and efficient integrators for the underlying high-dimensional nonlinear evolution equations.

In this research, we propose simple revisions to a new fourth-order scheme that improve its accuracy for the problem of water quality measurement in a non-uniform water flow in a stream. In the following sections, the formulation of a new fourth-order scheme is introduced. They proposed revision of a new fourth-order scheme with the Saulyev methd are described.

The results from the hydrodynamic model are the data of the water flow velocity for the 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 that guarantees the accuracy of the approximate solution is presented in [19], [20] and [22].

The stream has a simple one space dimension as shown in Fig.1. By averaging the equation over the depth, discarding the term due to the Coriolis force, it follows that the one-dimensional shallow water and the advection-dispersion-reaction equations are applicable. We use the Crank-Nicolson scheme, the traditional forward time central space scheme, and a couple of new fourth-order scheme and the Saulyev method to approximate the velocity, the elevation, and the pollutant concentration from the first and the second models, respectively.

2. Model Formulation

2.1. The Hydrodynamic Model

In this section, we derive a simple hydrodynamic model for describing water current and elevation by one-dimensional shallow water equation. We make the usual assumption in the continuity and momentum balance, i.e., we assume that the Coriolis, shearing stresses and the surface wind are small [16], [25], [19] and [20], we obtain the one-dimensional shallow water equations

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

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

where x is the longitudinal distance along the stream (m), t is time (s), $h(x)$ is the depth measured from the mean water level to the stream bed (m), $\zeta(x,t)$ is the elevation from the mean water level to the temporary water surface or the tidal elevation (m/s), and $u(x,t)$ is the velocity components (m/s), for all $x \in [0,l]$.

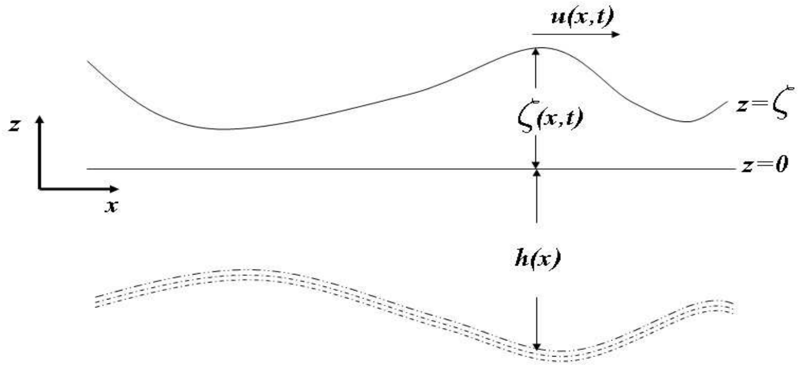

Figure 1: The shallow water system.

Assume that h is a constant and $\zeta \ll h$. Then the equations (1)-(2) lead to

$$\frac{\partial \zeta}{\partial t} + h\frac{\partial u}{\partial x} \doteq 0, \tag{3}$$
$$\frac{\partial u}{\partial t} + g\frac{\partial \zeta}{\partial x} = 0. \tag{4}$$

We will consider the equation in the dimensionless problem by letting $U = u/\sqrt{gh}, X = x/l, Z = \zeta/h$ and $T = t\sqrt{gh}/l$. Substituting them into the equations(3)-(4) lead to

$$\frac{\partial Z}{\partial T} + \frac{\partial U}{\partial X} = 0, \tag{5}$$
$$\frac{\partial U}{\partial T} + \frac{\partial Z}{\partial X} = 0. \tag{6}$$

In [19], [20] and [22], they introduce a damping term into Eqs.(5)-(6) to represent the frictional forces due to the drag of sides of the stream,

$$\frac{\partial Z}{\partial T} + \frac{\partial U}{\partial X} = 0, \tag{7}$$
$$\frac{\partial U}{\partial T} + \frac{\partial Z}{\partial X} = -U, \tag{8}$$

with the initial conditions at $t = 0$ and $0 \leq X \leq 1$ are $Z = 0$ and $U = 0$. The boundary conditions for $t > 0$ are specified: $Z = e^{it}$ at $X = 0$ and $\frac{\partial Z}{\partial X} = 0$

at $X = 1$. The system of Eqs.(7-8) is called the damped equation. We solve the damped equation by using the finite difference method. In order to solve the equations (7-8) in $[0, 1] \times [0, T]$, it is convenient to use u, d for U and Z respectively,

$$\frac{\partial u}{\partial t} + \frac{\partial d}{\partial x} = -u, \tag{9}$$

$$\frac{\partial d}{\partial t} + \frac{\partial u}{\partial x} = 0, \tag{10}$$

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 $x = 1$.

2.2. Dispersion Model

In a stream water quality model, the governing equations are the dynamic one-dimensional advection-dispersion equations (ADE). A simplified representation by averaging the equation over the depth is shown in [5], [12], [17], [20] and [23] as

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2}, \tag{11}$$

where $C(x, t)$ is the concentration averaged in depth at the point x and at time t (mg/L), D is the diffusion coefficient (m^2/s), and $u(x, t)$ is the velocity component (m/s), for all $x \in [0, L]$. The initial condition and the left boundary conditions are usually determined by observations. The potential pollutant concentration as the initial condition $C(x, 0) = C_0$ at $t = 0$ for all $x > 0$. The released pollutant concentration on the left boundary condition $C(0, t) = r(t)$ at $x = 0$. The observed rate of change of pollutant concentration on the right boundary is assumed to be a constant $\frac{\partial C}{\partial x} = S_0$ at $x = L$.

3. Crank-Nicolson method for the hydrodynamic model

The hydrodynamic model provides the velocity field and elevation of the water. Then the calculated results of the model will be the input into the dispersion model which provides the pollutant concentration field. We will follow the numerical techniques of [19]. To find the water velocity and water elevation from equations (9)-(10), we make the following change to variables $v = e^t u$ and substitute it into Eqs.(9)-(10). Therefore,

$$\frac{\partial v}{\partial t} + e^t \frac{\partial d}{\partial x} = 0, \tag{12}$$

$$\frac{\partial d}{\partial t} + e^{-t} \frac{\partial v}{\partial x} = 0. \tag{13}$$

The equations (12)-(13) can be written in the matrix form

$$\begin{pmatrix} v \\ d \end{pmatrix}_t + \begin{bmatrix} 0 & e^t \\ e^{-t} & 0 \end{bmatrix} \begin{pmatrix} v \\ d \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{14}$$

That is

$$U_t + AU_x = \bar{0}, \tag{15}$$

where

$$A = \begin{bmatrix} 0 & e^t \\ e^{-t} & 0 \end{bmatrix}, \tag{16}$$

$$U = \begin{pmatrix} v \\ d \end{pmatrix} \text{ and } \begin{pmatrix} v \\ d \end{pmatrix}_t = \begin{pmatrix} \partial v/\partial t \\ \partial d/\partial t \end{pmatrix}, \tag{17}$$

with the initial condition $d = v = 0$ at $t = 0$. The left boundary condition for $x = 0, t > 0$ is specified: $d(0,t) = f(t)$ and $\frac{\partial v}{\partial x} = -e^t \frac{df}{dt}$, and the right boundary condition for $x = 1, t > 0$ is 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 $0 \le i \le M$ and $0 \le n \le N$, and similarly defined for v_i^n and U_i^n. The grid point (x_n,t_n) is defined by $x_i = i\Delta x$ for all $i = 0,1,2,\ldots,M$ and $t_n = n\Delta t$ for all $n = 0,1,2,\ldots,N$ in which M and N are positive integers. Using the Crank-Nicolson method [15] to Eq.(15), the following finite difference equation can be obtained:

$$[I - \frac{1}{4}\lambda A(\Delta_x + \nabla_x)]U_i^{n+1} = [I + \frac{1}{4}\lambda A(\Delta_x + \nabla_x)]U_i^n, \tag{18}$$

where

$$U_i^n = \begin{pmatrix} v_i^n \\ d_i^n \end{pmatrix}, \Delta_x U_i^n = U_{i+1}^n - U_i^n \text{ and } \nabla_x U_i^n = U_i^n - U_{i-1}^n, \tag{19}$$

I is the unit matrix of order 2 and $\lambda = \Delta t/\Delta x$. Applying the initial and boundary conditions given in Eqs.(12)-(13), it can be obtained the general form

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

where

$$G^{n+1} = \begin{bmatrix} 1 & 0 & 0 & -\frac{\lambda}{4}a_1^{n+1} & 0 & 0 & \\ \frac{\lambda}{4}a_2^{n+1} & 1 & -\frac{\lambda}{4}a_2^{n+1} & 0 & 0 & 0 & \\ 0 & \frac{\lambda}{4}a_1^{n+1} & 1 & 0 & 0 & -\frac{\lambda}{4}a_1^{n+1} & \\ \frac{\lambda}{4}a_2^{n+1} & 0 & 0 & 1 & -\frac{\lambda}{4}a_2^{n+1} & 0 & \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & 0 & 0 & 0 & \frac{\lambda}{4}a_1^{n+1} & 1 & -\frac{\lambda}{4}a_1^{n+1} \\ & 0 & 0 & \frac{\lambda}{4}a_2^{n+1} & 0 & 0 & 1 \end{bmatrix},$$

$$E^n = \begin{bmatrix} 1 & 0 & 0 & -\frac{\lambda}{4}a_1^n & 0 & 0 & \\ -\frac{\lambda}{4}a_2^n & 1 & \frac{\lambda}{4}a_2^n & 0 & 0 & 0 & \\ 0 & -\frac{\lambda}{4}a_1^n & 1 & 0 & 0 & \frac{\lambda}{4}a_1^n & \\ -\frac{\lambda}{4}a_2^n & 0 & 0 & 1 & \frac{\lambda}{4}a_2^n & 0 & \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & 0 & 0 & 0 & -\frac{\lambda}{4}a_1^n & 1 & \frac{\lambda}{4}a_1^n \\ & 0 & 0 & -\frac{\lambda}{4}a_2^n & 0 & 0 & 1 \end{bmatrix}, \bar{U}^n = \begin{pmatrix} U_1^n \\ U_2^n \\ \vdots \\ U_{M-1}^n \end{pmatrix},$$

$$F^n = \begin{pmatrix} -\frac{\lambda}{4}a_1^{n+1}f(t_{n+1}) - \frac{\lambda}{4}a_1^n f(t_n) \\ -\frac{\lambda}{4}a_2^{n+1}\Delta x e^{-t_{n+1}}\frac{df}{dt}(t_{n+1}) - \frac{\lambda}{4}a_2^n\Delta x e^{-t_n}\frac{df}{dt}(t_n) \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix},$$

where $a_1^n = e^{t_n}, a_2^n = e^{-t_n}$ and $t_n = n\Delta t$ for all $n = 0, 1, 2, \ldots, N$. The Crank-Nicolson scheme is unconditionally stable [15, 4].

4. A new fouth-order scheme with a Saulyev method for the advection-dispersion equation

Taking a new fourth-order technique [7] into Eq.(11), the discretization for each terms are obtained as follows,

$$\begin{aligned} C &\cong C_i^n, && (21)\\ \frac{\partial C}{\partial t} &\cong \frac{C_i^{n+1}-C_i^n}{\Delta t}, && (22)\\ \frac{\partial C}{\partial x} &\cong F_i^n\frac{C_{i+2}^n-C_i^n}{2\Delta x}+G_i^n\frac{C_i^n-C_{i-2}^n}{2\Delta x}-H_i^n\frac{C_{i+1}^n-C_{i-1}^n}{2\Delta x}, && (23)\\ \frac{\partial^2 C}{\partial x^2} &\cong P_i^n\frac{C_{i+1}^n-2C_i^n+C_{i-1}^n}{(\Delta x)^2}+Q_i^n\frac{C_{i+2}^n-2C_i^n+C_{i-2}^n}{(\Delta x)^2} && (24)\\ u &\cong \widehat{U}_i^n, && (25) \end{aligned}$$

where

$$\begin{aligned} \lambda &= \frac{D\Delta t}{(\Delta x)^2},\\ \gamma_i^n &= \frac{\Delta t}{\Delta x}\widehat{U}_i^n,\\ F_i^n &= \frac{(12\lambda+2(\gamma_i^n)^2-3\gamma_i^n-2)}{12},\\ G_i^n &= \frac{(12\lambda+2(\gamma_i^n)^2+3\gamma_i^n-2)}{12},\\ H_i^n &= \frac{((\gamma_i^n)^2+6\lambda-4)}{3},\\ P_i^n &= \frac{(-(\gamma_i^n)^4+4(\gamma_i^n)^2-12\lambda^2-12\lambda(\gamma_i^n)^2+8\lambda)}{6\lambda},\\ Q_i^n &= \frac{((\gamma_i^n)^4-4(\gamma_i^n)^2+12\lambda^2+12\lambda(\gamma_i^n)^2-2\lambda)}{6\lambda}. \end{aligned}$$

Substitute Eqs.(21)-(25) into Eq.(11), we get

$$\begin{aligned} &\frac{C_i^{n+1}-C_i^n}{\Delta t}+\widehat{U}_i^n(F_i^n\frac{C_{i+2}^n-C_i^n}{2\Delta x}+G_i^n\frac{C_i^n-C_{i-2}^n}{2\Delta x}-H_i^n\frac{C_{i+1}^n-C_{i-1}^n}{2\Delta x})\\ &\qquad = D(P_i^n\frac{C_{i+1}^n-2C_i^n+C_{i-1}^n}{(\Delta x)^2}+Q_i^n\frac{C_{i+2}^n-2C_i^n+C_{i-2}^n}{(\Delta x)^2}), \qquad (26) \end{aligned}$$

for $2 \le i \le M-2$ and $0 \le n \le N-1$. The Eq.(26) can be written in an explicit form of finite difference equation as follows,

$$\begin{aligned} C_i^{n+1} &= (\frac{1}{2}\gamma_i^n G_i^n + \lambda Q_i^n)C_{i-2}^n + (-\frac{1}{2}\gamma_i^n H_i^n + \lambda P_i^n)C_{i-1}^n \\ &+(1+\frac{1}{2}\gamma_i^n F_i^n - \frac{1}{2}\gamma_i^n G_i^n - 2\lambda P_i^n - \lambda Q_i^n)C_i^n + (\frac{1}{2}\gamma_i^n H_i^n + \lambda P_i^n)C_{i+1}^n \\ &+(-\frac{1}{2}\gamma_i^n F_i^n + \lambda Q_i^n)C_{i+2}^n, \qquad (27) \end{aligned}$$

for $2 \le i \le M-2$ and $0 \le n \le N-1$. For $i = 1, M-1$ and M, the new fourth-order finite difference equation Eq.(27) cannot be employed to calculate the value C_i^n on the grid point next to left and right boundaries of the domain of solution. The alternate appropriate finite difference method such as the Saulyev method will be employed to approximate them as the following section.

4.0.1. The employment of a Saulyev method to the left and the right boundary conditions

The Saulyev scheme is unconditionally stable [6] and [7]. It is clear that the non-strictly stability requirement of Saulyev scheme is the main of advantage and economical to use. Taking Saulyev technique [6] into Eq.(11), it can be obtained the following discretization:

$$C \cong C_i^n, \qquad (28)$$

$$\frac{\partial C}{\partial t} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \qquad (29)$$

$$\frac{\partial C}{\partial x} \cong \frac{C_{i+1}^n - C_{i-1}^{n+1}}{2\Delta x}, \qquad (30)$$

$$\frac{\partial^2 C}{\partial x^2} \cong \frac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}, \qquad (31)$$

$$u \cong \widehat{U}_i^n. \qquad (32)$$

Substitute Eqs.(28)-(32) into Eq.(11), we get

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} + \widehat{U}_i^n(\frac{C_{i+1}^n - C_{i-1}^{n+1}}{2\Delta x}) = D(\frac{C_{i+1}^n - C_i^n - C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}), \qquad (33)$$

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

For $i = 1$, plug the known value of the left boundary $C_0^{n+1} = r_0^{n+1}$ to

Eq.(33) in the right hand side, we obtain

$$C_1^{n+1} = (\frac{1}{1+\lambda})((\frac{1}{2}\gamma_1^n + \lambda)r_0^{n+1}) + (1-\lambda)C_1^n + (\lambda - \frac{1}{2}\gamma_1^n)C_2^n). \tag{34}$$

For $i = M-1$, we can obtain an explicit form of Eq.(33),

$$C_{M-1}^{n+1} = (\frac{1}{1+\lambda})((\frac{1}{2}\gamma_{M-1}^n + \lambda)C_{M-2}^{n+1} + (1-\lambda)C_{M-1}^n + (\lambda - \frac{1}{2}\gamma_{M-1}^n)C_M^n). \tag{35}$$

For $i = M$, substitute the approximate unknown value of the right boundary by a traditional central difference method [3] with the known derivative right boundary condition,

$$C_{M+1}^n = C_{M-1}^n + 2\Delta x S_0. \tag{36}$$

Substituting Eq.(36) into Eq.(33), we can obtain

$$C_{M+1}^{n+1} = (\frac{1}{1+\lambda})(2\lambda C_{i-1}^n + (1-\lambda)C_i^n + (\lambda - \frac{1}{2}\gamma_i^n)(2\Delta x S_0)). \tag{37}$$

From Eqs.(34-37), it can be obtained that the technique does not generate their fictitious points along the both side of the solution domain. It follows that the new fourth-order finite difference equation Eq.(27) with the employed Saulyev finite difference equations Eqs.(34-35, 37) can be used to calculate the value C_i^n entire their grid points of the solution domain.

5. Numerical Experiment

The uniform flow of an advection-diffusion is considered in a uniform stream of constant cross-section and bottom slope. Flow velocity and diffusion coefficient are taken to be $U = 0.01$ m/s and $D = 0.002$ m^2/s. Assume that the length of the considered stream is $L = 100$ m. Let the pollutant concentration level that released at the left-end is

$$C(0,1) = 1. \tag{38}$$

There is no rate of change of pollutant on the right-end as follows

$$\frac{\partial C}{\partial x}(L,t) = 0. \tag{39}$$

The theoretical solution of the problem is [9], [24]

$$C(x,t) = \frac{1}{2}\text{erfc}(\frac{x-Ut}{\sqrt{4Dt}}) + \frac{1}{2}e^{\frac{Ux}{D}}\text{erfc}(\frac{x+Ut}{\sqrt{4Dt}}). \tag{40}$$

The accuracy of the proposed new fourth-order scheme with employed Saulyev method to the boundary and the theoretical methods are compared in Fig.2.

6. Application to a nonuniform flow stream water quality assessment problem

Suppose that the measurement of pollutant concentration C in a non-uniform flow stream is considered. A stream is aligned with longitudinal distance, 1.0 (km.) total length and 1.0 (m.) depth. There is a plant which discharges waste water into the stream and the pollutant concentration at the discharge point is $C(0,t) = C_0 = 1$ (mg/L) at $x = 0$ for all $t > 0$, there is no rate of change of pollutant level $\frac{\partial C}{\partial x} = 0$ at $x = 1.0$ for all $t > 0$, and there is no initial pollutant $C(x,0) = 0$ (mg/L) at $t = 0$. The elevation of water at the discharge point can be described as a function $d(0,t) = f(t) = \sin t$ (m.) for all $t > 0$, and the elevation does not change at $x = 1.0$ (km.) The physical parameters of the stream system is a diffusion coefficient $D = 0.1$ (m^2/s). In the analysis conducted in this study, meshing the stream into 40 elements with $\Delta x = 0.05$, and the time increment is 0.4 (s) with $\Delta t = 0.00125$, characterizing a one-dimensional flow. Using the Crank-Nicolson method of [19], [20] and [22], it can be obtained the water velocity $u(x,t)$ in Table 1 and Fig 3. Next, the approximate water velocity can be plugged new fourth-order scheme and employing the Saulyev method to the left boundary near the discharge point and the right boundary in Eq.(27). The approximation of pollutant concentrations C of the proposed scheme is shown in Table **??** and Fig.4.

Table 1: The velocity of water flow $u(x,t)$

t	$x=0$	$x=0.1$	$x=0.2$	$x=0.3$	$x=0.4$	$x=0.5$	$x=0.6$	$x=0.7$	$x=0.8$	$x=0.9$	$x=1.0$
10	0.5421	0.5505	0.5421	0.5202	0.4859	0.4362	0.3701	0.2901	0.1998	0.1029	0.0000
20	1.3284	1.2315	1.1228	1.0041	0.8766	0.7416	0.6001	0.4538	0.3042	0.1526	0.0000
30	0.3291	0.2628	0.2058	0.1578	0.1182	0.0861	0.0606	0.0405	0.0246	0.0116	0.0000
40	-1.1343	-1.0752	-0.9995	-0.9086	-0.8044	-0.6884	-0.5627	-0.4290	-0.2894	-0.1457	0.0000

Table 2: The pollutant concentration $C(x,t)$ using the new fourth-order scheme and employing Saulyev scheme, $\Delta x = 0.05$, $\Delta t = 0.00125$

t	$x=0$	$x=0.1$	$x=0.2$	$x=0.3$	$x=0.4$	$x=0.5$	$x=0.6$	$x=0.7$	$x=0.8$	$x=0.9$	$x=1.0$
10	1.00000	0.98707	0.96381	0.92269	0.85430	0.75311	0.62458	0.48989	0.38012	0.31931	0.30376
20	1.00000	0.99226	0.97058	0.92379	0.84269	0.72904	0.60095	0.48632	0.40726	0.36902	0.35910
30	1.00000	0.81678	0.67155	0.60392	0.58238	0.57723	0.57518	0.57294	0.57033	0.56750	0.56423
40	1.00000	0.73266	0.71148	0.71812	0.71721	0.71552	0.71391	0.71215	0.71013	0.70778	0.70470

7. Discussion and Conclusions

In this paper, the traditional Crank-Nicolson has bee used to solved a one-dimensional hydrodynamic model with damped force due to the drag of side of a stream. The one-dimensional advection-diffusion equation in a non-uniform flow in the stream are solved by using the new fourth-order scheme and employing the Saulyev method to their near left and right boundary conditions.

Acknowledgements

This work is supported by the Thailand Research Fund (TRG5780016).

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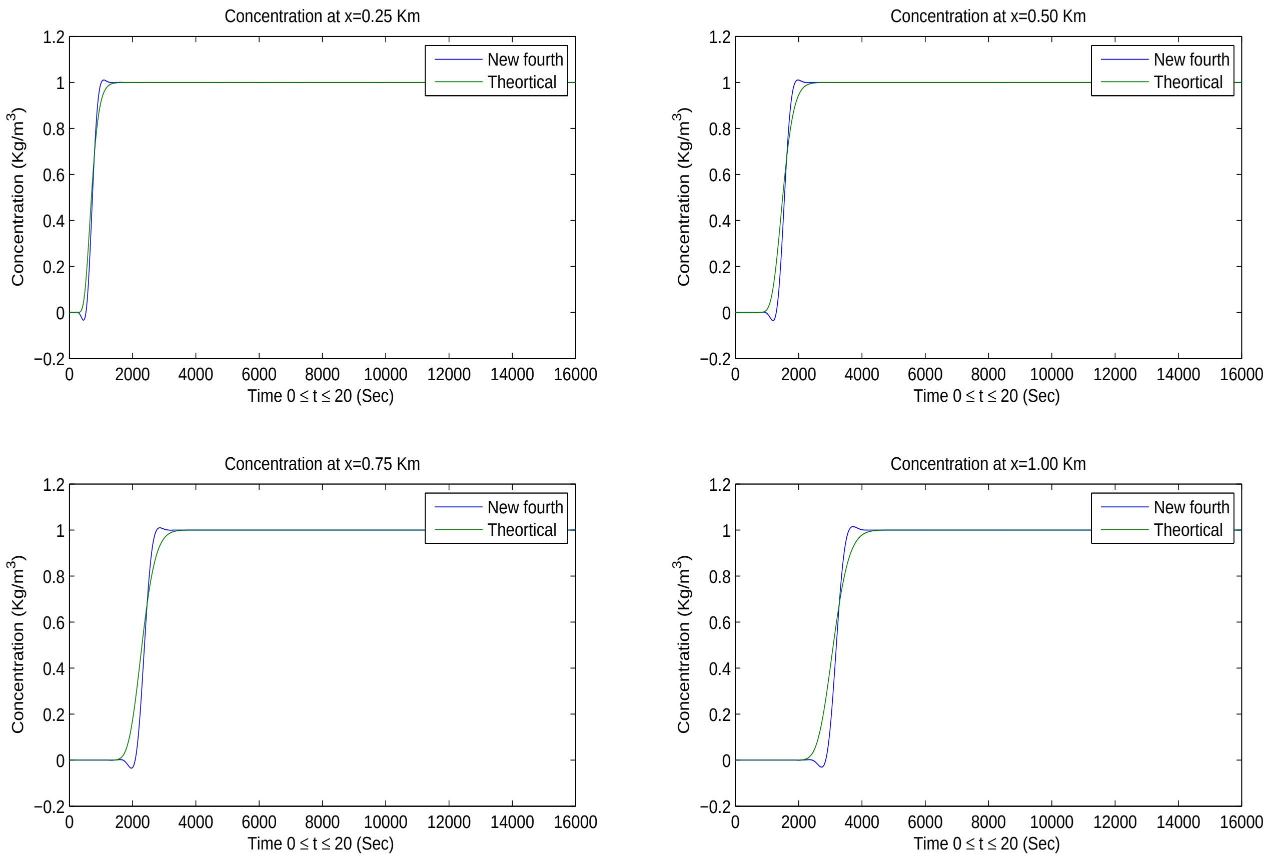

Figure 2: The comparison of exact solution and new fourth-order scheme

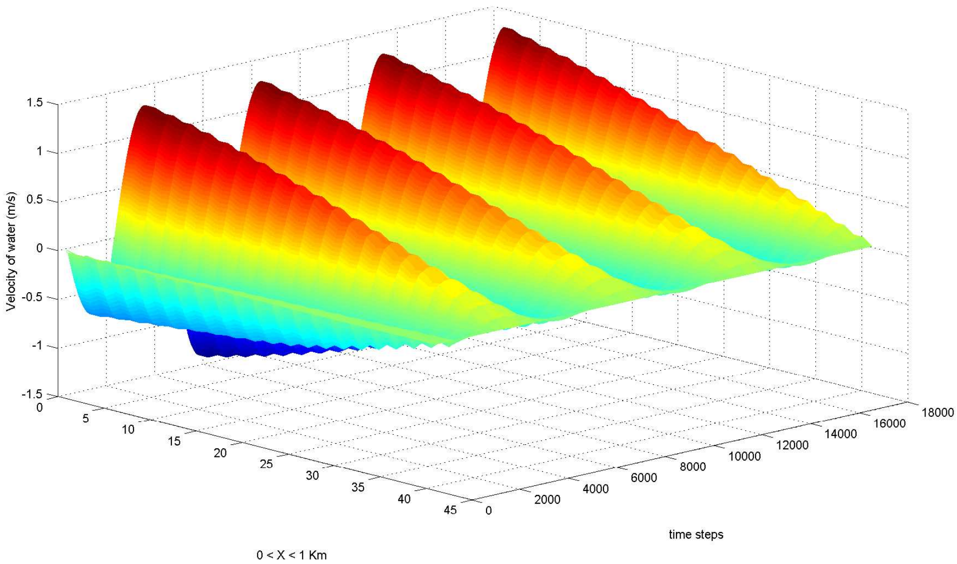

Figure 3: The water velocity $u(x, t)$ m/s

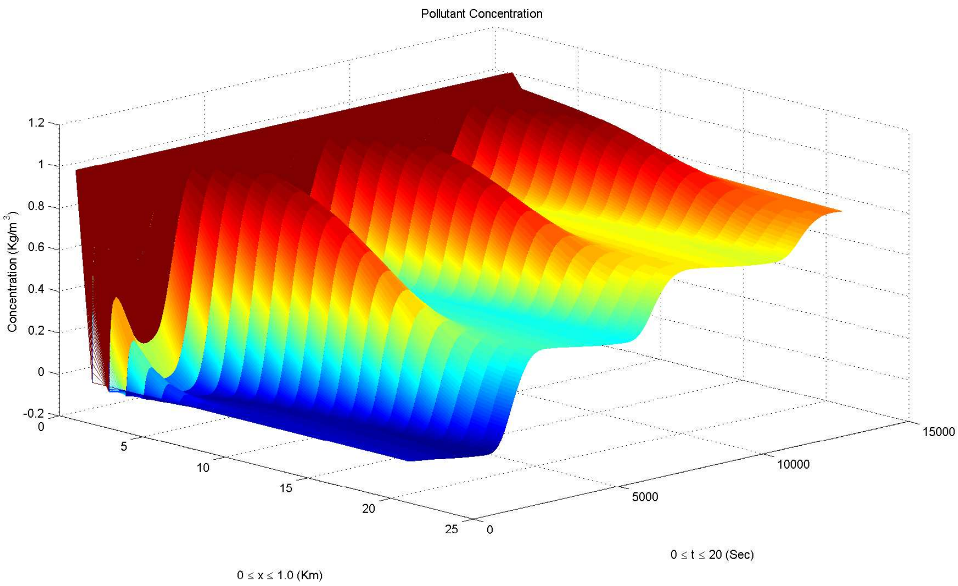

Figure 4: The pollutant concentration $C(x, t)$ (mg/L) using new fourth-order scheme and employing Saulyev scheme