รายงานการวิจัย

การคำนวณเชิงตัวเลขของตัวแบบเชิงคณิตศาสตร์ของการตรวจวัดคุณภาพน้ำเสียในทางน้ำไหลไม่เอกรูปโดยใช้ระเบียบวิธีแมกคอร์แมกดัดแปลง

A Numerical Computation of a Mathematical Model of Water Quality Measurement in a Non-uniform Stream by using Modified MacCormack Scheme

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ขอขอบคุณคณะวิทยาศาสตร์ สถาบันเทคโนโลยีพระจอมเกล้าเจ้าคุณทหารลาดกระบัง ที่ให้การสนับสนุนทุนวิจัย ประเภทส่งเสริมนักวิจัยด้วยเงินรายได้คณะวิทยาศาสตร์ ประจำปีงบประมาณ 2554 จำนวน 35,000 บาท จนงานวิจัยนี้สำเร็จลุล่วงไปได้ด้วยดี

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ทุนอุดหนุนการวิจัย

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บทความวิจัยที่ได้รับการตอบรับและกำลังอยู่ระหว่างการพิจารณาเพื่อลงตีพิมพ์ 27

CHAPTER I

Numerical Treatment of Modified MacCormack Scheme in a Non-dimensional Form of Water Quality Model in a Non-Uniform Flow Stream

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. The second is the dispersion 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 input into the second model as the field data. A modified MacCormack method is subsequently employed in the second model. This research propose a simply remarkable alteration to the MacCormack method so as to make it more accurate without any significant loss of computational efficiency. The results obtained indicates that the proposed modified MacCormack scheme does improve the prediction accuracy compared to that of the traditional MacCormack method.

1 Introduction

In generally, 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 [10], 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 [4], [6], [9], [5] and [15].

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 [16, 13], [11] and [12], 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 [1], [3].

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 [11], [12], [14].

The numerical techniques to solves the non-uniform flow of stream water quality model, one-dimensional advection-dispersion-reaction equation have been presented in [12] 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 [14], 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[6].

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 [3]. 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 [6].

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 [11], [12] and [14].

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 [8], [16], [11] and [12], 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 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

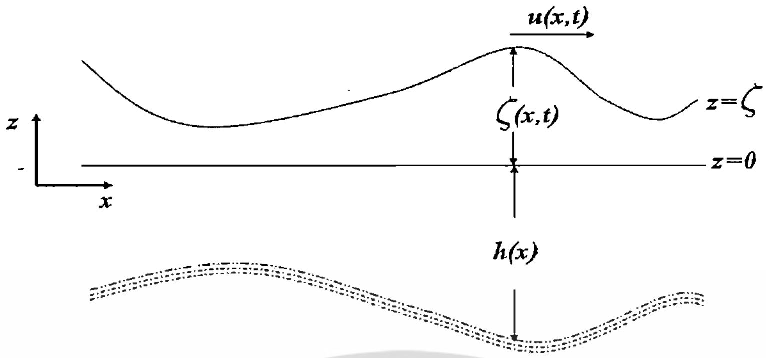

Figure 1: The shallow water system.

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

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

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

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

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

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

In [11], [12] and [14], they introduce a damping term into Eqs.(5)-(6) to represent frictional forces due to the drag of sides of the stream,

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

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

with the initial conditions at $t = 0$ and $0 \leq X \leq 1$ are 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,

$$\begin{aligned}\frac{\partial u}{\partial t}+\frac{\partial d}{\partial x} &= -u, &(9)\\ \frac{\partial d}{\partial t}+\frac{\partial u}{\partial x} &= 0, &(10)\end{aligned}$$

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 [4], [6], [9], [12] and [15] 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

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 input into the dispersion model which provides the pollutant concentration field. We will follow the numerical techniques of [11]. 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 $0 \le i \le M$ and $0 \le n \le N$, and similarly defined for v_i^n and U_i^n. The grid point (x_n, t_n) 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 [7] 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

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

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 [7, 3].

CHAPTER III

Modified MacCormack Scheme for the Advection-Dispersion-Reaction Equation

Traditional MacCormack scheme

First of all, we will 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 $0 \leq i \leq M$ 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. Taking the forward time forward space technique [7] and [6] into Eq.(11), we get the following discretization:

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

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

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

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

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

Note that $\widehat{U}_i^n$ are obtained by using Crank-Nicolson method with the hydrodynamic model of Eqs.(9)-(10) that are presented in [11], [12] and [14].

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

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

for $1 \leq i \leq M$ and $0 \leq n \leq N-1$. Substitute the difference equation into Eq.(26), and then define slope S_{i_1} as,

$$S_{i_1} = -\widehat{U}_i^n(\frac{C_{i+1}^n - C_i^n}{\Delta x}) + D(\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2}) - KC_i^n, \tag{27}$$

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.(27) takes a simplified form:

$$S_{i_1} = -\acute{\gamma}_i^n(C_{i+1}^n - C_i^n) + \acute{\lambda}(C_{i+1}^n - 2C_i^n + C_{i-1}^n) - KC_i^n, \tag{28}$$

or

$$S_{i_1} = (\acute{\lambda} - \acute{\gamma}_i^n)C_{i+1}^n - (2\acute{\lambda} - \acute{\gamma}_i^n + K)C_i^n + \acute{\lambda}C_{i-1}^n. \tag{29}$$

For upper boundary, where $i = 1$, plug the known value of the left boundary $C_0^n = C_0$ to Eq.(29) in the right hand side, we obtain

$$S_{1_1} = (\acute{\lambda} - \acute{\gamma}_1^n)C_2^n - (2\acute{\lambda} - \acute{\gamma}_1^n + K)C_1^n + \acute{\lambda}C_0. \tag{30}$$

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

$$S_{M_1} = -(\acute{\lambda} + K)C_{M-1}^n + \acute{\lambda}C_{M-2}^n. \tag{31}$$

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

$$C_i^{n+1} = C_i^n + S_{i_1}\Delta t. \tag{32}$$

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:

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

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:

$$S_{i_2} = \acute{\lambda} C_{i+1}^{n+1} - (2\acute{\lambda} + \acute{\gamma}_i^{n+1} + K) C_i^{n+1} + (\acute{\lambda} + \acute{\gamma}_i^{n+1}) C_{i-1}^{n+1}. \tag{37}$$

For upper boundary, where $i = 1$, plug the known value of the left boundary $C_0^{n+1} = C_0$ to Eq.(37) in the right hand side, we obtain

$$S_{1_2} = \acute{\lambda} C_2^{n+1} - (2\acute{\lambda} + \acute{\gamma}_1^{n+1} + K) C_1^{n+1} + (\acute{\lambda} + \acute{\gamma}_1^{n+1}) C_0. \tag{38}$$

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

$$S_{M_2} = \acute{\lambda} C_M^{n+1} - (2\acute{\lambda} + \acute{\gamma}_M^{n+1} + K) C_M^{n+1} + (\acute{\lambda} + \acute{\gamma}_M^{n+1}) C_{M-1}^{n+1}. \tag{39}$$

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

$$C_i^{n+1} = C_i^n + \frac{\Delta t}{2}(S_{i_1} + S_{i_2}). \tag{40}$$

The MacCormack scheme is conditionally stable subject to constraints in Eq.(26). The stability requirement for the scheme are [2]

$$\lambda = \frac{D\Delta t}{(\Delta x)^2} < \frac{1}{2}, \tag{41}$$

$$\gamma_i^n = \frac{\hat{U}_i^n \Delta t}{\Delta x} < 0.9, \tag{42}$$

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

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 valued obtained by subtracting the numerical dispersion from the real data of the stream. The amounts of numerical dispersion introduced by backward space denoted by Dn_1, and forward time denoted by Dn_2 schemes as follow [3], [6],

$$Dn_{1_i}^n = \frac{\Delta x}{2}\widehat{U}_i^n, \quad (43)$$

$$Dn_{2_i}^n = -\frac{\Delta x}{2}(\widehat{U}_i^n)^2. \quad (44)$$

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.(43)-(44), the numerical dispersion for forward time forward space prediction step and backward time backward space correction step are

$$D_{n_{prd}}{}_i^n = -\frac{\Delta x}{2}\widehat{U}_i^n - \frac{\Delta t}{2}(\widehat{U}_i^n)^2, \quad (45)$$

$$D_{n_{crc}}{}_i^n = \frac{\Delta x}{2}\widehat{U}_i^n + \frac{\Delta t}{2}(\widehat{U}_i^n)^2. \quad (46)$$

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

$$D_{1_i}^n = D_{real} - D_{n_{prd}}{}_i^n, \quad (47)$$

$$D_{2_i}^n = D_{real} - D_{n_{crc}}{}_i^n, \quad (48)$$

where $D_{1_i}^n$ is the dispersion coefficient used in prediction step, and $D_{2_i}^n$ is the dispersion coefficient used in correction step.

The Modified MacCormack scheme is conditionally stable subject to constraints in Eq.(26). The stability requirement for the scheme are

$$\lambda = \frac{D_{max}\Delta t}{(\Delta x)^2} < \frac{1}{2}, \quad (49)$$

$$\gamma_i^n = \frac{\widehat{U}_i^n \Delta t}{\Delta x} < 0.9, \quad (50)$$

where the maximum of numerical dispersion coefficients is $D_{max} = \max\{D_{1_i}^n, D_{2_i}^n : 0 \le i \le M, 0 \le n \le N\}$.

CHAPTER IV
Numerical Experiments

The accuracy of the hydrodynamic approximation

It is not hard to find the analytical solution $d(x,t)$ in the equations (9)-(10) with $f(t) = \sin t$. By changing of variables, $d(x,t) = e^{it}\mathcal{D}(x)$ and $u(x,t) = e^{it}\mathcal{U}(x)$ for some $\mathcal{D}(x), \mathcal{U}(x) \in C_0^2[0,1]$ and substitute into equations (9)-(10). Using a separable variables technique, we can obtain $d(1,t)$ a solution [12]

$$d(1,t) = \frac{\sin t \cos\beta \cosh\alpha - \cos t \sin\beta \sinh\alpha}{\cos^2\beta \cosh^2\alpha + \sin^2\beta \sinh^2\alpha} \qquad (51)$$

where $\alpha = 2^{1/4}\cos(3\pi/8)$ and $\beta = 2^{1/4}\sin(3\pi/8)$. Anyhow, it is not easy to find the analytical solution $u(x,t)$ of Eqs.(9)-(10). We use the solution $d(1,t)$ obtained in Eq.(51) to verify to our approximate solution obtained by the Crank-Nicolson method Eq.(20). Actually when using the Crank-Nicolson method, we get the approximate solution both $d(x,t)$ and $u(x,t)$. We assume that when we get a good approximation for $d(x,t)$ this implied that the method gives a good approximation for $u(x,t)$. The verification of the approximate solution $\bar{d}(1,t)$ is shown in Fig. 2.

Fig.2 shows the comparison between the analytical solutions $d(1,t)$ and the approximate solutions $\bar{d}(1,t)$ only at the end of the domain.

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 points on the domain as well.

Application to the 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 discharge point is $C(0,t) = C_0 = 1$ (mg/L) at $x = 0$ for all $t > 0$ and $C(x,0) = 0$ (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 is not change at $x = 1.0$ (km.) The physical parameters of the stream system are diffusion coefficient $D = 0.0125$ (m^2/s), and a first-order reaction rate $10^{-5}s^{-1}$. In the analysis conducted in this study, meshes the stream into 40 elements with $\Delta x = 0.025$, and time increment is 0.4 (s) with $\Delta t = 0.00125$, characterizing a one-dimensional flow. Using the Crank-Nicolson method of [11], [12] and [14], it can be obtained the water velocity $u(x, t)$ on Table 1 and Fig 3. Next, it can be plug the approximate water velocity into the traditional MacCormack scheme on Eq.(40). We also plug the approximate water velocity into the modified MacCormack scheme Eq.(40) with numerical dispersion coefficients Eqs.(47)-(48). The approximation of pollutant concentrations C of both schemes are shown in Tables 2-3 and Fig.4-5. The comparison of traditional MacCormack and modified MacCormack is shown in Fig.6.

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	1.3125	1.2187	1.1125	0.9960	0.8704	0.7372	0.5977	0.4530	0.3041	0.1525	0.0000
20	-1.0899	-1.0355	-0.9644	-0.8782	-0.7784	-0.6670	-0.5456	-0.4162	-0.2808	-0.1414	0.0000
30	0.5200	0.5224	0.5088	0.4801	0.4380	0.3839	0.3196	0.2471	0.1683	0.0852	0.0000
40	0.2172	0.1586	0.1105	0.0723	0.0433	0.0226	0.0091	0.0014	-0.0015	-0.0015	0.0000

Table 2: The pollutant concentration $C(x, t)$ of traditional MacCormack scheme, $\Delta x = 0.025$, $\Delta t = 0.00125$

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	1.000000	0.174513	0.029152	0.004634	0.000697	0.000099	0.000013	0.000002	0.000000	0.000000	0.000000
20	1.000000	0.054532	0.003068	0.000180	0.000011	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
30	1.000000	0.125937	0.015943	0.002012	0.000251	0.000031	0.000004	0.000000	0.000000	0.000000	0.000000
40	1.000000	0.105911	0.010827	0.001074	0.000104	0.000010	0.000001	0.000000	0.000000	0.000000	0.000000

Table 3: The pollutant concentration $C(x, t)$ of modified MacCormack scheme, $\Delta x = 0.025$, $\Delta t = 0.00125$

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	1.000000	0.146939	0.021001	0.002907	0.000388	0.000050	0.000006	0.000001	0.000000	0.000000	0.000000
20	1.000000	0.059627	0.003656	0.000233	0.000015	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
30	1.000000	0.117948	0.013959	0.001648	0.000193	0.000022	0.000003	0.000000	0.000000	0.000000	0.000000
40	1.000000	0.103863	0.010501	0.001038	0.000101	0.000010	0.000001	0.000000	0.000000	0.000000	0.000000

CHAPTER V

Discussion and Conclusions

The approximation of the pollutant concentrations of the traditional and modified MacCormack schemes are shown in Tables 2-3. 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 [14].

In [14], 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.

We proposed the modified MacCormack scheme by adding simple revision to the traditional MacCormack scheme. The numerical dispersion has been introduced because the derivative approximation during discretization is not centered. The traditional MacCormack scheme shows excessive dispersion effects for large time and space step lengths, significantly decreasing the efficiency of the traditional MacCormack scheme [6]. To eliminate the numerical dispersion effect, the modified MacCormack scheme for nonuniform flow is proposed. The revision show a good agreement in accuracy to the original one. Though the modified MacCormack scheme became less efficient than the traditional MacCormack scheme.

In this paper, 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 both if traditional and modified MacCormack schemes can be used in the dispersion model since the scheme is very simple to implement. By the both of traditional and modified MacCormack finite difference formulations, we obtain that the proposed technique is applicable and economical to be used in the real-world 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.

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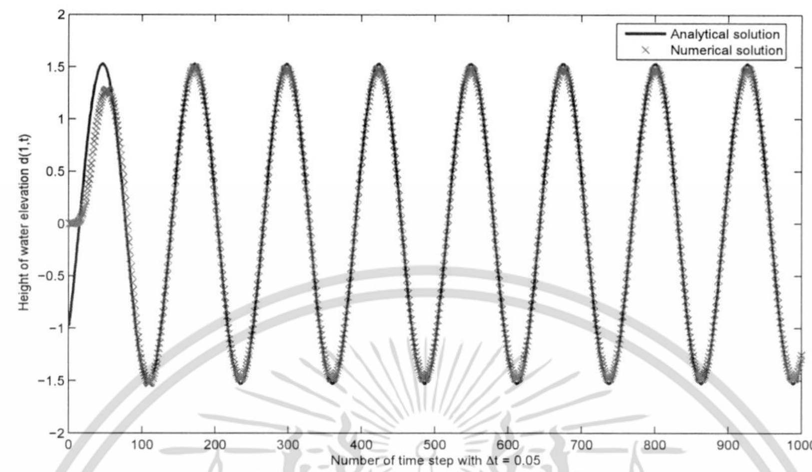

Figure 2: Comparison of analytical solution for height of water elevation with results obtained by numerical technique at the end point of the domain.

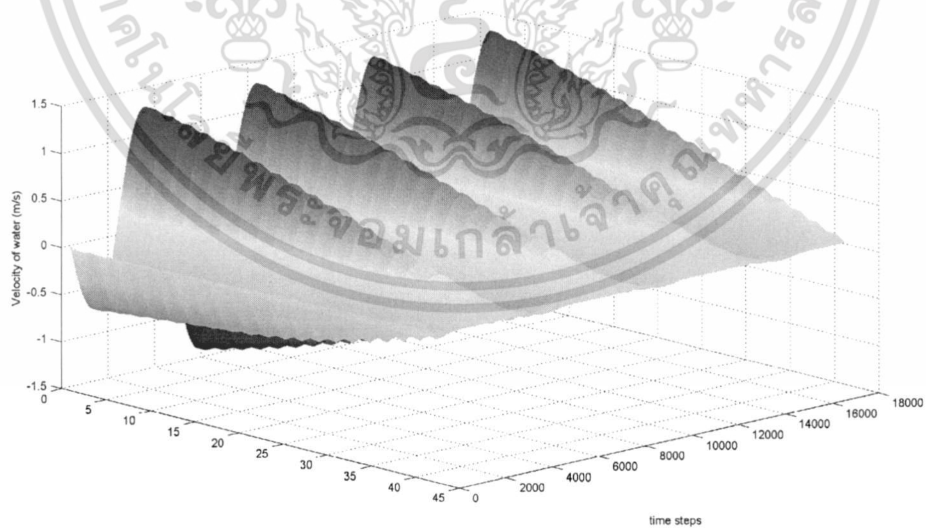

Figure 3: The water velocity $u(x,t)$ m/s

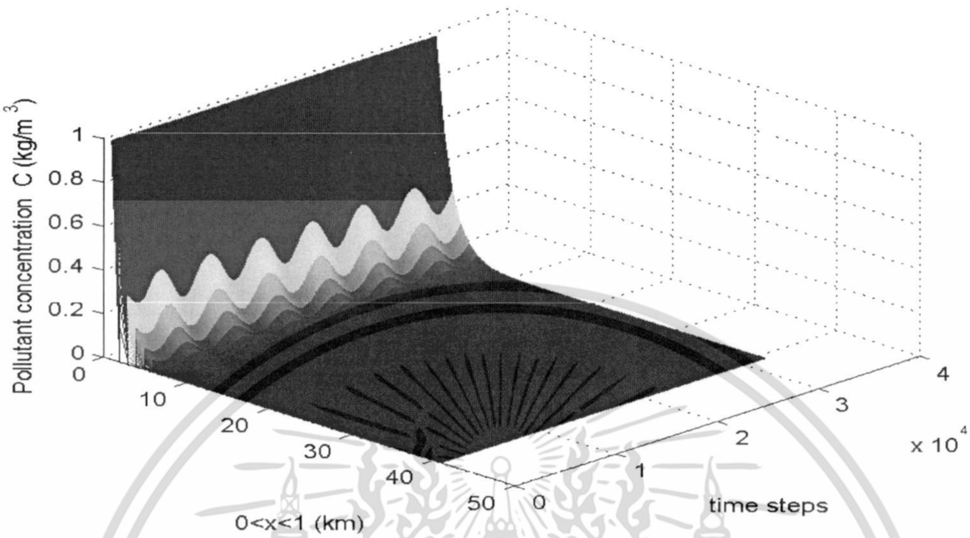

Figure 4: The pollutant concentration $C(x, t)$ (mg/L) using traditional MacCormack scheme

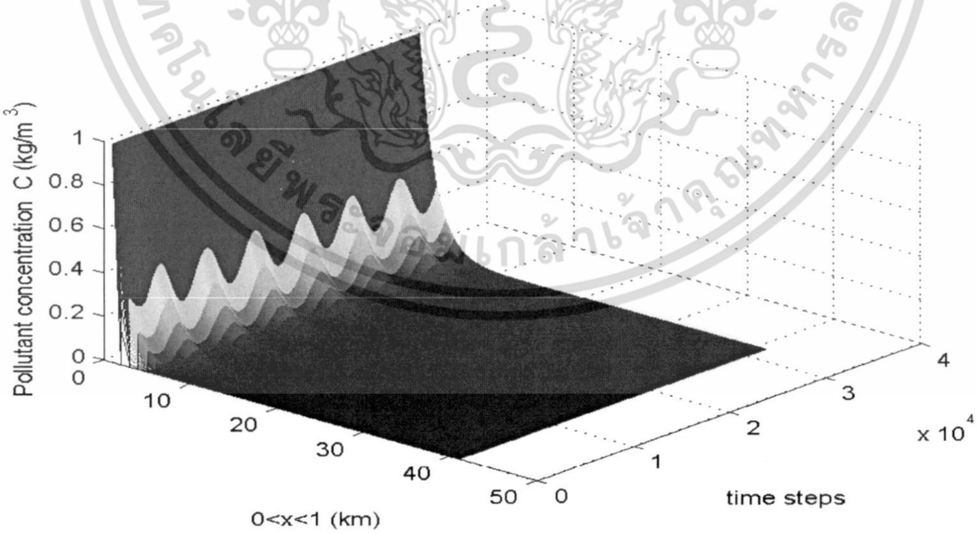

Figure 5: The pollutant concentration $C(x, t)$ (mg/L) using modified MacCormack scheme

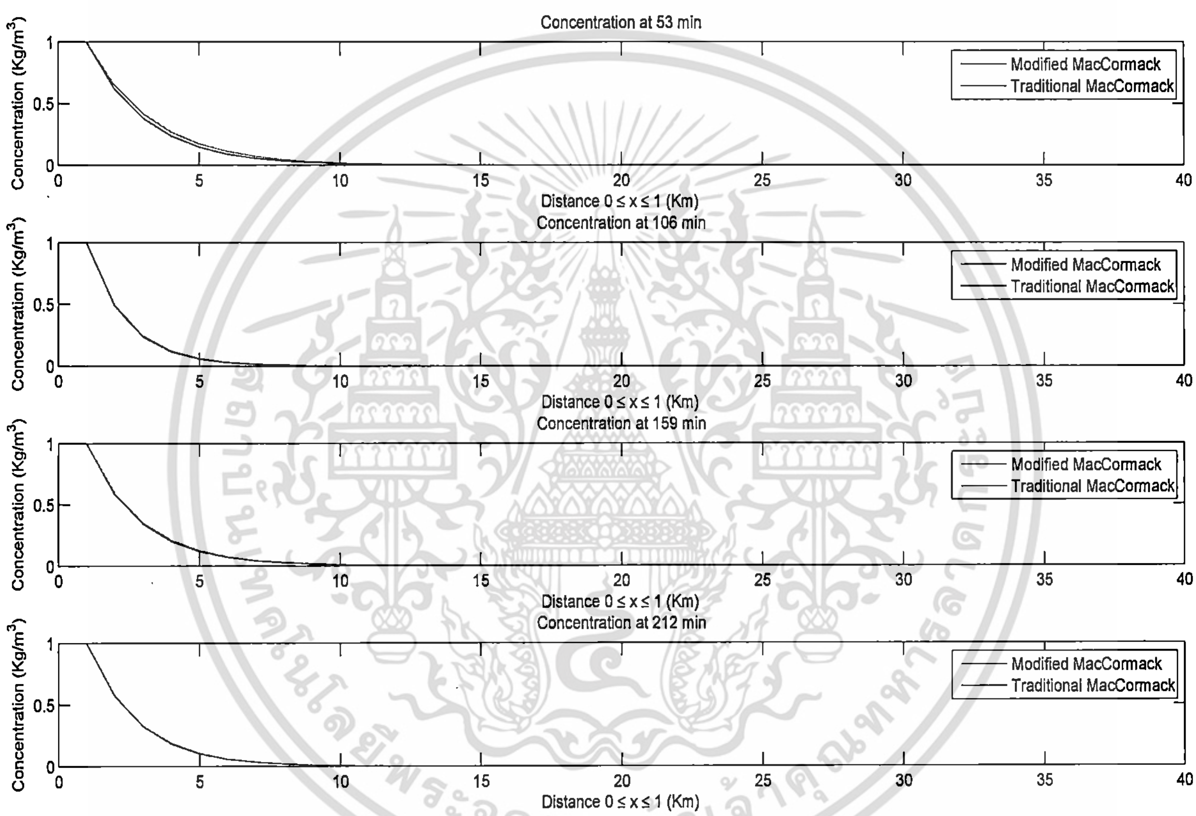

Figure 6: The comparison of concentration at 4 different time instants of Modified MacCormack and Traditional MacCormack methods

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Numerical Treatment of Modified MacCormack Scheme in a Non-dimensional Form of Water Quality Model in a Non-Uniform Flow Stream

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Abstract

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. The second is the dispersion 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 input into the second model as the field data. A modified MacCormack method is subsequently employed in the second model. This paper propose a simply remarkable alteration to the MacCormack method so as to make it more accurate without any significant loss of computational efficiency. The results obtained indicates that the proposed modified MacCormack scheme does improve the prediction accuracy compared to that of the traditional MacCormack method.

Key words: Finite differences/ Crank-Nicolson scheme/ MacCormack scheme/ Modified MacCormack scheme One-dimensional/ Hydrodynamic model/ Shallow water equation/ Dispersion model/ Advection-dispersion-reaction equations

Mathematics Subject Classification: 65M06, 62P12

1. Introduction

In generally, 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

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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 [10], 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 [4], [6], [9], [5] and [15].

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 [16, 13], [11] and [12], 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 [1], [3].

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 [11], [12], [14].

The numerical techniques to solves the non-uniform flow of stream water quality model, one-dimensional advection-dispersion-reaction equation have been presented in [12] 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 [14], 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 equations(3)-(4) leads to

$$\begin{aligned} \frac{\partial Z}{\partial T} + \frac{\partial U}{\partial X} &= 0, & (5) \\ \frac{\partial U}{\partial T} + \frac{\partial Z}{\partial X} &= 0. & (6) \end{aligned}$$

In [11], [12] and [14], they introduce a damping term into Eqs.(5)-(6) to represent frictional forces due to the drag of sides of the stream,

$$\begin{aligned} \frac{\partial Z}{\partial T} + \frac{\partial U}{\partial X} &= 0, & (7) \\ \frac{\partial U}{\partial T} + \frac{\partial Z}{\partial X} &= -U, & (8) \end{aligned}$$

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,

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial d}{\partial x} &= -u, & (9) \\ \frac{\partial d}{\partial t} + \frac{\partial u}{\partial x} &= 0, & (10) \end{aligned}$$

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-reaction equations (ADRE). A simplified representation by averaging the equation over the depth is shown in [4], [6], [9], [12] and [15] as

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

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.

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 input into the dispersion model which provides the pollutant concentration field. We will follow the numerical techniques of [11]. 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 $0 \le i \le M$ and $0 \le n \le N$, and similarly defined for v_i^n and U_i^n. The grid point (x_n, t_n) 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 [7] 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

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

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 [7, 3].

4. Modified MacCormack scheme for the advection-dispersion-reaction equation

4.1. Traditional MacCormack scheme

First of all, we will 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 $0 \leq i \leq M$ 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. Taking the forward time forward space technique [7] and [6] into Eq.(11), we get the following discretization:

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

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

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

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

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

Note that $\widehat{U}_i^n$ are obtained by using Crank-Nicolson method with the hydrodynamic model of Eqs.(9)-(10) that are presented in [11], [12] and [14].

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

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

for $1 \leq i \leq M$ and $0 \leq n \leq N-1$. Substitute the difference equation into Eq.(26), and then define slope S_{i_1} as,

$$S_{i_1} = -\widehat{U}_i^n\left(\frac{C_{i+1}^n - C_i^n}{\Delta x}\right) + D\left(\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2}\right) - KC_i^n, \tag{27}$$

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.(27) takes a simplified form:

$$S_{i_1} = -\acute{\gamma}_i^n(C_{i+1}^n - C_i^n) + \acute{\lambda}(C_{i+1}^n - 2C_i^n + C_{i-1}^n) - KC_i^n, \tag{28}$$

or

$$S_{i_1} = (\acute{\lambda} - \acute{\gamma}_i^n)C_{i+1}^n - (2\acute{\lambda} - \acute{\gamma}_i^n + K)C_i^n + \acute{\lambda}C_{i-1}^n. \tag{29}$$

For upper boundary, where $i = 1$, plug the known value of the left boundary $C_0^n = C_0$ to Eq.(29) in the right hand side, we obtain

$$S_{1_1} = (\acute{\lambda} - \acute{\gamma}_1^n)C_2^n - (2\acute{\lambda} - \acute{\gamma}_1^n + K)C_1^n + \acute{\lambda}C_0. \tag{30}$$

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

$$S_{M_1} = -(\acute{\lambda} + K)C_{M-1}^n + \acute{\lambda}C_{M-2}^n. \tag{31}$$

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

$$C_i^{n+1} = C_i^n + S_{i_1}\Delta t. \tag{32}$$

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:

$$C \cong \frac{1}{2}(C_i^n + C_i^{n+1}), \tag{33}$$

$$\frac{\partial C}{\partial t} \cong \frac{C_i^{n+1} - C_i^n}{\Delta t}, \tag{34}$$

$$\frac{\partial C}{\partial x} \cong \frac{C_i^{n+1} - C_{i-1}^{n+1}}{\Delta x}, \tag{35}$$

$$\frac{\partial^2 C}{\partial x^2} \cong \frac{1}{2}\left(\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} + \frac{C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta x)^2}\right). \tag{36}$$

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:

$$S_{i_2} = \acute{\lambda}C_{i+1}^{n+1} - (2\acute{\lambda} + \acute{\gamma}_i^{n+1} + K)C_i^{n+1} + (\acute{\lambda} + \acute{\gamma}_i^{n+1})C_{i-1}^{n+1}. \tag{37}$$

For upper boundary, where $i = 1$, plug the known value of the left boundary $C_0^{n+1} = C_0$ to Eq.(37) in the right hand side, we obtain

$$S_{1_2} = \acute{\lambda}C_2^{n+1} - (2\acute{\lambda} + \acute{\gamma}_1^{n+1} + K)C_1^{n+1} + (\acute{\lambda} + \acute{\gamma}_1^{n+1})C_0. \tag{38}$$

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

$$S_{M_2} = \acute{\lambda} C_M^{n+1} - (2\acute{\lambda} + \acute{\gamma}_M^{n+1} + K) C_M^{n+1} + (\acute{\lambda} + \acute{\gamma}_M^{n+1}) C_{M-1}^{n+1}. \tag{39}$$

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

$$C_i^{n+1} = C_i^n + \frac{\Delta t}{2}(S_{i_1} + S_{i_2}). \tag{40}$$

The MacCormack scheme is conditionally stable subject to constraints in Eq.(26). The stability requirement for the scheme are [2]

$$\lambda = \frac{D\Delta t}{(\Delta x)^2} < \frac{1}{2}, \tag{41}$$

$$\gamma_i^n = \frac{\widehat{U}_i^n \Delta t}{\Delta x} < 0.9, \tag{42}$$

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

4.2. 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 valued obtained by subtracting the numerical dispersion from the real data of the stream. The amounts of numerical dispersion introduced by backward space denoted by Dn_1, and forward time denoted by Dn_2 schemes as follow [3], [6],

$$Dn_{1i}^{\ n} = \frac{\Delta x}{2} \widehat{U}_i^n, \tag{43}$$

$$Dn_{2i}^{\ n} = -\frac{\Delta x}{2} (\widehat{U}_i^n)^2. \tag{44}$$

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.(43)-(44), the numerical dispersion for forward time forward space prediction step and backward time backward space correction step are

$$D_{n_{prd}}{}_i^n = -\frac{\Delta x}{2}\widehat{U}_i^n - \frac{\Delta t}{2}(\widehat{U}_i^n)^2, \tag{45}$$

$$D_{n_{crc}}{}_i^n = \frac{\Delta x}{2}\widehat{U}_i^n + \frac{\Delta t}{2}(\widehat{U}_i^n)^2. \tag{46}$$

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

$$D_1{}_i^n = D_{real} - D_{n_{prd}}{}_i^n, \tag{47}$$

$$D_2{}_i^n = D_{real} - D_{n_{crc}}{}_i^n, \tag{48}$$

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

The Modified MacCormack scheme is conditionally stable subject to constraints in Eq.(26). The stability requirement for the scheme are

$$\lambda = \frac{D_{max}\Delta t}{(\Delta x)^2} < \frac{1}{2}, \tag{49}$$

$$\gamma_i^n = \frac{\widehat{U}_i^n \Delta t}{\Delta x} < 0.9, \tag{50}$$

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

5. The accuracy of the hydrodynamic approximation

It is not hard to find the analytical solution $d(x,t)$ in the equations (9)-(10) with $f(t) = \sin t$. By changing of variables, $d(x,t) = e^{it}\mathcal{D}(x)$ and $u(x,t) = e^{it}\mathcal{U}(x)$ for some $\mathcal{D}(x), \mathcal{U}(x) \in C_0^2[0,1]$ and substitute into equations (9)-(10). Using a separable variables technique, we can obtain $d(1,t)$ a solution [12]

$$d(1,t) = \frac{\sin t \cos\beta \cosh\alpha - \cos t \sin\beta \sinh\alpha}{\cos^2\beta \cosh^2\alpha + \sin^2\beta \sinh^2\alpha} \tag{51}$$

where $\alpha = 2^{1/4}\cos(3\pi/8)$ and $\beta = 2^{1/4}\sin(3\pi/8)$. Anyhow, it is not easy to find the analytical solution $u(x,t)$ of Eqs.(9)-(10). We use the solution $d(1,t)$

obtained in Eq.(51) to verify to our approximate solution obtained by the Crank-Nicolson method Eq.(20). Actually when using the Crank-Nicolson method, we get the approximate solution both $d(x,t)$ and $u(x,t)$. We assume that when we get a good approximation for $d(x,t)$ this implied that the method gives a good approximation for $u(x,t)$. The verification of the approximate solution $\bar{d}(1,t)$ is shown in Fig. 2.

Fig.2 shows the comparison between the analytical solutions $d(1,t)$ and the approximate solutions $\bar{d}(1,t)$ only at the end of the domain.

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 points on the domain as well.

6. Application to the 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 discharge point is $C(0,t) = C_0 = 1$ (mg/L) at $x = 0$ for all $t > 0$ and $C(x,0) = 0$ (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 is not change at $x = 1.0$ (km.) The physical parameters of the stream system are diffusion coefficient $D = 0.0125$ (m^2/s), and a first-order reaction rate $10^{-5}s^{-1}$. In the analysis conducted in this study, meshes the stream into 40 elements with $\Delta x = 0.025$, and time increment is 0.4 (s) with $\Delta t = 0.00125$, characterizing a one-dimensional flow. Using the Crank-Nicolson method of [11], [12] and [14], it can be obtained the water velocity $u(x,t)$ on Table 1 and Fig 3. Next, it can be plug the approximate water velocity into the traditional MacCormack scheme on Eq.(40). We also plug the approximate water velocity into the modified MacCormack scheme Eq.(40) with numerical dispersion coefficients Eqs.(47)-(48). The approximation of pollutant concentrations C of both schemes are shown in Tables 2-3 and Fig.4-5. The comparison of traditional MacCormack and modified MacCormack is shown in Fig.6.

7. Discussion and Conclusions

The approximation of the pollutant concentrations of the traditional and modified MacCormack schemes are shown in Tables 2-3. The real-world

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	1.3125	1.2187	1.1125	0.9960	0.8704	0.7372	0.5977	0.4530	0.3041	0.1525	0.0000
20	-1.0899	-1.0355	-0.9644	-0.8782	-0.7784	-0.6670	-0.5456	-0.4162	-0.2808	-0.1414	0.0000
30	0.5200	0.5224	0.5088	0.4801	0.4380	0.3839	0.3196	0.2471	0.1683	0.0852	0.0000
40	0.2172	0.1586	0.1105	0.0723	0.0433	0.0226	0.0091	0.0014	-0.0015	-0.0015	0.0000

Table 2: The pollutant concentration $C(x,t)$ of traditional MacCormack scheme, $\Delta x = 0.025$, $\Delta t = 0.00125$

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	1.000000	0.174513	0.029152	0.004634	0.000697	0.000099	0.000013	0.000002	0.000000	0.000000	0.000000
20	1.000000	0.054532	0.003068	0.000180	0.000011	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
30	1.000000	0.125937	0.015943	0.002012	0.000251	0.000031	0.000004	0.000000	0.000000	0.000000	0.000000
40	1.000000	0.105911	0.010827	0.001074	0.000104	0.000010	0.000001	0.000000	0.000000	0.000000	0.000000

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 [14].

In [14], 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.

We proposed the modified MacCormack scheme by adding simple revision to the traditional MacCormack scheme. The numerical dispersion has been introduced because the derivative approximation during discretization is not centered. The traditional MacCormack scheme shows excessive dispersion effects for large time and space step lengths, significantly decreasing the efficiency of the traditional MacCormack scheme [6]. To eliminate the numerical dispersion effect, the modified MacCormack scheme for nonuniform flow is proposed. The revision show a good agreement in accuracy to the original one. Though the modified MacCormack scheme became less efficient than the traditional MacCormack scheme.

In this paper, it can be combined the hydrodynamic model and the convection-diffusion-reaction equation to approximate the pollutant concen-

Table 3: The pollutant concentration $C(x,t)$ of modified MacCormack scheme, $\Delta x = 0.025$, $\Delta t = 0.00125$

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	1.000000	0.146939	0.021001	0.002907	0.000388	0.000050	0.000006	0.000001	0.000000	0.000000	0.000000
20	1.000000	0.059627	0.003656	0.000233	0.000015	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
30	1.000000	0.117948	0.013959	0.001648	0.000193	0.000022	0.000003	0.000000	0.000000	0.000000	0.000000
40	1.000000	0.103863	0.010501	0.001038	0.000101	0.000010	0.000001	0.000000	0.000000	0.000000	0.000000

tration in a stream when the current reflects water in the stream is not uniform. The technique developed in this paper 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 both if traditional and modified MacCormack schemes can be used in the dispersion model since the scheme is very simple to implement. By the both of traditional and modified MacCormack finite difference formulations, we obtain that the proposed technique is applicable and economical to be used in the real-world 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.

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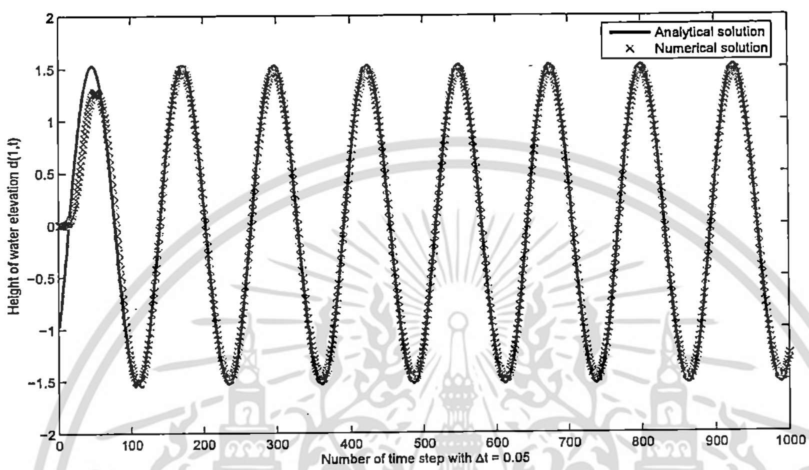

Figure 2: Comparison of analytical solution for height of water elevation with results obtained by numerical technique at the end point of the domain.

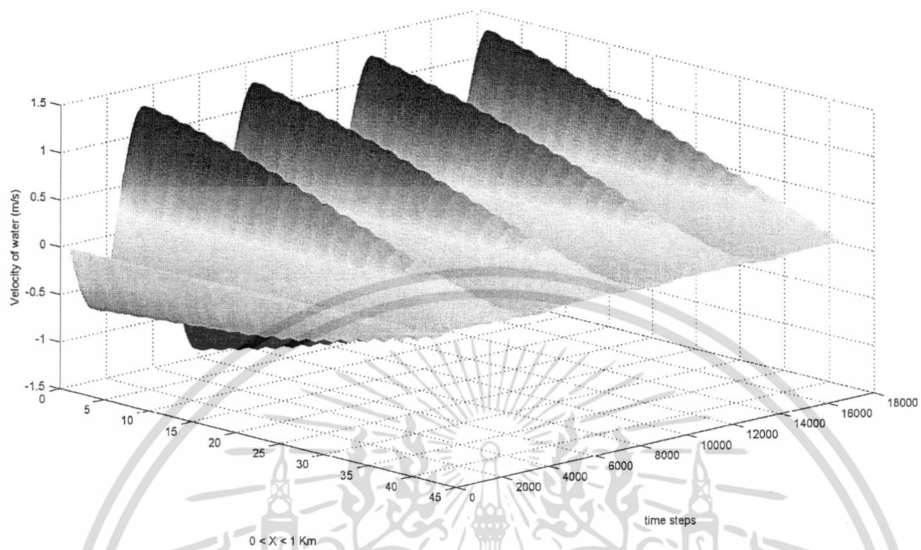

Figure 3: The water velocity $u(x,t)$ m/s

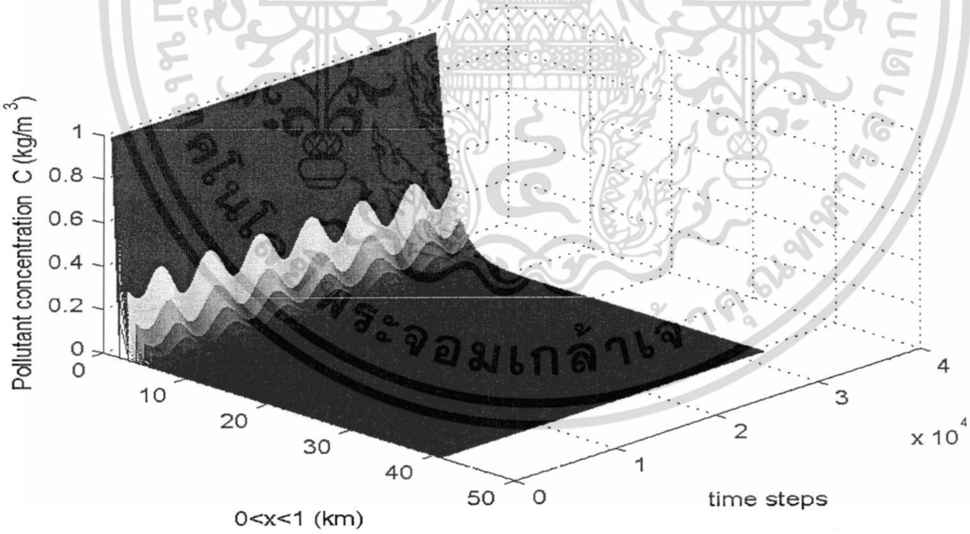

Figure 4: The pollutant concentration $C(x,t)$ (mg/L) using traditional MacCormack scheme

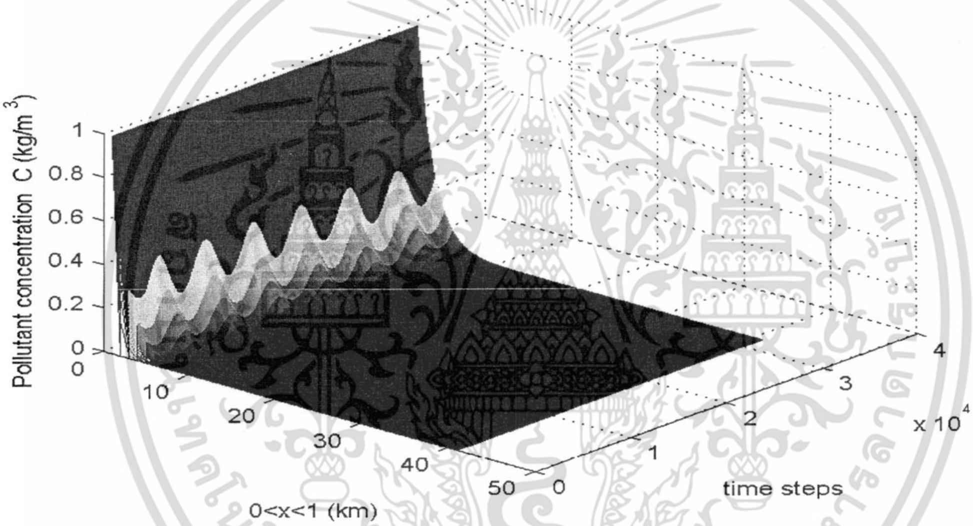

Figure 5: The pollutant concentration $C(x,t)$ (mg/L) using modified MacCormack scheme

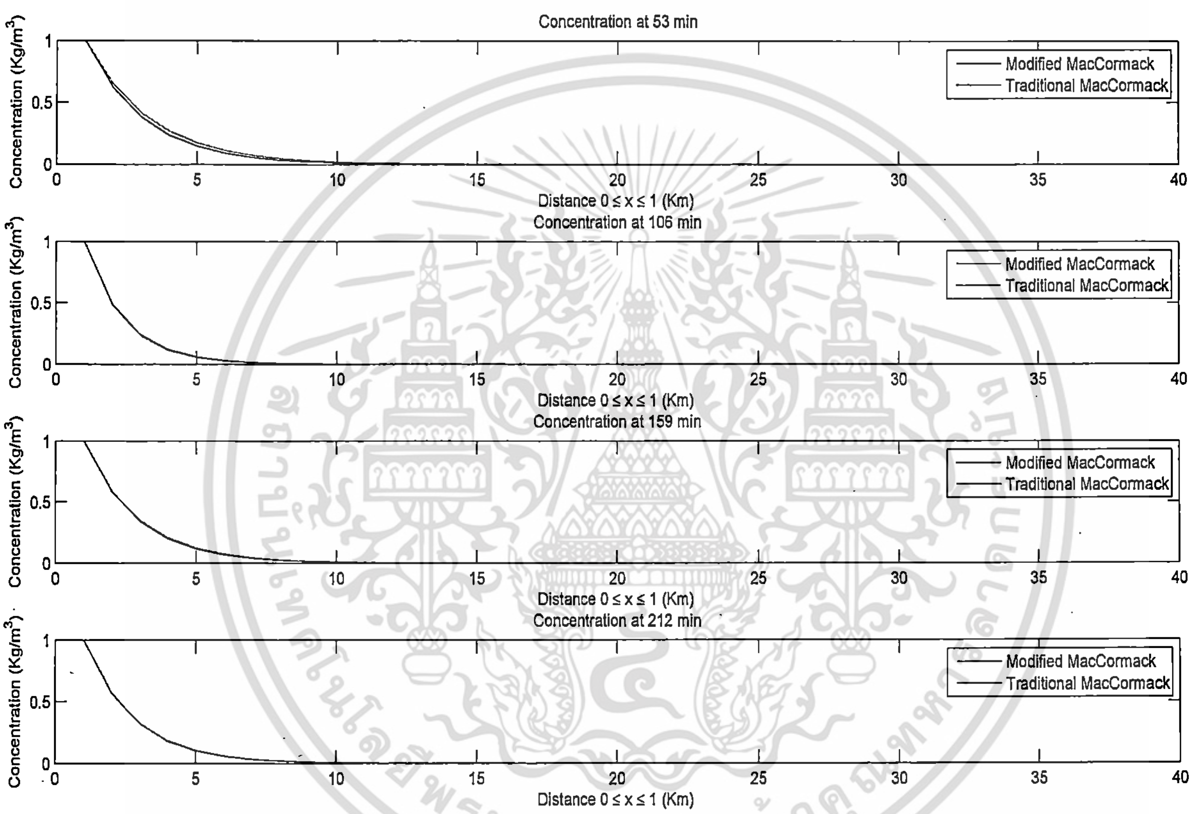

Figure 6: The comparison of concentration at 4 different time instants of Modified MacCormack and Traditional MacCormack methods