Finite Difference Formulation for Prediction of Water Pollution

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Abstract. Water is an important component of the earth. Human being and living organisms are demand for the quality of water. Human activity is one of the causes of the water pollution. The pollution happened give bad effect to the physical and characteristic of water contents. It is not practical to monitor all aspects of water flow and transport distribution. So, in order to help people to access to the polluted area, a prediction of water pollution concentration must be modelled. This study proposed a one-dimensional advection diffusion equation for predicting the water pollution concentration transport. The numerical modelling will be produced in order to predict the transportation of water pollution concentration. In order to approximate the advection diffusion equation, the implicit Crank Nicolson is used. For the purpose of the simulation, the boundary condition and initial condition, the spatial steps and time steps as well as the approximations of the advection diffusion equation have been encoded. The results of one dimensional advection diffusion equation have successfully been used to predict the transportation of water pollution concentration by manipulating the velocity and diffusion parameters.

1. Introduction
Water is an important component of the earth. It covered two thirds of the earth’s surface. Almost all earth’s population, especially human being depend on freshwater to continue their growth. Nowadays, people are not only demand for the quantity of the water but also the quality of the water. Many aspect of social life depend on the economic availability and acceptable quantity of water. Therefore, water quality has become an issue of increasing by the years [1].

Water pollution can be defined in many ways. The pollution happened when there exist modification or changes in the physical, chemical and biological characteristics of water which gives bad effects on living things. Surface waters and groundwater are the two types of water resources which affected by pollution. Surface water such as rivers, lakes and oceans are the most useful sources to the human being and wildlife habitats [2]. Most of water pollutions are caused by human activities. Human activities can give bad effects on the quality of water environment. As stated by the World Health Organization (WHO) and United Nations Environment Programme (UNEP), some examples of the activities which can cause water pollution are chemical fertilizers and chemical release by smokestacks. Farmers fertilized the fields and the chemical from the fertilizer used are washed by rain
and moves to the surface water nearby. Pollution also happen when chemical released by the smokestacks enter the atmosphere and they fall back to the earth as rain and entering the rivers, ocean or lake [1]. Water pollution gives bad impacts especially to the human health because water is the important resources for human to use in daily life. Besides, water pollution also affects the animals live in the water when poisoned through pollutant. Furthermore, this pollution will result in a lot of cost to treat and recover the polluted water contents [2].

[3] stated that there are two techniques which can be applied to water transport problem, which are experimental and numerical modelling. Numerical modelling is considered to be more portable than experimental model. This is because, the parameters can be simply adjusted which make it easier to handle in industrial side. There are many numerical methods to solve the mathematical equations in order to deal with the water pollution problem. The mathematical models introduced can contribute to save the cost of human effort and material for a large number of chemical experiments to some degree. Moreover, it is inaccessible for on-site experiments in some cases due to environmental pollution issues [4].

Advection diffusion equation (ADE) is one of the most important partial differential equations that has been used in transport of pollutants. An appropriate numerical method can give an accurate information on the concentration of pollution at different times and at different location efficiently and quickly [5]. Therefore, many researchers have studied the numerical methods to solve the ADE in predicting the water pollution problem. One of the method to predict water pollution concentration is finite difference method (FDM). According to [6], FDM has been used to solve the flow equations in order to obtain the flow rate and flow direction of water pollution concentration. In this study, FDM will be used for solving 1D ADE because of its ability to predict the concentration of pollutant as stated by [7].

2. Mathematical Formulation

2.1. Advection Diffusion Equation

In this present paper, the mathematical formulation for advection diffusion equation will be presented.

\[ \frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} \]  

where, \( c \) is the concentration, \( x \) is the position on the water, \( t \) is the amount of time that passes, \( D \) is the diffusion rate in \( x \) direction, and \( u \) is the fluid velocity.

With an initial condition,

\[ c(x,0) = f(x) \]  

And boundary conditions,

\[ c(0,t) = g_0(x) \]  

\[ \frac{\partial c(l,t)}{\partial x} = g_l \quad \text{for} \quad 0 \leq x \leq l \]
3. The Finite Difference Method

3.1. The FTCS Techniques
The Equation (1) forms the Equation (5) which is a forward time approximation. Equation (6) and 
Equation (7) shows the discretization of the spatial derivative by using second ordered central 
difference approximation. Let the solution \( c(x_i, t_j) \) be denoted \( C_i^j \) and its approximate value by \( c_i^j \).

\[
\frac{\partial c}{\partial t} = \frac{C_i^{j+1} - C_i^j}{\Delta t}
\]

(5)

\[
\frac{\partial c}{\partial x} = \frac{C_{i+1}^j - C_{i-1}^j}{2\Delta x}
\]

(6)

\[
\frac{\partial^2 c}{\partial x^2} = \frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{\Delta x^2}
\]

(7)

Equation (5), (6) and (7) then are substituted into Equation (1) and form Equation (8). Equation (8) is a 
combination of the time and spatial derivative that have been discretized and substitute to form one 
explicit method.

\[
\frac{c_i^{j+1} - c_i^j}{\Delta t} + u \frac{c_{i+1}^j - c_{i-1}^j}{2\Delta x} = D \frac{c_{i+1}^j - 2C_i^j + C_{i-1}^j}{\Delta x^2}
\]

(8)

After substitute and rearrange the equation according the time level \( (j+1) \), lead to form equation (9),

\[
c_i^{j+1} = c_i^j + D \left( \frac{\Delta t}{\Delta x^2} \right) (c_{i+1}^j - 2c_i^j + c_{i-1}^j) - u \left( \frac{\Delta t}{2\Delta x} \right) (c_{i+1}^j - c_{i-1}^j)
\]

\[
c_i^{j+1} = (\alpha + \beta)c_i^{j+1} + (1 - 2\alpha)c_i^j + (\alpha - \beta)c_{i+1}^{j+1}
\]

(9)

where,

\[
\alpha = D \left( \frac{\Delta t}{\Delta x^2} \right), \quad \beta = u \left( \frac{\Delta t}{\Delta x} \right)
\]

3.2. The Crank Nicolson Techniques
The implicit Crank Nicolson scheme approximations the Equation (1) by using forward finite differences approximation in time and the spatial derivatives by using second ordered central difference approximation are estimated by the average of their values at time step \( j \) and \( j+1 \).

\[
\frac{\partial c}{\partial x} = \frac{1}{2} \left[ \frac{C_{i+1}^{j+1} - C_{i-1}^{j+1}}{2\Delta x} + \frac{C_{i+1}^j - C_{i-1}^j}{2\Delta x} \right]
\]

(10)
Then, discretization of \( \frac{\partial^2 c}{\partial x^2} \) is obtained equation (11) from implicit second order centered difference in space.

\[
\frac{\partial^2 c}{\partial x^2} = \left( \frac{1}{2} \right) \left[ \frac{C_{i+1}^{j+1} - 2C_i^{j+1} + C_{i-1}^{j+1}}{(\Delta x)^2} + \frac{C_{i+1}^{j} - 2C_i^{j} + C_{i-1}^{j}}{(\Delta x)^2} \right]
\]  

(11)

Substituting equation (5), (10) and (11) into equation (1) and rearrange according to the time level \((j+1)\) and \(j\), lead to equation (12)

\[
\frac{C_i^{j+1} - C_i^{j}}{\Delta t} = D \left[ \frac{1}{2} \left( \frac{C_{i+1}^{j+1} - 2C_i^{j+1} + C_{i-1}^{j+1}}{(\Delta x)^2} + \frac{C_{i+1}^{j} - 2C_i^{j} + C_{i-1}^{j}}{(\Delta x)^2} \right) \right] \\
- u \left[ \frac{1}{2} \left( \frac{C_{i+1}^{j+1} - C_{i-1}^{j+1}}{2\Delta x} + \frac{C_{i+1}^{j} - C_{i-1}^{j}}{2\Delta x} \right) \right]
\]

(12)

Rearrange equation (12) of the time level \((j+1)\) at the LHS and time level \(j\) at the RHS, then will obtained equation (13).

\[
(-2\alpha + \beta)C_i^{j+1} + (4 + 4\alpha)C_i^{j+1} + (-2\alpha - \beta)C_i^{j+1} = (2\alpha - \beta)C_i^{j+1} + (4 - 4\alpha)C_i^{j+1} + (2\alpha + \beta)C_i^{j+1}
\]

(13)

where,

\[
\alpha = D \frac{(\Delta t)}{(\Delta x)^2}, \quad \beta = u \frac{(\Delta t)}{(\Delta x)}
\]

3.3. Error Estimation of the Numerical Scheme

In this section, the numerical solution of FTCS and CAN are validated with the analytical solution by [8]. The stability condition of the explicit and implicit difference scheme of 1D advection diffusion equation are: \(0 \leq u \frac{\Delta t}{\Delta x} \leq 1\), \(0 \leq D \frac{\Delta t}{\Delta x} \leq 2\) and \(\left( \frac{u\Delta t^2}{\Delta x} \right) \leq 2D \frac{\Delta t}{\Delta x} \leq 1\). The spatial grid, and time step, were provided by [8] are stated as follows,

\[
\Delta x = 0.05 \text{ and } 0.025 \text{ m} \quad \text{(14)}
\]

\[
\Delta t = 0.01, 0.025 \text{ and } 0.005 \text{ s} \quad \text{(15)}
\]
The selection of $\Delta t$ and $\Delta x$ has been tested based on the stability requirement. The Courant number, $r$ must satisfy $r \leq 0.5$, if the Courant number greater than 0.5 the result is unstable. Thus, the values of $\Delta x$ and $\Delta t$ is set based on (14) and (15) which is more stable.

Then, the numerical solution will be compared with the analytical solution in equation (16) as follows,

$$C(x,t) = \left(\frac{1}{2}\right) \left[ \text{erfc} \left( \frac{x-ut}{\sqrt{4Dt}} \right) + \exp \left( \frac{xt}{D} \right) \text{erfc} \left( \frac{x+ut}{\sqrt{4Dt}} \right) \right]$$ (16)

Based on these comparison, the error is determined as follow:

Absolute error = |Approximate value - Analytical value|

Figure 1 (a), (b) and (c) shows the error of the numerical solutions for this problem when compared with the analytical solution for $\Delta x = 0.05$ and $\Delta x = 0.025$. The values in Figure 3.18 are plotted at $t = 3s$ between $0 \leq x \leq 1$.

From Figure 1 (a), (b) and (c), we can see that the absolute errors for the FTCS and Crank Nicolson method are decreasing as the time step size decreases. However, the absolute errors for the FTCS is greater than the absolute errors for the Crank Nicolson method. Hence, the Crank Nicolson is the best method for solving ADE with as stated by the [8] and [9].
Figure 1. Comparison of the errors in the numerical solutions with analytical solution at $t = 3\text{s}$.

(a) $dt = 0.01$ [(i) $dx = 0.05$ (ii) $dx = 0.025$]
(b) $dt = 0.025$ [(i) $dx = 0.05$ (ii) $dx = 0.025$]
(c) $dt = 0.005$ [(i) $dx = 0.05$ (ii) $dx = 0.025$]

4. Results and Discussions

4.1. Numerical Simulation using Crank Nicolson Method

Based on the validation in section 3.3, it shows that the Crank Nicolson method is better than FTCS method. Therefore, the Crank Nicolson is used to predict the concentration of water pollution transport. By using the advection diffusion equation, which is varying the two parameters $D$ and $u$ that represent the diffusion rate and velocity rate respectively. In this study, it considered the specific 1D water pollution model problem as in Equation (17). Then it was discretized using the implicit method with an initial and boundary condition based on [10], which stated that,

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2}$$  \hspace{1cm} (17)

Initial condition:
$$c(x,0) = 0 , \quad 0 \leq x \leq 100$$  \hspace{1cm} (18)

Boundary condition:
$$c(0,t) = 1 \quad 0 \leq t \leq 24\text{min}$$  \hspace{1cm} (19)
$$c(100,t) = 0 \quad 0 \leq t \leq 24\text{min}$$  \hspace{1cm} (20)

By using the initial and boundary condition mention in Equation (17-20), the numerical simulation is presented in Figure 2. The Figure 2 shown the validation of the concentration distribution profile of water pollution between two difference methods. The calculated values are showed for times $0 \leq t \leq 24\text{min}$ . The plotted graph show that the pollutant concentration distribution profile at different time for Crank Nicolson. It can be observed that the pollutant concentration is decrease with respect to distance. As mentioned before, the Crank Nicolson method gives better accuracy result compare to the FTCS method.
Based on the results in Figure 2, the concentration pollutant transport is changing within the time. When the time increased, the further the distance of concentration pollutant moves and the amount of water pollution concentration reduced. The transport of water pollution concentration involves velocity and diffusion rate. Therefore, these two parameters are manipulated to see the effect towards the speed of the pollutant transport and concentration of pollutant travel at a certain distance.

4.2 Result and Effect of Water Pollution Transport on Velocity and Diffusion Rate
The numerical simulation results are represented for estimating the water pollution concentration transport by varying the water flow velocity, $u$ and the diffusion rate coefficient, $D$. The Crank Nicolson method is implemented to the advection diffusion equation that modelled the transport of the pollutant in the water. The aim of the result is to show that the advection term and diffusion term give the effect to the spreading of pollutant concentration in the water. Therefore, the varying of these two parameters, $D$ and $u$ need to satisfy the stability conditions as mentioned in section 3.2. From the stability conditions, the result is shown in Figure 3 by selecting the velocity rate and diffusion rate as follows, velocity rate, $u = 0.01 \text{m/s}$ and $0.05 \text{m/s}$ and diffusion rate, $D = 0.05 \text{m}^2 \text{s}^{-1}$ and $0.25 \text{m}^2 \text{s}^{-1}$.

Figure 2. Validation of concentration distribution profile at different time between FTCS and Crank Nicolson method.

Figure 3. Concentration distribution for varying velocity rate and diffusion rate at time $t = 24 \text{min}$.
Figure 3 shows the concentration distribution profile was calculated at $t = 24\text{min}$ by increasing the values of velocity rate from $u = 0.01 \text{ms}^{-1}$ to $u = 0.05 \text{ms}^{-1}$ and value of diffusion rate from $D = 0.05 \text{m}^2\text{s}^{-1}$ to $D = 0.25 \text{m}^2\text{s}^{-1}$. Figure 4 shows that, when the velocity and diffusion rate is high, the pollution concentration movement tend to spread faster. Besides that, the concentration of pollutant also decreases when it travels further along the distance of certain area.

It can be observed that at lower rate of velocity and diffusion, at concentration $0.9 \text{mg/l}$, the distance of pollutant travelled is approximately 8 meters long and the concentration continue decreasing to $0.4 \text{mg/l}$ when the distance travelled is approximately 22 meters. However, when the velocity and diffusion rate is higher, at concentration $0.9 \text{mg/l}$ the pollutant spread further which is approximately 45 meters and concentration reduce to $0.4 \text{mg/l}$, the distance of pollution travelled is approximately 85 meters.

Figure 4 shows the concentration distribution for each velocity rate at $t = 24\text{min}$. The velocity is varying at rate $u = 0.01 \text{ms}^{-1}$ and $u = 0.05 \text{ms}^{-1}$. Figure 5 shows the pollution concentration is spreading faster by increasing the velocity rate even though the diffusion rate is kept at constant rate, $D = 0.5\text{m}^2\text{s}^{-1}$. This is the same as the studies by [10], where the author fixed the value of diffusion rate and varying the value of velocity rate. The result gives faster rate of spreading of the pollutants on the water contents.

In that case, the water pollution concentration transport is predicted through the rate of velocity. At velocity $0.01 \text{m/s}$, the concentration distribution is smooth and pollutant concentration slowly decreases. At $0.4 \text{mg/l}$, the pollutant concentration travel approximately until 42 meters long. However, at high velocity $0.05 \text{m}^2\text{s}^{-1}$ the pollutant concentration travel about 85 meters in distance and concentration of pollutant reduces rapidly. For this reason, the pollutant move in a longer more distance with higher rate of velocity than lower velocity, even though the diffusion rate is constant.
Figure 5. Concentration distribution for varying diffusion rate at $t = 24\text{min}$.

Figure 5 shows the concentration distribution for each velocity rate at $t = 24\text{min}$. The diffusion rate is varying at $D = 0.05\text{m}^2\text{s}^{-1}$ and $D = 0.5\text{m}^2\text{s}^{-1}$. Fig.4.4 shows when the diffusion rate is high, the pollution is spreading faster while the velocity rate is kept at constant rate, $u = 0.01\text{m/s}$. As discussed in [10], even the velocity is constant, the spreading of the pollutants is faster with higher rate of diffusion rate.

The diffusion rate also give the impact to the prediction of the water pollution concentration transport. At diffusion rate $0.05\text{m}^2\text{s}^{-1}$, for concentration $0.4\text{mg/l}$, the pollutant concentration travel approximately about 23 meters long. However, when the diffusion rate is high at $0.5\text{m}^2\text{s}^{-1}$, the pollutant concentration travel approximately 43 meters in distance. For this reason, the concentration of pollutant spread further with the higher rate of diffusion than the lower rate, even though the velocity rate is constant. As a result, the concentration of pollutants is travel long distance then take slowly reduce its movements and existence. Based on the Figure 2, Figure 3 and Figure 4, the results show that when the two important parameters, velocity and diffusion rate in transport of pollutants are varying, the spreading of the pollutant will be affected as have been discussed in [10] and [11]. As a result, the water pollution concentration transport with higher rate of velocity or diffusion will spread faster than the lower rate.

5. Conclusions

In this paper, the prediction of the water pollution concentration transport has been studied through the numerical simulation. Based on the simulation results, the implicit Crank Nicolson method is successfully used to solve the 1D ADE. This method is great for solving the ADE after doing the error comparison with FTCS. It is successfully validated with the FTCS method on the water pollution concentration distribution. Therefore, this implicit Crank Nicolson method can be considered as one of the methods to solve one dimensional ADE specifically on water pollution problem. The water pollutants transport is affected by the advection and diffusion term when the velocity and diffusion rate are manipulated. In the real case, the water area such as river, lake and others inland have their own velocity and diffusion rate of pollutants moved along the streams. So, by these parameters the water pollution transport is predicted.

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