Numerical Modelling of Pollutant Transport in a Straight Narrow Channel using Upwind Finite Difference Method

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Abstract. River pollution has become an increasingly severe issue, resulting in the rapid depletion of freshwater resources. An accurate prediction of the transport of the pollutants is vital for effective mitigation measures. This paper presents the numerical modelling of pollutant transport in a straight narrow channel. The pollutant transport is modelled using an advection-diffusion equation. The equation is discretized using Finite Difference Method (FDM) with an explicit upwind scheme for the temporal term. The resulting system of simultaneous equations is solved using a direct method. The numerical model is validated against an existing analytical solution, and the results show good agreement between numerical prediction and analytical solution. The validated numerical model is applied to different cases of pollutant release mechanisms involving continuous and instantaneous pollutant releases. In both cases, the numerical model can capture the physics of the problem and able to provide valuable information on the time and spatial evolution of pollutant concentration. The model is extendable to higher dimension owing to its simplicity of discretization.

1. Introduction
Over the past few decades, we have been facing serious issue with river [1]. This issue is critical as river is one of the main water resources for our daily activities. River pollutant not only affect the environment but human wellbeing as well. If this problem is not resolved quickly, it is expected that we will be facing a serious depletion in clean water resources in near future. In order to mitigate this problem, we need a tool that can be used to predict the transport of pollutant effectively.

Experiments, measurements and observations have been widely used to investigate the physical process of pollutant transport [2]. However, the drawbacks with experimental investigation are cost and control. The cost of running even a simple experiment is not cheap. The total cost includes the cost of material, construction and manpower. Additionally, in an experimental setup, it is difficult to control or separate all the unnecessary variables and time-consuming. Extra effort is needed to filter the undesirable effect from the experimental result. In most cases, some of this uncertainty cannot be eliminated and remains in the result. Moreover, the experiment provides limited information and the results may be subjected to human and measurement errors.

With the advancement of computer and technology, numerical field has been developed rapidly and a remarkable progress has been done in the development of numerical methods such as finite difference, finite element and finite volume [2]. This allows the application of mathematical or partial differential equations that describe the physics of natural phenomenon on every flow problem. In the context of pollutant transport problem, numerical simulation has been used to predict the behaviour of pollutant pattern under specific environmental conditions [3,4]. From the perspective of numerical
method, the transport of pollutant can be modelled using advection-diffusion equation (ADE) [5]. Advection is the transport of a property due to the background fluid velocity. In the case of pollutant, this property is the pollutant concentration. Diffusion on the other hand, is the net movement of this concentration from high concentration to low concentration. ADE has been used to predict the diffusion of pollutant concentration as it is being carried away by the velocity of the water.

The pollutant transport phenomenon is extremely complex. Traditionally, the prediction of such transport quantities was limited to the laboratory studies and simplified theories. This former is used to model the realistic case but is expensive and time consuming. The latter on the other hand is simple and easy to use but limited to simple problem and in most cases does not provide a real representation of the problem. With the advancement of computer technology and numerical method, a numerical model is developed to enhance the understanding of the physical process that governs the pollutant transport phenomenon. This numerical model serves as an alternative tool to both experimental and simplified theories. A numerical method provides a much more realistic representation of the problem at a fraction of the cost of running a full experimental work.

The aim of this study is to solve a one-dimensional pollutant transport model using ADE. The objectives are to discretize a one-dimensional ADE using an explicit upwind FDM, to validate the numerical model against existing analytical solution and to determine the behaviour of pollutant concentration for different pollutant release mechanisms. In this study, the numerical modelling of pollutant transport is undertaken. The ADE is used as the governing equation of the problem. The ADE is discretized using an explicit upwind finite difference method. The numerical solution is validated with existing analytical solution before being used to simulate few cases of pollutant transports problems in a straight narrow channel.

2. Literature Review
In the context of pollutant transport, there are four mechanisms that need to be accounted. These are advection, shear flow dispersion, turbulent diffusion, and molecular (Fickian) diffusion. If the flow is laminar, the effect of shear and turbulence is not significant. In this case, only the advection and diffusion play an active role. These mechanisms can be modelling using ADE. ADE describe combined effect of advection and diffusion in fluid medium. Separately, advection is the transport mechanism of a substance or conserved property by a fluid due to the fluid’s bulk motion while diffusion is the net movement of particles from high concentration to low concentration. The theoretical behaviour of both advection and diffusion is presented in Figure 1(a) and 1(b) respectively.

![Figure 1. The behaviour of (a) advection and (b) diffusion transport mechanism.](image)

The simplest and most widely used numerical method to solve directly differential equations is the FDM. The solution of differential equation using FDM is called a strong form solution. The strong form stem from the fact that the FDM discretized the differential equation without reducing the order of the differential equation like most recent numerical techniques, for example Finite Element Method (FEM), Finite Volume Method (FVM) and Boundary Element Method (BEM), do. Most people use FDM due to its simple discretization and implementation [6]. Higher order solution can be obtained by simply by changing the order of discretization and does not alter much the subsequence step of the overall algorithm. The implementation of both the initial and boundary condition in FDM is also
straightforward intuitive. Both the Dirichlet (variable) and Neumann (derivative of variable) boundary condition can be implemented using a simple substitution in the discretized matrix. Although FDM are usually used for problems involving simple domain, the method is undoubtedly able to provide valuable information that cannot be obtained from analytical solution alone. This is especially true when the boundary condition is complex and not smooth. Taking these advantages into consideration, the FDM is used for the modelling of pollutant transport in this study.

3. Mathematical Model

3.1. Governing equation
The general equation for one-dimensional solute transport considering advection-diffusion without source or sink term is as follow:

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x}$$

(1)

where, $c$ is the concentration of solute, $u$ is the velocity and $D$ is the diffusion coefficient. This is so called advection-diffusion equation (ADE). The first term on the right-hand side of Equation (1) is the diffusion term while the second one is called the advection term. Due to unsteady nature of the equation, both boundary and initial conditions are required to properly defined the problem.

Finite difference approximations can be used to represent the derivatives in ADE. The derivation of ADE will be discussed in the following section.

3.2. Finite Difference Methods

3.2.1. Discretization of advection term. Advection can be defined as the process of transporting mass which being carried by the flow from one point to another. Equation (2) is the pure advection term in the ADE. $\partial c/\partial x$ is represented by backward finite difference approximation. $u$ is assumed as a constant which represent the flow velocity in the channel.

$$-u \frac{\partial c}{\partial x} = -u \frac{c_i - c_{i-1}}{\Delta x}$$

(2)

3.2.2. Discretization of diffusion term. Diffusion is the mixing of dissolved chemical due to the random motion of molecules within the fluid. The solute moves from high concentration region to low concentration region based on Fick’s first law of diffusion.

$$D \frac{\partial^2 c}{\partial x^2} = D \frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2}$$

(3)

Equation (3) is the diffusion term in the ADE. Equation (3) is represented by finite difference equation using the second-order central differencing of order $(\Delta x)^2$. $D$ is assumed as a constant which represent diffusion coefficient of the pollutant transport in medium such as liquid and air. In Equation (2) and (3) above, the subscript $i$ represent the spatial index of the variables. The summation and subtraction of $i$ means that the variables are location either to the right or the left of the main variables, respectively.
3.2.3. Discretization of temporal term. There are two methods for the discretization of temporal term in finite difference such as explicit and implicit method. The implicit method assumes that all or most of the spatial variables are unknowns that need to be solved at each time steps. This requires that all the variables to solve simultaneously, resulting in the creation of a system of simultaneous equation. In any numerical method, the solution to the simultaneous equation is the most expensive part of the whole solution. Explicit method on the other hand assumed that all spatial variables are known and only one variable need to be solved at any given time step. Therefore, it simpler and requires less computational effort as compared to implicit method. In this study, the explicit method is used. The general form of the explicit method is given as

\[
\frac{\partial c}{\partial t} = f(c) \tag{4}
\]

\[
\frac{c_i^{n+1} - c_i^n}{\Delta t} = f(c)^n \tag{5}
\]

where the subscript \( n \) and \( n + 1 \) represent the previous and current time step, respectively.

3.2.4. Full discretization of ADE. Equation (1) can be fully discretized by substituting Equation (2), (3) and (5) resulting in the following discretized equation.

\[
\frac{c_i^{n+1} - c_i^n}{\Delta t} = D \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta x)^2} - u \frac{c_i^n - c_{i-1}^n}{\Delta x} \tag{6}
\]

Equation (6) can be solved by rearranging all the terms with superscript \( n \) to the right-hand side and solving for the term \( n + 1 \) only. Although the explicit method is easy to solve, it suffers from stability issue. The method is only stable if the following criteria is fulfilled.

\[
D \frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2} \tag{7}
\]

\[
u \frac{\Delta t}{\Delta x} \leq 1 \tag{8}
\]

Equation (8) and (9) are called the diffusion and Courant numbers, respectively.

3.3. Numerical simulation

3.3.1. Initial and boundary conditions. In order for the problem to be well defined, initial and boundary conditions is required. The initial condition is related to the temporal term in the ADE, represented by the superscript \( n \). Because the temporal term is only first derivatives, only one initial condition is required. This is given by:

\[
c(0, x) = c(x) \tag{9}
\]
where \( C(0, x) \) represent all the spatial variables at time step, \( t = 0 \). The boundary condition on the other hands is related to the spatial variables and because the highest derivatives in the ADE is second order, the boundary condition needed to be fully defined the problem is two. In the case where the inlet is prescribed with known value and the pollutant is allowed to exit at the outlet boundary, the boundary conditions are given as

\[
C(t, 0) = c(t) \tag{10}
\]

\[
\frac{\partial c}{\partial t}(t, L) = 0 \tag{11}
\]

Equation (10) and (11) are called Dirichlet and Neumann boundary conditions, respectively.

4. Numerical Experiments and Discussion

This study assumed that the pollutant is transported downstream in a straight narrow channel. The unknown quantity is the concentration. The concentration is assumed to varies in just one direction. Therefore, the problem is assumed to be one-dimensional. As the concentration varies at each time step, the problem is considered as unsteady. The transport of the pollutant is modelled using an ADE. A simple explicit upwind FDM is used to solve the advection diffusion equation. The numerical solution of ADE provides a prediction of pollutant concentration distributions along the straight channel.

4.1. Model validation

The discretized ADE using FDM is given by Equation (7). In order to ensure that both the derivation and code is correct, validation need to be undertaken. For the ADE, an analytical solution exists. The analytical solution assumed that the initial condition of the concentration is given by the following equation.

\[
C(0, x) = e^{\frac{-(x-x_0)^2}{D}} \tag{12}
\]

where \( x_0 \) is the location of the peak concentration.

The diffusion coefficient, \( D \), is assumed to be 0.005m²/min while the background velocity, \( u \), is given by 0.05m/min. The length of the domain is assumed to be 2.5m. The domain is discretised into 313 nodes with a spacing of 0.008m. The total duration of the simulation is 50min and the time step used is 0.001min. In this case, the diffusion and Courant numbers are given by 0.0781 and 0.0063, respectively. As both values are lower than their critical limit, the solution is stable.

Figure 2 shows the concentration at various time steps between numerical results and analytical solution. At time \( t = 0 \) min, the pollutant concentration is given by a symmetric bell shape. This concentration is given by Equation (12). The concentration has a maximum value of 1 kg/m³, located at \( x = 0.5 \) m. As time progresses, the concentration drops rapidly at first due to diffusion and advected to the right due to the background velocity. At \( t = 10 \) min, the maximum concentration value reduces to 0.2kg/m³ and occur at \( x = 1 \) m. At the next time step, \( t = 20 \) min, the reduction in the maximum concentration value is very subtle. However, the maximum concentration value has been advected further to the right at \( x = 1.6 \) m.
Figure 2. Concentration at various time steps between numerical result and analytical solution.

At each time steps, it can be seen that the agreement between numerical prediction and analytical solution is excellent. This shows that the FDM discretization of the ADE is correct and the numerical code is free from error.

4.2. Simulation 1: Continuous Pollutant Release

Having validated the numerical model against existing analytical solution, this section seeks to provide the simulation of pollutant transport for a continuous pollutant release. It is important to find out the behaviour of the pollutant concentration at various part of the domain if say, a pollutant is release continuously. Before the simulation is undertaken, it is important that a correct initial and boundary conditions is imposed so that the correct physics is simulated.

Initially, it is assumed that the river or channel is not polluted yet. In this case, the pollutant concentration over the entire domain is zero. The initial condition that needs to be imposed is given as:

\[ C (0, x) = 0 \]  \hspace{1cm} (13)

As we need to impose continuous pollutant release at the inlet, the boundary condition at the inlet needs to be a function of time. Initially, the value is zero. As the pollutant is released at the inlet, the pollutant concentration increases. After some time, the concentration reaches maximum value and plateaued. The boundary condition at the inlet is given as follows:

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

\[ 0 < t < 10, \quad c(x) = \frac{1}{10} t \]

\[ t > 10, \quad c(x) = 1 \]

At the outlet, the pollutant concentration is allowed to exit the boundary. Therefore, Neumann boundary condition is applied as given by Equation (11).
The concentration of pollution at \( x = 0 \text{m}, x = 1 \text{m} \) and \( x = 2 \text{m} \) are given in Figure 3. The inlet is located at \( x = 0 \text{m} \). From the figure, it is clear that the correct boundary condition is imposed at the inlet. At \( t = 0 \text{min} \), the concentration at all these locations are zero, as time progresses, the concentration starts to increase. Because the location differs, the time required for the concentration to initiate is slightly delayed. At \( x = 1 \text{m} \), the concentration starts to increase at around \( t = 10 \text{min} \) while for \( x = 2 \text{m} \), this occurs at around \( t = 20 \text{min} \).

Another interesting observation that can be made from Figure 3 is the shape of the concentration profile. At the inlet, the pollutant concentration has a distinct profile, a sharp change in profile at \( t = 10 \text{min} \). This profile changes completely for second and third location; the profile is much smoother than the inlet profile. These smooth changes are caused by the diffusion term in the ADE. As the advection term is only responsible for the movement of the concentration, the only plausible explanation for the changes in the profile is due to the diffusion.

The spatial variation of the concentration over the whole domain at different time steps is given in Figure 4. From the figure, we can clearly see the evolution of the concentration over the whole domain. Initially, the concentration is zero over the whole domain, as time progresses, the concentration at the inlet increases due to continuous release of pollutant. At the same time, due the
background velocity, the concentration is being advected to the right. As explained earlier, the diffusion term in the ADE has a smoothing effect and forces the profile varies smoothly over the whole domain. With further increase in time, the pollutant concentration starts to reach peak the maximum value. If the simulation is continued further, the value of concentration will reach a maximum value of 1kg/m³ over the whole domain.

4.3. Simulation 2: Pollutant Release Over a Short Period

The exact solution for pollutant release over a short period is

\[
\begin{align*}
  & t = 0, \quad c(x) = 0 \\
  & 0 < t < 10, \quad c(x) = \frac{1}{10}t \\
  & 10 < t < 15, \quad c(x) = 1 \\
  & 15 < t < 25, \quad c(x) = \frac{1}{10}t + 2.5 \\
  & t > 25, \quad c(x) = 0
\end{align*}
\]

In this section, the test case also divided into two types; concentration time-histories at various location for pollutant release over a short period and concentration over the whole domain at various time steps for pollutant release over a short period. In this case, the pollutant is released in a limited time period.

In concentration time-histories at various location for continuous pollutant release, the time is set as \(0 \leq t \leq 50\)s. In concentration over the whole domain at various time steps for continuous pollutant release, the value of the distance is set as \(0 \leq L \leq 2\)m. The velocity in all direction is assumed constant. The dispersion pattern and behaviour of the pollutant concentration are observed in Figure 5 and 6.

![Figure 5. Concentration time-histories at various location for pollutant release over a short period](image-url)
5. Conclusion
In this paper, a one-dimensional transport of pollutants is solved using finite difference method (FDM). The pollutant transport dependent on few key parameters such as diffusion coefficient and the background velocity. The results obtained using FDM shows good agreement when compared to analytical solution. Numerical simulations of pollutant transport for continuous and fixed period release shows that the numerical model is capable of simulating the physics of the problems correctly.

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