A numerical model for pollutant distribution on a closed lagoon with inlet and outlet

Zaitun, Mahie A G, and Khaeruddin
Department of Mathematics Hasanuddin University, Indonesia
Email: zet.zaitun@gmail.com

Abstract. This research obtains a model of the distribution of pollutants in a closed lagoon with inlet and outlet. The model is made and solved by the DuFort-Frankel scheme. This research produces a flow equation or stream function model on the closed lagoon, stated in the 2-D Laplace equation and pollutant distribution model using a 2-D advection-diffusion equation. The DuFort-Frankel numerical modeling was carried out in two different cases of pollutants injection, namely instantaneous and continuous injection on the closed lagoon, resulted that pollutants spreading in all directions and tend to flow toward the outlet of the lagoon. The Lax-Richtmyer equivalency theorem carries out the convergence analysis of the DuFort-Frankel scheme.

1. Introduction
Partial Differential Equation (PDE) is a base of the mathematical model of many phenomena. The advection-diffusion equation as one of PDE can model physical phenomena like pollutant distribution. We have to estimate the solution because usually in more cases of pollutants have no exact solution. The numerical solution is an alternative solution to the modeling of pollutant distribution [1–4].

One of the numerical methods that widely used is the finite difference method. This method has been used to solve various differential equations, even with a more complex problem. In Sampera (2016), the numerical modeling is used cause it is quite practical and possible accuracy in the case of physical identified pollutant distribution [4]. A numerical solution with the DuFort-Frankel scheme and its stability had been carried out by Hutomo et al., (2019) and Alman et al., (2013) [2,3]. Consistency and convergence of some numerical schemes are discussed by [5–7]. Pollutants distribution on the lagoon with the constant flow is carried out in [1,3,4], and the uniform flow is carried out in [2]. With consistent flows, we have to describe with the flow equation like a stream function. The stream function can be made constant or somewhat natural to produce a better mathematical model.

In this paper, the pollutant distribution of the closed lagoon is modeled by a 2-D advection-diffusion equation and solve by the DuFort-Frankel scheme the flow of the lagoon we made by 2-D Laplace’s equation to obtain the advection coefficient. In the closed lagoon, we made inlets and outlets for forming a flow. The convergence of the DuFort-Frankel scheme is carried out by the Lax-Richtmyer equivalency theorem to produce convergent computation. The numerical solution in this study we made an injection of pollutants is instantaneous and continue.

2. Literature Review
The finite difference method is available for solving Partial Differential Equations (PDE), which model heat and mass transfer in fluid [6]. Starting the discretization of PDE through Taylor’s series, various PDE problems can be evaluated, either explicit or implicit.
2.1. Stream Function and Discretization

Continuity equation in the form of a partial differential equation has been developed by Anderson (2010) [8], for \( \rho \) density and the continuity equation are

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0
\]  

(1)

Where \( \nabla \) said “del” is a Laplace operator where \( \nabla = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}) \), \( \mathbf{V} = (u, v, w) \) denote a vector velocity in 3-Dspace, and time \( t \geq 0 \). Generally, fluid flow is a steady-state where \( \rho(x, y, z, t) = \rho \) constant for \( x, y, z, t \geq 0 \), so the density at that point will be a fixed value, invariant with time. Hence, the equation (1) for 2-D fluid flow will be

\[
\frac{\partial}{\partial x} u(x, y) + \frac{\partial}{\partial y} v(x, y) = 0
\]  

(2)

We define the stream function \( \psi \) for incompressible flow in 2-D fluid flow (see [8] and [9])

\[
u = \frac{\partial \psi}{\partial y} \quad \text{and} \quad v = -\frac{\partial \psi}{\partial x}
\]

(3) (4)

and the new parameter vorticity \( \Omega \). In a velocity field, the curl of the velocity is equal to the vorticity (see [8])

\[
\Omega = \nabla \times \mathbf{V}
\]

(5)

for incompressible flow, it is required that the motion of fluid elements is a pure translation at every point in a flow, or this is called “irrotational” flow. So \( \Omega \) are equal to zero, and hence the equation (5) will be

\[
\frac{\partial}{\partial x} v(x, y) - \frac{\partial}{\partial y} u(x, y) = 0
\]  

(6)

By substitution equation (3) and (4) in the equation (6), we obtain

\[
\frac{\partial}{\partial x} \left( \frac{\partial \psi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{\partial \psi}{\partial y} \right) = 0
\]

(7)

Equation (7) is called Laplace’s equation, or it can be said that the stream function is similar to Laplace’s Equation. The Laplace’s equation (see [10]) can determine values for the potential (temperature, voltage, concentration, or other potential quantity) at points within a rectangular region subject to conditions that are specified on the boundaries of a rectangular region.

The stream function or Laplace’s equation (see [11]) by the equation (7) has a discretization from Taylor’s series are

\[
\frac{\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j}}{(\Delta x)^2} + \frac{\psi_{i,j+1} - 2\psi_{i,j} + \psi_{i,j-1}}{(\Delta y)^2} = 0
\]

(8)

and rearranging equation (8) above, we obtain
The difference equation (9) above is an implicit scheme. Therefore, we have to evaluate by another method. In order to be easy and efficient, we will use the iterative method for solving the linear equation. The iterative method has been introduced and carried out in [11], we use that method for solving this implicit scheme, and the advection coefficients in $x$ and $y$ respectively, is evaluated.

The analysis convergence of these schemes are clearly by [5], where the parameter of $\Delta x$ and $\Delta y$ go to zero, respectively. The analytical and numerical solution for Laplace’s equation with FDM for the Dirichlet boundary condition has been compared in [12], where the numerical solution is convergence to the analytical solution.

2.2. Advection-diffusion Equation and Discretization

The two-dimensional (2-D) advection-diffusion equation (see [2]) can be written as:

$$\frac{\partial}{\partial t} C(x, y, t) + \frac{\partial}{\partial x} (u(x, y, t)C(x, y, t)) + \frac{\partial}{\partial y} (v(x, y, t)C(x, y, t)) = \frac{\partial}{\partial x} \left( D_x(x, y, t) \frac{\partial}{\partial x} C(x, y, t) \right)$$

$$+ \frac{\partial}{\partial y} \left( D_y(x, y, t) \frac{\partial}{\partial y} C(x, y, t) \right)$$

where $u, v$ are velocity coefficients in $x$ and $y$ direction; and $D_x, D_y$ are the diffusion coefficients in $x$ and $y$ direction, respectively.

For the velocity coefficients $u, v$ are independent by time $t$ and the diffusion coefficients $D_x, D_y$ are constant, the Equation (12) will be
\[ \frac{\partial}{\partial t} C(x, y, t) + \frac{\partial}{\partial x} (u(x, y) C(x, y, t)) + \frac{\partial}{\partial y} (v(x, y) C(x, y, t)) = D_x \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} C(x, y, t) \right) + D_y \frac{\partial}{\partial y} \left( \frac{\partial}{\partial y} C(x, y, t) \right) \]  

Equation (13) can be developed if the continuity

\[ \frac{\partial}{\partial x} u(x, y) + \frac{\partial}{\partial y} v(x, y) = 0 \]

is applied and hence the Equation (13) will be

\[ \frac{\partial}{\partial t} C(x, y, t) + u(x, y) \frac{\partial}{\partial x} C(x, y, t) + v(x, y) \frac{\partial}{\partial y} C(x, y, t) = D_x \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} C(x, y, t) \right) + D_y \frac{\partial}{\partial y} \left( \frac{\partial}{\partial y} C(x, y, t) \right) \]

Equation (15) has a discretization by the DuFort-Frankel method. The DuFort-Frankel process (see [6]) is that developed by DuFort and Frankel. This is a modification of Richardson’s way in which the central grid-point value \( C^n_{i,j} \) in the finite difference approximation for the diffusion term in the 1-D diffusion equation. The discretization of the 2-D advection-diffusion equation using the DuFort-Frankel scheme is carried out in [2, 3]. In a similar way, discretization of Equation (15) can be developed to:

\[ \frac{C_{i,j}^{n+1} - C_{i,j}^{n-1}}{2\Delta t} + u_{i,j} \frac{C_{i+1,j}^n - C_{i-1,j}^n}{2\Delta x} + v_{i,j} \frac{C_{i,j+1}^n - C_{i,j-1}^n}{2\Delta y} = D_x \frac{C_{i+1,j}^n - C_{i-1,j}^n}{(\Delta x)^2} + D_y \frac{C_{i,j+1}^n - C_{i,j-1}^n}{(\Delta y)^2} \]

and rearranging gives the difference equation

\[ C_{i,j}^{n+1} = \left( 1 - \frac{2B_x - 2B_y}{1 + 2B_x + 2B_y} \right) C_{i,j}^{n-1} + \left( -\frac{A_x + 2B_x}{1 + 2B_x + 2B_y} \right) C_{i+1,j}^n + \left( \frac{A_x + 2B_x}{1 + 2B_x + 2B_y} \right) C_{i-1,j}^n \]

\[ + \left( -\frac{A_y + 2B_y}{1 + 2B_x + 2B_y} \right) C_{i,j+1}^n + \left( \frac{A_y + 2B_y}{1 + 2B_x + 2B_y} \right) C_{i,j-1}^n \]

where

\[ A_x = \frac{u \Delta t}{\Delta x}, \ A_y = \frac{v \Delta t}{\Delta y}, \ B_x = \frac{D_x \Delta t}{(\Delta x)^2}, \ B_y = \frac{D_y \Delta t}{(\Delta y)^2} \]
As in Hutomo et al., (2019), the DuFort-Frankel scheme is using a two-level approximation for evaluating the third grids in time [2]. The schemes above are used for the third level at the inner points. The second level in time is evaluated by Forward in Time and Central in Space (FTCS); therefore, the DuFort-Frankel scheme is used.

The DuFort-Frankel scheme has stability criteria unconditionally stable for the advection-diffusion equation in [3], different within [2], the DuFort-Frankel scheme have a stable condition. Using the von Neumann method in [3], the DuFort-Frankel scheme in equation (17) has a stability condition

$$
\xi = \frac{\sqrt{4(B_x + B_y)^2 - (A_x + A_y)^2 + \sqrt{1 - (A_x + A_y)^2}}}{(1 + 2B_x + 2B_y)}
$$

for $\xi$ is a wave number and required $|\xi|^2 \leq 1$ to obtain a stable scheme, where $A_x$, $A_y$, $B_x$, and $B_y$ given by Equation (18).

Checking consistency in DuFort-Frankel schemes is carried out in [6] for a one-dimensional diffusion equation. In a similar way to obtain consistency, Equation (17) are consistence to 2-D advection-diffusion equation as follows

$$
\frac{\partial C^n}{\partial t_{i,j}} + u_{i,j} \frac{\partial C^n}{\partial x_{i,j}} + v_{i,j} \frac{\partial C^n}{\partial y_{i,j}} = D_x \frac{\partial^2 C^n}{\partial x^2_{i,j}} + D_y \frac{\partial^2 C^n}{\partial y^2_{i,j}} + E^n_{i,j} \tag{20}
$$

where truncation error $E^n_{i,j}$ as follows

$$
E^n_{i,j} = -D_x \left( \frac{\Delta t^2}{\Delta x^2} \right) \frac{\partial C^n}{\partial x_{i,j}} - D_y \left( \frac{\Delta t^2}{\Delta y^2} \right) \frac{\partial C^n}{\partial y_{i,j}} - \left( \frac{(\Delta t)^2}{6} \right) \frac{\partial^3 C^n}{\partial x^3_{i,j}} - u_{i,j} \left( \frac{(\Delta t)^2}{6} \right) \frac{\partial^3 C^n}{\partial x^3_{i,j}} \\
- v_{i,j} \left( \frac{(\Delta t)^2}{6} \right) \frac{\partial^3 C^n}{\partial y^3_{i,j}} + D_x \left( \frac{(\Delta x)^2}{12} \right) \frac{\partial^4 C^n}{\partial x^4_{i,j}} + D_y \left( \frac{(\Delta y)^2}{12} \right) \frac{\partial^4 C^n}{\partial y^4_{i,j}} + O((\Delta t)^3, (\Delta x)^3, (\Delta y)^3) \tag{21}
$$

Therefore the Equation (20) from Equation (17) is consistent with the 2-D advection-diffusion equation for $E^n_{i,j}$ approaches zero as $\Delta x$, $\Delta y$, $\Delta t$ $\rightarrow$ 0. In this scheme $\Delta t << \Delta x$ and $\Delta t << \Delta y$ is
required in order, the finite difference Equation (20) is consistent with Equation (15).

By the Lax-Richtmyer equivalency theorem (see [7]) within Equation (17), the criteria stability and consistency is used to produce a convergent computation.

3. Results and Discussion

We begin to design of closed lagoon with a square domain $0 \leq x \leq 1$ and $0 \leq y \leq 1$. Taking $\Delta x = \Delta y = 0.05$, we have 21 grid in $x$ and $y$. To made inlet and outlet, we have to arrange the boundary condition of the domain where the Equation (7) is applied to produce the advection coefficient and used in Equation (15). The boundary condition of the domain is shown in Table 1 and Figure 3.

![Figure 3. The domain of closed lagoon with inlet and outlet](image)

| Domain side | Flow | Interval | Neumann | Dirichlet |
|-------------|------|----------|---------|-----------|
| Bottom      | Inlet| $i \in [1,7]$ | $\psi_{i,1} = 0.0025$ | $\frac{\partial \psi}{\partial y}_{i,i} = 0$, $\frac{\partial \psi}{\partial x}_{i,1} = 0$ |
|             |      | $i = 8$   |         | $\frac{\partial \psi}{\partial y}_{8,1} = 0$ |
|             |      | $i \in [9,21]$ | $\psi_{i,1} = 0$ | $\frac{\partial \psi}{\partial y}_{i,i} = 0$, $\frac{\partial \psi}{\partial x}_{i,1} = 0$ |
| Left        | Outlet| $j \in [1,10]$ | $\psi_{1,j} = 0.0025$ | $\frac{\partial \psi}{\partial y}_{1,j} = 0$, $\frac{\partial \psi}{\partial x}_{1,1} = 0$ |
|             |      | $j = 11$  |         | $\frac{\partial \psi}{\partial x}_{1,11} = 0$ |
After solving the Equation (7) using a finite difference scheme in Equations (9), (10), and (11) with boundary conditions as before, we obtain a vector field of velocity flow are shown in Figure 4.

3.1. Simulation I
In this first simulation, we consider the same domain as before and the advection-diffusion equation

\[
\frac{\partial}{\partial t} \text{C}(x, y, t) + u(x, y) \frac{\partial}{\partial x} \text{C}(x, y, t) + v(x, y) \frac{\partial}{\partial y} \text{C}(x, y, t) = D_x \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \text{C}(x, y, t) \right) + D_y \frac{\partial}{\partial y} \left( \frac{\partial}{\partial y} \text{C}(x, y, t) \right)
\]

with the advection coefficient are evaluated before are shown in Figure 4, diffusion coefficient \(D_x = D_y = 0.0004\), the initial condition

\[
\text{C}(x, y, 0) = 1, \quad 0 < x < 1, \quad 0 < y < 1
\]

\[
\text{C}(x_0, y_0, 0) = 10, \text{ for } x_0 = 8, \ y_0 = 2
\]
and the boundary condition

\[ C(0,y,t) = 1 \]
\[ C(1,y,t) = 1 \]
\[ C(x,0,t) = 1 \]
\[ C(x,1,t) = 1 \]

\[ 0 \leq x \leq 1, \quad 0 \leq y \leq 1, \quad t \geq 0 \]

with \( \Delta t = 0.025 \) we obtain the results, the pollutants distribution for \( t = 3, t = 5, t = 15, t = 60, \) and \( t = 300 \) are in Figures 5, 6, 7, 8, and 9.

**Figure 5.** Pollutant distribution on the lagoon with \( t=3 \) (time step 120)

**Figure 6.** Pollutant distribution on the lagoon with \( t=5 \) (time step 200)

**Figure 7.** Pollutant distribution on the lagoon with \( t=15 \) (time step 600)
3.2. Simulation II
In the second simulation, we consider the same parameter as before (simulation 1) is used. The 2-D advection-diffusion equation

\[
\frac{\partial}{\partial t} C(x,y,t) + u(x,y) \frac{\partial}{\partial x} C(x,y,t) + v(x,y) \frac{\partial}{\partial y} C(x,y,t) = D_x \frac{\partial^2}{\partial x^2} C(x,y,t) + D_y \frac{\partial^2}{\partial y^2} C(x,y,t)
\]

to produce a continue injection of pollutants, we consider the initial condition is

\[
C(x,y,0) = 1, \quad 0 < x < 1, \quad 0 < y < 1
\]
\[
C(x_0,y_0, t) = 10, \quad t \geq 0, \quad \text{for } x_0 = 8, \quad y_0 = 2
\]

and the boundary condition

\[
C(0,y,t) = 1
\]
\[
C(1,y,t) = 1
\]
\[
C(x,0,t) = 1
\]
\[
C(x,1,t) = 1
\]

\[
0 \leq x \leq 1, \quad 0 \leq y \leq 1, \quad t \geq 0
\]

we obtain the results the distribution of the pollutant for \( t = 3, t = 5, t = 15, t = 60, \) and \( t = 300 \) are in Figures 10, 11, 12, 13, and 14.

Figure 8. Pollutant distribution on the lagoon with \( t=60 \) (time step 2400)

Figure 9. Pollutant distribution on the lagoon with \( t=300 \) (time step 12000)

Figure 10. Pollutant distribution on the lagoon with \( t=3 \) (time step 120)
3.3. Simulation III

Here we consider the inlet and outlet in the closed lagoon area at the corner of the domain. All parameters in simulation 1 and 2 are used with $x_0 = 3$, $y_0 = 3$. We obtain the vector field of velocity flow shown in Figure 15, and pollutants distribution on the closed lagoon for instantaneous and continue injection is
shown in Figures 16, 17, 18, and 19.

Figure 15. Velocity flow on the lagoon with inlet and outlet at the corner domain

Figure 16. Pollutant distribution of continue injection (left) and instantaneous injection (right) with t=5 (time step 200)

Figure 17. Pollutant distribution of continue injection (left) and instantaneous injection (right) with t=15 (time step 600)
Figure 18. Pollutant distribution of continue injection (left) and instantaneous injection (right) with t=60 (time step 2400)

Figure 19. Pollutant distribution of continue injection (left) and instantaneous injection (right) with t=300 (time step 12000)

4. Conclusion

Using the DuFort-Frankel scheme as a finite difference method, we obtained good results and presented in some figures. Some vector field of velocity flow with inlet and outlet has been evaluated by the finite difference method and presented as in Figures 4 and 15 based on the boundary condition in Table 1. Figures 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, and 19 show pollutant distribution is spreading in all directions and tend to flow toward the outlet of the closed lagoon. Based on the results, it can be concluded that the DuFort-Frankel scheme is good to solve pollutant distribution problems by the 2-D advection-diffusion equation.

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