Numerical solution of 2-d advection-diffusion equation with variable coefficient using du-fort frankel method

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Abstract. The advection-diffusion equation or transport equation is investigated further. A simple numerical approximation such as Du-Fort Frankel methods for advection-diffusion equation with variable coefficient is employed. The obtained results are compared with its analytical solution in a simple unit square domain. The method and results are then being used to solve advection-diffusion in the real-world problems for the more complicate irregular domain.

1. Introduction

The solution of the partial differential equation and their associated boundary and initial condition play an important role in the modeling of phenomena in fields as diverse as physics, chemistry, geology, biology, engineering, and economics. One of the physics phenomena is pollutant transport. The transport of pollutant occurs in a large variety of environmental, agricultural and industrial processes. Accurate prediction of the transport of these pollutants is crucial to the effective management of these pollutants processes. The transport of these pollutants can be adequately described by the advection-diffusion equation.

Only very few partial differential equations have the analytical or exact solution, anyone who wants to develop and use models based on such equations and their associated conditions, must be able to obtain numerical solutions efficiently and accurately. Because exact analytical solutions are not generally able to be found, it is often necessary to resort to numerical methods to find approximate solutions of these partial differential equations, in order to investigate the predictions of the mathematical models.

Finite difference method is the oldest and most commonly used for the numerical solution of the partial differential equation. While more recently developed techniques such as those based on finite elements (see [1] and [2]) or on boundary elements (see [3]) are appropriate for the solution of equilibrium type problems, the finite difference remains the most appropriate for solving time-dependent phenomena.

There are numerous numerical solutions to 2-D or 3-D advection-diffusion equation with the uniform flow and constant coefficients (see [4 – 7]). Recently, a generalized finite difference method to solve the advection-diffusion equation is shown in [8], and a numerical solution 2-D advection-diffusion equation for the irregular domain had been studied in [9]. Although practical problems generally involve non-uniform velocity fields.

In this paper, we solve the 2-D advection-diffusion equation with variable coefficient by using Du-Fort Frankel method, that is the development of the finite difference method. The numerical solution in
this study starts with a simple domain. The results obtained are compared with the analytical solution. Later, then the methods and results are then being used to solve advection-diffusion for more complicated irregular domain.

2. Transport Equation
Hundsdorfer [10] explain the standard advection-diffusion-reaction model deals with the time evolution of chemical or biological species in a flowing medium such as water or air. The mathematical equations describing this evolution are partial differential equations that can be derived from mass balances. Consider a concentration \( C(x, t) \) of a certain species, with space variable \( x \in \mathbb{R} \) and time \( t \geq 0 \). Let \( h > 0 \) be a small number, and consider the average concentration \( \bar{C}(x, t) \) in a domain \( [x - \frac{1}{2}h, x + \frac{1}{2}h] \),

\[
\bar{C}(x, t) = \frac{1}{h} \int_{x-\frac{1}{2}h}^{x+\frac{1}{2}h} C(s, t) \, ds = C(x, t) + \frac{1}{24} h^2 \frac{\partial^2}{\partial x^2} C(x, t) + \cdots \tag{2.1}
\]

If the species is carried along by a flowing medium with velocity \( u(x, t) \), then the mass conservation law implies that the change of \( \bar{C}(x, t) \) per unit of time is the net balance of inflow and outflow over the domain boundaries,

\[
\frac{\partial}{\partial t} \bar{C}(x, t) = \frac{1}{h} \left[ u \left( x - \frac{1}{2}h, t \right) C \left( x - \frac{1}{2}h, t \right) - u \left( x + \frac{1}{2}h, t \right) C \left( x + \frac{1}{2}h, t \right) \right] \tag{2.2}
\]

where \( u \left( x \pm \frac{1}{2}h, t \right) C \left( x \pm \frac{1}{2}h, t \right) \) are the mass fluxes over the left and right domain boundaries. Now, if we let \( h \to 0 \), it follows that the concentration satisfies

\[
\frac{\partial}{\partial t} C(x, t) + \frac{\partial}{\partial x} \left( u(x, t) C(x, t) \right) = 0 \tag{2.3}
\]

this is called an advection equation (or convection equation). In a similar way, we can consider the effect of diffusion. The change of \( \bar{C}(x, t) \) is caused by gradients in the solution and the fluxes across the domain boundaries are \(-D \left( x \pm \frac{1}{2}h, t \right) C \left( x \pm \frac{1}{2}h, t \right)\) with \( D(x, t) \) the diffusion coefficient. The corresponding diffusion equation is

\[
\frac{\partial}{\partial t} C(x, t) = \frac{\partial}{\partial x} \left( D(x, t) \frac{\partial}{\partial x} C(x, t) \right) \tag{2.4}
\]

The overall change in concentration is described by combining these three effects, leading to the advection-diffusion equation.

\[
\frac{\partial}{\partial t} C(x, t) + \frac{\partial}{\partial x} \left( u(x, t) C(x, t) \right) = \frac{\partial}{\partial x} \left( D(x, t) \frac{\partial}{\partial x} C(x, t) \right) \tag{2.5}
\]

We will consider (2.5) in a spatial interval \( \Omega \subset \mathbb{R} \) with time \( t > 0 \). An initial profile \( C(x, 0) \) will be given and we also assume that suitable boundary conditions are provided. Equation (2.5) is known as the 1-D form of the advection-diffusion equation.
In a similar way, 2-D advection-diffusion can be developed as:

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

$$\frac{\partial}{\partial x} \left( D_x(x, y, t) \frac{\partial}{\partial x} C(x, y, t) \right) + \frac{\partial}{\partial y} \left( D_y(x, y, t) \frac{\partial}{\partial y} C(x, y, t) \right)$$ (2.6)

where $u, v$ are velocity coefficients in $x$ and $y$ direction, $D_x, D_y$ 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 (2.6) will be

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

$$\frac{\partial}{\partial x} \left( D_x \frac{\partial}{\partial x} C(x, y, t) \right) + \frac{\partial}{\partial y} \left( D_y \frac{\partial}{\partial y} C(x, y, t) \right)$$ (2.7)

3. Du-Fort Frankel Method

Du-Fort and Frankel (see [11]) proposed a modification of the Centred Time Centred Space (CTCS) discretization to ensure second order accuracy while improving numerical stability. The idea is to replace the middle term in the numerator on CTCS Method with an average value, and after substituted in equation (2.7), yielding

$$\frac{C_{i,j}^{n+1} - C_{i,j}^{n-1}}{2\Delta t} + \left( \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} \right) C_{i,j}^{n} + \left( \frac{v_{i,j+1} - v_{i,j-1}}{2\Delta y} \right) C_{i,j}^{n} =$$

$$\frac{D_x}{(\Delta x)^2} \left( \frac{C_{i+1,j}^{n+1} - 2C_{i,j}^{n+1} + C_{i-1,j}^{n+1}}{(\Delta x)^2} \right) + \frac{D_y}{(\Delta y)^2} \left( \frac{C_{i,j+1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j-1}^{n+1}}{(\Delta y)^2} \right)$$ (3.1)

Rearranging, we obtain

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

$$+ \left( \frac{-A_y + 2B_y}{1 + 2B_x + 2B_y} \right) C_{i+1,j}^{n} + \left( \frac{A_y + 2B_y}{1 + 2B_x + 2B_y} \right) C_{i-1,j}^{n}$$ (3.2)

where

$$u_x = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x}, v_y = \frac{v_{i,j+1} - v_{i,j-1}}{2\Delta y},$$

$$A_x = \frac{u\Delta t}{\Delta x}, A_y = \frac{v\Delta t}{\Delta y}, B_x = \frac{D_x\Delta t}{(\Delta x)^2}, B_y = \frac{D_y\Delta t}{(\Delta y)^2}, E = (u_x + v_y)\Delta t,$$ (3.3)
Figure 1. Grid points of Du-Fort Frankel Method

The Du-Fort Frankel method used here is stable if $\sqrt{\alpha^2 + \beta^2} - \alpha \leq E$. For $2B_x + 2B_y = \alpha$, and $A_x + A_y = \beta$, where $A_x, A_y, B_x, B_y, E$ given by equation (3.3).

The Du-Fort Frankel scheme is using a two-level approximation in time, so the Du-Fort Frankel scheme as described above is used for the second level at the inner points. For the first level of inner points and the boundaries points, we use a combination approach of Finite Difference Method such as Forward Time Centred Space (FTCS), Forward Time Forward Space (FTFS), Forward Time Backward Space (FTBS) which depend on the availability of the grids.

4. Comparison of Numerical Solutions and Analytical Solutions

In order to compare the analytical solutions with the numerical solutions of Du-Fort Frankel method in 2-D advection-diffusion equation, we consider a simple square domain $0 \leq x \leq 1, 0 \leq y \leq 1$.

Here, the 2-D advection-diffusion equation

$$\frac{\partial C}{\partial t} + \left( \frac{\partial u}{\partial x} \right) C + u \frac{\partial C}{\partial x} + \left( \frac{\partial v}{\partial y} \right) C + v \frac{\partial C}{\partial y} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} \quad (4.1)$$

It is not difficult to prove that the analytical solution $C(x, y, t) = e^{\alpha t + \beta x + \gamma y}$, where

$$u(x, y) = \left( D_x \beta - \frac{\alpha}{\beta} \right) + pe^{-\beta x},$$

$$v(x, y) = \left( D_y \gamma - \frac{\alpha}{\gamma} \right) + qe^{-\gamma y}, \quad (4.2)$$

satisfy (4.1), where $\alpha, \beta, \gamma, p, q, D_x, D_y$ are constants. Taking the values of the constants as $\alpha = -0.029, \beta = 0.500, \gamma = 0.500, p = 0.050, q = 0.050, D_x = 0.004, D_y = 0.004$, we obtain the numerical and analytical solution as in table 1 and table 2.
Based on Table 1 and Table 2, it is clear that when computational grids are reduced, numerical errors get smaller too. This also shows that the solution generated from the Du-Fort Frankel method converges to its analytical or exact solution when computational grids are reduced.

### 5. Numerical Simulation

We begin the simulation from a simple domain that is a square domain with domain areas $0 \leq x \leq 1$ and $0 \leq y \leq 1$, then to an irregular domain, in this case, Hasanuddin University’s lake, with initial condition 10 at the specific grid, and for the other grids are 1. The chosen of these initial conditions mainly for visualization effect. The boundary condition along the lakeside is $\frac{\partial C}{\partial n} = 0$, where $n$ denotes unit normal vector outward from the boundary domain.

#### Simulation I

In this first simulation, we consider a simple unit square domain $0 \leq x \leq 1$ and $0 \leq y \leq 1$, with advection coefficients $u(x, y) = 0.01 + 0.005x - 0.005y$, $v(x, y) = -0.01 - 0.005x + 0.005y$, and diffusion coefficients $D_x = D_y = 0.0004$. Taking $\Delta x = \Delta y = 0.05$, $\Delta t = 0.05$, the initial condition of pollutant source at grid $C(10,10,1) = 10$, and the other grids of the initial conditions are 1. We obtain the results are in figure 2, figure 3, figure 4, and figure 5.
Figure 2. The vector field of velocity flow for the square domain

Figure 3. Pollutant distribution for $T = 1$ (time step 20)

Figure 4. Pollutant distribution for $T = 3$ (time step 60)
Figure 5. Pollutant distribution for $T = 5$ (time step 100)

**Simulation II**

The second simulation, we consider a simple unit square domain $0 \leq x \leq 1$ and $0 \leq y \leq 1$, with advection coefficients $u(x, y) = 0.007 + 0.003x^2 - 0.004y^2$, $v(x, y) = -0.007 - 0.03x^2 + 0.03y^2$, and diffusion coefficients $D_x = D_y = 0.00012$. Taking $\Delta x = \Delta y = 0.025$, $\Delta t = 0.005$, the initial condition of pollutant source at grids $C(20, 20, 1) = C(20, 21, 1) = C(20, 22, 1) = C(21, 20, 1) = C(21, 21, 1) = C(21, 22, 1) = C(22, 20, 1) = C(22, 21, 1) = C(22, 22, 1) = 10$, and the other grids of the initial conditions are 1. We obtain the results are on the figure 6, figure 7, figure 8, and figure 9.

Figure 6. The vector field of velocity flow for the square domain

Figure 7. Pollutant distribution for $T = 1$ (time step 200)
Here, we consider an irregular domain in this third simulation. The lake of Hasanuddin University which is located at Tamalanrea Campus in Makassar have the ±400m length (y) and ±320m wide (x). These physical dimensions are divided into 33 equal grids of the x-axis, and 41 equal grids of y-axis (see [6] and [9]). These are equally by taking $\Delta x = 0.025$, $\Delta y = 0.03125$, and $\Delta t = 0.005$. Here advection coefficients, in general, are the unknown functions. However in this simulation, we took the function $u(x, y)$, and $v(x, y)$ are shown as in figure 10. Taking the diffusion coefficients $D_x = D_y = 0.00013$, the initial condition for the pollutant source at grids $C(13,22,1) = C(13,23,1) = C(13,24,1) = C(14,22,1) = C(14,23,1) = C(14,24,1) = 10$, and the other grids of the initial conditions are 1. We obtain the results are in figure 11, figure 12, and figure 13.

Figure 8. Pollutant distribution for $T = 3$ (time step 600)

Figure 9. Pollutant distribution for $T = 5$ (time step 1000)

Simulation III

Here, we consider an irregular domain in this third simulation. The lake of Hasanuddin University which is located at Tamalanrea Campus in Makassar have the ±400m length (y) and ±320m wide (x). These physical dimensions are divided into 33 equal grids of the x-axis, and 41 equal grids of y-axis (see [6] and [9]). These are equally by taking $\Delta x = 0.025$, $\Delta y = 0.03125$, and $\Delta t = 0.005$. Here advection coefficients, in general, are the unknown functions. However in this simulation, we took the function $u(x, y)$, and $v(x, y)$ are shown as in figure 10. Taking the diffusion coefficients $D_x = D_y = 0.00013$, the initial condition for the pollutant source at grids $C(13,22,1) = C(13,23,1) = C(13,24,1) = C(14,22,1) = C(14,23,1) = C(14,24,1) = 10$, and the other grids of the initial conditions are 1. We obtain the results are in figure 11, figure 12, and figure 13.

Figure 10. The vector field of velocity flow for the domain of Hasanuddin University’s lake
Simulation IV

Here, we consider the same irregular domain with the third simulation. The lake of Hasanuddin University which is located at Tamalanrea Campus in Makassar. Taking $\Delta x = 0.025$, $\Delta y = 0.03125$, $\Delta t = 0.005$ and advection coefficients as in figure 14. These advection coefficients are more natural than the previous simulation in order to make better mathematical models. Taking the diffusion coefficients $D_x = D_y = 0.00028$, the initial condition for the pollutant source at grids $C(29, 21, 1) = C(29, 22, 1), C(30, 21, 1) = C(30, 22, 1) = 10$, and the other grids of the initial conditions are 1. We obtain the results are in figure 15, figure 16, and figure 17.
Figure 14. The vector field of velocity flow for the domain of Hasanuddin University’s lake

Figure 15. Pollutant distribution for $T = 2$ (time step 400)

Figure 16. Pollutant distribution for $T = 3$ (time step 600)

Figure 17. Pollutant distribution for $T = 6$ (time step 1200)
6. Conclusions and Discussions
We have obtained and compared the analytical and numerical solutions using Du-Fort Frankel method. The numerical solutions converge to its analytical solutions when computational grids size being reduced. Using Du-Fort Frankel method for the 2-D advection-diffusion equation, simulations have been presented. Several kinds of velocity vector $u$ and $v$ are used as in figures 2, 6, 10, 14. figures 3, 4, 5, 7, 8, 9, 11, 12, 13, 15, 16, and 17, explained that the pollutants will move together with the flow, diffuses, and the concentration will fade with respect to time. Based on the results, it can be concluded that the Du-Fort Frankel method has been good for solving 2-D advection-diffusion equation problems with variable coefficients.

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