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The 2^{nd}, 4^{th}, and 6^{th}-Order Finite Difference Schemes for Pollutant Transport Equation

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ABSTRACT
In this paper, we study the pollutant transport phenomenon using an advection-diffusion equation. To solve the model numerically, we apply the finite difference method. Here we use the second, fourth, and sixth-order explicit finite difference schemes. To validate our numerical models, we compare the numerical results with the existing analytical solution. Further, we conclude that the methods can best approximate the exact solution when using a small Courant number and spatial grid partition. Amongst the three finite difference methods, we observe that the fourth-order FTCS is the best method to simulate the pollutant transport phenomena.

Keywords: *Pollutant transport, Advection-diffusion equation, FTCS.*

1. INTRODUCTION

A pollutant is a substance or energy such as chemical substance, salt, temperature, and light that disturbs a location and becomes unwanted existence [1]. The pollutants move in the water or atmosphere through diffusion and advection. The word diffusion is related to the phenomena when the pollutant moves from a high-concentrated area to the lower one. The term advection refers to the substance movement due to fluid flow. In the case of pollutant transport in the river area, it is hard to say that only the diffusion movement is involved. It is because the water in the river is rarely static. Therefore in this study, we consider the advection-diffusion equation to investigate the pollutant transport phenomena.

Recently, the pollutant transport phenomenon has been a popular object to study. Many mathematicians and civil engineers pay attention to develop numerical models. Some of them use the modified finite difference schemes such as the compact finite difference [2] and the high-order finite-difference combined with 4th-order Runge-Kutta [3]. The Runge-Kutta method itself is applied to solve the advection-reaction-diffusion equation in [4]. Another modification of the finite difference technique is used by [5]. Several methods have also been implemented by [6–8] to simulate the transport phenomenon using spreadsheets. The finite element method has also been applied by [9] to construct the advection-diffusion equation's numerical model. Other researchers have also examined various numerical methods to simulate the transport phenomenon [10–13]. However, amongst other numerical methods, the explicit finite difference is the most popular. It can be fastly computed and less expensive because it does not require large matrices in each time step. In addition to that, since the explicit finite difference scheme has the same form as the mathematical equation, it becomes the simplest method. This study will discuss the numerical simulations using the explicit finite difference method (FTCS) of the second, fourth, and sixth-order. We aim to see these methods' performance in solving the advection-diffusion problem, which makes them more stable, and the differences of each FTCS despite their order of accuracy.

This paper consists of four main sections. We start with a brief overview of this problem in the first section. Next, in the second section, we will present the mathematical model and the numerical method used in this research. In the third section, we will establish the numerical simulation result. Finally, we draw our conclusions in the last part.

2. FINITE DIFFERENCE METHOD

In this section, we observe the one-dimensional pollutant transport phenomenon by considering the advection and diffusion movement. The observation time is T, and the spatial domain is defined by $[0, L]$. The governing equation is

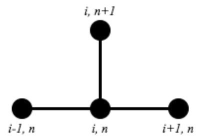

Figure 1 Second-order FTCS stencil.

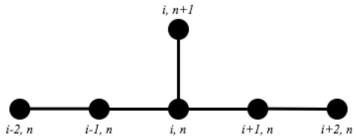

Figure 2 Fourth-order FTCS stencil.

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} - D\frac{\partial^2 C}{\partial x^2} = 0, \quad (1)$$

where U and D denote constant water velocity and diffusion coefficient, respectively. The function $C(x,t)$ is the concentration of the pollutant. In this study, we only consider the constant coefficients. Another researcher has discussed the use of variable coefficients [14].

Then we implement the finite difference method to solve Equation (1) numerically. Here, we consider a simple explicit finite difference scheme called the Forward Time Central Space (FTCS) of second, fourth, and sixth-order. We obtain the scheme by approximating the derivative terms from the Taylor series expansion. The difference between various accuracy orders lies in the number of spatial grids used in approximating the derivatives. The second-order FTCS (or FD2 to shorten the name) requires grids x_{i-1} , x_i , and x_{i+1} to approximate the C's derivative at x_i as shown in Figure 1, whereas the FD4 uses more grids, i.e., x_{i-2}, x_{i-1}, x_i, x_{i+1}, and x_{i+2}. Table 1 presents the complete central finite difference coefficients for the first and second derivatives with various accuracy orders [15].

After applying the stencil in Figures 1–3 to Equation (1) with the coefficients from Table 1, we obtain the FTCS scheme for the second, fourth, and sixth-order respectively, as follows:

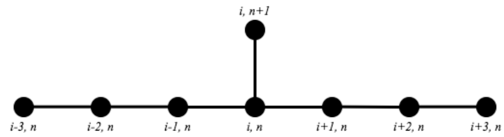

Figure 3 Sixth-order FTCS stencil.

$$C_i^{n+1} = C_i^n + D\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{\Delta x^2}\Delta t - U\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}\Delta t, \quad (2)$$

$$C_i^{n+1} = C_i^n + D\frac{-C_{i+2}^n + 16C_{i+1}^n - 30C_i^n + 16C_{i-1}^n - C_{i-2}^n}{12\Delta x^2}\Delta t - U\frac{C_{i+2}^n - 8C_{i+1}^n + 8C_{i-1}^n - C_{i-2}^n}{12\Delta x}\Delta t, \quad (3)$$

$$C_i^{n+1} = C_i^n + D\frac{2C_{i+3}^n - 27C_{i+2}^n + 270C_{i+1}^n}{180\Delta x^2}\Delta t - D\frac{490C_i^n - 270C_{i-1}^n + 27C_{i-2}^n - 2C_{i-3}^n}{180\Delta x^2}\Delta t - U\frac{C_{i+3}^n - 9C_{i+2}^n + 45C_{i+1}^n}{60\Delta x}\Delta t - U\frac{45C_{i-1}^n - 9C_{i-2}^n + C_{i-3}^n}{60\Delta x}\Delta t. \quad (4)$$

The symbol C_i^n denotes $C(x_i, t^n)$ for $i = 1, 2, \ldots, Nx$ and $n = 1, 2, \ldots, Nt$, where Nx and Nt are the number of spatial and time grid points, respectively. By using Von Neumann's stability analysis, the above schemes are stable if $0 \le D\frac{\Delta t}{\Delta x^2} \le \frac{1}{2}, U\frac{\Delta t}{\Delta x} \le 1$ for FD2; $D\frac{\Delta t}{\Delta x^2} \le \frac{3}{8}, U\frac{\Delta t}{\Delta x} \le \sqrt{\frac{51}{128}}$ for FD4; and $D\frac{\Delta t}{\Delta x^2} \le \frac{90}{272}, U\frac{\Delta t}{\Delta x} \le \frac{273}{1642}$ for FD6. Let us define $Cr = U\frac{\Delta t}{\Delta x}$ as the Courant number for numerical analysis.

3. NUMERICAL SIMULATION AND RESULT

The numerical schemes (Equations (2)–(4)) are applied to Equation (1) to simulate the pollutant transport

Table 1. Central finite difference coefficient

Derivative	Accuracy	-3	-2	-1	0	1	2	3
1	2			-1/2	0	1/2		
	4		1/12	-2/3	0	2/3	-1/12	
	6	-1/60	3/20	-3/4	0	3/4	-3/20	1/60
2	2			1	-2	1		
	4		-1/12	4/3	-5/2	4/3	-1/12	
	6	1/90	-3/20	3/2	-49/18	3/2	-3/20	1/90

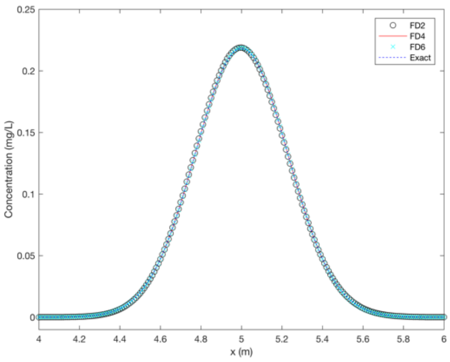

Figure 4 The Gaussian pulse distribution from the numerical result using $Cr = 0.008$.

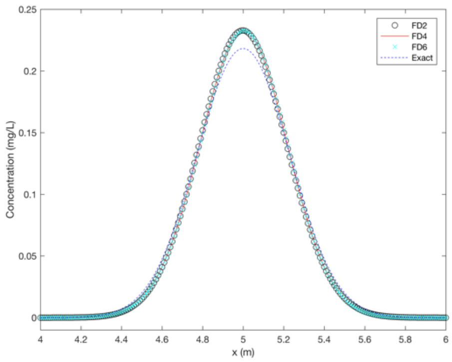

Figure 5 The Gaussian pulse distribution from the numerical result using $Cr = 0.16$.

phenomenon. We study the same one-dimensional advection-diffusion cases used in [2]. We will compare the accuracy of FD2, FD4, and FD6 by calculating the absolute error (E) and norm error (L_2 and L_∞) of each method using the formula:

$$E = \left|C_i^{\text{exact}} - C_i^{\text{numerical}}\right|, \quad (5)$$

$$L_2 = \sqrt{\sum_{i=1}^{Nx} \left|C_i^{\text{exact}} - C_i^{\text{numerical}}\right|^2}, \quad (6)$$

$$L_\infty = \max_i \left|C_i^{\text{exact}} - C_i^{\text{numerical}}\right|. \quad (7)$$

Here, we present two cases to observe the spreading of pollutant transport phenomena.

Case 1. Consider a channel with length of L = 9 m. The water velocity is U = 0.8 m/s and the diffusion coefficient is D = 0.005 m^2/s. As written in [2], the obtained exact solution is

$$C(x,t) = \frac{1}{\sqrt{4t+1}} \exp\left[-\frac{(x-1-Ut)^2}{D(4t+1)}\right], \quad (8)$$

and the boundary conditions are

$$C(0,t) = \frac{1}{\sqrt{4t+1}} \exp\left[-\frac{(-1-Ut)^2}{D(4t+1)}\right], \quad (9)$$

$$C(9,t) = \frac{1}{\sqrt{4t+1}} \exp\left[-\frac{(8-Ut)^2}{D(4t+1)}\right]. \quad (10)$$

We take the initial condition from the exact solution where t = 0. For the computation, we use $\Delta x = 0.01$. The numerical simulation shows that the Gaussian pulse distribution at t = 5 s confirms the exact solution, as

Table 2. The absolute error of each finite difference methods with $Cr = 0.008$

x	Exact	FD2	FD4	FD6	Absolute error		
					FD2	FD4	FD6
4.0	0.000016	0.000010	0.000015	0.000015	5.88E-06	6.62E-07	6.89E-07
4.5	0.020177	0.019507	0.019958	0.019959	6.70E-04	2.19E-04	2.18E-04
5.0	0.218218	0.218885	0.218885	0.218884	6.67E-04	6.67E-04	6.67E-04
5.5	0.020177	0.020356	0.019933	0.019932	1.79E-04	2.44E-04	2.45E-04
6.0	0.000016	0.000022	0.000015	0.000015	5.77E-06	1.07E-06	1.05E-06

Table 3. The norm error of each finite difference methods using various Cr

Cr	FD2		FD4		FD6	
	L_2	L_∞	L_2	L_∞	L_2	L_∞
0.008	0.011010	0.001942	0.003690	0.000670	0.003691	0.000670
0.064	0.031597	0.005804	0.030348	0.005534	0.030349	0.005535
0.16	0.079762	0.014705	0.079703	0.014685	0.079704	0.014686

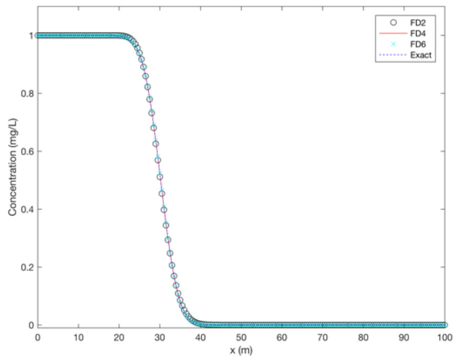

Figure 6 The comparison between the numerical solution and the exact solution using $\Delta t = 0.5$ and $\Delta x = 0.5$ ($Cr = 0.01$) after $t = 3000$ s.

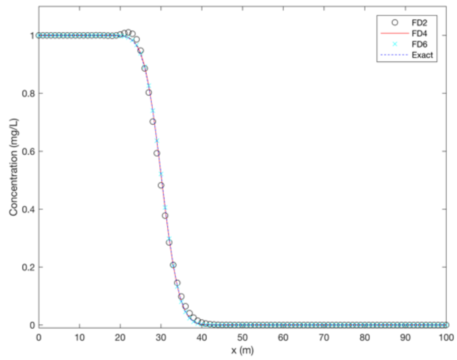

Figure 7 The comparison between the numerical solution and the exact solution using $\Delta t = 1$ and $\Delta x = 1$ ($Cr = 0.01$) after $t = 3000$ s.

shown in Figures 4 and 5. We observe that we get a better result when we use smaller Cr. Quantitatively, we calculate the norm error as presented in Table 3. From Tables 2 and 3, we can interpret that FD2 has the biggest error in each simulation.

Case 2. Here we assume that the water moves with velocity $U = 0.01$ m/s in the channel whose length of $L = 100$ m. The diffusion coefficient is $D = 0.002$ m^2/s. The exact solution is

$$C(x,t) = \frac{1}{2}\operatorname{erfc}\left(\frac{x - Ut}{\sqrt{4Dt}}\right) + \frac{1}{2}\exp\left(\frac{Ux}{D}\right)\operatorname{erfc}\left(\frac{x + Ut}{\sqrt{4Dt}}\right), \quad (11)$$

where $\operatorname{erfc}(x)$ is the complementary error function. The pollutant concentration at the boundary must follows these conditions:

$$C(0,t) = 1, \quad (12)$$

$$-D\left(\frac{\partial C}{\partial x}\right)(L,t) = 0. \quad (13)$$

As used in Case 1, the initial condition is also obtained from the exact solution. Figure 6 presents the comparison between the numerical results using FDMs and the exact solution. It says that they are in a good agreement. As shown in Table 4, the norm errors of the methods with $Cr = 0.01$ and $\Delta x = 0.5$ are small. But when we change Δx to 1, the same number of Cr produces different result as displayed in Figure 7 and Table 5. The figure also shows that FD2 method seems give a wiggle at the wave front 20 m $< x <$ 30 m while FD4 and FD6 perform a more accurate result.

From the numerical simulations, we can see that FD2 consistently becomes the least accurate method of all, while the results from FD4 and FD6 are barely distinguishable. The computation of FD6 is more complicated than FD4 because it involves seven grid points in total, whereas FD4 only uses five. Yet, the two methods perform similarly. These become the main reasons why FD4 is the best method to choose.

Table 4. The norm error of each finite difference methods using various Cr and $\Delta x = 0.5$

Cr	FD2		FD4		FD6	
	L_2	L_∞	L_2	L_∞	L_2	L_∞
0.01	0.035118	0.011567	0.006096	0.001545	0.006162	0.001505
0.02	0.035183	0.011388	0.012393	0.003090	0.012489	0.003068
0.1	0.065731	0.016980	0.065482	0.016342	0.065621	0.016476

Table 5. The norm error of each finite difference methods using various Cr and $\Delta x = 1$

Cr	FD2		FD4		FD6	
	L_2	L_∞	L_2	L_∞	L_2	L_∞
0.01	0.097148	0.043042	0.010674	0.004391	0.009083	0.003399
0.1	0.124831	0.047238	0.095794	0.035722	0.097184	0.034842

4. CONCLUSION

We successfully derive the second, fourth, and sixth-order explicit FDM schemes for solving the advection-diffusion equation. These methods can best approximate the exact solution when we use a small number of Cr and Δx. On the overall, amongst the three finite difference methods, FD4 is the best to use. For further study, the numerical modification of an explicit finite difference scheme should be considered in order to gain a better result.

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