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Abstract

This study used the finite difference method to develop a numerical model for pollutant transport phenomenon simulation. Mathematically, the phenomenon is often described by the advection–diffusion differential equation, which is obtained from a combination of the continuity equation and Fick’s first law. The Forward Time Central Space (FTCS) scheme is one of the explicit finite difference methods and is used in this study to solve the model due to its simplicity in solving a differential equation. Yet, this method is currently unstable, which results in oscillations in the model. Thus, a numerical filter (Hansen) is added to the FTCS method to improve the stability of the model. The developed numerical model is applied to several 1D and 2D pollutant transport test cases. Simulation results are compared with those of existing analytical solutions to verify the developed model, and they show that the developed model can simulate the pollutant transport phenomenon well. Moreover, the numerical filter can increase the model stability.

Abstrak

Pengembangan Model Numerik 2D untuk Transpor Polutan dengan Skema FTCS dan Numerical Filter. Studi ini menggunakan metode beda hingga untuk mengembangkan suatu model numerik pada simulasi fenomena transpor polutan. Secara matematis, fenomena ini seringkali digambarkan dengan persamaan differensial adveksi-difusi yang merupakan gabungan dari persamaan kontinuitas dan hukum pertama Fick. Skema *Forward Time Central Space* (FTCS) adalah salah satu metode eksplisit beda hingga dan digunakan dalam pemodelan pada studi ini karena kesederhanaannya dalam menyelesaikan suatu persamaan differensial. Namun, metode ini kurang stabil sehingga dapat menimbulkan osilasi pada model. Oleh karena itu, suatu *numerical filter* (Hansen) digunakan pada metode FTCS ini untuk meningkatkan stabilitas dari model. Model numerik yang telah dikembangkan diaplikasikan pada beberapa kasus transpor polutan 1D dan 2D. Hasil simulasi model dibandingkan dengan solusi analitik untuk memverifikasi model yang telah dikembangkan. Hasil tersebut menunjukkan bahwa model yang telah dikembangkan dapat mensimulasikan fenomena transpor polutan dengan baik. Selain itu, *numerical filter* juga dapat meningkatkan stabilitas model.

Keywords: FTCS, hansen filter, pollutant transport

1. Introduction

The study of pollutant transport is an important part of water quality management and can be conducted by designing a model. Thus, an accurate model is required for water quality management [1]. Such a model can be described by the advection–diffusion equation [2],

which is derived from a combination of the continuity equation and Fick’s first law [3].

The governing equation in this study is the differential equation. Numerical methods, such as shallow water equation [4–6] and advection–diffusion [7, 8], are able to solve differential equations. The commonly used

numerical method is the finite difference method, which is a well-established numerical method for transport modeling [9] that has a simple algorithm and is easy to apply.

Several studies used finite difference methods in pollutant transport modeling. For example, pollutant distribution in a lake was simulated by [7] using a two-dimensional form of the advection–diffusion equation. Sea–sand mining pollution distribution was simulated by [8] using a three-dimensional form of the equation. The finite difference method has two types of schemes: implicit and explicit. Explicit schemes are easier to evaluate numerically [10] and more cost effective than implicit schemes [11].

The Forward Time Central Space (FTCS) scheme is one of the explicit finite difference methods. This scheme is very simple [12] but unconditionally unstable [13]. Its stability has been studied in [14], which compared its result with the numerical simulation result that was obtained by using the Forward Time Backward Space and Centered Space (FTBSCS) Scheme. Findings show that FTCS can give better pointwise solutions than FTBSCS.

This study develops an FTCS scheme by adding a numerical filter to the model to increase stability. The numerical filter by Hansen will be used in this study because of its simple application in numerical models. This numerical filter has been applied to the finite difference model, as shown in [6, 15–18]. Results show that the Hansen filter successfully increased the stability of the model.

In this paper, the developed FTCS scheme is used to solve 1D and 2D pollutant transport cases. Then, the numerical results are compared with the analytical results. In brief, this study aims to determine the performance of the simple developed model in simulating pollutant transport.

2. Methods

Governing equation. The pollutant transport phenomenon can be explained and described by a mathematical equation. The advection–diffusion equation is commonly used in pollutant transport cases. The two-dimensional form of the equation is given as follows:

$$\frac{\partial C}{\partial t} + \frac{\partial(UC)}{\partial x} + \frac{\partial(VC)}{\partial y} = \frac{\partial}{\partial x} \left(D_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_y \frac{\partial C}{\partial y} \right) \quad (1)$$

where C is a concentration of pollutant; U and V are depth-integrated velocities in the x - and y -directions, respectively; D_x and D_y are dispersion coefficients in the

x - and y -directions, respectively; x and y are spatial coordinates; and t is time.

Numerical scheme. This study uses the FTCS scheme to address the case numerically. This scheme approximates the time derivative by using the first-order forward difference, while the central difference is used for the space derivative. The scheme is given in Figure 1.

According to the FTCS scheme, the discretization for each component in (1) is as follows:

$$\frac{\partial C}{\partial t} = \frac{C_{i,j}^{t+1} - C_{i,j}^t}{\Delta t} \quad (2)$$

$$\frac{\partial(UC)}{\partial x} = \frac{U_{i+1,j}^t C_{i+1,j}^t - U_{i-1,j}^t C_{i-1,j}^t}{2\Delta x} \quad (3)$$

$$\frac{\partial(VC)}{\partial y} = \frac{U_{i,j+1}^t C_{i,j+1}^t - U_{i,j-1}^t C_{i,j-1}^t}{2\Delta y} \quad (4)$$

$$\frac{\partial}{\partial x} \left(D_x \frac{\partial C}{\partial x} \right) = D_x \frac{C_{i+1,j}^t - 2C_{i,j}^t + C_{i-1,j}^t}{\Delta x^2} \quad (5)$$

$$\frac{\partial}{\partial y} \left(D_y \frac{\partial C}{\partial y} \right) = D_y \frac{C_{i,j+1}^t - 2C_{i,j}^t + C_{i,j-1}^t}{\Delta y^2} \quad (6)$$

Therefore, the whole equation can be written as

$$\begin{aligned} & \frac{C_{i,j}^{t+1} - C_{i,j}^t}{\Delta t} + \frac{U_{i+1,j}^t C_{i+1,j}^t - U_{i-1,j}^t C_{i-1,j}^t}{2\Delta x} \\ & + \frac{U_{i,j+1}^t C_{i,j+1}^t - U_{i,j-1}^t C_{i,j-1}^t}{2\Delta y} \\ & = D_x \frac{C_{i+1,j}^t - 2C_{i,j}^t + C_{i-1,j}^t}{\Delta x^2} \\ & + D_y \frac{C_{i,j+1}^t - 2C_{i,j}^t + C_{i,j-1}^t}{\Delta y^2} \end{aligned} \quad (7)$$

Figure 1. FTCS Scheme

Numerical filter. A numerical filter, namely, Hansen filter, is applied to increase the model's stability. This filter is easier to apply in the model. The filters are used in each time step. For each iteration at each node, the concentration is updated by the following equation:

$$F_{ij} = C_f \times F_{ij} + \frac{F_{i-1,j} + F_{i+1,j} + F_{i,j-1} + F_{i,j+1}}{4} \times (1 - C_f) \quad (8)$$

where F corresponds to the filtered parameters, and C_f (correction factor) is taken to be 0.99. Previous studies [16–19] showed that this value provides satisfactory and stable results.

3. Result and Discussion

In this study, the FTCS scheme is applied to pollutant transport cases for either the 1D or the 2D case. The 1D cases (examples 1–3) were analyzed by [20] using the compact finite difference method. The 2D cases (example 4) were analyzed using a high-order finite difference scheme by [21]. Norm error (L_2 and L_∞) and absolute error (E) are used to validate the model. The equations used to calculate these errors are as follows:

$$E = |C_i^{\text{exact}} - C_i^{\text{numerical}}| \quad (9)$$

$$L_2 = \sqrt{\sum_{i=1}^N |C_i^{\text{exact}} - C_i^{\text{numerical}}|^2} \quad (10)$$

$$L_\infty = \max |C_i^{\text{exact}} - C_i^{\text{numerical}}| \quad (11)$$

Example 1. The first case is the pure advection equation, which was studied by [20] using a compact finite difference method. The domain is considered an infinitely 9000 m long channel with a constant cross section and bottom slope. The parameters are velocity (U) = 0.5 m/s, Gaussian distribution of ρ , and initial peak location $x_0 = 2000$ m. The initial distribution of pollutants is transported downstream in a regular long channel over a simulation time of 9600 s. This straight channel is simulated by dividing it into 360 elements ($\Delta x = 25$), similar to that in a previous study [20]. The case is simulated with the following boundary condition:

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

$$-D \frac{\partial C}{\partial x}(9000,t) = 0 \quad (13)$$

The initial condition can be taken from the exact solution below

$$C(x,t) = 10 \exp\left(-\frac{(x-x_0-Ut)^2}{2\rho^2}\right) \quad (14)$$

The result obtained by numerical simulation without a numerical filter is greater than the exact solution (Table 1). However, after the numerical filter is applied, the numerical simulation result is similar to the exact solution.

The previous study conducted the simulation by using several methods and found that the sixth-order compact finite difference (CD6) method gives better results than other finite difference and finite element methods, with a norm error (L_2 and L_∞) of 0.0029 and 0.0007 respectively. Compared with the previous results, the norm error value of simulations in this study is still greater than the CD6 error for $\Delta x = 25$.

Example 2. The second case is the advection–diffusion case, with velocity (U) = 0.01 m/s and $D = 0.002$ m²/s. The channel has a length (L) = 100 m and is divided into 100 uniform elements ($\Delta x = 1$ m). The initial condition is taken from the exact solution below.

$$C(x,t) = \frac{1}{2} \operatorname{erfc}\left(\frac{x-Ut}{\sqrt{4Dt}}\right) + \frac{1}{2} \exp\left(\frac{Ux}{D}\right) \operatorname{erfc}\left(\frac{x+Ut}{\sqrt{4Dt}}\right) \quad (15)$$

Table 1. Example 1 Numerical and Exact Solution

Method	Peak Concentration (mg/L)	L_2	L_∞
Exact	10.0000		
FTCS	10.9377	4.06164	1.12127
FTCS with Filter	9.9715	1.63218	0.39256

Figure 2. Example 1 Result

The boundary conditions for the simulation are

$$C(0,t) = 1 \quad (16)$$

$$-D \frac{\partial C}{\partial x}(L,t) = 0 \quad (17)$$

The simulation shows that the numerical model with the additional filter gives a similar result as the exact solution unlike the numerical simulation without filter (Figure 3). The previous results obtained by using the CD6 scheme have excellent agreement with the exact solution. Yet, a few differences remain between the numerical and exact solutions if FTCS is used.

Table 2. Example 2 Comparison between Exact and Numerical Solution

Distance (m)	Concentration (mg/L)			Distance (m)	Concentration (mg/L)		
	Exact	FTCS	FTCS with Filter		Exact	FTCS	FTCS with Filter
0	1.000	1.000	1.000	30	0.523	0.464	0.481
18	1.000	0.997	0.999	31	0.408	0.352	0.377
19	0.999	0.997	1.001	32	0.301	0.255	0.284
20	0.998	1.000	1.003	33	0.208	0.177	0.206
21	0.996	1.008	1.006	34	0.135	0.118	0.144
22	0.991	1.017	1.007	35	0.082	0.075	0.097
23	0.982	1.021	1.000	36	0.046	0.046	0.063
24	0.964	1.009	0.980	37	0.024	0.027	0.039
25	0.934	0.975	0.941	38	0.012	0.016	0.024
26	0.889	0.911	0.880	39	0.005	0.009	0.014
27	0.823	0.821	0.798	40	0.002	0.005	0.008
28	0.738	0.709	0.700	41	0.001	0.002	0.004
29	0.636	0.587	0.591	42	0.000	0.001	0.002
L ₂ Norm Error					0.14124 0.09647		
L _∞ Norm Error					0.05874 0.04481

Figure 3. Example 2 Result

Example 3. The third case is about a one-dimensional Gaussian pulse. $U = 0.8$ m/s and $D = 0.005$ m²/s are set. The exact solution is

$$C(x,t) = \frac{1}{\sqrt{4t+1}} \exp\left(-\frac{(x-1-Ut)^2}{D(4t+1)}\right) \quad (18)$$

Then, the boundary conditions of this case are

$$C(0,t) = \frac{1}{\sqrt{4t+1}} \exp\left(-\frac{(1-Ut)^2}{D(4t+1)}\right) \quad (19)$$

$$C(9,t) = \frac{1}{\sqrt{4t+1}} \exp\left(-\frac{(8-Ut)^2}{D(4t+1)}\right) \quad (20)$$

The Gaussian pulse distribution is simulated for $t = 5$ s. On the basis of the simulation, the same result as that of examples 1 and 2 is obtained. The numerical simulation without filter obtains a greater result than the exact solution. When the numerical filter is applied, the numerical simulation has a similar result as the exact solution. However, the previous study still had better results because it used a higher-order finite difference method.

Figure 4. Example 3 Result

Table 3. Example 3 Comparison of Exact and Numerical Solution

Distance (m)	Concentration (mg/L)			Absolute Error	
	Exact	FTCS	FTCS with Filter	FTCS	FTCS with Filter
3.5	0.000000	0.000000	0.000000	1.02E-10	6.66E-11
4.0	0.000016	0.000005	0.000012	1.05E-05	3.61E-06
4.5	0.020177	0.016903	0.019893	3.27E-03	2.84E-04
5.0	0.218218	0.227036	0.218222	8.82E-03	3.70E-06
5.5	0.020177	0.017583	0.020448	2.59E-03	2.71E-04
6.0	0.000016	0.000010	0.000020	5.65E-06	4.39E-06
6.5	0.000000	0.000000	0.000000	4.93E-11	1.55E-10

Example 4. The domain of this dimensionless 2D case is $0 < x, y < 2$ with the velocity 0.8 for the x- and y-directions. The initial condition is Gaussian pulse, which is located at (0.5, 0.5) with a pulse height of 1. It is presented by using Equation (21).

$$C(x,y,0) = \exp\left(-\frac{(x-0.5)^2}{D_x} - \frac{(y-0.5)^2}{D_y}\right) \quad (21)$$

The appropriate boundary condition can be obtained from the exact solution. The exact solution is given by [22] by considering

$$C(x,y,t) = \frac{1}{1+4t} \exp\left(-\frac{(x-Ut-0.5)^2}{D_x(1+4t)} - \frac{(y-Vt-0.5)^2}{D_y(1+4t)}\right) \quad (22)$$

The parameter of this numerical simulation is taken as $\Delta x = \Delta y = h = 0.025$, $D_x = D_y = 0.01$, and $t = 1.25$ s with $\Delta t = 0.001$. The simulation results are shown in Figures 5 and 6. The result of the numerical simulation is similar to that of the analytic (exact) solution. The contour of the concentration (Figure 6) shows that a good agreement exists between the numerical and analytic solutions.

The numerical simulation, which is conducted by adding a filter to the FTCS scheme, gives a smaller absolute error than a numerical simulation without a filter. This numerical filter is similar to the moving average principle. Consequently, if the filter is overused, then the model will return a uniform value for the corresponding parameter.

Table 4. Pulse Height of Analytical and Numerical Solution

Method	Analytical	FTCS with Filter	FTCS
Peak Height	0.166667	0.167725	0.171315
Absolute Error		0.001058	0.004648

Figure 5. 2D Simulation Result

Figure 6. Concentration Contour

4. Conclusions

In this study, the numerical model for pollutant transport cases is developed. The model deals with the advection-diffusion equation by using FTCS scheme. Results show that this simple scheme can simulate 1D and 2D cases and return a similar result with the exact solution. Then, a numerical filter is applied to increase the model stability. The results are better than those of the numerical simulation without a numerical filter.

However, the overall results of these simulations still have greater errors than those of the previous study. Thus, sensitivity analysis and implementation in other cases are required to further verify this developed model by simulating a real case of pollutant transport as either a 1D or a 2D problem.

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