

Numerical Simulation of Effects of Velocity and Diffusion Coefficient on Concentration of Contaminants in the Fluid Flow

K. Langat, J. Shichikha, and J. Bitok

Abstract — The study developed and implemented Implicit and explicit schemes for solving convection –diffusion equation in one dimension on concentration of contaminant in a fluid flow. The stability of the scheme was analyzed and the accuracy of the solution of the contaminant transport equation was validated by exact available solution. Graphical presentation of the solution for varying velocity and diffusion coefficient was given. The explicit method (EM) involved one unknown on left hand side (LHS) while implicit method (IM) involved several unknowns on LHS. The study analyzed the effect of velocity and diffusion coefficient on concentration of contaminant in a fluid flow. The developed schemes were solved numerically using MATLAB to generate the result and in analysis of results. Results showed that concentration of contaminants increased inversely with velocity and directly to diffusion coefficient. Therefore, for proper treatment of water for example, it is necessary to reduce the flow velocities to reduce the trend of contaminants. As Velocity increases the concentration of contaminant decreases and as diffusion coefficient increases the concentration of contaminant increases.

Keywords — diffusion coefficient, explicit method, implicit backward method, velocity.

I. INTRODUCTION

A. Background Information

Numerical simulations of partial differential equations have a great significant in environmentalists, hydrologist and mathematical modelers in a real life application process are required to address current situation and problem solving approaches in science and engineering. The application process of simulating this equation by numerical discretization method for example finite difference method (FDM) become a greater point of concern due to time and computation consuming on complexity of the method used to solve convection-diffusion equation. The convection-diffusion equation (CDE) is a parabolic partial differential equation combining the diffusion equation and advection equation. Most problem on CDE occur frequently in transport of a ground water pollutants where mass, momentum and heat are fundamental transfer phenomena in the universe and inside a physical system due to two processes namely diffusion and convection whereby diffusion is the movement of particles spread from a region of high concentration to a region of low concentration and convection is the movement

of particles within fluids due to physical movement of particles. To study the effects of velocity and diffusion coefficient on the concentration contaminant through porous medium by numerically solving the parabolic partial differential equation using finite difference approximation (FDA). Pollutants are unwanted materials in a substance that can cause harm to human health and contaminants are inputs of alien and potentially toxic substances into the environment for example untreated sewage discharge. Authors used various methods to solve CDE, for example, Rizwan [1] used second order space with time Nodal method, Dehghan [2] used new fourth-order explicit formula and Perez used change of valuable and integral transform technique to generated analytical solution with constant coefficient. None of them analyzed the effects of velocity and diffusion coefficient using implicit method and explicit method

B. Mathematical model of CDE

The mathematical model consider one dimension time dependent convection-diffusion equation with velocity and diffusion coefficient are two parents to be investigated and with assumption that the constant velocity and diffusion coefficient are positive, for a general scalar variable and subjected to appropriate initial and Dirichlet boundary condition is given as:

$$C_t + \mu C_x = DC_{xx} \quad 0 \leq x \leq L, \quad 0 \leq t \leq T \quad (1)$$

with initial conditions:

$$C(x, 0) = f(x) = \exp \left[\frac{-(x-2)^2}{80D} \right] \quad 0 \leq x \leq L \quad (2)$$

and Dirichlet boundary conditions.

Left boundary condition:

$$C(0, t) = g_o(t) = \sqrt{\frac{20}{t+20}} \exp \left[\frac{-(2+\mu t)^2}{4D(t+20)} \right] \quad 0 \leq t \leq T \quad (3)$$

Right boundary condition:

$$C(1, t) = g_L(t) = \sqrt{\frac{20}{t+20}} \exp \left[\frac{-(1+\mu t)^2}{4D(t+20)} \right] \quad 0 \leq t \leq T \quad (4)$$

where the function f , $g_o(t)$ and $g_L(t)$ are known. The function values of $C(x, t)$ are to be determined and used to

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validate the methods used with the assumption that the constants μ and D are positive and parameters to be investigated

Dehghan [2] solves (1) with new fourth-order explicit formula to obtain analytical solution.

C. Numerical Schemes

The section presents the formulation of the three numerical schemes to CDE using FDM

1) Scheme 1: Implicit Backward Euler method

A difference schemes is implicit if the several unknown values can be expressed in terms of the known values. Generally, we can express Crank-Nicolson method that space derivative is averaged.

$$\frac{c_{i,j+1} - c_{i,j}}{\Delta t} = \frac{D}{2} \left(\frac{u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}}{\Delta x^2} + \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} \right) + \frac{u}{2} \left(\frac{c_{i+1,j+1} - c_{i-1,j+1}}{\Delta x^2} + \frac{c_{i+1,j} - c_{i-1,j}}{\Delta x^2} \right) \quad (5)$$

2) Explicit scheme

A difference scheme is explicit if one unknown value can be expressed in terms of the known values.

$$\frac{c_{i,j+1} - c_{i,j}}{\Delta t} + \mu \left(\frac{c_{i,j+1} - c_{i-1,j}}{\Delta x} \right) = D \left(\frac{c_{i+1,j+1} - 2c_{i,j+1} + c_{i-1,j+1}}{\Delta x^2} \right) \quad (6)$$

II. METHOD OF SOLUTION

A. Implicit Backward Euler Method

The Implicit Backward Euler method is the best method because of its unconditionally stable. The stability condition was derived by Mehdi [3] stability is ratio between the mesh sizes Δx and Δt beyond which the schemes will not hold.

Replacing (1) with partial derivative forward in t , forward in x and central in x :

$$\frac{C_i^k - C_i^{k-1}}{\Delta t} = \frac{-\mu(C_{i+1}^k - C_{i-1}^k)}{2\Delta x} + \frac{D(C_{i-1}^k - 2C_i^k + C_{i+1}^k)}{(\Delta x)^2} \quad (7)$$

where k is variable of time and i is variable in x .

Multiply equation (7) on both sides by Δt :

$$C_i^k - C_i^{k-1} = \frac{-\mu \Delta t (C_{i+1}^k - C_{i-1}^k)}{2\Delta x} + D \Delta t \left(\frac{C_{i-1}^k - 2C_i^k + C_{i+1}^k}{(\Delta x)^2} \right) \quad (8)$$

$$C_i^k - C_i^{k-1} = \frac{-\mu \Delta t}{2\Delta x} (C_{i+1}^k - C_{i-1}^k) + \frac{D \Delta t}{(\Delta x)^2} (C_{i-1}^k - 2C_i^k + C_{i+1}^k) \quad (9)$$

We define $\alpha = \frac{\mu \Delta t}{2\Delta x}$, $\beta = \frac{D \Delta t}{(\Delta x)^2}$ and β are stability ratios. Replacing α and β in equation (9) gives:

$$C_i^k - C_i^{k-1} = -\alpha (C_{i+1}^k - C_{i-1}^k) + \beta (C_{i-1}^k - 2C_i^k + C_{i+1}^k) \quad (10)$$

$$C_i^k - C_i^{k-1} = -\alpha C_{i+1}^k + \alpha C_{i-1}^k + \beta C_{i-1}^k - 2\beta C_i^k + \beta C_{i+1}^k \quad (11)$$

$$-C_i^{k-1} = -\alpha C_{i+1}^k + \alpha C_{i-1}^k + \beta C_{i-1}^k - 2\beta C_i^k + \beta C_{i+1}^k - C_i^k \quad (12)$$

Dividing (12) on both side by negative, we have:

$$C_i^{k-1} = \alpha C_{i+1}^k - \alpha C_{i-1}^k - \beta C_{i-1}^k + 2\beta C_i^k - \beta C_{i+1}^k + C_i^k \quad (13)$$

$$C_i^{k-1} = -\alpha C_{i-1}^k - \beta C_{i-1}^k + C_i^k + 2\beta C_i^k + \alpha C_{i+1}^k - \beta C_{i+1}^k \quad (14)$$

$$C_i^k - C_i^{k-1} = \frac{-\mu \Delta t}{2\Delta x} (C_{i+1}^k - C_{i-1}^k) + \frac{D \Delta t}{(\Delta x)^2} (C_{i-1}^k - 2C_i^k + C_{i+1}^k) \quad (15)$$

We define $\alpha = \frac{\mu \Delta t}{2\Delta x}$, $\beta = \frac{D \Delta t}{(\Delta x)^2}$ and β are stability ratios. Replacing α and β in (9) gives:

$$C_i^k - C_i^{k-1} = -\alpha (C_{i+1}^k - C_{i-1}^k) + \beta (C_{i-1}^k - 2C_i^k + C_{i+1}^k) \quad (16)$$

$$C_i^k - C_i^{k-1} = -\alpha C_{i+1}^k + \alpha C_{i-1}^k + \beta C_{i-1}^k - 2\beta C_i^k + \beta C_{i+1}^k \quad (17)$$

$$C_i^k - C_i^{k-1} = \frac{-\mu \Delta t}{2\Delta x} (C_{i+1}^k - C_{i-1}^k) + \frac{D \Delta t}{(\Delta x)^2} (C_{i-1}^k - 2C_i^k + C_{i+1}^k) \quad (18)$$

We define $\alpha = \frac{\mu \Delta t}{2\Delta x}$, $\beta = \frac{D \Delta t}{(\Delta x)^2}$ and β are stability ratios. Replacing α and β in (9) gives:

$$C_i^k - C_i^{k-1} = -\alpha (C_{i+1}^k - C_{i-1}^k) + \beta (C_{i-1}^k - 2C_i^k + C_{i+1}^k) \quad (19)$$

$$C_i^k - C_i^{k-1} = -\alpha C_{i+1}^k + \alpha C_{i-1}^k + \beta C_{i-1}^k - 2\beta C_i^k + \beta C_{i+1}^k \quad (20)$$

$$-C_i^{k-1} = -\alpha C_{i+1}^k + \alpha C_{i-1}^k + \beta C_{i-1}^k - 2\beta C_i^k + \beta C_{i+1}^k - C_i^k \quad (21)$$

Dividing (21) on both side by negative, we have:

$$C_i^{k-1} = \alpha C_{i+1}^k - \alpha C_{i-1}^k - \beta C_{i-1}^k + 2\beta C_i^k - \beta C_{i+1}^k + C_i^k \quad (22)$$

$$C_i^{k-1} = -\alpha C_{i-1}^k - \beta C_{i-1}^k + C_i^k + 2\beta C_i^k + \alpha C_{i+1}^k - \beta C_{i+1}^k \quad (23)$$

Re-arranging equation (23) we get:

$$C_i^{k-1} = -(\alpha + \beta) C_{i-1}^k + (1+2\beta) C_i^k + (\alpha - \beta) C_{i+1}^k \quad (24)$$

$$-C_i^{k-1} = -\alpha C_{i+1}^k + \alpha C_{i-1}^k + \beta C_{i-1}^k - 2\beta C_i^k + \beta C_{i+1}^k - C_i^k \quad (25)$$

Dividing (25) on both side by negative, we have:

$$C_i^{k-1} = \alpha C_{i+1}^k - \alpha C_{i-1}^k - \beta C_{i-1}^k + 2\beta C_i^k - \beta C_{i+1}^k + C_i^k \quad (26)$$

$$C_i^{k-1} = -\alpha C_{i-1}^k - \beta C_{i-1}^k + C_i^k + 2\beta C_i^k + \alpha C_{i+1}^k - \beta C_{i+1}^k \quad (27)$$

Re-arranging (27) we get:

$$C_i^{k-1} = -(\alpha + \beta) C_{i-1}^k + (1+2\beta) C_i^k + (\alpha - \beta) C_{i+1}^k \quad (28)$$

B. Explicit Method (EM)

The unknown $C_{i,j+1}$ is on the LHS alone and the knowns are on the RHS.

By discretizing the PDE in (1) approximated by the FDA as:

$$\frac{C_{i,j+1}-C_{i,j}}{\Delta t} + \mu \frac{(C_{i-1,j}-C_{i+1,j})}{2\Delta x} = \frac{D(C_{i-1,j}-2C_{i,j}+C_{i+1,j})}{(\Delta x)^2} \quad (29)$$

Multiply (29) on both sides by Δt :

$$C_{i,j+1} - C_{i,j} + \mu \Delta t \frac{(C_{i-1,j}-C_{i+1,j})}{2\Delta x} = \frac{D\Delta t(C_{i-1,j}-2C_{i,j}+C_{i+1,j})}{(\Delta x)^2} \quad (30)$$

$$C_{i,j+1} - C_{i,j} = \frac{\mu \Delta t}{2\Delta x} (C_{i-1,j} - C_{i+1,j}) + \frac{D\Delta t}{(\Delta x)^2} (C_{i-1,j} - 2C_{i,j} + C_{i+1,j}) \quad (31)$$

$$C_{i,j+1} = \frac{\mu \Delta t}{2\Delta x} (C_{i-1,j} - C_{i+1,j}) + \frac{D\Delta t}{(\Delta x)^2} (C_{i-1,j} - 2C_{i,j} + C_{i+1,j}) + C_{i,j} \quad (32)$$

We define $r_1 = \frac{\mu \Delta t}{2\Delta x}$, $r_2 = \frac{D\Delta t}{(\Delta x)^2}$ and r_2 are stability ratios; Replacing (32) with stability ratios gives:

$$C_{i,j+1} = -r_1 (C_{i-1,j} - C_{i+1,j}) + r_2 (C_{i-1,j} - 2C_{i,j} + C_{i+1,j}) + C_{i,j} \quad (33)$$

$$C_{i,j+1} = -r_1 C_{i-1,j} + r_1 C_{i+1,j} + r_2 C_{i-1,j} - 2r_2 C_{i,j} + r_2 C_{i+1,j} + C_{i,j} \quad (34)$$

$$C_{i,j+1} = -r_1 C_{i-1,j} + r_2 C_{i-1,j} + C_{i,j} - 2r_2 C_{i,j} + r_1 C_{i+1,j} + r_2 C_{i+1,j} \quad (35)$$

Re-arranging (35) we get:

$$C_{i,j+1} = (r_2 - r_1)C_{i-1,j} + (1 - 2r_2)C_{i,j} + (r_1 + r_2)C_{i+1,j} \quad (36)$$

as the numerical scheme.

Hindmarsh [4] and Sousa [5] showed that the condition for stability is:

$$\frac{2D\Delta t}{(\Delta x)^2} \leq 1 \text{ and } \left(\frac{\mu \Delta t}{\Delta x}\right)^2 \leq \frac{2D\Delta t}{(\Delta x)^2}$$

$$r_1 = 0.2, r_2 = 0.5, \Delta t = 0.05, \Delta x \leq 0.1$$

where D and μ are varied to study effect of concentration of contaminants.

III. RESULTS

The data of numerical schemes presented in Table I and II for objective one: To analyze the effect of velocity on the concentration of contaminant are obtained from (15) and (36) respectively for analysis.

TABLE I: IMPLICIT VALUES OF C(x, t); D=0.1, T=1

Length x (m)	Concentration C(x, t)		
	Velocity μ (m/s)		
	0.8	0.9	1.0
0	0.3838	0.3586	0.3343
0.1	0.4098	0.3839	0.3587
0.2	0.4366	0.4099	0.384
0.3	0.4640	0.4367	0.4100
0.4	0.4919	0.4641	0.4368
0.5	0.5202	0.4919	0.4642
0.6	0.5488	0.5203	0.4921
0.7	0.5776	0.5489	0.5203
0.8	0.6064	0.5776	0.5489
0.9	0.6352	0.6064	0.5776
1	0.6636	0.6350	0.6062

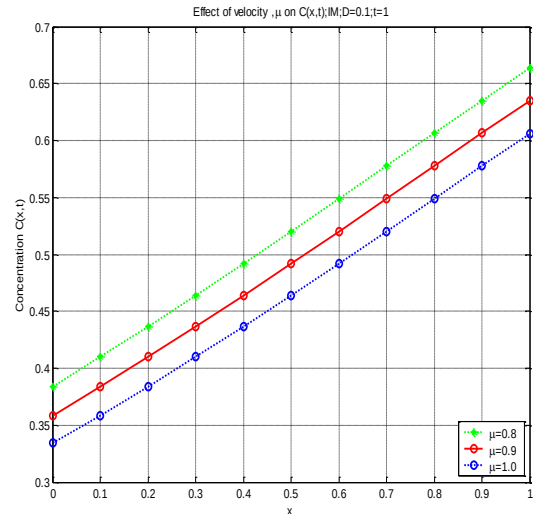


Fig. 1. Implicit analysis.

Fig. 1 of implicit values of concentration above clearly shows there is general linear increase of concentration with distance and also with respect with time. As velocity increases from 0.9 to 1.0 the concentration of contaminant decreases. The rate of increase of concentration are nearly the same, take at $x = 0.1$ m the difference rate of concentration of contaminant is 0.025(3dp).

TABLE II: EXPLICIT VALUES OF C(x, t); D=0.1; T=1

x	$\mu=0.8$	$\mu=0.9$	$\mu=1.0$
0	0.5764	0.5794	0.5824
0.1	0.6578	0.6549	0.6521
0.2	0.6952	0.6922	0.6892
0.3	0.7254	0.7225	0.7195
0.4	0.7540	0.7512	0.7483
0.5	0.7816	0.7789	0.7762
0.6	0.8079	0.8054	0.8028
0.7	0.8319	0.8298	0.8276
0.8	0.8513	0.8500	0.8486
0.9	0.8616	0.8619	0.8620
1	0.8581	0.8605	0.8628

Fig. 2 of explicit values of concentration above clearly shows there is general linear increase of concentration with distance and also with respect with time. As velocity increases from 0.9 to 1.0 the concentration of contaminant decreases. The rate of increase of concentration are nearly the same. The effect of velocity was notes after amplification of results.

The data of numerical schemes presented in Table III and IV for objective two: to analyze the effect of diffusion coefficient on the concentration of contaminant are obtained from (15) and (36) respectively for analysis.

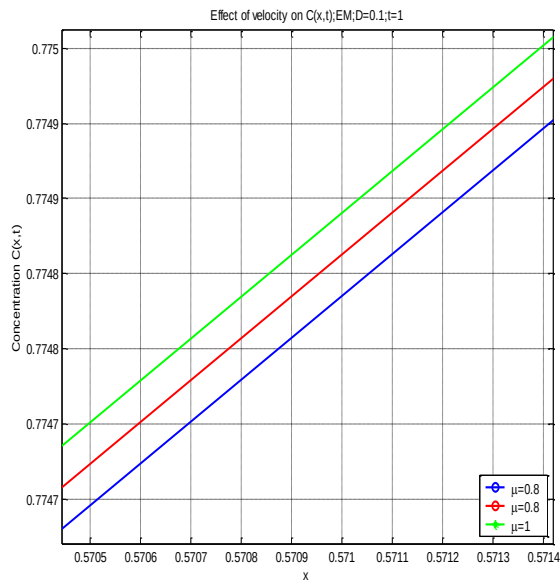


Fig. 2. Explicit analysis.

x	D=0.1	D=0.2	D=0.3
0	0.3838	0.715	0.612
0.1	0.4098	0.7307	0.6324
0.2	0.4366	0.7463	0.6526
0.3	0.464	0.7615	0.6727
0.4	0.4919	0.7765	0.6926
0.5	0.5202	0.7911	0.7123
0.6	0.5488	0.8053	0.7316
0.7	0.5776	0.8192	0.7506
0.8	0.6064	0.8326	0.7691
0.9	0.6352	0.8456	0.7872
1	0.6636	0.8582	0.8047

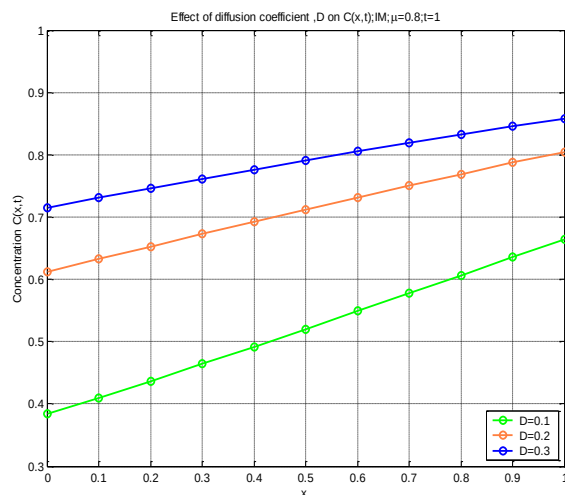


Fig. 3. Implicit analysis.

x	D=0.1	D=0.2	D=0.3
0	0.6041	0.7771	0.8452
0.1	0.6391	0.7992	0.861
0.2	0.6693	0.818	0.8746
0.3	0.6991	0.836	0.8874
0.4	0.7284	0.8534	0.8996
0.5	0.757	0.87	0.9112
0.6	0.7848	0.8858	0.9222
0.7	0.8116	0.9007	0.9326
0.8	0.8371	0.9148	0.9423
0.9	0.8611	0.9278	0.9511
1	0.8806	0.9383	0.9583

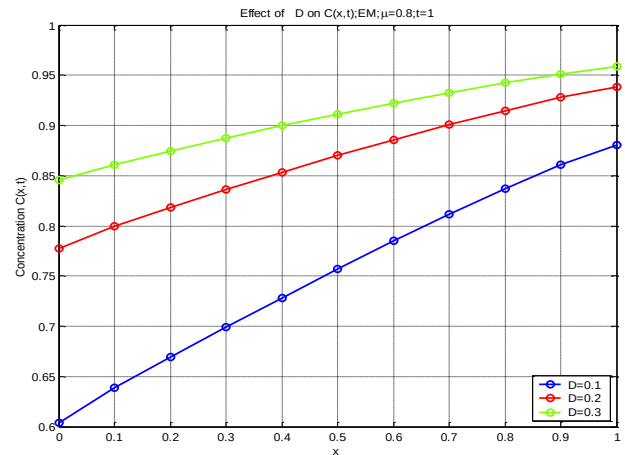


Fig. 4. Explicit analysis.

Fig. 3 of implicit values of concentration above clearly shows there is linear increase of concentration with distance and also with respect with time. As D increases from 0.1 to 0.3 the concentration of contaminant increases. The rate of increase of concentration at $D=0.1$ is sharp compare when the $D=0.2, 0.3$.

Fig. 4 of explicit values of concentration above clearly shows there is linear increase of concentration with distance and also with respect with time. As D increases from 0.1 to 0.3 the concentration of contaminant increases. The effect of D was notes after amplification of results.

IV. DISCUSSION AND CONCLUSION

A. Conclusion

The study has successfully developed and implemented the numerical simulations using Implicit Backward Euler method (IM) and explicit method (EM) schemes from FDM. The schemes proved to satisfy the stability ratio, r , must fall within a certain range for the scheme to be useful.

$$\frac{2D\Delta t}{(\Delta x)^2} \leq 1 \text{ and } \left(\frac{\mu\Delta t}{\Delta x}\right)^2 \leq \frac{2D\Delta t}{(\Delta x)^2} \quad [4], [5]$$

Generally, the methods showed the following effects:

- (i) As the velocity of the flow increases the concentration of the contaminants decreases.
- (ii) As the diffusion coefficient increases the concentration of contaminants increases.

LIST OF ABBREVIATIONS, ACRONYMS AND SYMBOLS

PDE	Partial Differential Equation
EM	Explicit method
FDA	Finite Difference Approximation
CNM	Crank-Nicolson method
$C(x, t)$	Concentration (dependent variable)
1D	One Dimensional
μ	Velocity of flow
ICs	Initial conditions
D	Diffusion constant
C_x	First spatial derivative of concentration
C_{xx}	Second spatial derivative of concentration
C_t	ime derivative of concentration

T	Time of flow (independent variable) in second
BCs	Boundary condition
L	Length of channel (independent variable) in meters
RHS	Right hand side
CDE	Convection-Diffusion Equation
LHS	Left hand side
α	courant constant
MATLAB	Matrix Laboratory
$\beta, r_1, r_2, r_3, r_4$	ratio of stability
IM	Implicit Method

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