

Consistency And Stability Analysis of a Mathematical Model of Chlorine Concentration in Contact Tanks Using Numerical Solution of A 1- Dimensional Convection-Diffusion Equation

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Abstract- In this paper we consider the consistency and stability analysis of the modified convection diffusion equation: $u_t + mu_x - n_L u_{xx} = 0$, which describes the mass transfer of chlorine in contact tank water disinfectant. We employ the concept of Dufort-Frankel based on Richardson's scheme to discretize the modified equation. This resulted to a numerical scheme algorithm. The consistency was analyzed by Taylor's expansion of the discretized scheme, which was found to be consistent with the original modified equation. In addition, stability was analyzed by using matrix method. The numerical computation results showed that the scheme was conditionally stable. This has been concluded by numerical computations to illustrate the consistence and stability of the scheme.

Indexed Terms- Consistency analysis, Coupled convection-diffusion equation, discretized schemes, stability analysis.

I. INTRODUCTION

Lack of access to clean and safe water remains a worldwide problem as in [1]. Disinfection is done to ensure water is of a safe quality for consumption. The study was focused on chlorination as the method of disinfection, since it's cheaper and more effective against a vast range of pathogens. However, there was arising concerns about chlorine disinfection by-products during the process of chlorination as in [3]. Studies done by Villanueva *et al.* [6] showed that there is a risk to diseases for those exposed to chlorine disinfection by-products. Therefore, the study focused

on chlorination of water in contact tanks before the distribution.

Convection-diffusion equation is a parabolic equation which was derived based on Fick's 1st law as in the study of Mudde and Akker, [4s]. The study modified the equation to incorporate the characteristic length of diffusion denoted by "L" in the equation: $u_t + mu_x - n_L u_{xx} = 0$, which represented the model of the physical phenomena in the contact tank. Before the discretized numerical scheme could be used to generate the solution, consistency and stability of the scheme was analysed.

II. EQUATION MODIFICATION

$$u_t - nu_{xx} = 0 \quad (2.1)$$

$$u_t + mu_x = 0 \quad (2.2)$$

$$u_t + mu_x - nu_{xx} = 0 \quad (2.3)$$

$$u_t + mu_x - n_L u_{xx} = 0 \quad (2.4)$$

Equations 2.1, 2.2, 2.3, 2.4 shows the diffusion, convection, coupled convection-diffusion and the modified convection-diffusion equations respectively. On the whole line of $-\infty < x < +\infty$, the flow and the diffusion don't interact. For the velocity m, the convection carries along the diffusion solution. Hence, the coupling of the convection and diffusion equations.

III. DUFORT-FRANKEL SCHEME

Richardson's scheme involves three-time levels $i-1$, (i) and $i+1$. Modification of this method by replacing $u_{i,j}$ with $\frac{u_{i,j+1} - u_{i,j-1}}{2}$ in finite difference of the space derivative in Richardson's scheme. This results to a 3-level explicit Dufort-Frankel scheme which is conditionally stable.

IV. DISCRETIZATION

Assuming u is smooth, partially differentiable and bounded i.e $-\infty < u < +\infty$. The paper replaced:

(i) $u_t = \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta t}$ central difference in time.

(ii) $u_x = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x}$ central difference in space.

(iii) $u_{xx} = \frac{u_{i+1,j} - u_{i,j+1} + u_{i,j-1} + u_{i-1,j}}{\Delta x^2}$ spatial

coupled with time derivative.

Setting $\Delta x = h$, $\Delta t = k$, the equation (2.4) then becomes:

$$\frac{1}{2k} \{u_{i,j+1} - u_{i,j-1}\} + \frac{m}{2h} \{u_{i+1,j} - u_{i-1,j}\} - \frac{n_L}{h^2} \{u_{i+1,j} - u_{i,j+1} - u_{i,j-1} + u_{i-1,j}\} = 0 \quad (2.41)$$

Multiplying through by $2k$ and letting $r = \frac{kn_L}{h^2}$, b

$$= \frac{2km}{2h}. \text{ The equation (2.41) then results to:}$$

$$u_{i,j+1} + u_{i,j-1} = 2ru_{i+1,j} - 2ru_{i-1,j} \quad (2.42)$$

$$-2ru_{i,j+1} + 2ru_{i,j-1} - bu_{i+1,j} + bu_{i-1,j}$$

$$(1+2r)u_{i,j+1} = (2r-b)u_{i+1,j} + (2r+b)u_{i-1,j} \quad (2.43)$$

$$+ (1-2r)u_{i,j-1} + 2ru_{i-1,j} \\ (1+2r)u_{i,j+1} = 4r(u_{i+1,j} + u_{i-1,j}) + (1-2r)u_{i,j-1} \quad (2.44)$$

Equation (2.44) is the algorithm used in this paper. Using the initial condition: $u_t = 0$, $u_{i,j+1} = u_{i,j-1}$ for central difference in time. Hence, $u_{i,1} = u_{i,-1}$ for all (I's).

Setting $j = 0, i = 1, 2, 3 \dots 9$ into the algorithm

(i) $j = 0, i = 1: 4ru_{1,1} = 4ru_{2,0} + 4ru_{0,0}$

(ii) $j = 0, i = 2: 4ru_{2,1} = 4ru_{3,0} + 4ru_{1,0}$

⋮

(ix) $j = 0, i = 9: 4ru_{9,1} = 4ru_{10,0} + 4ru_{8,0}$

This resulted to a $M_{(N-1) \text{ by } (N-1)}$ represented as:

$$\begin{pmatrix} a_{1,1} & \dots & a_{1,8} \\ \vdots & \ddots & \vdots \\ a_{8,1} & \dots & a_{8,8} \end{pmatrix}$$

where $a_{1,1}, a_{8,8} = 4r$ while other elements of the matrix = 0.

$$(u_{1,1}, u_{2,1} \dots u_{8,1})^T$$

$((4ru_{2,0} + 4ru_{0,0}) \dots (4ru_{9,0} + 4ru_{7,0}))^T$. The algorithm was then represented as

$$\begin{pmatrix} a_{1,1} & \dots & a_{1,8} \\ \vdots & \ddots & \vdots \\ a_{8,1} & \dots & a_{8,8} \end{pmatrix} (u_{1,1}, u_{2,1} \dots u_{8,1})^T = ((4ru_{2,0} + 4ru_{0,0}) \dots (4ru_{9,0} + 4ru_{7,0}))^T \quad (2.45)$$

This was computed severally at different i^{th} and j^{th} levels.

V. CONSISTENCY ANALYSIS

By Taylor's series, the following expressions are used to expand equation (2.41) further.

(i) $u_{i,j+1} = u_{i,j} + \frac{\Delta t \partial u}{\partial t} + \frac{\Delta t^2 \partial^2 u}{2! \partial t^2} + \frac{\Delta t^3 \partial^3 u}{3! \partial t^3} + \dots$

(ii) $u_{i,j-1} = u_{i,j} - \frac{\Delta t \partial u}{\partial t} + \frac{\Delta t^2 \partial^2 u}{2! \partial t^2} - \frac{\Delta t^3 \partial^3 u}{3! \partial t^3} + \dots$

(iii)

$$u_{i+1,j} = u_{i,j} + \frac{\partial x \partial u}{\partial x} + \frac{\partial x^2 \partial^2 u}{2! \partial x^2} + \frac{\partial x^3 \partial^3 u}{3! \partial x^3} + \dots$$

$$(iv) u_{i-1,j} = u_{i,j} - \frac{\partial x \partial u}{\partial x} + \frac{\partial x^2 \partial^2 u}{2! \partial x^2} - \frac{\partial x^3 \partial^3 u}{3! \partial x^3} + \dots$$

The paper substituted these into the equation:

$$\frac{1}{2\Delta t} \{u_{i,j+1} - u_{i,j-1}\} + \frac{m}{2\Delta x} \{u_{i+1,j} - u_{i-1,j}\} - \frac{n_L}{(\Delta x)^2} \{u_{i+1,j} - u_{i,j+1} - u_{i,j-1} + u_{i-1,j}\} = 0$$

. This

resulted to:

$$\begin{aligned} & \frac{1}{2\Delta t} \left\{ u_{i,j} + \frac{\partial t \partial u}{\partial t} + \frac{\partial t^2 \partial^2 u}{2! \partial t^2} + \frac{\partial t^3 \partial^3 u}{3! \partial t^3} - \right. \\ & u_{i,j} - \frac{\partial t \partial u}{\partial t} + \frac{\partial t^2 \partial^2 u}{2! \partial t^2} - \frac{\partial t^3 \partial^3 u}{3! \partial t^3} \left. \right\} + \\ & \frac{m}{2\Delta x} \left\{ u_{i,j} + \frac{\partial x \partial u}{\partial x} + \frac{\partial x^2 \partial^2 u}{2! \partial x^2} + \frac{\partial x^3 \partial^3 u}{3! \partial x^3} \right. \\ & \left. - u_{i,j} - \frac{\partial x \partial u}{\partial x} + \frac{\partial x^2 \partial^2 u}{2! \partial x^2} - \frac{\partial x^3 \partial^3 u}{3! \partial x^3} \right\} \\ & = \frac{n_L}{(\Delta x)^2} \left\{ u_{i,j} + \frac{\partial x \partial u}{\partial x} + \frac{\partial x^2 \partial^2 u}{2! \partial x^2} \right. \\ & + \frac{\partial x^3 \partial^3 u}{3! \partial x^3} - u_{i,j} + \frac{\partial t \partial u}{\partial t} + \frac{\partial t^2 \partial^2 u}{2! \partial t^2} + \frac{\partial t^3 \partial^3 u}{3! \partial t^3} \\ & - u_{i,j} - \frac{\partial t \partial u}{\partial t} + \frac{\partial t^2 \partial^2 u}{2! \partial t^2} - \frac{\partial t^3 \partial^3 u}{3! \partial t^3} + u_{i,j} \\ & \left. - \frac{\partial x \partial u}{\partial x} + \frac{\partial x^2 \partial^2 u}{2! \partial x^2} - \frac{\partial x^3 \partial^3 u}{3! \partial x^3} \right\} \end{aligned}$$

Through simplification, the paper obtained:

$$\begin{aligned} & \frac{\partial t \partial u}{\partial t} + \frac{\partial t^3 \partial^3 u}{3! \partial t^3} + 2r \frac{\partial t^2 \partial^2 u}{2! \partial t^2} + m \frac{\partial u}{\partial x} + m \frac{\partial x^2 \partial^3 u}{3! \partial x^3} \\ & = 4r \frac{\partial x^2 \partial^2 u}{2! \partial x^2} - \frac{\partial t \partial u}{\partial t} - \frac{\partial t^3 \partial^3 u}{3! \partial t^3} - 2r \frac{\partial t^2 \partial^2 u}{2! \partial t^2} \end{aligned}$$

Then,

$$\begin{aligned} m \frac{\partial u}{\partial x} &= -2 \frac{\partial t \partial u}{\partial t} - \frac{\partial t^3 \partial^3 u}{3! \partial t^3} - r \frac{\partial t^2 \partial^2 u}{\partial t^2} - \\ & m \frac{\partial x^2 \partial^3 u}{3! \partial x^3} + 2r \frac{\partial x^2 \partial^2 u}{\partial x^2} \\ & - \frac{\partial t^3 \partial^3 u}{3! \partial t^3} - 2r \frac{\partial t^2 \partial^2 u}{2! \partial t^2} \end{aligned} \quad (2.46)$$

From $r \Delta x^2 = \Delta t n_L$, we then substitute this into equation (2.46) and simplifying it further by dividing through by $2\Delta t$ to get:

$$\begin{aligned} m \frac{\partial u}{\partial x} &= \frac{\partial u}{\partial t} - \frac{\partial t^2 \partial^3 u}{12! \partial t^3} - r \frac{\partial t \partial^2 u}{2 \partial t^2} - \\ & m \frac{\partial x^2 \partial^3 u}{12 \Delta t \partial x^3} + n_L \frac{\partial^2 u}{\partial x^2} - \frac{\partial t^2 \partial^3 u}{12 \partial t^3} - r \frac{\partial t \partial^2 u}{2 \partial t^2} \end{aligned} \quad (2.47)$$

Rearranging the equation 2.47, we obtained:

$$\begin{aligned} \frac{\partial u}{\partial t} + m \frac{\partial u}{\partial x} - n_L \frac{\partial^2 u}{\partial x^2} &= \\ -r \frac{\partial t \partial^2 u}{\partial t^2} - m \frac{\partial x^2 \partial^3 u}{12 \Delta t \partial x^3} \\ - \frac{\partial t^2 \partial^3 u}{6 \partial t^3} \end{aligned} \quad (2.48)$$

Since the left hand side of equation (2.48) is the convection equation we had initially, it follows that:

$$-r \frac{\partial t \partial^2 u}{\partial t^2} - m \frac{\partial x^2 \partial^3 u}{12 \Delta t \partial x^3} - \frac{\partial t^2 \partial^3 u}{6 \partial t^3} \quad (2.49)$$

as the truncation error (T.E).

Since $\lim_{T.E \rightarrow 0} = 0$, it follows that the scheme is consistent with the original partial differential equation.

VI. STABILITY ANALYSIS

The paper has used matrix method to analyze the stability of the discretize scheme as computed below. From the algorithm equation $(1+2r)u_{i,j+1} = 4r(u_{i+1,j} + u_{i-1,j}) + (1-2r)u_{i,j-1}$ equation (2.44), the paper used known boundary values and $i = 1, 2, 3, \dots, N-1$, the matrix form of equation (2.41) shall be:

$$\begin{aligned} & (1+2r) \left(u_{1,j+1} \cdots u_{N-1,j+1} \right)^T + 4r \\ & \begin{pmatrix} a_{1,1} & \cdots & a_{1,8} \\ \vdots & \ddots & \vdots \\ a_{8,1} & \cdots & a_{8,8} \end{pmatrix} \left(u_{1,j} \cdots u_{N-1,j} \right)^T - (1-2r) \\ & \left(u_{1,j-1} \cdots u_{N-1,j-1} \right)^T = 0 \end{aligned} \quad (2.50).$$

Where,

$$A = \begin{pmatrix} a_{1,1} & \cdots & a_{1,8} \\ \vdots & \ddots & \vdots \\ a_{8,1} & \cdots & a_{8,8} \end{pmatrix}$$

With elements

$$a_{1,2}, a_{2,3}, a_{3,4}, a_{4,5}, a_{5,6}, a_{6,7}, a_{7,8} = -1,$$

$$a_{2,1}, a_{3,2}, a_{4,3}, a_{5,4}, a_{6,5}, a_{7,6}, a_{8,7} = -1$$

while, the remaining elements and $a_{n,n} = 0$.

The eigenvalues is given as:

$$a - 2 + 4 \sin^2 \left(\frac{i\pi}{2N} \right) \quad (2.51)$$

Since the element a in the leading diagonal $= 0$, the eigenvalue equation is given by:

$$-2 + 4 \sin^2 \left(\frac{i\pi}{2N} \right) \quad (2.52).$$

Taking, $\left(u_{1,j+1} \cdots u_{N-1,j+1} \right)^T$, $\left(u_{1,j-1} \cdots u_{N-1,j-1} \right)^T$ and $\left(u_{1,j} \cdots u_{N-1,j} \right)^T$ as:

e_{j+1} , e_{j-1} , and e_j respectively. We then substitute these into equation (2.50) to get:

$$(1+2r)e_{j+1} - (1-2r)e_{j-1} + 4rAe_j = 0 \quad (2.53).$$

Substituting the eigenvalues of matrix A into (2.53), we get:

$$\begin{aligned} & (1+2r)e_{j+1} - (1-2r)e_{j-1} \\ & + 4r \left\{ 2 + 4 \sin^2 \left(\frac{i\pi}{2N} \right) \right\} e_j = 0 \end{aligned}$$

By simplification, we get:

$$\begin{aligned} & (1+2r)e_{j+1} - (1-2r)e_{j-1} \\ & - 8r \left\{ 1 + 2 \sin^2 \left(\frac{i\pi}{2N} \right) \right\} e_j = 0 \end{aligned} \quad (2.54).$$

From, $1 - 2 \sin^2 \theta = \cos 2\theta$, we substitute this into equation (2.54) to get:

$$\begin{aligned} & (1+2r)e_{j+1} - (1-2r)e_{j-1} \\ & - 8r \left\{ \cos 2 \left(\frac{i\pi}{2N} \right) \right\} e_j = 0 \end{aligned} \quad (2.55).$$

Letting $\varphi^2, 1, \varphi$ to be e_{j+1}, e_{j-1}, e_j respectively, equation (2.55) becomes:

$$\begin{aligned} & (1+2r)\varphi^2 - 8r \left\{ \cos 2 \left(\frac{i\pi}{2N} \right) \right\} \varphi \\ & - (1-2r) = 0 \end{aligned} \quad (2.56).$$

Since equation (2.51) is a quadratic equation, it has two roots, it has two roots φ_1 and φ_2 .

For stability, $|\varphi_1| \& |\varphi_2| < 1$. This implies that:

$$\left| \frac{8r \left\{ \cos 2 \left(\frac{i\pi}{2N} \right) \right\}}{(1-2r)} \right| < 2.$$

Multiplying both side of the inequality by $(1-2r)$, we get:

$$8r \left\{ \cos 2 \left(\frac{i\pi}{2N} \right) \right\} < 2(1-2r) \quad (2.57).$$

Dividing through by 2 to simplify equation (2.57), we get:

$$4r \left\{ \cos 2 \left(\frac{i\pi}{2N} \right) \right\} < (1-2r) \quad (2.58)$$

Which is true always as:

$$\left| \left\{ \cos 2\left(\frac{i\pi}{2N}\right) \right\} \right| < 1 \quad (2.59).$$

Hence the scheme is conditionally stable for all values of r .

CONCLUSION

By using Dufort-Frankel scheme based on the Richardson's scheme, the paper successfully discretized the modified convection-diffusion equation by employing the principle of Taylor's series expansion for the approximation of the derivatives of concerned variables. After all these substitutions, the paper obtained the algorithm – equation (2.44). The spatial and time change inside the domain was represented by change in i^{th} and j^{th} levels respectively. The computations in this paper showed that Dufort-Frankel scheme based on the Richardson's scheme is consistent and conditionally stable.

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