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EFFICIENT EXPLICIT NUMERICAL TECHNIQUE FOR MODELING ADVECTION DIFFUSION REACTION FOR A WATER QUALITY MODEL IN AN OPENED UNIFORM FLOW - A 1D PERSPECTIVE

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Abstract

This research paper presents a novel and efficient explicit numerical technique for modeling advection diffusion reactions in an opened uniform flow from a one-dimensional perspective. The proposed hybrid scheme combines the benefits of explicit finite difference schemes, resulting in an accurate and fast solution for the advection-diffusion equation in water stream problems. The effectiveness of the scheme is demonstrated through its successful implementation in the solution of the water quality problems, where the advection-diffusion equation plays a crucial role. The results obtained using this technique show improved accuracy and computational efficiency. Overall, this research offers a valuable contribution to the field of numerical modeling in water quality and provides a useful tool for researchers and practitioners working in the area of approximating the one-dimensional diffusion equation for the measurement of pollutant concentration.

Keywords: Explicit, Finite Difference, One Dimensional Advection Diffusion Equation, Uniform Flow

I. Introduction

The study of partial differential equations has been a major concern in the history of mathematics used in many various fields of science and engineering so the one-dimensional Advection Diffusion Equation is also one of them, having many applications as mathematical models in different areas of science. Such as form transporting, in literature scholars used 1-D (ADRE) as a mathematical model for different applications such as transport, diffusion problems, and many more as in [II, III, V, VI, and VII]. The authors considered the (ADE) in one dimension and simulated numerical results by an explicit (FDM) and finally compared the approximate solution with the exact solution [I].

In [II], authors used one-dimensional (ADE) with Finite difference method (FDM) using spreadsheet simulation (ADESS) with various weighted values in the model, and obtained solutions through Formwart Time Center Space (FTCS), Upwind and Lax-Wendroff schemes along with two examples already existing in literature, results obtained numerically as well as analytically solutions, and found Lax-Wendroff scheme is in good satisfaction with the Exact solution also determined accuracy of model. Authors combined (ADR) equation for a transport problem in which contamination in a porous medium is described, evaluated results by using numerical methods (such as (FDM), (EM) and splitting technique) comparing results with the exact solution, also stability and convergence was under discussion [III].

Authors in [IV] used various two-level explicit and implicit numerical schemes such as Forward Time Center Space scheme (FTCS), Upwind, and Lax-Wendroff and also discussed new numerical techniques for 1-D (ADE), also determined the accuracy, and stability of these schemes. In [V], authors used (ADRE) as a model for an opened uniform flow stream and also determined a non-uniform velocity field using Saulyev's Explicit Scheme with an unconditionally stable method and computed results within three θ values, found for $\theta = 0$ gave a smooth solution compared to the other values.

In this research, the main objective is the successful implementation of an efficient explicit finite difference scheme to approximate the one-dimensional advection diffusion reaction for measurement of the pollutant concentration in open uniform flow stream water. For this purpose, section II describes the mathematical model of 1D (ADRE). Section III presents the numerical techniques to approximate the equation 1D ADRE which includes both the existing schemes and the proposed hybrid scheme. Section IV presents the application of 1D (ADRE) for the flow of stream water with an open right boundary along with three cases to approximate the pollutant concentration. The results and discussion for three cases have been enclosed in section V and finally, the conclusion is presented in section VI.

II. Mathematical Model

Consider the mathematical model describing the transport and diffusion processes as a One-dimensional advection diffusion reaction equation (1D ADRE) [V].

$$\frac{\partial u}{\partial t} + \beta \frac{\partial u}{\partial x} = \alpha \frac{\partial^2 u}{\partial x^2} - Ku \tag{1}$$

Initial condition,

$$u(x, 0) = f(x), \quad 0 \leq x \leq L \tag{2}$$

And boundary conditions

$$u(0, t) = g_0(t), \quad 0 \leq t \leq T \tag{3}$$

$$\left(\frac{\partial u}{\partial x}\right)_{x=L} = g_1(t), \quad 0 \leq t \leq T \tag{4}$$

In equations (1)-(4), $f(x)$, are known. Constants α, β are diffusion, and advection and K are reaction rates respectively. The only u is an unknown numerical solution of differential equation 1D ADRE together with conditions (1)-(4).

III. Numerical Technique

In literature explicit and implicit schemes are available to solve the model problem (1)-(4). The FTCS, Upwind, Lax-Wendroff, and (BTCS), Upwind schemes respectively as in [IV]. We mention some existing explicit with new Hybrid schemes with applications in this section.

Discussion of Few Existing Schemes Present Literature

Three schemes with forward difference quotient for time derivative approximation and first spatial derivative term with a weight ϕ and second order derivative term central difference approximation are [IV] given as

$$\frac{\partial u}{\partial t} = \frac{u_i^{n+1} - u_i^n}{\Delta t} \tag{5}$$

$$\frac{\partial u}{\partial x} = \phi \frac{(u_i^n - u_{i-1}^n)}{\Delta x} + (1-\phi)\frac{(u_{i+1}^n - u_{i-1}^n)}{2\Delta x} \tag{6}$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \tag{7}$$

Putting equations (5) (6) and (7) in (1) yields the following general scheme,

$$u_i^{n+1} = \frac{1}{2}\big(2s + c(1+\phi)\big)u_{i-1}^n + (1 - 2s - c\phi)u_i^n + \frac{1}{2}(2s - c(1-\phi))u_{i+1}^n \tag{8}$$

Where $\mathbf{c} = \boldsymbol{\beta}\frac{\Delta \mathbf{t}}{\Delta \mathbf{x}}$, $\mathbf{s} = \boldsymbol{\alpha}\frac{\Delta \mathbf{t}}{(\Delta \mathbf{x})^2}$ as in [IV]

Substituting $\boldsymbol{\phi} = \mathbf{0}$, $\boldsymbol{\phi} = \mathbf{1}$, $\boldsymbol{\phi} = \boldsymbol{c}$ in (8) yields the Forward Time Center Space scheme (FTCS), Upwind, and Lax Wendorff respectively as in [IV].

Hybrid Scheme

In this scheme, for time derivative approximation we use for forward difference quotient as in (5) and the first-order spatial derivative term $\boldsymbol{\phi} = \boldsymbol{c}$ in equation(6), and second order derivative term as in [VII] is replaced by $\boldsymbol{\theta} = \boldsymbol{s}^{\mathbf{2}}$ are given as;

$$\frac{\partial u}{\partial x} = c\frac{(u_i^n - u_{i-1}^n)}{\Delta x} + (1-c)\frac{(u_{i+1}^n - u_{i-1}^n)}{2\Delta x} \tag{9}$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{s^2}{(\Delta x)^2}\left(u_{i-1}^{n+1} - u_i^{n+1} - u_i^n + u_{i+1}^n\right) + \frac{(1-s^2)}{(\Delta x)^2}\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right) \tag{10}$$

Where $\boldsymbol{\phi}, \boldsymbol{\theta}$are weighted functions

Now, substituting (5), (9) and (10) in (1) yields the following,

$$u_i^{n+1} = \frac{1}{1+s\theta}\begin{bmatrix} \left(\frac{c\phi}{2} - \frac{c}{2} + s\right)u_{i+1}^n + (1 - c\phi - 2s + s\theta)u_i^n \\ + \left(\frac{c\phi}{2} + \frac{c}{2} + s - s\theta\right)u_{i-1}^n + s\theta u_{i-1}^{n+1} \end{bmatrix} \tag{11}$$

IV. Application regarding Flow of Stream Water

In this section, we implement the new explicit schemes (11) in the water stream problem to know the concentration of pollution in the water stream. The problem is taken from [V] and is described as that the pollutant concentration measurement u for a uniform flow stream is aligned with longitudinal distance, length 1.0 (km) along x, and 1 (m) of depth. Wasted water flows into the stream through the plant with pollutant concentration at the discharge point is

$u(0,t) = 2 + sin(t)\ at\ x = 0$ for all $t > 0$ positive.

$u(x,0) = 2 + x(1-x)(mg/L)$ at $t = 0$ at $x = L$

Then opening the right boundary the three cases are under consideration for the different rates of change of pollutants, which are:

Case 1. $\frac{\partial u}{\partial x} = 0$(No rate of change of pollutant concentration.)
Case 2. $\frac{\partial u}{\partial x} = 0.05$(Increase in rate of change of pollutant concentration.)
Case 3. $\frac{\partial u}{\partial x} = -0.05$(Decrease in rate of change of pollutant concentration.)

The numerical approximations of pollutant concentration with these three cases are summarized in tables (1)-(3) respectively and Figure 1.

Table 1 : Pollutant Concentration $u(x,t)$ (kg/m^3) of case 1)

T(sec)/x(km)	0	20	40	60	80	100
0	2.0000	2.1600	2.2400	2.2400	2.1600	2.0000
5	1.0411	2.0877	2.6663	2.1629	2.2005	2.2402
10	1.4560	2.8120	1.8564	1.5382	2.4282	2.3974
15	2.6503	2.3732	1.3204	2.1761	2.3516	1.6649
20	2.9129	1.3997	1.7580	2.5624	1.8087	1.7128
25	1.8676	1.2862	2.5423	2.1430	1.5399	2.1728

Table 2 : Pollutant Concentration $u(x,t)$ (kg/m^3) of case 2)

T(sec)/x(km)	0	20	40	60	80	100
0	2.0000	1.0411	1.4560	2.6503	2.9129	1.8676
5	2.1600	2.0877	2.8120	2.3732	1.3997	1.2862
10	2.2400	2.6663	1.8564	1.3204	1.7580	2.5423
15	2.2400	2.1629	1.5382	2.1761	2.5624	2.1430
20	2.1600	2.2005	2.4282	2.3516	1.8087	1.5399
25	2.0000	2.2406	2.3978	1.6652	1.7132	2.1732

Table 3 : Pollutant Concentration $u(x,t)$ (kg/m^3) of case 3)

T(sec)/x(km)	0	20	40	60	80	100
0	2.0000	1.0411	1.4560	2.6503	2.9129	1.8676
5	2.1600	2.0877	2.8120	2.3732	1.3997	1.2862
10	2.2400	2.6663	1.8564	1.3204	1.7580	2.5423
15	2.2400	2.1629	1.5382	2.1761	2.5624	2.1430
20	2.1600	2.2005	2.4282	2.3516	1.8087	1.5399
25	2.0000	2.2398	2.3971	1.6645	1.7124	2.1724

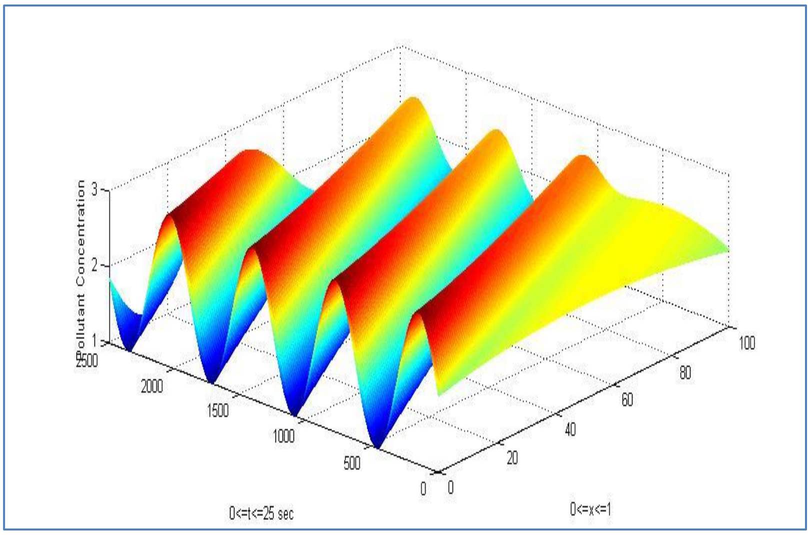

Fig. 1. Pollutant Concentration u(x,t) (kg/m^3) of case 1

V. Results and Discussion

In the research, the new explicit finite difference scheme is implemented to approximate the unknown pollutant concentration with opened right end of the water stream as the application of the one-dimensional advection-diffusion equation.

The tables (1-3) are computed with assumed values of diffusion $\alpha = 0.001$, advection $\beta = 0.1$, and reaction rate *K=0.18*. The spatial step size is h=0.01 and with temporal step size is 0.005. It is clear from these tables provide a better approximation of pollutant concentration along with three cases of small change in the concentration which are effects of the rate of change in concentration at opened right end.

Figure-1 is captured with step size *h=0.01* in spatial variable *x* and *k = 0.01* step size in temporal variable t. Figure-1 well summarized the transport of pollutant concentration in water stream flow at opened right end of case 1 along with these step sizes overall (25 seconds). All the results are in good agreement with work as in [V].

VI. Conclusion

In this paper, an explicit scheme was implemented to solve the one-dimensional diffusion reaction equation for the measurement of the concentration of water pollutants along with three cases at the open right boundary. The pollutant concentration at 25th second were measured to vary 1.8676 to 2.1728, 2.0000 to 2.1732 and 2.0000 to 2.1724 (kg/m^3) in cases 1, 2 and 3 respectively. The proposed scheme worked well to compute all three cases as described in tables (1-3) and figure -1. The proposed scheme is explicit in nature hence easy to implement and programmable and works well with various step sizes, advection, and diffusion coefficients. The results show that the numerical measurements obtained by the proposed scheme are reasonable approximations, hence scheme can be used in real-world applications for advection-diffusion equations.

Conflict of Interest:

There was no relevant conflict of interest regarding this paper.

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