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A Saulyev Explicit Scheme for an One-Dimensional Advection-Diffusion-Reaction Equation in an Opened Uniform Flow Stream

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Abstract The one-dimensional advection-diffusion-reaction equation is a mathematical model describing the transport and diffusion problems such as pollutants and suspended matter in a river or channel. If the velocity field is non-uniform the model cannot be theoretically manipulated, there for numerical techniques are required. The object of this research is to propose a simple advection-diffusion-reaction numerical simulation by using the Saulyev schemes. The proposed numerical technique uses an unconditionally stable method. It is the large or small of time step and/or grid size can be employed in the techniques. Among examples are calculated for three θ values. The case of $\theta = 0$ gives a smooth solution compare to the another values. Increasing the mass decay rate affects the maximum concentration level. The numerical experiments show that the calculated results are reasonable approximations.

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1. Introduction

Models are used to express the characteristics of reality which are considered important and to neglect those which seem secondary. These simplifications, good models allow to obtain an easily understandable, mathematically calculable image of the real world. A model is formulated with the aid of mathematical relation that is a mathematical model. A model is a set of rules, or formulas, which try to represent the behaviour of a given phenomenon. Several classes of mathematical models three classes appear: Models which come from laws of physics, this is the case for gravitation laws, Maxwell equations. Navier-Stokes equations, and so on; Model which come from empirical laws, such as air resistance for a movement. Model which come from statistical laws, for instance that

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fit a line between several points and assume the response to be linear. There are three reasons that why we build mathematical models. It gives a better understanding of the phenomenon, which leads to a more precise tuning of the parameters; It warns you get off limits for instance, An empirical knowledge usually is not enough to answer the questions. It allows you find the values of the parameters, which lead to a given result. So building a mathematical model usually means better control upon the phenomenon, which, in turns, mean more precision, cheaper results and better quality output. Those are the reasons to use mathematical model and how different from the fieldwork.

In [1], the Parabolic partial differential equations with nonstandard initial condition, feature in the mathematical modeling of many phenomena. While a significant body of knowledge about the theory and numerical methods for parabolic partial differential equations with classical initial condition has been accumulated, not much has been extended to parabolic partial differential equations with nonstandard initial condition. The Saulyev's explicit schemes are an economical implement to use. These unconditionally explicit schemes are very simple to program and compute. The new explicit schemes developed are very efficient and they need less CPU time than the implicit methods. The explicit finite difference schemes are very easy to implement for similar higher dimensional problems. In [2], a user friendly and a flexible solution algorithm is proposed for the numerical solution of the one-dimensional advection-diffusion equation (ADE), explicit spreadsheet simulation (ESS) technique is used instead of computer code. In the numeric solution of ADE by using finite differences, either the small values of a Courant number such as 0.05-0.10 is used for oscillation free results or an artificial diffusion is used in order to reduce oscillation. In order to provide for small Courant numbers, it is necessary to choose a small time step and/or grid size; however this increases the computer time. While the proposed ADEESS solution technique uses an unconditional stable Saulyev scheme, it is gives highly accurate results even for the values of the Courant numbers as high as 2-3. By changing only the values of the temporal weighted parameter(θ) are solved three θ values, 0, 0.5 and 1, respectively. The model results for the values of $\theta = 0$ are in good agreement with the analytical solution.

In [3], a better finite difference scheme to solve the dynamic one dimensional advection-dispersion-reaction equations (ADRE) is focused, and the effect of non-uniform water flows in a stream is considered. There are two mathematical models used to simulate pollution due to sewage effluent. First, is a hydrodynamic model for numerical techniques, we used the Crank-Nicolson method. Second, is a advection-dispersion-reaction model, we used explicit schemes. The revised explicit schemes are modified from two computation techniques of uniform flow stream problems, forward time central space (FTCS) and Saulyev schemes for dispersion model. A comparison of both schemes regarding stability aspect is provided so as to illustrate their applicability to the real-world problem.

The dispersion model that provides the pollutant concentration field. A modified MacCormack method is subsequently employed in the dispersion model. This proposed a simply remarkable alteration to the MacCormack method so as to make it more accurate without any significant loss of computational efficiency. The results obtained indicate that proposed modified MacCormack scheme does improve the prediction accuracy compared to that the tradition MacCormack method [4]. We propose and explores the simple revision to the MacCormack and Saulyev schemes that improve their accuracy for high Peclet number problems, which are named the Saulyevc and MacCormack schemes respectively, greatly improved the prediction accuracy over the original ones [5]. We propose a new

scheme that guarantees the positivity of the solutions for arbitrary step sizes. We develop for one advection-diffusion reaction equation in one spatial dimension with constant velocity and diffusion and state how to generalize it [6]. The simple explicit schemes have the advantages of simplicity in computing without losing more accuracy and these schemes are precedent for several model applications. To identify the best one these simple schemes, comparative studies of these are necessary.

The object of this research is to propose a simple advection-diffusion-reaction numerical simulation by using the Saulyev schemes. The proposed numerical technique uses an unconditionally stable method. It is the large or small of time step and/or grid size can be employed in the techniques. We apply the method to three problems with different derivative right boundary conditions. The results of the model are show that the calculated results are reasonable approximations.

2. The Governing Equation

In this section, we consider the parabolic equation. The mathematical model describing the transport and diffusion processes is a one-dimensional advection-diffusion-reaction equation (ADRE)

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} - KC, \quad 0 < x < L, 0 < t \leq T, \tag{2.1}$$

with initial conditions

$$c(x,0) = f(x), \quad 0 \leq x \leq L, \tag{2.2}$$

and boundary conditions

$$c(0,t) = g(t), \quad 0 \leq t \leq T, \tag{2.3}$$

$$\left.\frac{\partial c}{\partial x}\right|_{x=L} = h(t), \quad 0 \leq t \leq T, \tag{2.4}$$

where x is the longitudinal distance along the stream, t is time, T is the stationary time, $f(x)$ and $g(t)$ and $h(t)$ are known functions, while $c(x,t)$ is the concentration averaged in depth at the point x and at time t, the function c is unknown, $u(x,t)$ is a known velocity function of the water in the x direction for all $x \in [0,1]$ at time t, D is a dispersion coefficient and K is the mass decay rate. We will consider the model with the following conditions, that $u(x,t)$ and D are positive constant values. The initial conditions $c(x,0) = f(x)$ at $t = 0$ for all $x > 0$. The boundary conditions are $c(0,t) = g(t)$ at $t = 0$ and $\partial c/\partial x = 0$ at $x = 1$.

3. Numerical Technique

The solution domain of the problem is covered by a mesh of grid-lines. The grid point (x_i, t_n) is defined by $x_i = i\Delta x$ for all $i = 0, 1, 2, ..., M$ and $t_n = n\Delta t$ for all $n = 0, 1, 2, ..., N$ in which M and N are positive integers, where x_i and t_n are parallel to the space and time coordinate axes. The constant spatial and temporal grid-spacing are $\Delta x = L/M$ and $\Delta t = T/N$.

Consider the following approximations of the derivative in the advection - diffusion equation which incorporate time weights θ as follows

$$\frac{\partial c}{\partial t} = \frac{c_i^{n+1} - c_i^n}{\Delta t}, \tag{3.1}$$

$$u\frac{\partial c}{\partial x} = u_i^{n+1}\left(\frac{1}{2\Delta x}\right)\left[c_i^{n+1} - c_{i-1}^{n+1} + c_{i+1}^n - c_i^n\right], \tag{3.2}$$

$$\begin{aligned} D\frac{\partial^2 c}{\partial x^2} &= D\left(\frac{\theta}{(\Delta x)^2}\right)\left[c_{i-1}^{n+1} - c_i^{n+1} + c_{i+1}^n - c_i^n\right] \\ &\quad + D\left(\frac{(1-\theta)}{(\Delta x)^2}\right)\left[c_{i+1}^n - 2c_i^n + c_{i+1}^n\right], \end{aligned} \tag{3.3}$$

where $\theta \in [0,1]$ is the weighting factor. Substituting the equations (3.1)–(3.3) into the equation (2.1).

$$\begin{aligned} &\left[1 + \frac{Cr}{2} + \theta\left(\frac{Cr}{Pe}\right)\right]c_i^{n+1} - \left[\frac{Cr}{2} + \theta\left(\frac{Cr}{Pe}\right)\right]c_{i-1}^{n+1} \\ &= \left(\frac{Cr}{Pe} - \theta\left(\frac{Cr}{Pe}\right)\right)c_{i-1}^n + \left[1 + \frac{Cr}{2} - 2\left(\frac{Cr}{Pe}\right) + \theta\left(\frac{cr}{Pe}\right) + K\Delta t\right]c_i^n \\ &\quad + \left[\frac{Cr}{Pe} - \frac{Cr}{2}\right]c_{i+1}^n, \end{aligned} \tag{3.4}$$

for $1 \le i \le M-1$ and $1 \le n \le N-1$, where $Cr = \frac{u\Delta t}{\Delta x}$ is a Courant number and $Pe = \frac{u\Delta x}{D}$ is a Pelet number.

Although the equation (3.4) does not seem explicit, because c_{i-1}^{n+1} and c_i^{n+1} are on the left-hand side, a suitable use of the equation makes it explicit.

Therefore, equation (3.4) can be written in the following form

$$\begin{aligned} c_i^{n+1} = &\left\{\left[\frac{Cr}{2} + \theta\left(\frac{Cr}{Pe}\right)\right]c_{i-1}^{n+1} + \left[\frac{Cr}{Pe} - \theta\left(\frac{Cr}{Pe}\right)\right]c_{i-1}^n \right. \\ &\left. + \left[1 + \frac{Cr}{2} - 2\left(\frac{Cr}{Pe}\right) + \theta\left(\frac{Cr}{Pe}\right) + K\Delta t\right]c_i^n + \left[\frac{Cr}{Pe} - \frac{Cr}{2}\right]c_{i+1}^n\right\} \\ &/\left[1 + \frac{Cr}{2} + \theta\left(\frac{Cr}{Pe}\right)\right]. \end{aligned} \tag{3.5}$$

This scheme is an explicit. In this case, only a single value, c_i^{n+1} will be unknown. This scheme is known as Saulyev's formula and the main advantage of it is that it is unconditionally stable and explicit [2, 3].

4. Application to a Stream Water Assessment Problem

Suppose that the measurement of pollutant concentration C in a non-uniform flow steam is aligned with longitudinal distance, 1.0 (km) total length and 1.0 (m) depth. There is a plant which discharges waste water into the stream and the pollutant concentration at the discharge point is $C(0,t) = C_0 = 2 + \sin(t)(\text{mg/L})$ at $x = 0$ for all $t > 0$ and $C(x,0) = 2 + x(1-x)(\text{mg/L})$ at $t = 0$. We will consider 3 cases of difference rate of change of pollutant concentration at the opened right end of a stream as following.

Case 1: There is not rate of change of pollutant concentration at $x = L$. These means that $\frac{\partial c}{\partial x} = 0$.

Case 2: If the rate of change of pollutant concentration at $x = L$ is increase. These can be assumed that $\frac{\partial c}{\partial x} = 0.05$.

Case 3: If the rate of change of pollutant concentration at $x = L$ is decrease. We can be assumed that $\frac{\partial c}{\partial x} = -0.05$.

The approximation of pollutant concentrations C of all schemes are shown in Tables 1, 2 and 3 and Figure 1.

TABLE 1. Pollutant Concentration $c(x,t)(kg/m^3)$ 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	2.8222	2.1687	2.2387	2.2588	2.1997
10	1.4560	1.7149	2.1427	2.1112	2.2332	2.2726
15	2.6503	1.0077	2.6532	2.1862	1.3591	2.2192
20	2.9129	1.74088	1.4384	3.0381	1.3591	2.2164
25	1.8676	2.8574	1.0617	2.3877	2.5125	1.0404

TABLE 2. Pollutant Concentration $c(x,t)(kg/m^3)$ of case 2

t(sec)\x(km)	0	20	40	60	80	100
0	2.0000	2.1600	2.2400	2.2500	2.1600	2.0000
5	1.0411	2.8222	2.1382	2.1985	2.2588	2.2122
10	1.4560	1.7149	2.9803	2.1546	2.2398	2.2852
15	2.6503	1.0077	2.6532	1.0615	2.0994	2.2318
20	2.9129	1.74088	1.4384	1.5235	1.3658	2.2290
25	1.8676	2.8574	1.0640	2.7136	2.5191	1.0530

TABLE 3. Pollutant Concentration $c(x,t)(kg/m^3)$ of case 3

t(sec)\x(km)	0	20	40	60	80	100
0	2.0000	2.1600	2.2400	2.2400	2.1630	2.0050
5	1.0411	2.8222	2.1382	2.2387	2.2588	2.2121
10	1.4560	1.7149	2.9803	2.1112	2.2266	2.2849
15	2.6503	1.0077	2.6532	2.1861	2.0859	2.2316
20	2.9129	1.74088	1.4384	3.0344	1.3524	2.2288
25	1.8676	2.8574	1.0594	2.3840	2.5060	1.0528

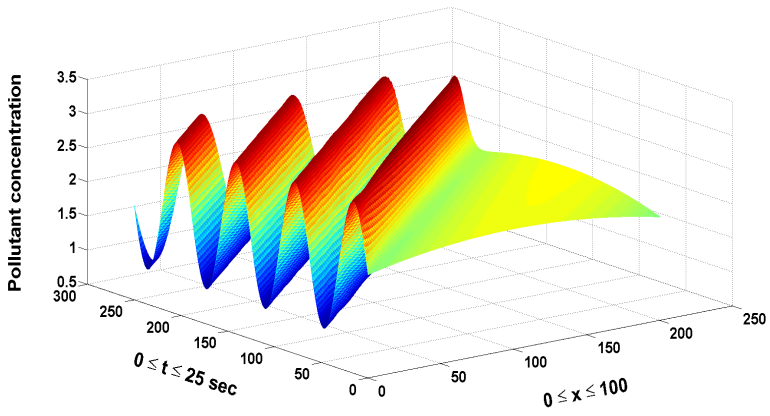

FIGURE 1. Pollutant Concentration $c(x,t)(kg/m^3)$ of case 1

5. Discussion and Conclusion

In this research, the approximation of the pollutant concentrations of a simple advection-diffusion-reaction numerical simulation by using the Saulyev schemes is shown in Tables 1, 2 and 3 and Figure 1. The numerical techniques are proposed for three θ values, 0, 0.5 and 1, respectively. The case of $\theta = 0$ gives a smooth solution compare to another values. Increasing the mass decaying rate affects the maximum concentration level. The proposed numerical technique uses are unconditionally stable methods. It is the large or small of time step and/or grid size can be employed in the techniques. The numerical experiments show that the calculated results are reasonable approximations. The revision shows good agreement solutions. The proposed technique is suitable to be used in the real-world problem due to it easily to program and the straight forwardness of the implementation.

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