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A semi-lagrangian scheme for advection-diffusion equation

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Abstract. This study proposes a semi-Lagrangian scheme for numerical simulation of advection-diffusion equation. The proposed method provides unconditional stability and highly accurate solutions even at large time steps. Another advantage of this method is that it requires a low computational time. Accuracy of the method is tested by a numerical application.

Keywords: Advection-diffusion; contaminant transport; method of characteristics; Saulyev scheme.

1 Introduction

The significant applications of advection-diffusion equation can be seen in fluid dynamics [1], heat transfer [2] and mass transfer [3]. The 3-D advection-diffusion equation without source is given by

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} + V\frac{\partial C}{\partial y} + W\frac{\partial C}{\partial z} = D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2} \quad (1)$$

Where t is time, x, y and z are spatial directions in cartesian coordinates, C is concentration of substance, U, V and W are velocity components of flow in each direction and D represents the diffusivity coefficent in each direction.

In this paper, we consider one-dimensional advection-diffusion equation is given by:

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} \quad (2)$$

with U and D is constant, $0 \leq x \leq L$, and $0 \leq t \leq T$. L and T represent spatial and temporal boundaries of computational domain, respectively.

We denote the spatial and temporal step sizes by Δx and Δt, respectively. Also Courant number, Cr, is computed as $U\Delta t/\Delta x$ and the Peclet number, Pe, is obtained as $U\Delta x/D_x$.

The initial condition is $C(x,0) = f(x)$ and boundary conditions are

$$C(0,t) = g_0(t), \quad 0 \leq t \leq T \quad (3)$$

$$C(L,t) = g_1(t), \quad 0 \leq t \leq T \quad (4)$$

Where f, g_0, g_1 are known functions.
Accurate solution of equation (2) is very important for reducing existing pollutant concentrations or taking precautions by predicting pollution formation in water resources, which is the basic requirement of human beings. However, since this equation contains two different physical processes such as advection and diffusion, the precise numerical solution is quite difficult. To overcome this difficulty such as classical finite difference method [4], high-order finite element method [5], high-order finite difference methods [6, 7], green element method [8], cubic and extended B-spline collocation methods [9-11], cubic, quartic and quintic B-spline differential quadrature methods [12, 13], method of characteristics unified with splines [14-16], cubic trigonometric B-spline approach [17] Taylor collocation and Taylor-Galerkin methods [18] , Lattice Boltzmann method [19] have been developed. In addition, with the help of operator splitting methods, the appropriate methods for the physical processes of the problem can be combined.

In the scope of the study, equation (2) will be divided into two processes as the advection and diffusion by the operator splitting method. Method of characteristics with cubic spline interpolation (MOC-CS) and Saulyev scheme will be used for the solution of advection and diffusion processes, respectively. Though Saulyev scheme is an explicit method, it has the same order as the Crank-Nicolson scheme which is an implicit method. Saulyev scheme will shorten the computation time because it is explicit, but the precision of the solutions must be examined. For this purpose, the results obtained with Saulyev scheme will be compared with other methods in the literature and analytical solution of the problem.

2 Numerical Discretization

2.1. Operator Splitting Approach

Lie-Trotter operator splitting method is a first-order splitting method and solves problems sequentially. Its application to the equation (2) separates advection-diffusion equation into the two sub-problem such as advection and diffusion. Mathematical formulation of the application is as follows:

$$\frac{\partial \hat{C}_1}{\partial t} + U\frac{\partial \hat{C}_1}{\partial x} = 0, \qquad \hat{C}_1(t_n, x) = C(t_n, x), \quad t \in [t_n, t_{n+1}] \tag{5}$$

$$\frac{\partial \hat{C}_2}{\partial t} = D_x\frac{\partial^2 \hat{C}_2}{\partial x^2}, \qquad \hat{C}_2(t_n, x) = \hat{C}_1(t_{n+1}, x), \quad t \in [t_n, t_{n+1}] \tag{6}$$

Equation (5) and equation (6) represent advection and diffusion equations, respectively. These problems are solved consecutively, but are combined through the initial conditions. First, Equation (5) will be solved by the MOC-CS method at the time interval of Δt using the initial condition of the general advection-diffusion problem and the result obtained from this will be used as the initial condition of the diffusion process. Then equation (6) will be solved in the time interval of Δt with the help of the explicit Saulyev method and thus the solution of the advection-diffusion problem in the time interval of Δt will be obtained.

2.2. Numerical Discretization of Advection Part

By multiplying both sides of the advection equation given in equation (5) by dt, this partial differential equation can be transformed into two ordinary differential equations as follows:

$$\frac{d\hat{C}_1}{dt} = 0 \tag{7}$$

$$\frac{dx}{dt} = U \tag{8}$$

Thus, the equation (5) which is a partial differential equation can be solved as a simple ordinary differential equation along the line defined in the equation (8) in the plane (x, t). As a result of equation (7), there is no change in the concentration along the characteristic line shown in Figure 1. In this case, the exact solution of equation (5) can be expressed as follows.

$$\hat{C}_1(x_{i+1}, t_{n+1}) = \hat{C}_1(\hat{x}_i, t_n) = \hat{C}_1\left(x_{i+1} - \int_{t_n}^{t_{n+1}} U dt, t_n\right) \tag{9}$$

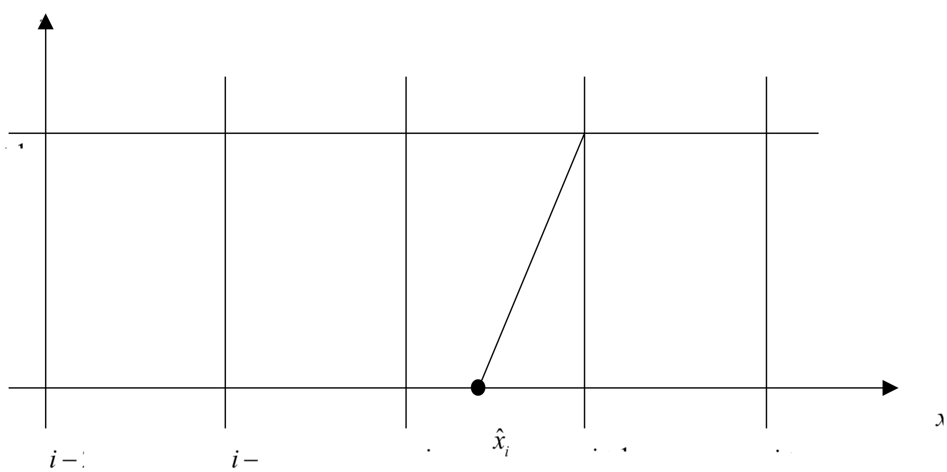

Figure 1 Finite difference grid and trajectory line of concentration in one-dimension

Since the coordinate of the point $\hat{x}_i$ is between the nodal points, interpolation must be made using the concentration values which are known from initial condition in the nodal points so that the concentration value at this point can be calculated. The only error encountered in solving the advection process is the interpolation. For this purpose, cubic spline polynomials with pretty low interpolation error will be used. Cubic spline polynomials can be written in the form

$$C(x) = C_i + \alpha_i(x - x_i) + \beta_i(x - x_i)^2 + \gamma_i(x - x_i)^3, \quad x_i \leq x \leq x_{i+1} \qquad (10)$$

Where C_i is the concentration value of at node i and $\alpha_i, \beta_i, \gamma_i$ are polynomial coefficients determined from values at nodes. The detailed description about construction of the cubic spline polynomials and calculation of coefficients in the polynomials are given, for example, at [20].

After the polynomial is calculated in equation (10), the concentration values in all nodes at time t_{n+1} can be calculated as follows.

$$\hat{C}_1(x_{i+1}, t_{n+1}) = \hat{C}_1(x_i, t_n) + \alpha_i(\hat{x}_i - x_i) + \beta_i(\hat{x}_i - x_i)^2 + \gamma_i(\hat{x}_i - x_i)^3 \qquad (11)$$

As stated in equation (7), this method is time-independent and therefore does not have any stability condition. Solutions can be produced by selecting very large time steps.

2.3. Numerical Discretization of Diffusion Part

Although the Saulyev scheme is an explicit scheme, it uses values from the new time step. Thus, the quality of the solution is improving. There are two ways of solutions, from left to right and from right to left. The left to right version was used in the study. Spatial discretization of diffusion process via Saulyev scheme as follows:

$$\left.\frac{\partial^2 \hat{C}_2}{\partial x^2}\right|_{i,n} \approx \frac{\left.\frac{\partial \hat{C}_2}{\partial x}\right|_{i+1/2,n} - \left.\frac{\partial \hat{C}_2}{\partial x}\right|_{i-1/2,n}}{\Delta x}, \qquad (12)$$

we can replace the left hand side derivate term at time level n with derivative term at time level $n + 1$ as the solution process goes from left to right. Similar modification can be done for right to left solution procedure.

$$\left.\frac{\partial^2 \hat{C}_2}{\partial x^2}\right|_{i,n} \approx \frac{\left.\frac{\partial \hat{C}_2}{\partial x}\right|_{i+1/2,n} - \left.\frac{\partial \hat{C}_2}{\partial x}\right|_{i-1/2,n+1}}{\Delta x}, \qquad (13)$$

Also following approximations are used

$$\left.\frac{\partial \hat{C}_2}{\partial x}\right|_{i+1/2,n} \approx \frac{\left.\hat{C}_2\right|_{i+1,n} - \left.\hat{C}_2\right|_{i,n}}{\Delta x} \tag{14}$$

$$\left.\frac{\partial \hat{C}_2}{\partial x}\right|_{i-1/2,n+1} \approx \frac{\left.\hat{C}_2\right|_{i,n+1} - \left.\hat{C}_2\right|_{i-1,n+1}}{\Delta x} \tag{15}$$

$$\left.\frac{\partial \hat{C}_2}{\partial t}\right|_{i,n} \approx \frac{\left.\hat{C}_2\right|_{i,n+1} - \left.\hat{C}_2\right|_{i,n}}{\Delta t} \tag{16}$$

Combining these equations gives us the solution of diffusion equation using left to right Saulyev scheme as follows:

$$\left.\hat{C}_2\right|_{i,n+1} = \frac{\theta \left.\hat{C}_2\right|_{i-1,n+1} + (1-\theta)\left.\hat{C}_2\right|_{i,n} + \theta \left.\hat{C}_2\right|_{i+1,n}}{(1+\theta)} \tag{17}$$

where $\theta = \Delta t/\Delta x^2$.

At each unknown time level, $n+1$, at $i=1$ the term $\left.\hat{C}_2\right|_{0,n+1}$ is known from boundary conditions. Thus for $i>1$ the value of $\left.\hat{C}_2\right|_{i-1,n+1}$ is computed from equation (17), hence this method is explicit method.

3 Numerical Applications

In this section, we consider two one-dimensional advection-diffusion problems. One of them has a sharp gradient and the other one has smooth behavior. Obtained numerical results are compared with exact solution and the solutions of the other researchers in the literature. Many analyses have been done to test our numerical method's efficiency for a wide range of Courant numbers. Also error norms are compared and computed as follows:

$$L_\infty = \max_i \left| C_i^{exact} - C_i^{numerical} \right| \quad (18)$$

$$L_2 = \sqrt{\sum_{i=1}^{M} \left| C_i^{exact} - C_i^{numerical} \right|^2} \quad (19)$$

Example: Flow velocity and diffusion coefficient are taken as $U = 0.01\ m/s$ and $D = 0.002\ m^2/s$ in this experiment. Length of the channel picked as $L = 100\ m$. Exact solution of this problem given as follows [21]:

$$C(x,t) = \frac{1}{2} erfc\left(\frac{x - Ut}{\sqrt{4Dt}}\right) + \frac{1}{2} exp\left(\frac{Ux}{D}\right) erfc\left(\frac{x + Ut}{\sqrt{4Dt}}\right) \quad (20)$$

Following boundary conditions are used:

$$C(0,t) = 1 \quad (21)$$

$$-D\left(\frac{\partial C}{\partial x}\right)(L,t) = 0 \quad (22)$$

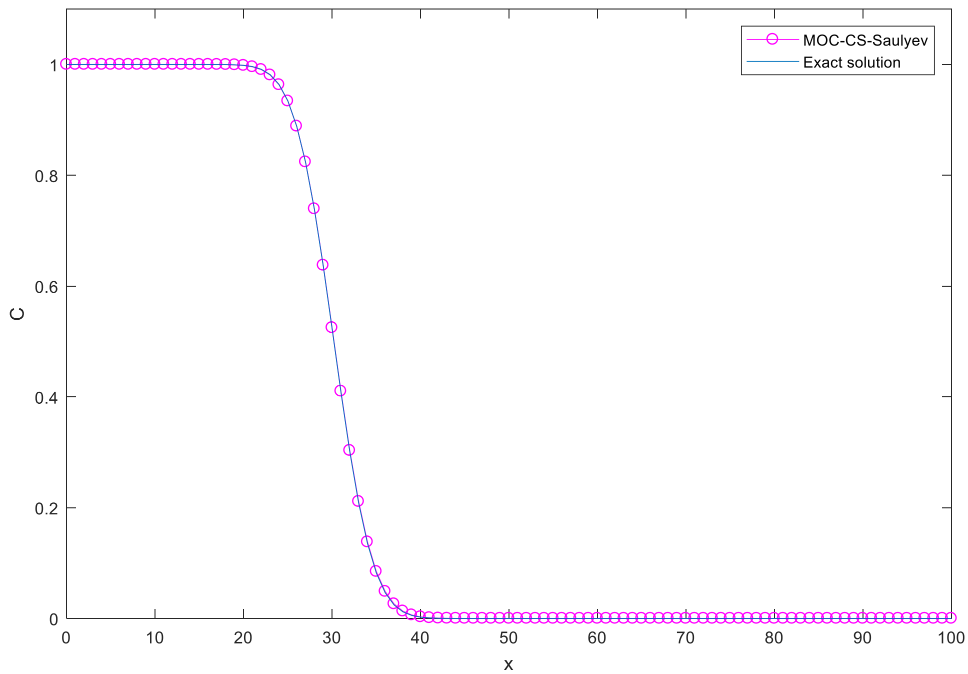

Figure 2 Comparison of the exact solution and the numerical solution obtained with MOC-CS-Saulyev method for $\Delta x = 1\ m$ and $\Delta t = 10\ s$

In all calculations the spatial step size picked as $\Delta x = 1\ m$. Also maximum computational time taken as $3000\ s$. As maximum computational time remain same in all analyzes, critical concentration values can be observed at from $18\ m$ to $42\ m$ (Figure 2). Also it should be taken to consideration that this problem is advection dominant $(Pe = 5)$ and has sharp shape. This makes the solution difficult for almost all numerical methods.

In Table 1, all concentration values obtained for the time interval of $\Delta t = 10\ s$. This makes Courant number equals to 0.1. It clearly can be seen that MOC-CS-Saulyev scheme has closer results to exact solution compare to other numerical methods. This situation can also be recognized by looking at the error norms. It should be noted that even though MOC-CS-Saulyev has low order discretization compare to the sixth order compact finite difference it has smaller error norm values.

Table 1 Comparison between numerical solutions and exact solution ($\Delta t = 10\ s$)

x (m)	[7] MC-CD6	[6] RK4-CD6	[17] CuTBSM	MOC-CS Saulyev	Exact
0	1.000	1.000	1.000	1.000	1.000
18	1.000	1.000	1.000	1.000	1.000
19	0.999	0.999	0.999	0.999	0.999
20	0.998	0.998	0.998	0.998	0.998
21	0.996	0.996	0.996	0.996	0.996
22	0.991	0.992	0.991	0.991	0.991
23	0.982	0.982	0.982	0.981	0.982
24	0.965	0.965	0.963	0.964	0.964
25	0.936	0.936	0.933	0.934	0.934
26	0.891	0.891	0.885	0.889	0.889
27	0.827	0.827	0.818	0.824	0.823
28	0.743	0.743	0.732	0.739	0.738
29	0.642	0.641	0.631	0.636	0.636
30	0.529	0.528	0.517	0.524	0.523
31	0.414	0.413	0.404	0.409	0.408
32	0.306	0.306	0.298	0.302	0.301
33	0.213	0.212	0.207	0.211	0.208
34	0.138	0.138	0.134	0.138	0.135
35	0.084	0.084	0.081	0.085	0.082
36	0.048	0.048	0.045	0.049	0.046
37	0.025	0.025	0.023	0.027	0.024
38	0.012	0.012	0.011	0.014	0.012
39	0.006	0.006	0.005	0.006	0.005
40	0.002	0.002	0.002	0.003	0.002
41	0.001	0.001	0.001	0.001	0.001
42	0.000	0.000	0.000	0.000	0.000
L_2	0.0148	0.0142	-	0.0071	-
L_∞	0.0060	0.0055	-	0.0031	-

In Table 2, infinity error norms of MOC-CS-Saulyev, cubic B-spline and extended cubic B-spline collocation methods are compared for different time interval values. When Table 2 is examined it can be seen that MOC-CS-Saulyev scheme always has smaller error norm values except for extended cubic B-spline collocation method at the time interval of $\Delta t = 1\ s$.

Table 2 Comparison of L_∞ error norms ($\Delta x = 1\ m$)

Δt (s)	[11] BSCM	[11] ECuBSCM	MOC-CS Saulyev
60	0.04330	0.04250	0.01235
30	0.01962	0.01961	0.00635
20	0.01270	0.01260	0.00471
10	0.00685	0.00608	0.00314
5	0.00409	0.00307	0.00243
1	0.00224	0.00127	0.00193

4 Conclusions

This paper deals with the advection-diffusion equation with the help of Lie-Trotter opeator splitting method. The problem splits into advection and diffusion processes. Each process solved by suitable methods for physical processes. Method of characteristics with cubic spline and Saulyev scheme is used for advection and diffusion, respectively. The effectiveness of method was tested using a one-dimensional problem. The problem has a sharp gradient which is quite difficult to solve accurately. Obtained results are compared with exact solution and other researcher's solutions available in the literature.

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