A Comparison of Some Numerical Schemes for Modified Advection Diffusion Equation

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Abstract

In the present paper, we present a comparison of two standard finite difference schemes such as explicit finite difference scheme with forward time backward space and centered space (FTBSCS) and forward time centered space (FTCS) for solving modified advection diffusion equation (ADE) where the solutions of Burgers' equation are incorporated into the ADE. The numerical solutions are implemented with appropriate initial and Neumann boundary conditions. The numerical results are compared with analytical solutions by setting two problems.

Keywords— Advection Diffusion Equation, Burger's Equation, Explicit Finite Difference Schemes, Exact Solutions..

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1 Introduction

Advection Diffusion Equation is one of the most important partial differential equation and observed in a wide range of engineering and industrial applications. This equation reflects physical phenomena where in the diffusion process particles are moving with certain velocity from higher concentration to lower concentration. The analyti-cal/numerical solutions along with an initial condition and two boundary conditions help to understand the contaminant or pollutant concentration distribution behavior through an open medium like air, rivers, lakes and porous medium like aquifer. It has wide applications in other disciplines too, like soil physics, petroleum engineering, chemical engineering and biosciences.

Burgers' equation is a fundamental partial differential equation that was originally proposed as a simplified model of turbulence as exhibited by the full-fledged Navier-Stockes equation. The turbulent behavior especially of a stochastically forced Burger's equation is sometimes dubbed Burgulence. It is a nonlinear equation for which exact solutions are known and is therefore important as a benchmark problem for numerical methods. Many researchers have already been worked on it.

A N S Al-Niami N S and K R Ruston [1] obtained an analysis of flow against dispersion in porous media. Anderson, P. Mary, and W. William [2] Woessner presented a simulation on Groundwater Modeling of Flow and Advective Transport. M. M. Aral and B. Liao [3] obtained an Analytical solution for two-dimensional transport equation with time-dependent disper-sion coefficients. Atul Kumar, Dilip Kumar Jaiswal and Naveen Kumar [4] presented an analytical solution of the one-dimensional ADE by reducing the original ADE into a diffusion equation by using Laplace transformation technique. Banks and Ali [5] obtained an analytical solution of the one-dimensional ADE by reducing the original ADE into a diffu-sion equa-tion by introducing another dependent variable. Bender and Edward [6] presented an Introduction to Math-ematical Model-ing. Changiun Zhu, Liping Wa and Sha Li [7] presented a numerical simulation of hybrid finite analytic methods for ground water pollution. Changjun and Shuwen [8] made a numerical simulation on river water pollution by using grey dif-ferential model. They corrected the model in finding the truncation error and found that the obtained results from the grey model are excellent and reasonable. Donea, Guilinai and Laval. Quartpelle [9] studied on Time accurate solution of ad-vection-diffusion problems by finite elements". Aksan and Ozdes [10] studied a numerical solution of Brger's equa-tion. Agusta and Bamingbola [11] studied on the numerical treatment of the mathematical model for water pollution. This study was examined by various mathematical models involving water pollution [12]. Leon and Austria [13] obtained a Stability Criterion for Explicit Scheme on the solution of Advection-Diffusion Equation. Abdou and Soliman [14] applied variational iteration method for solving Burger's and coupled Burger's equation. Thongmoon and Mckibbin [15] compared some numerical methods for the advection-diffusion equation. Nicholas J. Higham [16] studied on accuracy and stability of Nu-merical Algorithms. Ogata and Banks [17] obtained an analytical solution of the one-dimensional ADE by reducing the orig-inal ADE into a diffusion equation by applying moving coordinates. In [12, 18 – 22] analytical and numerical solutions have been obtained by applying different method. Azad, Begum and Andallah [23] studied an explicit finite difference scheme for solving the advection diffusion equation (ADE). Numerical solution of the ADE is obtained by using FTBSCS and FTCS techniques for prescribed initial and boundary data. Numerical results for both the schemes are com-pared in terms of accuracy by error estimation with respect to exact solution of the ADE and also the numerical features of the rate of convergence are presented graphically.

With the above discussion in view, we present a comparison of two numerical schemes such as FTBSCS and FTCS for solving modified ADE where the solutions of Burgers' equation are incorporated into the ADE. The numerical solutions are implemented with appropriate initial and Neumann boundary conditions. The numerical results are compared with analytical solutions by using two examples.

2 Governing Equation and Numerical Methods

2.1 Governing Equation

In this study, we consider one-dimensional motion with advective speed u, the solutions of Burgers' equation are incorporated and dispersion D which gives the 1-D advection-diffusion equation [20]:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2}, \qquad x \in [a, b], \qquad t \in [0, T] \qquad (1),$$

and the Burger's equation is [12]

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = D\frac{\partial^2 u}{\partial x^2}, \qquad x \in [a, b], \qquad t \in [0, T] \qquad (2)$$

where c(t, x) represents the solute concentration at x ($0 \le x \le L$) and time t.

Appended with initial condition

$$c(x,0) = f(x); \; u(x,0) = f(x) \qquad 0 \le x < l$$

and Neumann boundary conditions

$$c(t,a) = c_a(t) \,; u(t,a) = u_a(t) \qquad t_0 \le t \le T$$

$$\frac{\partial}{\partial x}c(t,b) = c_b(t) \,; \; \frac{\partial}{\partial x}u(t,b) = u_b(t) \qquad t_0 \le t \le T$$

$$\frac{\partial}{\partial x}c(t,b) = c_b(t) \,; \; \frac{\partial}{\partial x}u(t,b) = u_b(t) \qquad t_0 \le t \le T$$

where ca(t), cb(t) are constant concentration values at the left-hand end and right-hand end respectively.

2.2 Analytic solution

The exact solution of the advection-diffusion equation as IVP with initial condition

c(x, 0) = f(x) is given [20]

$$c(x,t) = \frac{M}{A\sqrt{4\pi D t}} exp\left(-\frac{(x - (x_0 + ut))^2}{4Dt}\right) \qquad (3)$$

where M = mass of tracer

A = uniformly cross section area at the point x = 0, at time t = 0.

2.3 Finite difference method for ADE

We consider the one–dimensional ADE as an initial and boundary value problem.

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2}$$

With initial condition,

$$c(t_0, x) = c_0(x); \qquad a \le x \le b$$

and Neumann boundary conditions

$$c(t, a) = c_a(x)\ ; \qquad t_0 \le t \le T$$

$$\frac{\partial}{\partial x} c(t, b) = c_b(x)\ ; \qquad t_0 \le t \le T$$

FDMs are the efficient approach to numerical solutions of partial differential equations. A finite difference method proceeds by replacing the derivatives in the differential equation by the finite difference approximations. This gives a large algebraic system of equation to be developing a computer programming code.

2.4 Explicit finite difference scheme for ADE

For the numerical solution of the one –dimensional linear advection- diffusion equation we consider the IBVP

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \tag{4}$$

With initial condition

$$c(x, 0) = f(x) \qquad 0 \le x < l$$

and Neumann boundary conditions

$$c(t, x = 0) = g_0(x) \qquad 0 < t \le T$$

$$\frac{\partial}{\partial x} c(t, x = l) = 0 \qquad 0 < t \le T$$

In order to develop the scheme, we discretize the x-t plane by choosing a mesh width h = Δx space size and a time step size k = Δt. The finite difference methods, we will develop, produce approximations $c_i^n \in R^n$ to the solution $c(x_i, t_n)$ in the discrete points by

$$x_i = ih, i = 0, 1, 2, 3, \dots \dots \dots$$

$$t_n = nk, n = 0, 1, 2, \dots \dots \dots$$

3 Finite Difference Formulae

The forward difference in time

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

The backward space difference formula

$$\frac{\partial c}{\partial x} = \frac{c_i^n - c_{i-1}^n}{\Delta x} \tag{6}$$

The centered space difference formula

$$\frac{\partial c}{\partial x} = \frac{c_{i+1}^{n} - c_{i-1}^{n}}{2\Delta x} \tag{7}$$

And centered space difference formula

$$\frac{\partial^2 c}{\partial x^2} = \frac{c_{i+1}^{n} - 2c_{i}^{n} + c_{i-1}^{n}}{\Delta x^2} \tag{8}$$

3.1 Explicit Centered Difference Scheme by FTBSCS Techniques

Substituting equations (5 - 6) into equation (4) and rearrange according the time level,

Implies to

$$c_{i}^{n+1} = (1 - 2\lambda)c_{i}^{n} - \gamma u_{i}^{n}(c_{i}^{n} - c_{i-1}^{n}) + \gamma(c_{i+1}^{n} + c_{i-1}^{n}) \tag{9}$$

In which

$$\gamma = \frac{\Delta t}{\Delta x}\,, \qquad \lambda = \frac{D\Delta t}{\Delta x^2}$$

3.2 Explicit Centered Difference Scheme by FTCS techniques

Substituting equations (5, 7, 8) into equation (4) and rearrange according the time level, lead to

$$c_{i}^{n+1} = (1 - 2\lambda)c_{i}^{n} - \frac{1}{2}\gamma u_{i}^{n}(c_{i+1}^{n} - c_{i-1}^{n}) + \gamma(c_{i+1}^{n} + c_{i-1}^{n}) \tag{10}$$

In which,

$$\gamma = \frac{u\Delta t}{\Delta x}\,, \qquad \lambda = \frac{D\Delta t}{\Delta x^2}$$

4 Stability Analysis

After surveying the relevant literature on the subject, we discover that no practical stability criterion exists for the schemes (9) and (10). We developed stability conditions for both the schemes and maintaining the criteria we verify the results of the schemes by setting an example.

4.1 Stability condition

Stability condition for the scheme by FTBSCS scheme (9) is given by

$$0 \le \frac{\Delta t}{\Delta x} \le 1 \text{ and } 0 \le \frac{D\Delta t}{\Delta x^2} \le \frac{1}{2}$$

4.2 Stability condition

Stability condition for the scheme by FTCS Scheme (10) is given by

$$0 \le \frac{\Delta t}{\Delta x} \le \frac{1}{2} \text{ and } 0 \le \frac{D\Delta t}{\Delta x^2} \le \frac{1}{2}$$

5 COMPARISON AND DISCUSSIONS

Various finite difference equations were used to approximate the parabolic model equation (1). It is interesting to experiment with these numerical techniques. It is hoped that by writing computer codes and analyzing the results, additional insights into the solution procedures are gained. Therefore, this section proposes an example and presents a comparison between the solutions obtained by the described schemes.

5.1 Problem description

Estimation of pollutant in a river of length l = 6 meters at all time t = 1minute to t = 6 minutes with diffusion coefficient, D = 0.01*m²/s*=36 *m²/h*.

The advection diffusion equation for this problem is

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2}$$

Various values of spatial nodes size and time steps are to be used to investigate the numerical schemes and the effect of steps on stability and accuracy.

An attempt is made to solve the stated problem subject to the imposed initial and Neumann boundary conditions by the following:

The FTBSCS and FTCS schemes with parameters

Δx = 0.5,	nx = 120Δt = 0.07,	nt = 3600, T= 60×4 sec
Δx = 0.5,	nx = 120Δt = 0.08,	nt = 3600 T= 60×5 sec
Δx = 5,	nx = 120Δt = 0.1,	nt = 3600 T= 60×6 sec
Δx = 5,	nx = 120Δt = 0.126,	nt = 3600 T = 60×7.507 sec

Case *I*. When the step sizes are Δx = 0.5, Δt = 0.07.

In this case, both the schemes are to be used as stated previously:

The stability requirements of the FTBSCS scheme are

$$0 \le \frac{\Delta t}{\Delta x} \le 1 \text{ and } 0 \le \frac{D\Delta t}{\Delta x^2} \le \frac{1}{2}.$$

(The terms $\frac{\Delta t}{\Delta x} = \gamma$ and $\frac{D\Delta t}{\Delta x^2} = \lambda$ are known as the advection number and diffusion number respectively.)

$$\text{For this particular application, } \gamma = \frac{\Delta t}{\Delta x} = \frac{0.07}{0.5} = 0.14 \text{ and } \lambda = \frac{D\Delta t}{\Delta x^2} = \frac{1 \times 0.07}{(0.5)^2} = 0.000028$$

And the stability requirements of the FTCS scheme are

$$0 \le \frac{\Delta t}{\Delta x} \le \frac{1}{2} \text{ and } 0 \le \frac{D\Delta t}{\Delta x^2} \le \frac{1}{2}$$

For this particular application,

$$\frac{\Delta t}{\Delta x} = \frac{0.07}{0.05} = 1.4 \text{ and } \frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.07}{(0.05)^2} = 0.28 \le \frac{1}{2}$$

Therefore, the stability conditions for both the schemes are satisfied, and a stable solution is expected. The comparison of the solutions of the schemes are to be obtained up to t = 4 minutes are shown in Figure 5.1.

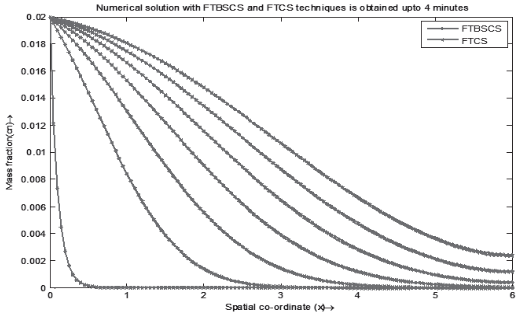

Figure 5.1 : The comparison the solutions with the schemes, *Δx* = 0.05, *Δt* = 0.07

Case *II*. When the step sizes are increased to Δx = 0.15, Δt = 0.1,

The stability requirements of the FTBSCS scheme are

$$0 \le \frac{D\Delta t}{\Delta x^2} \le 1 \text{ and } -\frac{D\Delta t}{\Delta x^2} \le \frac{u\Delta t}{\Delta x} \le 1 - 2\frac{D\Delta t}{\Delta x^2}$$

For this particular application,

$$\lambda = \frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.1}{(0.15)^2} = 0.044$$

$$\gamma = \frac{u\Delta t}{\Delta x} = \frac{0.01 \times 0.1}{0.15} = 0.007$$

$$\frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.1}{(0.15)^2} = 0.044 \le 1 \text{ and } -\frac{0.01 \times 0.1}{(0.15)^2} \le \frac{0.01 \times 0.1}{0.15} \le 1 - 2 \times \frac{0.01 \times 0}{(0.15)^{2}.1}$$

$$or, \frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.1}{(0.15)^2} = 0.044 \le 1 \text{ and } -0.044 \le 0.007 \le 0.912$$

And the stability requirements of the FTCS scheme are

$$0 \le \frac{D\Delta t}{\Delta x^2} \le \frac{1}{2} \text{ and } -2\frac{D\Delta t}{\Delta x^2} \le \frac{u\Delta t}{\Delta x} \le 2\left(1 - \frac{D\Delta t}{\Delta x^2}\right).$$

For this particular application,

$$\frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.1}{(0.15)^2} = 0.044 \le \frac{1}{2} \text{ and } 2 \times \frac{0.01 \times 0.1}{(0.15)^2} \le \frac{0.01 \times 0.1}{0.15} \le 2\left(1 - \frac{0.01 \times 0.1}{(0.15)^2}\right)$$

$$or, \quad \frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.1}{(0.15)^2} = 0.044 \le \frac{1}{2} \text{ and } -0.088 \le 0.007 \le 1.912.$$

Therefore, the stability condition is satisfied, and a stable solution is expected. The comparison of the solutions are to be obtained up to t = 6 minutes are shown in Figure 5.2.

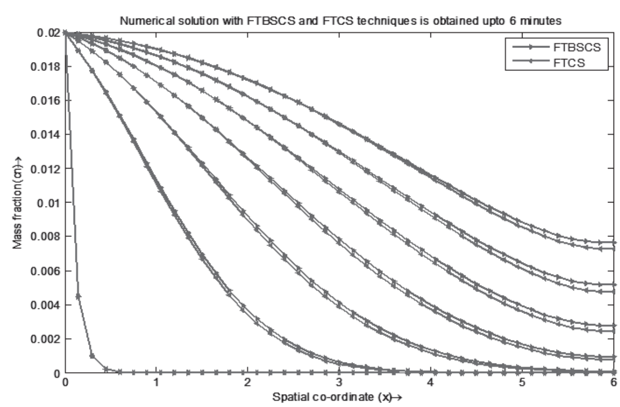

Figure 5.2 : The comparison of solutionswith the schemes, Δx = 0.15, Δt = 0.1

Case *III*. When the step sizes are increased to Δ*x* = 0.05, Δ*t* = 0.122, which is only a fraction of an increase over preceding cases. In this case, the stability requirements of the FTBSCS schemes are

$$0 \le \frac{D\Delta t}{\Delta x^2} \le 1 \text{ and} -\frac{D\Delta t}{\Delta x^2} \le \frac{u\Delta t}{\Delta x} \le 1 - 2\frac{D\Delta t}{\Delta x^2}.$$

For this particular application,

$$\lambda = \frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.122}{(0.05)^2} = 0.488$$

$$\gamma = \frac{u\Delta t}{\Delta x} = \frac{0.01 \times 0.122}{0.05} = 0.0244$$

$$\frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.122}{(0.05)^2} = 0.488 \le 1 \text{ and} -\frac{0.01 \times 0.122}{(0.05)^2} \le \frac{0.01 \times 0.122}{0.05} \le 1 - 2 \times \frac{0.01 \times 0.122}{(0.05)^2}$$

$$or, \quad \frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.122}{(0.05)^2} = 0.488 \le 1 \text{ and } -0.488 \le 0.0244 \le 0.024,$$

which exceeds the stability requirement.

And the stability requirements of the FTCS scheme are

$$0 \le \frac{D\Delta t}{\Delta x^2} \le \frac{1}{2} \text{ and } -2\frac{D\Delta t}{\Delta x^2} \le \frac{u\Delta t}{\Delta x} \le 2\left(1 - \frac{D\Delta t}{\Delta x^2}\right).$$

For this particular application,

$$\frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.122}{(0.05)^2} = 0.488 \le \frac{1}{2} \text{ and } -2 \times \frac{0.01 \times 0.122}{(0.05)^2} \le \frac{0.01 \times 0.122}{0.05} \le 2\left(1 - \frac{0.01 \times 0.122}{(0.05)^2}\right)$$

$$or, \quad \frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.122}{(0.05)^2} = 0.488 \le \frac{1}{2} \text{ and } -0.976 \le 0.0244 \le 1.024.$$

Therefore, at this stage one of the stability conditions for FTBSCS is not satisfied, and an unstable solution is appeared. With the step sizes indicated, an unstable solution is developed. The comparison of the solutions are to be obtained at t = 6 minutes are shown in Figure 5.3

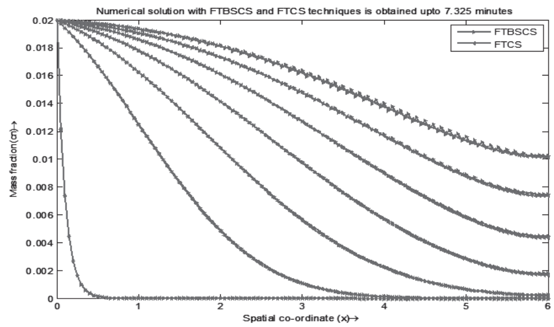

Figure 5.3 : The comparison of solutions with the schemes, Δx= 0.05, Δt = 0.122

6. Analysis

In the preceding section, two explicit finite difference schemes are applied to the advection diffusion equation and the solutions are presented. The effect of the stability imposed by the diffusion number on the FTBSCS and FTCS explicit schemes are clearly indicated. Therefore, for these schemes, the selection of step sizes is limited due to the stability requirement. However, the accuracy requirement limits the use of large time steps, since an increase in time steps will increase the truncation errors introduced in the approximation process of the PDE.

For the simple problem under consideration, an analytical solution may be obtained. The analytical solution of ADE with the imposed initial and boundary conditions is as follows-

6.1 Error Estimation and Convergence

We compute the relative error in L1-norm which is defined as

err = 〖‖c_e-c_n‖〗 _1/ 〖‖c_e‖〗 _1 (11)

where, ce is the exact solution, and cn is the numerical solution computed by the finite difference schemes for time t∈[0,6].The following Figure 6.1 shows the convergence of relative error by the scheme FTBSCS.

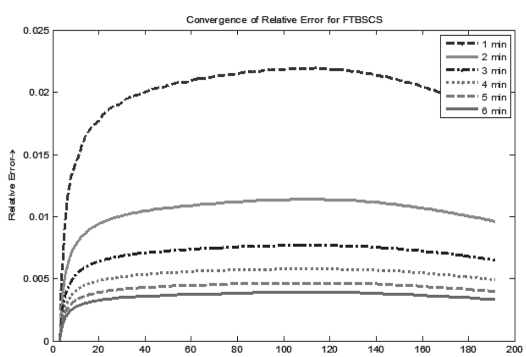

Figure 6.1: Rate of numerical feature of convergence by the scheme FTBSCS.

The following Figure 6.2 shows the convergence of relative error by the scheme FTCS.

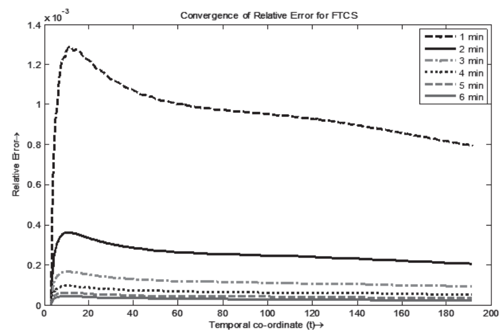

Figure 6.2 : Rate of numerical feature of convergence by the scheme FTCS.

The following Figure 6.3 shows the comparison of relative errors for the both schemes.

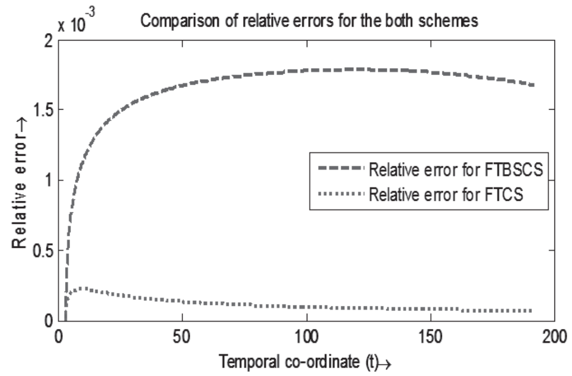

Figure 6.3 : Comparison of relative errors for the both FTBSCS and FTCS schemes

7. Conclusion

Numerical experiment in the comparison is presented graphically. The analytical result is used for code validation and for error comparison of both schemes. In addition, it is used to study the effect of step size on the accuracy of solutions. The results shown in Figure 5.1 – 5.3 are the error terms as defined above at time level [1, 6]. Two points to emphasize with regard to Figure 5.1-5.3 are: (1) for this application, the FTCS scheme has minimum error in comparison with FTBSCS scheme, and the amount of error is decreased for the both schemes as the solution is marched in time. This error reduction is due to a decrease in the influence of the initial data.

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