Analytical and Numerical Solutions of Modified Convection-Diffusion Equation by Explicit Finite Difference Method

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ABSTRACT

This paper investigates the analytical and numerical solutions of the convection-diffusion equation, emphasizing its theoretical foundations, solution methodologies, and applications in engineering and environmental sciences. The study highlights the roles of convection (advection and buoyancy) and diffusion in transport phenomena, derives analytical solutions for simplified cases, and introduces numerical methods for addressing more complex scenarios.

The convection velocity u(t, x) in the Convection-Diffusion Equation (CDE) is computed by solving the viscous Burgers' equation using consistent numerical schemes. The stability conditions for these schemes are analytically derived, demonstrating that the FTCS (Forward Time Central Space) scheme outperforms the FTBSCS (Forward Time Backward Space Central Space) scheme in terms of time step selection. These stability conditions are further validated through numerical verification. Numerical simulations are conducted for various parameters, and the results are presented to illustrate the behavior of the solutions. Additionally, error comparisons between the two schemes are provided to evaluate the accuracy of the numerical solutions.

Keywords: Convection-Diffusion Equation, Burger’s Equation, Finite Difference Schemes, Stability Conditions.

INTRODUCTION

Burger’s equation was first introduced by Bateman [1], who provided its steady solutions. Later, it was explored by Burger [3], who applied it as a mathematical model for turbulence, and it is now widely referred to as Burger’s equation. As a nonlinear equation with known exact solutions, Burger's equation is crucial as a benchmark problem for numerical methods. The study of its general properties has garnered significant attention due to its applications in diverse fields, including number theory, gas dynamics, heat conduction, elasticity, and more. Benton and Platzman [2] provided an extensive survey of the exact solutions for the one-dimensional form of the equation. Numerous other researchers have employed various numerical techniques, such as finite-difference, finite-element, and boundary element methods, to solve this equation, especially for small kinematic viscosities (ν), which correspond to steep fronts in the propagation of dynamic waveforms.

The Convection-Diffusion Equation (CDE) is another crucial partial differential equation widely observed in engineering and industrial applications. It describes physical phenomena where particles move with a certain velocity, transferring from regions of higher concentration to regions of lower concentration. Analytical and numerical solutions to this equation, accompanied by initial and boundary conditions, are essential for understanding the distribution of contaminants or pollutants through open mediums such as air, rivers, and lakes, as well as porous mediums like aquifers. The CDE is fundamental in fields such as environmental engineering, mechanical engineering, heat transfer, soil science, and biology, with additional applications in soil physics, petroleum engineering, chemical engineering, and biosciences.

Historically, analytical solutions of the Advection-Diffusion Equation (ADE) were obtained by simplifying the equation to a diffusion equation, often by eliminating the advective terms. This simplification was achieved either by introducing moving coordinates Aral and Liao, 1996 [5]; Al-Niami and Rushton, 1977 [4]). Kumar et al., 2009 [6]). Various methods for solving the ADE, both analytically and numerically, have been explored in the literature [7-13].

In their work, Azad et al. [14] and Azad and Andallah [15] presented finite difference schemes for solving the Advection-Diffusion Equation (ADE). They applied the FTBSCS and FTCS techniques to obtain numerical solutions for prescribed initial and boundary conditions. The accuracy of these schemes was evaluated through error estimation relative to the exact solution of the ADE, and the numerical features, such as the rate of convergence, were also presented graphically.

Building on the above, this study focuses on solving the one-dimensional convection-diffusion equation using two finite difference schemes: FTBSCS and FTCS. The convection velocity u(t,x) is computed by solving the viscous Burger's equation using the same numerical schemes. The stability conditions for the schemes are analyzed, and their stability is numerically verified.

GOVERNING EQUATION AND NUMERICAL SCHEMES

2.1 Governing Equation

In this study, we consider variable advection velocity u(t, x). The Convection Diffusion Equation (CDE) governing the solute concentration c(t, x) is given by $\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2}$ where $c(t, x)$ is the solute concentration, and $u(t, x)$ represents the advection velocity, which is itself a function of time and position.

Since u(t,x) is a variable that must be determined, we need to solve for u(t,x) using an additional equation. For this, we select the viscous Burger's equation $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}$ where $\nu > 0$ is the kinetic viscosity coefficient. This equation is used to compute the variable velocity $u(t, x)$.

Thus, our problem is to solve the following system of partial differential equations (PDEs) simultaneously, as an initial-boundary value problem (IBVP).

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}, \qquad a < x < b, \quad t > 0, \qquad (1)$$

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2}, \qquad a < x < b, \quad t > 0, \qquad (2)$$

Here, $c(t, x)$ represents the solute concentration in the longitudinal direction at time t, measured in units of $[ML^{-3}]$. The parameter $\nu > 0$ is the coefficient of kinematic viscosity, D is the solute dispersion, is assumed to be independent of both position and time, is called dispersion coefficient $[L^2T^{-1}]$, t = time$[T]$; x = distance$[L]$ and, $u(t, x)$ satisfies the equation (1) while the concentration c(t,x) satisfies equation (2).

The problem is computed with the following initial and boundary conditions:

Initial Conditions:

$$u(x, 0) = f(x); \qquad c(x, 0) = f(x) \qquad\qquad a \le x < b \qquad (3)$$

Boundary conditions

$$\frac{\partial}{\partial x}u(t, a) = u_a(t)\,; \qquad \frac{\partial}{\partial x}u(t, b) = u_b(t) \qquad\qquad t_0 \le t \le T \qquad (4)$$

$$\frac{\partial}{\partial x}c(t, a) = c_a(t)\,; \qquad \frac{\partial}{\partial x}c(t, b) = c_b(t) \qquad\qquad t_0 \le t \le T \qquad (5)$$

where c_a, c_b, u_a, u_b represent the prescribed values of the velocity and concentration gradients at the boundaries.

The system of equations (1) and (2) along with the initial and boundary conditions (3) to (5), defines the problem to be solved.

2.2 Analytic solution

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

$c(\mathrm{x}, 0) = f(x)$ is given [13]

$$c(x,t) = \frac{M}{A\sqrt{4\pi D\mathrm{t}}} exp\left(-\frac{(x - (x_0 + ut))^2}{4D\mathrm{t}}\right) \tag{6}$$

where M = mass of tracer

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

2.3 Finite Difference Scheme

We consider the one–dimensional CDE 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 $c(t_0, x) = c_0(x);$ $\quad a \le x \le b$

and Neumann boundary conditions

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

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

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 the numerical solution of the one –dimensional linear convection- diffusion equation, we consider the IBVP

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

with initial condition $c(x, 0) = 0.02 \times e^{-10x},$ $\quad 0 \le x < l$

and Neumann boundary conditions

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

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

In order to develop the schemes, we discretize the *x-t* plane by choosing a spatial grid size $h \equiv \Delta\mathrm{x}$ and temporal grid size $k \equiv \Delta\mathrm{t}$. Then we can define the discrete grid points

$x_i = a + ih,\ i = 0, 1, 2, 3, \dots\dots\dots, M$ and $t_n = nk, n = 0, 1, 2, \dots\dots\dots, N$ where $M = (b - a)/h$ and $N = T/k$. Now we present two finite difference schemes as follows-

FINITE DIFFERENCE FORMULAE

Derivatives in the convection- diffusion equation are approximated by truncated Taylor Series expansions, which are follows-

$$\frac{\partial c}{\partial t} = \frac{c_i^{n+1} - c_i^n}{\Delta t} \text{ (1st order forward difference in time)} \quad (7)$$

$$\frac{\partial c}{\partial x} = \frac{c_i^n - c_{i-1}^n}{\Delta x} \text{ (1st order backward space difference formula)} \quad (8)$$

$$\frac{\partial c}{\partial x} = \frac{c_{i+1}^n - c_{i-1}^n}{2\Delta x} \text{ (1st order centered space difference formula)} \quad (9)$$

and

$$\frac{\partial^2 c}{\partial x^2} = \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{\Delta x^2} \text{ (2nd order centered space difference formula)} \quad (10)$$

3.1 Finite Difference (FTBSCS) Scheme

Substituting equations (7), (8), (10) into equation (1), (2) and rearranging according the time level,

(1) tends to

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + u_i^n \frac{u_i^n - u_{i-1}^n}{\Delta x} = \nu \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2},$$

$$\Rightarrow u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x} u_i^n (u_i^n - u_{i-1}^n) + \frac{\nu \Delta t}{\Delta x^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n),$$

$$\Rightarrow u_i^{n+1} = u_i^n - \gamma (u_i^n - u_{i-1}^n) + r (u_{i+1}^n - 2u_i^n + u_{i-1}^n)$$

$$We\ get, u_i^{n+1} = (\gamma + r) u_{i-1}^n + (1 - \gamma - 2r) u_i^n + r u_{i+1}^n, \quad (11)$$

$$where, \quad \gamma = \frac{\Delta t}{\Delta x} u_i^n, \quad r = \frac{\nu \Delta t}{\Delta x^2}$$

(2) tends to

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + u_i^n \frac{c_i^n - c_{i-1}^n}{\Delta x} = D \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{\Delta x^2},$$

$$\Rightarrow c_i^{n+1} = c_i^n - \frac{\Delta t}{\Delta x} u_i^n (c_i^n - c_{i-1}^n) + \frac{D \Delta t}{\Delta x^2} (c_{i+1}^n - 2c_i^n + c_{i-1}^n),$$

$$\Rightarrow c_i^{n+1} = c_i^n - \gamma (c_i^n - c_{i-1}^n) + \frac{D \Delta t}{\Delta x^2} (c_{i+1}^n - 2c_i^n + c_{i-1}^n)$$

$$We\ get, c_i^{n+1} = (\gamma + \lambda) c_{i-1}^n + (1 - \gamma - 2\lambda) c_i^n + \lambda c_{i+1}^n, \quad (12)$$

$$where, \quad \gamma = \frac{\Delta t}{\Delta x} u_i^n, \quad \lambda = \frac{D \Delta t}{\Delta x^2}$$

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3.2 Finite Difference (FTCS) Scheme

Substituting equations (7), (8), (10) into equation (1), (2) and rearranging according the time level,

(1) tends to

$$\frac{u_i^{n+1}-u_i^n}{\Delta t}+u_i^n\frac{u_{i+1}^n-u_{i-1}^n}{2\Delta x}=\nu\frac{u_{i+1}^n-2u_i^n+u_{i-1}^n}{\Delta x^2},$$

$$\Rightarrow\ u_i^{n+1}=u_i^n-\frac{\Delta t}{2\Delta x}u_i^n(u_{i+1}^n-u_{i-1}^n)+\frac{\nu\Delta t}{\Delta x^2}(u_{i+1}^n-2u_i^n+u_{i-1}^n),$$

$$\Rightarrow\ u_i^{n+1}=u_i^n-\frac{\gamma}{2}(u_{i+1}^n-u_{i-1}^n)+r(u_{i+1}^n-2u_i^n+u_{i-1}^n),$$

$$We\ get,\ \ u_i^{n+1}=\left(r+\frac{\gamma}{2}\right)u_{i-1}^n+(1-2r)u_i^n+\left(\mathrm{r}-\frac{\gamma}{2}\right)u_{i+1}^n,\qquad (13)$$

$$where,\quad \gamma=\frac{\Delta t}{\Delta x}u_i^n\,,\qquad r=\frac{\nu\Delta t}{\Delta x^2}$$

(2) tends to

$$\frac{c_i^{n+1}-c_i^n}{\Delta t}+u_i^n\frac{c_{i+1}^n-c_{i-1}^n}{2\Delta x}=D\frac{c_{i+1}^n-2c_i^n+c_{i-1}^n}{\Delta x^2},$$

$$\Rightarrow\ c_i^{n+1}=c_i^n-\frac{\Delta t}{2\Delta x}u_i^n(c_{i+1}^n-c_{i-1}^n)+\frac{D\Delta t}{\Delta x^2}(c_{i+1}^n-2c_i^n+c_{i-1}^n),$$

$$\Rightarrow\ c_i^{n+1}=c_i^n-\frac{\gamma}{2}(c_{i+1}^n-c_{i-1}^n)+\lambda(c_{i+1}^n-2c_i^n+c_{i-1}^n)$$

$$We\ get,\quad c_i^{n+1}=\left(\lambda+\frac{\gamma}{2}\right)c_{i-1}^n+(1-2\lambda)c_i^n+\left(\lambda-\frac{\gamma}{2}u_i^n\right)c_{i+1}^n,\qquad (14)$$

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

It is seen that the truncation errors for the forward and backward differences are of first order; whereas the centered difference yields a second order truncation error (using by Taylor Series expansions). Therefore, both the schemes outlined above are consistent.

STABILITY ANALYSIS

After surveying the relevant literature on the subject, we discover that no practical stability criterion exists for the schemes. We have developed stability conditions for both the schemes in the following two propositions and maintaining the criteria we verify the results of the schemes numerically in the next sections.

4.1 proposition 1

Statement: The stability conditions for the FTBSCS scheme are

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

This is guaranteed by the simultaneous inequalities

$0\le\frac{D\Delta t}{\Delta x^2}\le 1$ and $-\frac{D}{\Delta x}\le\max\,(u_i^0)\le\frac{\Delta x}{\Delta t}-2\frac{D}{\Delta x}$

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Proof:

The explicit centered difference scheme using by FTBSCS for CDE (2) is given by

$$c_i^{n+1} = (\gamma + \lambda)c_{i-1}^n + (1 - \gamma - 2\lambda)c_i^n + \lambda c_{i+1}^n, \qquad (15)$$

where $\gamma = \frac{\Delta t}{\Delta x} u_i^n$, $\lambda = \frac{D\Delta t}{\Delta x^2}$

The equation (12) implies that if

$0 \le \gamma + \lambda \le 1$ (i)

$0 \le 1 - \gamma - 2\lambda \le 1$ (ii)

$0 \le \lambda \le 1$ (iii)

then the new solution is a convex combination of the two previous solutions. That is the solution at new time-step (n+1) at a spatial node i is an average of the solutions at the previous time-step at the spatial-nodes i-1, i and i+1. This means that the extreme value of the new solution is the average of the extreme values of the previous two solutions at the three consecutive nodes. Therefore, the new solution continuously depends on the initial value $c_i^0,\ i = 1, 2, 3, \dots\dots\dots, M$.

(ii) implies $\gamma \le 1 - 2\lambda \le 1 + \gamma$ (iv)

(i) implies $-\lambda \le \gamma \le 1 - \lambda$

$$\therefore -\lambda \le \gamma \le 1 - 2\lambda \text{ by (iv)}$$

Therefore, the conditions are $0 \le \lambda \le 1$ and $-\lambda \le \gamma \le 1 - 2\lambda$

That is $0 \le \frac{D\Delta t}{\Delta x^2} \le 1$ and $-\frac{D\Delta t}{\Delta x^2} \le \frac{\Delta t}{\Delta x} u_i^n \le 1 - 2\frac{D\Delta t}{\Delta x^2}$

This is guaranteed by the simultaneous inequality

$0 \le \frac{D\Delta t}{\Delta x^2} \le 1$ and $-\frac{D}{\Delta x} \le \max\,(u_i^0) \le \frac{\Delta x}{\Delta t} - 2\frac{D}{\Delta x}$

4.2 Proposition 2

Statement: The stability conditions for the FTCS scheme are

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

This is guaranteed by the conditions $0 \le \frac{D\Delta t}{\Delta x^2} \le \frac{1}{2}$ and $-\frac{2D}{\Delta x} \le \max\,(u_i^0) \le 2\left(\frac{\Delta x}{\Delta t} - \frac{D}{\Delta x}\right)$.

Proof:

The explicit centered difference scheme using by FTCS for CDE (2) is given by

$$c_i^{n+1} = \left(\lambda + \frac{\gamma}{2}\right)c_{i-1}^n + (1 - 2\lambda)c_i^n + \left(\lambda - \frac{\gamma}{2}u_i^n\right)c_{i+1}^n, \qquad (16)$$

where $\gamma = \frac{\Delta t}{\Delta x} u_i^n$, $\lambda = \frac{D\Delta t}{\Delta x^2}$

The equation (13) implies that if

$0 \leq \lambda + \frac{\gamma}{2} \leq 1$ (i)

$0 \leq 1 - 2\lambda \leq 1$ (ii)

$0 \leq \lambda - \frac{\gamma}{2} \leq 1$ (iii)

then the new solution is a convex combination of the two previous solutions. That is, the solution at new time-step (n+1) at a spatial node i is an average of the solutions at the previous time-step at the spatial-nodes i-1, i and i+1. This means that the extreme value of the new solution is the average of the extreme values of the previous two solutions at the three consecutive nodes. Therefore, the new solution continuously depends on the initial value $c_i^0,\ i = 1, 2, 3, \dots\dots\dots. M$.

(ii) implies $0 \leq \lambda \leq \frac{1}{2}$ (iv)

(iii) implies $\lambda - 1 \leq \frac{\gamma}{2}$ (v)

(i) implies $-\lambda \leq \frac{\gamma}{2} \leq 1 - \lambda$ (vi)

From (v) & (vi), it follows that $-\lambda \leq \frac{\gamma}{2} \leq 1 - \lambda$

$$\therefore -2\lambda \leq \gamma \leq 2(1 - \lambda)$$

Therefore, (from (v), (vi)) the conditions are $0 \leq \lambda \leq \frac{1}{2}$ and $-2\lambda \leq \gamma \leq 2(1 - \lambda)$

That is $0 \leq \frac{D\Delta t}{\Delta x^2} \leq \frac{1}{2}$ and $-2\frac{D\Delta t}{\Delta x^2} \leq \frac{\Delta t}{\Delta x} u_i^n \leq 2\left(1 - \frac{D\Delta t}{\Delta x^2}\right)$.

This is guaranteed by the conditions $0 \leq \frac{D\Delta t}{\Delta x^2} \leq \frac{1}{2}$ and $-\frac{2D}{\Delta x} \leq \max\,(u_i^0) \leq 2\left(\frac{\Delta x}{\Delta t} - \frac{D}{\Delta x}\right)$

NUMERICAL SIMULATION AND RESULTS DISCUSSIONS

Various finite difference equations were used to represent the parabolic model equation (2). It is extremely important to experiment with the application of 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 solutions by the described schemes.

5.1 Numerical verification of Stability Conditions:

In this study, we assume that the length of spatial domain, l = 6 meters at all time, t = 1minute to t = 6 minutes with viscosity, $\nu = 0.01 m^2/s = 36\ m^2/h$ and diffusion coefficient, $D = 0.01 m^2/s = 36\ m^2/h$.

The convection-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.

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

I. Spatial step size, Δx = 0.05 m Temporal step size, Δt = 0.033s, Time, T = 60×2 sec
II. Spatial step size, Δx = 0.05 m Temporal step size, Δt = 0.067s, Time, T = 60×4 sec
III. Spatial step size, Δx = 0.05 m Temporal step size, Δt = 0.01s, Time, T = 60×6 sec

IV. Spatial step size, Δx = 0.05 m   Temporal step size, Δt = 0.1192s, Time, T =60×7.152 sec

Solutions:

Case *I.* When the step sizes are $\Delta x = 0.05$, $\Delta t = 0.033$.

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

The stability conditions of FTBSCS is determined by equation (12) as

$0 \leq \lambda \leq 1$ and $-\lambda \leq \gamma \leq 1 - 2\lambda$

This is guaranteed by the simultaneous inequalities

$$0 \leq \frac{D\Delta t}{\Delta x^2} \leq 1 \; and -\frac{D}{\Delta x} \leq \max\,(u_i^0) \leq \frac{\Delta x}{\Delta t} - 2\frac{D}{\Delta x}$$

The stability conditions of FTCS is determined by equation (13) as

$$0 \leq \lambda \leq \frac{1}{2} \; and - 2\lambda \leq \gamma \leq 2(1-\lambda)$$

This is guaranteed by the conditions $0 \leq \frac{D\Delta t}{\Delta x^2} \leq \frac{1}{2} \; and -\frac{2D}{\Delta x} \leq \max\,(u_i^0) \leq 2\left(\frac{\Delta x}{\Delta t} - \frac{D}{\Delta x}\right)$

$$where, \;\; \gamma = \frac{\Delta t}{\Delta x}\max\,(u_i^0)\,, \qquad \lambda = \frac{D\Delta t}{\Delta x^2}$$

For this particular application,

The value of $\max\left(u_i^0\right) = 0.02$ which satisfies the guaranteed inequality in both the schemes.

$\gamma = \frac{\Delta t}{\Delta x}\max\left(u_i^0\right) = \frac{0.033}{0.05} \times 0.02 = 0.0132 \; and \; \lambda = \frac{D\Delta t}{\Delta x^2} = \frac{0.01\times 0.033}{(0.05)^2} = 0.132$

FTBSCS $\Rightarrow 0 \leq 0.132 \leq 1 \; and - 0.132 \leq 0.0132 \leq 1 - 2\times 0.132 = 0.736$

and

FTCS $\Rightarrow 0 \leq 0.132 \leq \frac{1}{2} \; and - 0.264 \leq 0.0132 \leq 1.736$

Therefore, the stability conditions for both the schemes are satisfied and a stable solution is expected. The concentration profiles are to be obtained up to t = 2 minutes are shown in figure 5.1.

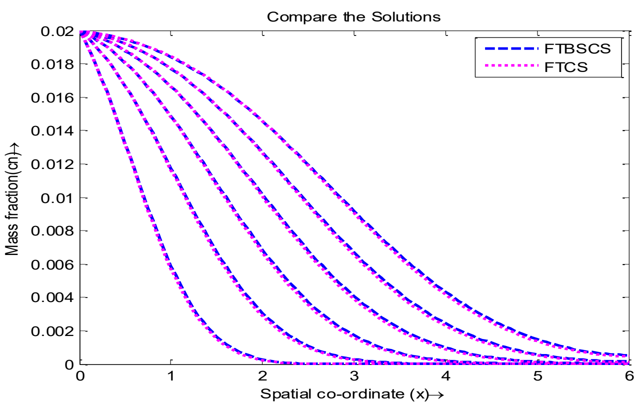

Figure 5.1: Concentration profiles with *Δx* = 0.05, *Δt* = 0.033

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Case *II*. When the step sizes are $\Delta x = 0.05$, $\Delta t = 0.067$.

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

The stability conditions of FTBSCS is determined by equation (12) as

$0 \leq \lambda \leq 1$ and $-\lambda \leq \gamma \leq 1 - 2\lambda$

This is guaranteed by the simultaneous inequalities

$0 \leq \frac{D\Delta t}{\Delta x^2} \leq 1$ and $-\frac{D}{\Delta x} \leq \max\left(u_i^0\right) \leq \frac{\Delta x}{\Delta t} - 2\frac{D}{\Delta x}$

The stability conditions of FTCS is determined by equation (13) as

$0 \leq \lambda \leq \frac{1}{2}$ and $-2\lambda \leq \gamma \leq 2(1 - \lambda)$

This is guaranteed by the conditions $0 \leq \frac{D\Delta t}{\Delta x^2} \leq \frac{1}{2}$ and $-\frac{2D}{\Delta x} \leq \max\left(u_i^0\right) \leq 2\left(\frac{\Delta x}{\Delta t} - \frac{D}{\Delta x}\right)$

where $\gamma = \frac{\Delta t}{\Delta x}\max\left(u_i^0\right)$, $\lambda = \frac{D\Delta t}{\Delta x^2}$

For this particular application,

The value of $\max\left(u_i^0\right) = 0.02$ which satisfies the guaranteed inequality in both the schemes.

$\gamma = \frac{\Delta t}{\Delta x}\max\left(u_i^0\right) = \frac{0.067}{0.05} \times 0.02 = 0.0268$ and $\lambda = \frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.067}{(0.05)^2} = 0.268$

FTBSCS $\Rightarrow 0 \leq 0.268 \leq 1$ and $-0.268 \leq 0.0268 \leq 1 - 2 \times 0.268 = 0.464$

and

FTCS $\Rightarrow 0 \leq 0.268 \leq \frac{1}{2}$ and $-0.536 \leq 0.0268 \leq 1.464$

Therefore, the stability conditions for both the schemes are satisfied and a stable solution is expected. The concentration profiles are to be obtained up to $t = 4$ minutes are shown in figure 5.2.

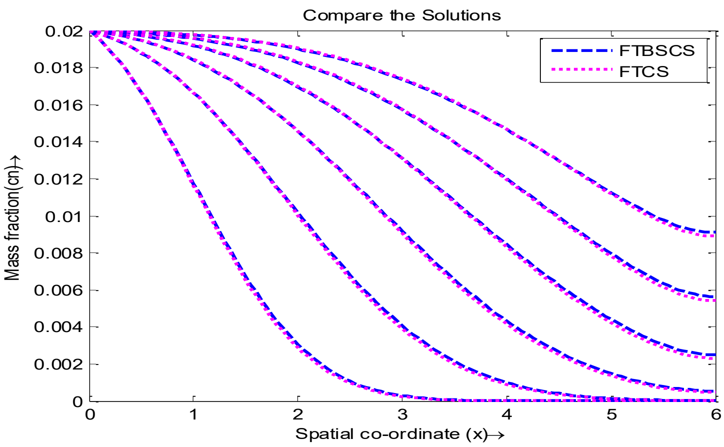

Figure 5.2: Concentration profiles with Δx = 0.05, Δt = 0.067

Case *III*. When the step sizes are $\Delta x = 0.05$, $\Delta t = 0.1$.

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

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The stability conditions of FTBSCS is determined by equation (12) as

$0 \leq \lambda \leq 1$ and $-\lambda \leq \gamma \leq 1 - 2\lambda$

This is guaranteed by the simultaneous inequalities

$0 \leq \frac{D\Delta t}{\Delta x^2} \leq 1$ and $-\frac{D}{\Delta x} \leq \max(u_i^0) \leq \frac{\Delta x}{\Delta t} - 2\frac{D}{\Delta x}$

The stability conditions of FTCS is determined by equation (13) as

$0 \leq \lambda \leq \frac{1}{2}$ and $-2\lambda \leq \gamma \leq 2(1 - \lambda)$

This is guaranteed by the conditions $0 \leq \frac{D\Delta t}{\Delta x^2} \leq \frac{1}{2}$ and $-\frac{2D}{\Delta x} \leq \max(u_i^0) \leq 2\left(\frac{\Delta x}{\Delta t} - \frac{D}{\Delta x}\right)$

where $\gamma = \frac{\Delta t}{\Delta x}\max(u_i^0)$, $\lambda = \frac{D\Delta t}{\Delta x^2}$

For this particular application,

The value of $\max(u_i^0) = 0.02$ which satisfies the guaranteed inequality in both the schemes.

$\gamma = \frac{\Delta t}{\Delta x}\max(u_i^0) = \frac{0.1}{0.05} \times 0.02 = 0.04$ and $\lambda = \frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.1}{(0.05)^2} = 0.4$

FTBSCS $\Rightarrow$ $0 \leq 0.4 \leq 1$ and $-0.4 \leq 0.04 \leq 1 - 2 \times 0.4 = 0.2$

and

FTCS $\Rightarrow 0 \leq 0.4 \leq \frac{1}{2}$ and $-0.8 \leq 0.04 \leq 1.2$

Therefore, the stability conditions for both the schemes are satisfied and a stable solution is expected. The concentration profiles are to be obtained up to t = 6 minutes are shown in figure 5.3.

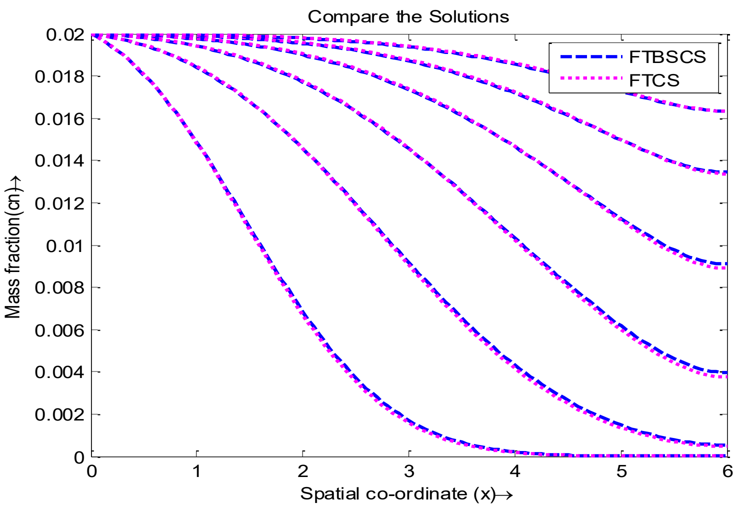

Figure 5.3: Concentration profiles with Δx = 0.05, Δt = 0.1

Case *IV*. When the step sizes are increased to Δx = 0.05, Δt = 0.1192,

The stability conditions of FTBSCS is determined by equation (12) as

$0 \leq \lambda \leq 1$ and $-\lambda \leq \gamma \leq 1 - 2\lambda$

This is guaranteed by the simultaneous inequalities

$0 \leq \frac{D\Delta t}{\Delta x^2} \leq 1$ and $-\frac{D}{\Delta x} \leq \max\,(u_i^0) \leq \frac{\Delta x}{\Delta t} - 2\frac{D}{\Delta x}$

The stability conditions of FTCS is determined by equation (13) as

$0 \leq \lambda \leq \frac{1}{2}$ and $-2\lambda \leq \gamma \leq 2(1-\lambda)$

This is guaranteed by the conditions $0 \leq \frac{D\Delta t}{\Delta x^2} \leq \frac{1}{2}$ and $-\frac{2D}{\Delta x} \leq \max\,(u_i^0) \leq 2\left(\frac{\Delta x}{\Delta t} - \frac{D}{\Delta x}\right)$

where $\gamma = \frac{\Delta t}{\Delta x}\max\,(u_i^0)$, $\lambda = \frac{D\Delta t}{\Delta x^2}$

For this particular application,

The value of $\max(u_i^0) = 0.02$ which satisfies the guaranteed inequality in both the schemes.

$\gamma = \frac{\Delta t}{\Delta x}\max\,(u_i^0) = \frac{0.1192}{0.05} \times 0.02 = 0.04768$ and $\lambda = \frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.1192}{(0.05)^2} = 0.4768$

FTBSCS $\Rightarrow 0 \leq 0.4768 \leq 1$ and $-0.4768 \leq 0.04768 \leq 0.0464$ which does not satisfy the stability condition of FTBSCS scheme, and

FTCS $\Rightarrow 0 \leq 0.4768 \leq \frac{1}{2}$ and $-0.9536 \leq 0.04768 \leq 1.0464$

In this case, FTBSCS of the CDE shows an instability which is shown in the following figure 5.4.

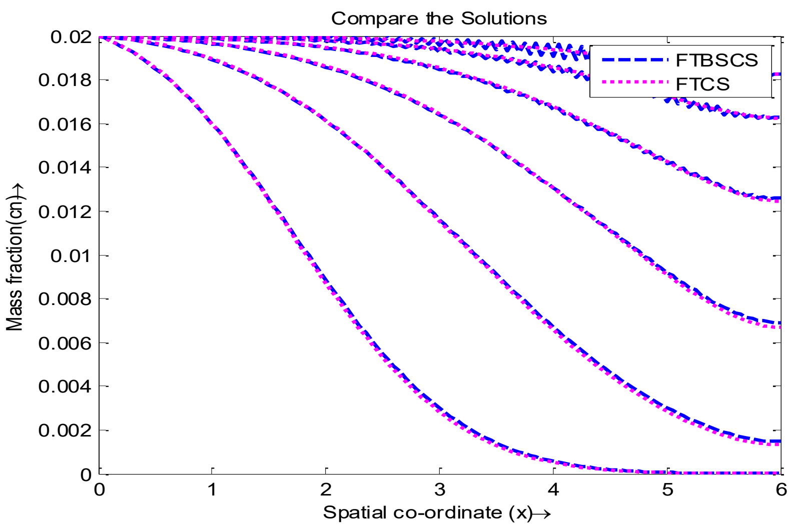

Figure 5.4: Concentration profiles with Δx = 0.05, Δt = 0.1192

ERROR ESTIMATION AND CONVERGENCE

We compute the relative error in L_1-norm which is defined as

$$err = \frac{\| c_e - c_n \|_1}{\| c_e \|_1} \quad (17)$$

where, c_e is the exact solution, and c_n is the numerical solution computed by the finite difference schemes for time $t \in [0, 6]$. The following **figure 6.1** shows the convergence of relative error by the scheme FTBSCS.

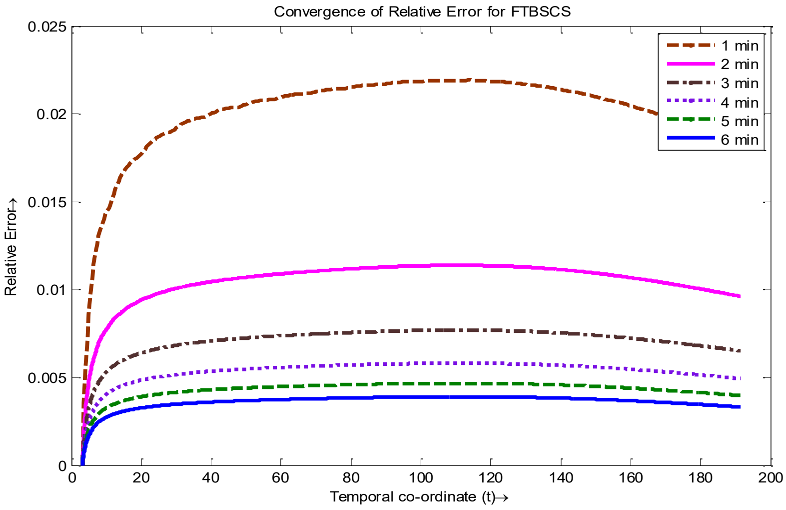

Figure 6.1 Rate of Numerical feature of Convergence

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

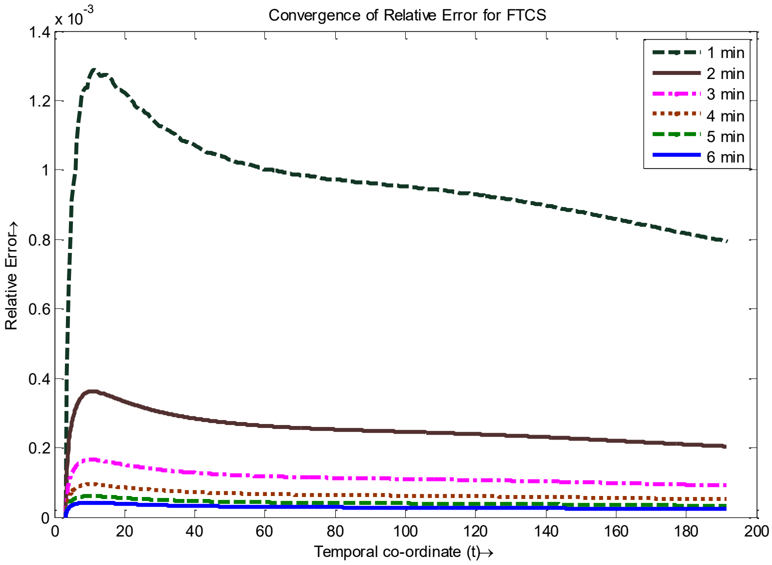

Figure 6.2 Rate of Numerical feature of Convergence

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

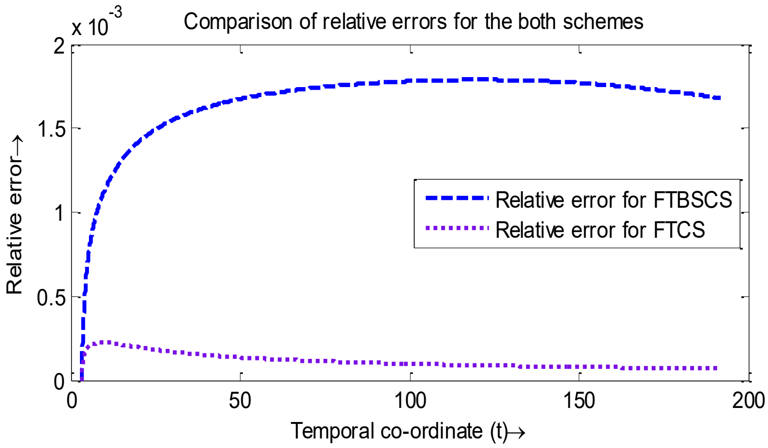

Figure 6.3 Comparison of relative errors for the both schemes

CONCLUSION

We have developed stability conditions and numerical solutions by using FTBSCS and FTCS schemes for convection diffusion equation with an initial condition and Neumann boundary conditions. The solution of Burger's equation is used as convection term in the CDE. Some numerical experiment is presented graphically.

In the Figure 5.1, 5.2, 5.3, it has been found that FTCS scheme gives better pointwise solution than FTBSCS scheme. In figure 5.4, an unstable solution is appeared by using FTBSCS scheme however, the solutions by using FTCS scheme is stable at the increased time step size $\Delta t = 0.1192$ and it is numerically shown that FTCS scheme is superior to FTBSCS scheme interms of time step selection.

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 6.1 – 6.3 are the error terms as defined above at time level [1, 6]. Two points to emphasize with regard to Figure 6.1-6.3 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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