COMPUTATION OF THE CONVECTION-DIFFUSION EQUATION BY THE FOURTH-ORDER COMPACT FINITE DIFFERENCE METHOD

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ABSTRACT

COMPUTATION OF THE CONVECTION-DIFFUSION EQUATION BY THE FOURTH-ORDER COMPACT FINITE DIFFERENCE METHOD

This dissertation aims to develop various numerical techniques for solving the one dimensional convection–diffusion equation with constant coefficient. These techniques are based on the explicit finite difference approximations using second, third and fourth-order compact difference schemes in space and a first-order explicit scheme in time. The suggested scheme has been seen to be very accurate and a relatively flexible solution approach in solving the contaminant transport equation for $Pe \leq 5$. For the solution, the combined technique has been used instead of conventional solution techniques. The accuracy and validity of the numerical model are verified. The computed results showed that the use of the current method in the simulation is very applicable for the solution of the convection-diffusion equation. The technique is seen to be alternative to existing techniques.

This dissertation is divided into six chapters: The derivation of the convective diffusion equation is given in Chapter 2. The main idea behind the higher order finite difference technique is given in Chapter 3. The numerical approximations to CDE described with ten different explicit schemes are introduced in Chapter 4. The results of numerical experiments using second, third and fourth-order compact difference schemes are presented in Chapter 5. Chapter 6 is devoted to a brief conclusion. Finally the references are introduced at the end.

ÖZET

KONVEKSİYON – DİFÜZYON DENKLEMİNİN DÖRDÜNCÜ MERTEBEDEN KOMPAK SONLU FARK METODU İLE ÇÖZÜMÜ

Bu tez, bir boyutlu sabit katsayılı konveksiyon-difüzyon denkleminin çözümü için bir çok sayısal metotlar geliştirmeyi amaçlamıştır. Bu teknikler sonlu zamanda birinci derece ve uzayda ikinci, üçüncü ve dördüncü dereceden kompak sonlu fark yaklaşımına dayanır. Sonlu fark denklemlerinin analizi Warming ve Hyett tarafından 1974'te geliştirilen, kısmi diferansiyel denklemine dayanır. Geliştirilen yöntem, Pe ≤ 5 için, kirlilik taşınım denkleminin çözümünde doğruluk ve esneklik özelliğine sahiptir. Çalışmada, geleneksel çözüm tekniği yerine, bileşik teknik kullanılmıştır. Uygulama sonuçları göstermiştir ki, kullanılan metot konveksiyon -difüzyon denkleminin çözümü için uygundur. Geliştirilen metot bu gibi denklemlerin çözümü için mevcut yöntemlere alternatif ve güvenilirdir.

Tez altı bölümden oluşmaktadır: Konveksiyon-difüzyon denkleminin elde edilişi Bölüm 2'de verilmiştir. Yüksek mertebeden sonlu fark tekniği Bölüm 3'te verilmiştir. CDE için on farklı açık şema sayısal çözümü metotları Bölüm 4'te verilmiştir. İkinci, üçüncü ve dördüncü dereceden kompak sonlu fark şeması kullanılarak yapılan sayısal çözüm sonuçları Bölüm 5'te verilmiştir. Sonuç kısmı Bölüm 6'da ve Kaynaklar tezin sonunda verilmiştir.

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CHAPTER 1

INTRODUCTION

Convection-Diffusion Equation (CDE) is a description of contaminant transport in porous media where advection causes translation of the solute field by moving the solute with the flow velocity and dispersion causes spreading of the solute plume. This equation reflects physical phenomena where in the diffusion process particles are moving with certain velocity form higher concentration to lower concentration. This process is described by the last term of the Convection-Diffusion Equation presented in equation (1.1). Second and third terms represent the concentration of the contaminant particles as respect to the change in distance and the acceleration in velocity gained over distance, respectively. The convection-diffusion equation in one-dimensional case, without source term, can be expressed as follows (Alkaya et al, 2013):

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} - D\frac{\partial^2 c}{\partial x^2} = 0 \quad , \text{where } 0 \le x \le L \text{ and } 0 \le t \le T \qquad (1.1)$$

The subscripts t and x stand for differentiation with respect to time and space, respectively. D is diffusion coefficient, $c(x,t)$ is concentration, $u(x,t)$ is velocity of water flow, and L is length of the channel, respectively. Equation (1.1) describes two processes: Convection and diffusion. Notice that $D > 0$ and $u > 0$ are considered to be positive constants quantifying the diffusion and convection processes, respectively. ADE is benefited in applications in different disciplines such as environmental engineering, mechanical engineering, soil science, petroleum engineering, chemical engineering and as well as in biology (Mazaheri et al,2013).

The initial condition can be: no concentration, constant concentration or a space-dependent concentration source as:

1. $c(x,0) = 0$ (1.2a)

2. $c(x,0) = c_0$ (1.2b)

3. $c(x,0) = c_0(x) \qquad where\ 0 \le x \le L$ (1.2c)

Boundary conditions can be fixed constant concentration and time–dependent concentration or fixed concentration and gradient B.C (or mixed) B.C:

$$\left.\begin{array}{l} 1.\ c(0,t) = f_0 \\ 2.\ c(L,t) = f_1(t) \\ 3.\ -D\frac{\partial c}{\partial x}|_{x=L} = g(t) \end{array}\right\} \quad where\ 0 \le t \le T \qquad (1.3)$$

where f_0, f_1 and g are prescribed functions whilst c is unknown function, concentration CDE is used in transfer of mass, heat, energy, velocity, etc. The solution of the equation models some of the phenomena such as the contaminant transport in groundwater, spread of pollutants in rivers, contaminant dispersion in shallow lakes and reservoirs. The slow progress has been made towards the analytical solutions of the ADE when initial and boundary conditions are intricate. Since many of the analytical solutions have not much easy use, many attempts have been carried out on developing the accurate numerical techniques. A number of numerical techniques have been recommended to illuminate physical phenomena described by the convection-diffusion equation in various fields of science. The difficulties arising in numerical solutions of the ADE results are due to the dominant convection that is for relatively high Peclet number (Sari et al,2010).

1.1. Related Works

In the following literature review, we present mathematical models used to solve the convection-diffusion equation and a critique is submitted to evaluate each model.

In (Juanes and Patzek, 2004), a numerical solution of miscible and immiscible flow in porous media was studied and focus was presented in the case of small diffusion; this turns linear convection-diffusion equation into hyperbolic equation.

In this effort, a stabilized finite element method was presented which arises from considering a multi-scale decomposition of the variable of interest into resolved and unresolved scales. This approach incorporates the effect of the fine (sub grid) scale onto the coarse (grid) scale. The numerical simulations clearly show the potential of the method for solving multiphase compositional flow in porous media.

In (Claassen, 2010), one-dimensional diffusion on the real line was studied through ignoring the effects of convection in the three dimensional equation, i.e. $u_t = k\nabla^2{}_u - \vec{v}.\nabla u$; was reduced to $u_t = ku_{xx} - vu_x$. The researcher made assumptions about k to be constant and $v = v(t)$ to be function of time only. The researcher obtained the one-dimensional diffusion equation by setting $v(t) \equiv 0$ to reach $u_t = ku_{xx}$. By coupling this equation with the initial condition $u(x,0) = \emptyset(x)$ and considering its domain to be the real line, he/she reached out the following initial value problem:

$$u_t = ku_{xx} \qquad (x \in R, t \in R^+)$$

$$u(x,0) = \emptyset(x)$$

One-dimensional diffusion equation was investigated against multiple properties such the invariance and the uniqueness of the solution. The solution to the convection-diffusion there was initiated by guessing a particular solution of the diffusion initial value problem; this guess was motivated by the invariance properties investigated earlier in the research. The researcher provides a methodology to solve the convection-diffusion equation by constructing solutions for any initial condition $\emptyset(x)$.

In (Ahmed, 2012), a novel finite difference method as well as a numerical scheme was presented to solve and analyze the convection-diffusion equation. The developed scheme was based on a mathematical combination between Siemieniuch and Gradwell approximation for time and Dehghan's approximation for spatial variable. In that work, a special discretization for the spatial variable was made in such a way that when applying the finite difference equation at any time level two nodes from both ends of the domain were left. Then, the unknowns at the two nodes adjacent to the boundaries were obtained from the interpolation technique. The proposed methodology was tested for their validity to solve advection-diffusion with constant and variable coefficients. Three different examples for advection-diffusion with constant coefficients were presented to study the effect of the some dependant variables. The results show a great agreement with analogue numerical methodologies.

In (Pereira et al, 2013), an evaluation of the first-order upwind and high-order flux-limiter for solving the advection-diffusion equation on unstructured grids, was accomplished. The numerical schemes were implemented as a module of an unstructured two-dimensional depth-averaged circulation model for shallow lakes (IPH-UnTRIM2D), and they were applied to the Guaiba River in Brazil. Their performances were evaluated by comparing mass conservation balance errors for two scenarios of a passive tracer released into the Guaiba River. The circulation model showed good agreement with observed data collected at four water level stations along the Guaiba River, where correlation coefficients achieved values up to 0.93. In addition, volume conservation errors were lower that 1% of the total volume of the Guaiba River. For all scenarios, the higher order flux-limiter scheme was shown to be less diffusive than a first-order upwind scheme.

Noye and Tan (1988) used a weighted discretization with the modified equivalent partial differential equation. Soon after, the authors extended this scheme to solve two- dimensional advection-diffusion equation (Noye and Tan, 1989). However, solution of two- and three- dimensional problems by using these methods was difficult due to requirement of matrix inversions at each time step. The upwind scheme (Spalding, 1972) and the flux-corrected scheme (Boris and Book, 1973) were available for the solution of the depth-averaged from of the advection-diffusion equation. An alternative widely used approach was the split-operation approach, in which the advection and diffusion terms were solved by two various numerical methods (Li and Chen, 1989; Sobey, 1983).

To solve the advection-diffusion equation accurately, various versions of the finite difference methods were used in the literature (Patel et al, 1985). Stability of their schemes for the advection-diffusion problems were carried out in several studies in the literature (Hindmarsh et al, 1984).

In (Kaya, 2010), the advection-diffusion equation (ADE) was solved using differential quadrature method (DQM), and results were compared to explicit finite difference method (EFDM), Implicit finite differences method (IFDM) and exact solution.

1.2. Definition of The Basic Terms of Advection – Diffusion Equation

In the following sections we present the definition of the basic terms of the advection-diffusion equation. It is essential to understand its physical meaning and mathematical representation in order to develop solution methodologies.

1.2.1. Diffusion

A fundamental transport process in environmental fluid mechanics is the diffusion. Diffusion differs from advection in that it is random in nature (i.e., it does not necessarily follow a fluid particle). A well-known example is the diffusion of perfume in an empty room. If a bottle of perfume is opened and allowed to evaporate into the air, soon the whole room will be scented. We know also from experience that the scent would be stronger near the source and weaker as we move away, but fragrance molecules would have wondered throughout space due to random molecular and turbulent motions. Thus, diffusion has two primary properties: it is random in nature, and transport occurs from regions of high concentration to low concentration, with an equilibrium state of uniform concentration.

In advection-diffusion equation (1.1), the term ($-D\frac{\partial^2 C}{\partial x^2}$) is the one-dimensional diffusive flux equation. It is important to note that diffusive flux is a vector quantity and, since concentrationis expressed in units of [$M/_{L^3}$], it has units of [$M/_{L^2T}$]. To compute the total mass flux rate m, in units [M/T], the diffusive flux must be integrated over a surface area (Sobey, 1983).

1.2.2. Advection (Convection)

Advection is the gradient of concentration of pollutant particles corresponding to distances and it is given by the term ($u\frac{\partial c}{\partial x}$), where u is flow velocity and can be constant. It is obvious that this term is one dimensional concentration gradient.

Both advection and diffusion move the pollutant from one place to another, but each accomplishes this in different ways. That is; advection moves in one way (i.e., in the flow direction downstream) while diffusion spreads out (i.e., regardless of a stream flow direction). Another important property is that advection is represented by first-order derivate, which means that if x is replaced by –x the term changes signs; this is the anti-symmetry, while by observing, diffusion term is introducing the symmetry property where if x is replaced by –x then the term does not change sign (Sobey, 1983).

1.2.3. Accumulation

This is the third term in the advection-diffusion equation as ($\frac{\partial c}{\partial t}$), represents the change of concentration over the time. This term is evaluated in term of the gradient (i.e., one direction or three dimensions). It represents the starting point to evaluate the movement of pollutant particles. It is important to mention that the advection and diffusion terms are proportional to each other and each term can dominate the entire system (Sobey, 1983).

CHAPTER 2

CONVECTION DIFFUSION EQUATION

In nature, transport occurs in fluids through the combination of convection and diffusion. The previous chapter introduced convection diffusion. This chapter gives the derivation of the convection diffusion equation.

2.1. Derivation of the Convective Diffusion Equation

Convection-Diffusion equation uses the mass balance approach. We form a continuity equation by equating the difference between the mass of material entering a volume element and that leaving the element (i.e., net influx of mass) to the rate of accumulation of mass inside the volume. The net influx is composed of terms involving dispersion and convection. The dispersion coefficient that appears in the dispersion component is assumed to be independent of concentration. In addition, it is assumed that the densities of viscosity of all the fluids in the system are the same and that no loss or addition of matter occurs within the system. For case of exposition, the development will be in terms of Cartesian coordinates. Consider a volume element of porous mediums in three - dimensional Cartesian coordinates (see Fig. 2.1). Since we are considering only convection and dispersion as the two modes of transport of a fluid within the porous medium, we can mathematically represent these two modes of transport (in the x-direction) as:

$$\text{transport by convection} = u\, C\, dA$$

$$\text{transport by dispersion} = D_x \frac{\partial C}{\partial x}\, dA$$

where dA is an elemental cross-sectional area of the cubic element, and D_x is the dispersion coefficient in the x-direction.

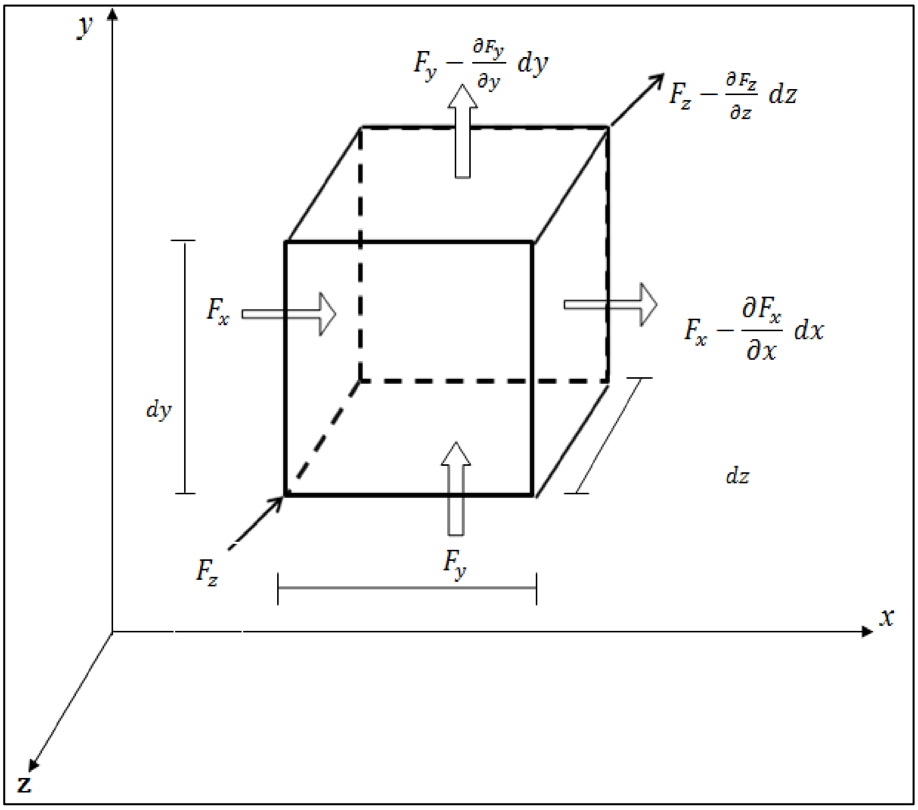


Figure 2.1. Mass balance in a volume element of a porous medium.

The total amount of fluid entering the volume element is:

$$\text{inflow} = F_x \text{dy dz} + F_y \text{ dz dx} + F_z \text{ dx dy}$$

where F_x , F_y, and F_z represent the total amount of mass per unit cross-sectional area transported in the x, y, and z directions, respectively.

Assuming that the two components (convection and dispersion) may be superposed, the total amount of material transported parallel to any given direction is obtained by summing the convective and dispersive transports. Thus,

$$F_x = uC \pm n\, D_x \left(\frac{\partial C}{\partial x}\right) \quad (2.1a)$$

$$F_y = vC \pm n\, D_y \left(\frac{\partial C}{\partial y}\right) \quad (2.1b)$$

$$F_z = wC \pm n\, D_z \left(\frac{\partial C}{\partial z}\right) \quad (2.1c)$$

where u, v, w are velocities in the x, y, and z directions, respectively, D_x , D_y , D_z are dispersion coefficients in the x, y, z directions, respectively, C is concentration of the material in the volume elements, n is porosity of the medium.

The negative sign indicates that the contaminant moves forward the zone of lower fluid concentration.

The total amount of solute leaving the volume element is:

$$\text{outflow} = (F_x - \frac{\partial F_x}{\partial_x}\text{dx})\,\text{dy dz} + (F_y - \frac{\partial F_y}{\partial_y}\text{dy})\,\text{dz dx} + (F_z - \frac{\partial F_z}{\partial_z}\text{dz})\,\text{dx dy}$$

where the partial terms indicate the spatial change of the fluid mass in the specified direction. Therefore,

$$\text{outflow} - \text{inflow} = -(\frac{\partial F_x}{\partial_x} + \frac{\partial F_y}{\partial_y} + \frac{\partial F_z}{\partial_z})\,\text{dx dy dz}$$

By continuity ($\Longrightarrow$ no loss in the mass of the liquid), the total difference between the outflow and the inflow of the volume element must be equal to the total change in time in the concentration of the material in the volume element. That is,

$$\text{outflow} - \text{inflow} = n\,\frac{\partial C}{\partial t} d_x d_y d_z$$

Yielding,

$$-\left(\frac{\partial F_x}{\partial_x} + \frac{\partial F_y}{\partial_y} + \frac{\partial F_z}{\partial_z}\right) = n\,\frac{\partial C}{\partial t} \qquad (2.2)$$

equation (2.2) is a mathematical statement of the law of conservation of mass under the conditions stipulated.

Substituting (2.1) into (2.2) gives:

$$\frac{\partial}{\partial_x}\left(n\,D_x\frac{\partial C}{\partial x} - uC\right) + \frac{\partial}{\partial y}\left(n\,D_y\frac{\partial C}{\partial y} - vC\right) + \frac{\partial}{\partial z}\left(n\,D_z\frac{\partial C}{\partial z} - wC\right) = n\,\frac{\partial C}{\partial t} \qquad (2.3)$$

If the flux per unit area is constant (i.e., u, v, and w are constants):

$$\frac{\partial}{\partial_x}\left(D_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right) = \frac{\partial C}{\partial t} + U\,\frac{\partial C}{\partial x} + V\,\frac{\partial C}{ay} + W\frac{\partial C}{\partial Z} \qquad (2.4)$$

where U, V, and W represent average velocities (i. e., U = u/n, V= v/n, and W= w/n).

Results of two-dimensional experiments indicate that the magnitudes of the dispersion coefficient depend on the direction of the flow, with the larger value oriented in the direction parallel to the flow. The inclusion of this directional dependency in the transport equations requires that the dispersion coefficient is to be represented as a tensor. Researchers have shown that for unidirectional flow in an isotropic porous medium the dispersion coefficient is described by a tensor composed of two components: longitudinal and transverse components (Marino, 1974).

The difficulties inherent in the application of the tensor to evaluate mass transport arise from difficulties in measuring the various components. Thus (as in heat flow or diffusions), it is generally necessary to assume that the dispersion coefficient is characterized by three independent components parallel to the chosen reference axes. Under this assumption, the dispersion tensor is a second-rank tensor consisting of nine components.

Using the standard notation for second-order tensors, the dispersion component of the transport equation can be expressed as:

$$-G_i = D_{ij}\frac{\partial C}{\partial x_j}(i, j = 1, 2, 3) \tag{2.5}$$

In other words, the three components of mass transport are written as:

$$-G_1 = D_{11}\frac{\partial C}{\partial x_1} + D_{12}\frac{\partial C}{\partial x_2} + D_{13}\frac{\partial C}{\partial x_3} \tag{2.6a}$$

$$-G_2 = D_{21}\frac{\partial C}{\partial x_1} + D_{22}\frac{\partial C}{\partial x_2} + D_{23}\frac{\partial C}{\partial x_3} \tag{2.6b}$$

$$-G_3 = D_{31}\frac{\partial C}{\partial x_1} + D_{32}\frac{\partial C}{\partial x_2} + D_{33}\frac{\partial C}{\partial x_3} \tag{2.6c}$$

and the dispersion tensor can be represented by a matrix:

$$D_{ij} = \begin{pmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{pmatrix}$$

The advantage of the tensor notation is that it provides a shorthand method of describing (in general) the physical phenomena. It can be shown that the general form of the convective-dispersion equation for a homogeneous and isotropic porous medium is expressed as follows:

$$\frac{\partial}{\partial x_j}\left(D_{ij}\frac{\partial C}{\partial x_j} - u_i c\right) = \frac{\partial C}{\partial t} \qquad , (i, j = 1, 2, 3) \tag{2.7}$$

The equation describing the field distribution for a system of anisotropic mass transport is expressed as:

$$D_{11}\frac{\partial^2 C}{\partial x^2} + D_{22}\frac{\partial^2 C}{\partial y^2} + D_{33}\frac{\partial^2 C}{\partial z^2} + (D_{12} + D_{21})\frac{\partial^2 C}{\partial x\,\partial y} + (D_{13} + D_{31})\frac{\partial^2 C}{\partial z\,\partial x} + (D_{23} + D_{32})\frac{\partial^2 C}{\partial y\,\partial z} = \frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} + V\frac{\partial C}{\partial y} + W\frac{\partial C}{\partial z} \tag{2.8}$$

Equation (2.8) is known as a quadric, and by the use of standard transformations it can be reduced to the form of Equation (2.4). This transformation involves rotating the coordinate axes so that the reference axes parallel the principal axes of dispersion.

Recent experimental and analytical studies point to the fact that in isotropic and homogeneous media, the principal axes of dispersion are oriented parallel and transverse to the mean direction of regional flow. This indicates that for homogeneous isotropic media, the mass transport system can be defined by two characteristic dispersion components that are specified when the mean direction of regional flow is known (Marino, 1974).

Assuming that the principal axes can be defined, the dispersion tensor can be transformed so that only the elements of the major diagonal remain, all others being zero. The matrix representation of the tensor then becomes:

$$D_{ij} = \begin{pmatrix} D_x & 0 & 0 \\ 0 & D_y & 0 \\ 0 & 0 & D_z \end{pmatrix}$$

In unidirectional flow, symmetry about the mean flow line exists so that Dy = Dz. For steady unidirectional flow in the x-direction, the mass transport equation can be written as:

$$D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} = \frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} \tag{2.9}$$

where D_x is longitudinal dispersion coefficient (also represented as D_L); D_y is transverse or lateral dispersion coefficient (also represented as D_T); U is average seepage velocity (U_{Darcy} / porosity).

If the lateral variation in concentration is assumed to be insignificant, then Eqution (2.9) becomes:

$$D_x \frac{\partial^2 C}{\partial x^2} = \frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} \tag{2.10}$$

2.2. Boundary and Initial Conditions

Boundary conditions associated with a linear second order partial differential equation: L(C) = G (t, x) for t, x ∈ R, can be written in the operator form as:

$$B(C) = f(t, x) \qquad \text{for } t, x \in \partial R, \tag{2.11}$$

where ∂R denotes the boundary of the region R and f (t, x) is a given function of t and x. If the boundary operator B(C) = C, the boundary condition represents the dependent variable being specified on the boundary. These types of boundary conditions are called Dirichlet conditions. If the boundary operator $B(C) = \frac{\partial C}{\partial n} = \text{grad } C \cdot \hat{n}$ denotes a normal derivative, then the boundary condition is that the normal derivative at each point of the boundary is being specified. These types of boundary conditions are called Neumann type conditions. Neumann conditions require the boundary to be such that one can calculate the normal derivative $\frac{\partial C}{\partial n}$ at each point of the boundary of the given region R. This requires that the unit exterior normal vector $\hat{n}$ be known at each point of the boundary. If the boundary operator is a linear combination of the Dirichlet and Neumann boundary conditions, then the boundary operator has the form $B(C) = \propto \frac{\partial C}{\partial n} + \beta C$, where α and β are constants. These types of boundary conditions are said to be of the Robin type. The partial differential equation together with a Dirichlet boundary condition is sometimes referred to as a boundary value problem of the second kind. A partial differential equation with a Neumann boundary condition is sometimes referred to as a boundary value problem of the second kind. A boundary value problem of the third kind is a partial differential equation with a Robin type boundary condition. A partial differential equation with a boundary condition of the form:

$$B(C) = \begin{cases} C, & \text{for } t, x \in \partial R_1 , \quad \partial R_1 \cap \partial R_2 = \emptyset \\ \dfrac{\partial C}{\partial n} & \text{for } t, x \in \partial R_2 , \quad \partial R_1 \cap \partial R_2 = \partial R \end{cases} \tag{2.12}$$

is called a mixed boundary value problem. If time t is one of the independent variables in a partial differential equation, then a given condition to be satisfied at the time t = 0 is referred to as an initial condition. A partial differential equation subject to both boundary and initial conditions is called a boundary-initial value problem (Alexander, 2005).

2.3. Robin Boundary Condition

The Robin boundary condition, or third type boundary condition, is a type of boundary condition, named after Victor Gustave Robin (1855–1897). When imposed on a partial differential equation, it is a specification of a linear combination of the values of a function and the values of its derivative on the boundary of the domain. Robin boundary conditions are a weighted combination of Dirichlet boundary conditions and Neumann boundary conditions. This contrasts to mixed boundary conditions, which are boundary conditions of different types specified on different subsets of the boundary. Robin boundary conditions are also called impedance boundary conditions, due to their application in electromagnetic problems.

If R is the domain on which the given equation is to be solved and ∂R denotes its boundary, the Robin boundary condition is expressed as:

$$\propto C + \beta \frac{\partial C}{\partial n} = g \quad , \text{on } \partial R \tag{2.13}$$

for some non-zero constants α and β and a given function g defined on ∂R. Here, C is the unknown solution defined on R and $\frac{\partial C}{\partial n}$ denotes the normal derivative at the boundary. More generally, α and β are allowed to be (given) functions, rather than constants.

In one dimension, if, for example, $R = [0,1]$ the Robin boundary condition becomes the conditions:

$$\propto C(0,t) - \beta \frac{\partial C}{\partial x}(0,t) = g(0,t) \tag{2.14a}$$

$$\propto C(1,t) + \beta \frac{\partial C}{\partial x}(1,t) = g(1,t) \tag{2.14b}$$

where $0 < t \leq T$. Notice the change of sign in front of the term involving a derivative: that is because the normal to [0,1] at 0 points in the negative direction, while at 1 it points in the positive direction.

The Robin boundary condition is a general form of the insulating boundary condition for convection–diffusion equations. Here, the convective and diffusive fluxes at the boundary sum to zero:

$$u_x(0,t)C(0,t) - D\frac{\partial C(0,t)}{\partial x} = 0 \tag{2.15}$$

where D is the diffusive constant, u is the convective velocity at the boundary and c is the concentration. The second term is a result of Fick's law of diffusion (Gustafson, 1998; Eriksson et al, 2004).

CHAPTER 3

HIGHER-ORDER FINITE DIFFERENCE SCHEMES

In this chapter, we review the calculus of finite differences. The Taylor expansion provides a very useful tool for the derivation of higher-order approximation to derivatives of any order.

3.1. Finite Difference Approximations of the Derivatives

The main idea behind the finite difference methods for obtaining the solution of a given partial differential equation is to approximate the derivatives appearing in the equation by a set of values of the function at a selected number of points. The most usual way to generate these approximations is through the use of Taylor series. The numerical techniques developed here are based on the modified equivalent partial differential equation as described by Warming and Hyett (1974).

This approach allows the simple determination of the theoretical order of accuracy, thus allowing methods to be compared with one another. Also from the truncation error of the modified equivalent equation, it is possible to eliminate the dominant error terms associated with the finite difference equations that contain free parameters (weights), thus leading to more accurate methods (Dehghan, 2004).

To derive a numerical approximation to the governing equation, one replaces derivatives by the difference equation using the discrete nodal values. Figure 3.1 schematically shows finite difference discretization in space and time. According to Figure 3.1, $\Delta t = k$ = time step, $\Delta x = h$ = space step and C(t,x) is solution at nodals

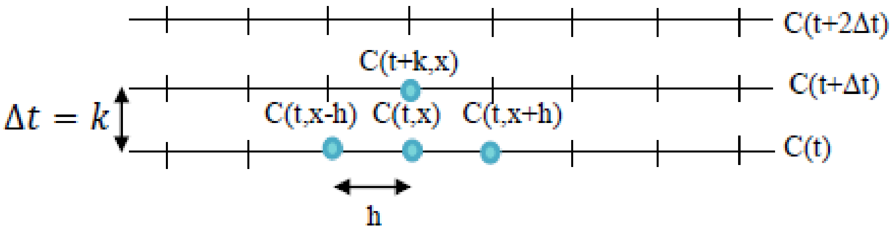


Figure 3.1. Scheme representation of finite difference

3.1.1. The Time Derivative

The approximation for the time derivative can be found by using Taylor series expansion as:

$$C(t+k) = C(t) + \frac{\partial C(t)}{\partial t} k + \frac{\partial^2 C(t)}{\partial t^2}\frac{k^2}{2!} + \cdots \tag{3.1}$$

where k = Δt discretization step size (see Figure 3.1). Solving equation (3.1) for the time derivative gives:

$$\frac{\partial C(t)}{\partial t} = \frac{C(t+k) - C(t)}{k} - \frac{\partial^2 C(t)}{\partial t^2}\frac{k}{2!} + \cdots$$

Considering only the first term a right hand side,

$$\left(\frac{\partial C}{\partial t}\right)_j = \frac{C_{j+1} - C_j}{k} + O(k) \tag{3.2}$$

where C_{j+1} = C (t+k), C_j = C (t) . In short; forward difference: $\left(\frac{\partial C}{\partial t}\right)_j = \frac{C_{j+1} - C_j}{k}$ and Truncation error = O (k) = $-\frac{k}{2}\frac{\partial^2 C(t)}{\partial t^2}$ are obtained.

3.1.2. Arbitrary-Order Approximations of Derivatives

Finite-difference approximations of arbitrary order can be obtained systematically (e.g., Celia and Gray 1992). The approximation of $\partial^m C/\partial x^m$, which is the mth derivative of C, can be obtained by expanding the derivative across q discrete nodes in the x-direction. If the independent variable is time, the derivative can be expanded along q time steps. The minimum number of nodes allowed in the expansion is m + 1. In general, the maximum order of approximation of a finite difference solution is q−m, although it may be smaller or larger for some individual cases. For instance, when m is even and the grid spacing is constant, the order of approximation can by increased to q − m + 1. Figure 3.2 shows the arbitrary grid spacing for the derivation to come.

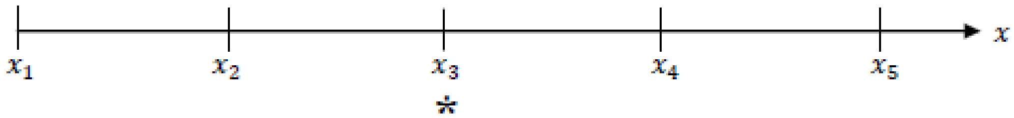


Figure 3.2. Grid spacing of an arbitrary-spaced grid where q=5. The derivative is taken at node point x_3, marked$*$.

The location at which the derivative is taken does not need to correspond to a node point, although in the figure the derivative is assumed to be taken at node point x_3. The distance between two node points is $\Delta x_i = x_{i+1} - x_i$, where i varies from 1 to q – 1 (Jacobson,2005).

For example; considering there are 6 points; for the 2^{nd} approximate, if m=2 (2^{nd}derivative) and q=10 (i.e. 10 nodes) then q-m=8 (i.e. we can have a maximum 8-order approximation for the second derivative)

3.2. Fourth– Order Difference Approximation of $\frac{\partial C}{\partial x}$

It would be beneficial to recall the single finite difference (1^{st}order) approximation to the 1^{st} derivatives as follows:

$$\left(\frac{\partial C}{\partial x}\right)_i \simeq \frac{C_{i+1}-C_i}{h} \qquad \text{Forward difference}$$

$$\left(\frac{\partial C}{\partial x}\right)_i \simeq \frac{C_i-C_{i-1}}{h} \qquad \text{Backward difference}$$

$$\left(\frac{\partial C}{\partial x}\right)_i \simeq \frac{C_{i+1}-C_{i-1}}{2h} \qquad \text{Central difference}$$

where $\Delta x = h$ (discretization step), $C_i = C(x_i)$, $C_{i+1} = C(x_i + h)$, $C_{i-1} = C(x_i - h)$ and x_i is discretization point. Taylor series expansion is always used to obtain higher order approximation as follows:

$$C(x) = \sum_{n=0}^{\infty} \frac{(x - x_i)^n}{n!} \left(\frac{\partial^n c}{\partial x^n}\right)_i \tag{3.3}$$

3.2.1. Fourth-Order Forward Difference Approximation of $\frac{\partial C}{\partial x}$

This is found by using a Taylor series (3.3). We start the procedure by expressing the value of C_{i+1}, C_{i+2}, $C_{i+3}$and C_{i+4} in terms of as Ci follows:

$$C_{i+1} = C_i + h\left(\frac{\partial C}{\partial x}\right)_i + \frac{h^2}{2}\left(\frac{\partial^2 C}{\partial x^2}\right)_i + \frac{h^3}{6}\left(\frac{\partial^3 C}{\partial x^3}\right)_i + \frac{h^4}{24}\left(\frac{\partial^4 C}{\partial x^4}\right)_i + \frac{h^5}{120}\left(\frac{\partial^5 C}{\partial x^5}\right)_i + \ldots \quad (3.4)$$

$$C_{i+2} = C_i + 2h\left(\frac{\partial C}{\partial x}\right)_i + \frac{(2h)^2}{2}\left(\frac{\partial^2 C}{\partial x^2}\right)_i + \frac{(2h)^3}{6}\left(\frac{\partial^3 C}{\partial x^3}\right)_i + \frac{(2h)^4}{24}\left(\frac{\partial^4 C}{\partial x^4}\right)_i + \frac{(2h)^5}{120}\left(\frac{\partial^5 C}{\partial x^5}\right)_i + \cdots \quad (3.5)$$

$$C_{i+3} = C_i + 3h\left(\frac{\partial C}{\partial x}\right)_i + \frac{(3h)^2}{2}\left(\frac{\partial^2 C}{\partial x^2}\right)_i + \frac{(3h)^3}{6}\left(\frac{\partial^3 C}{\partial x^3}\right)_i + \frac{(3h)^4}{24}\left(\frac{\partial^4 C}{\partial x^4}\right)_i + \frac{(3h)^5}{120}\left(\frac{\partial^5 C}{\partial x^5}\right)_i + \cdots \quad (3.6)$$

$$C_{i+4} = C_i + 4h\left(\frac{\partial C}{\partial x}\right)_i + \frac{(4h)^2}{2}\left(\frac{\partial^2 C}{\partial x^2}\right)_i + \frac{(4h)^3}{6}\left(\frac{\partial^3 C}{\partial x^3}\right)_i + \frac{(4h)^4}{24}\left(\frac{\partial^4 C}{\partial x^4}\right)_i + \frac{(4h)^5}{120}\left(\frac{\partial^5 C}{\partial x^5}\right)_i + \cdots \quad (3.7)$$

As such, we can express the first derivative by multiplying equations (3.4), (3.5), (3.6) and (3.7) by the coefficients β, γ, δ and θ respectively. Then taking the summation of these four equations, one obtains the following expressions:

$$\beta\, C_{i+1} + \gamma\, C_{i+2} + \delta\, C_{i+3} + \theta\, C_{i+4}$$

$$= \frac{1}{h}\Big[\beta C_i + h\beta\left(\frac{\partial C}{\partial x}\right)_i + \frac{h^2}{2}\beta\left(\frac{\partial^2 C}{\partial x^2}\right)_i + \frac{h^3}{6}\beta\left(\frac{\partial^3 C}{\partial x^3}\right)_i + \frac{h^4}{24}\beta\left(\frac{\partial^4 C}{\partial x^4}\right)_i$$

$$+ \frac{h^5}{120}\beta\left(\frac{\partial^5 C}{\partial x^5}\right)_i + \ \ldots + \gamma C_i + 2h\gamma\left(\frac{\partial C}{\partial x}\right)_i + 2h^2\gamma\left(\frac{\partial^2 C}{\partial x^2}\right)_i$$

$$+ \frac{8}{6}h^3\gamma\left(\frac{\partial^3 C}{\partial x^3}\right)_i + \frac{16}{24}h^4\gamma\left(\frac{\partial^4 C}{\partial x^4}\right)_i + \frac{32}{120}h^5\gamma\left(\frac{\partial^5 C}{\partial x^5}\right)_i + \cdots + \delta C_i$$

$$+ 3h\delta\left(\frac{\partial C}{\partial x}\right)_i + \frac{9}{2}h^2\delta\left(\frac{\partial^2 C}{\partial x^2}\right)_i + \frac{27}{6}h^3\left(\frac{\partial^3 C}{\partial x^3}\right)_i + \frac{81}{24}h^4\left(\frac{\partial^4 C}{\partial x^4}\right)_i$$

$$+ \frac{243}{120}h^5\left(\frac{\partial^5 C}{\partial x^5}\right)_i + \cdots + \theta C_i + 4h\theta\left(\frac{\partial C}{\partial x}\right)_i + \frac{16}{2}h^2\theta\left(\frac{\partial^2 C}{\partial x^2}\right)_i$$

$$+ \frac{64}{6}h^3\theta\left(\frac{\partial^3 C}{\partial x^3}\right)_i + \frac{256}{24}h^4\theta\left(\frac{\partial^4 C}{\partial x^4}\right)_i + \frac{1024}{120}h^5\theta\left(\frac{\partial^5 C}{\partial x^5}\right)_i + \cdots\Big] \qquad (3.8)$$

Upon rearrangement of equation (3.8):

$$\beta\, C_{i+1} + \gamma\, C_{i+2} + \delta\, C_{i+3} + \theta\, C_{i+4}$$

$$= \frac{1}{h}(\beta + \gamma + \delta + \theta)C_i + (\beta + 2\gamma + 3\delta + 4\theta)\left(\frac{\partial C}{\partial x}\right)_i$$

$$+ \frac{h}{2}(\beta + 4\gamma + 9\delta + 16\theta)\left(\frac{\partial^2 C}{\partial x^2}\right)_i + \frac{h^2}{6}(\beta + 8\gamma + 27\delta + 64\theta)\left(\frac{\partial^3 C}{\partial x^3}\right)_i$$

$$+ \frac{h^3}{24}(\beta + 16\gamma + 81\delta + 256\theta)\left(\frac{\partial^4 C}{\partial x^4}\right)_i$$

$$+ \frac{h^4}{120}(\beta + 32\gamma + 243\delta + 1024\theta)\left(\frac{\partial^5 C}{\partial x^5}\right)_i \qquad (3.9)$$

At this stage; in order to satisfy the accurate fourth order in equation (3.9), we need to find the values of the coefficients β, γ, δ and θ such that the coefficient of $\left(\frac{\partial C}{\partial x}\right)_i$ must equal 1 and the coefficients of $\left(\frac{\partial^2 C}{\partial x^2}\right)_i$, $\left(\frac{\partial^3 C}{\partial x^3}\right)_i$ and $\left(\frac{\partial^4 C}{\partial x^4}\right)_i$ must be zeros and the coefficient of $\left(\frac{\partial^5 C}{\partial x^5}\right)_i$ should be not zero. Thus, one obtains the following linear equations to be solved:

$$E_1: \quad \beta + 2\gamma + 3\delta + 4\theta = 1$$

$$E_2: \quad \beta + 4\gamma + 9\delta + 16\theta = 0 \tag{3.10}$$

$$E_3: \quad \beta + 8\gamma + 27\delta + 64\theta = 0$$

$$E_4: \quad \beta + 16\gamma + 81\delta + 256\theta = 0$$

where equation (3.10) has truncation error as:

$$(\mathrm{T.E}) = \frac{h^4}{120}(\beta + 32\gamma + 243\delta + 1024\theta)\left(\frac{\partial^5 C}{\partial x^5}\right)_i \tag{3.11}$$

The four equations (3.10) are solved for the unknowns α, β, γ, δ and θ. The first step is to use equation E2 to eliminate the unknown β from E3, E4 and E5 by performing:

$(E_2\text{-}E_1) \longrightarrow E_2$

$(E_3\text{-}E_1) \longrightarrow E_3$

$(E_4\text{-}E_1) \longrightarrow E_4$

The resulting system is:

$$E_1: \quad \beta + 2\gamma + 3\delta + 4\theta = 1$$

$$E_2: \quad 2\gamma + 6\delta + 12\theta = -1 \tag{3.12}$$

$$E_3: \quad 6\gamma + 24\delta + 60\theta = -1$$

$$E_4: \quad 14\gamma + 78\delta + 252\theta = -1$$

where the new equations (3.12) are for simplicity, again labeled E_1, E_2, E_3 and E_4. In the new system (3.12), E_2 is used to eliminate γ from E_3 and E_4 by the operations:

$(E_3\text{-}3E_2) \longrightarrow E_3$

$(E_4\text{-}7E_2) \longrightarrow E_4$

Resulting in the system

$$
\begin{aligned}
E_1: &\quad \beta + 2\gamma + 3\delta + 4\theta = 1 \\
E_2: &\quad 2\gamma + 6\delta + 12\theta = -1 \\
E_3: &\quad 6\delta + 24\theta = 2 \\
E_4: &\quad 36\delta + 168\theta = 6
\end{aligned}
\tag{3.13}
$$

where the new equations (3.13) are, for simplicity, again labeledE_1, E_2, $E_3$and E_4.

In the new system (3.13), E_3 is used to eliminate δ from E_4 by the operation:

$(E_4\text{-}6E_3) \longrightarrow E_4$

Resulting in the system:

$$
\begin{aligned}
E_1: &\quad \beta + 2\gamma + 3\delta + 4\theta = 1 \\
E_2: &\quad 2\gamma + 6\delta + 12\theta = -1 \\
E_3: &\quad 6\delta + 24\theta = 2 \\
E_4: &\quad 24\theta = -6
\end{aligned}
\tag{3.14}
$$

The system of equations (3.14) is now in reduced form and can easily be solved for the unknown by a backward-substation process:

Noting that E5 implies: $\theta = -\frac{3}{12}$

E_3 can be solved for δ:

$$\delta = \frac{1}{6}[2 - 24\theta] = \frac{1}{6}\left[2 - 24\left(-\frac{3}{12}\right)\right] = \frac{1}{6}[2 + 6]$$

$$\delta = \frac{16}{12}$$

Continuing E_2 and E_1 gives: $\gamma = -\frac{36}{12}$ and $\beta = \frac{48}{12}$

It can easily be verified that these values satisfies the equations in (3.9). Substituting solution into equations (3.8) and (3.9) yields:

The fourth-order forward-difference approximation of $\frac{\partial C}{\partial x}$

$$\left(\frac{\partial C}{\partial x}\right)_i \backsimeq \frac{-25C_i + 48C_{i+1} - 36C_{i+2} + 16\,C_{i+3} + 3\,C_{i+4}}{12\,h} \tag{3.15}$$

and the truncation error (T.E)= $O(h^4) = \frac{h^4}{120}(\beta + 32\gamma + 243\delta + 1024\theta)\left(\frac{\partial^5 C}{\partial x^2}\right)_i$

$$= \frac{h^4}{120}\left(\frac{48}{12} - \frac{32 * 36}{12} + \frac{243 * 16}{12} - \frac{3 * 1024}{12}\right)\left(\frac{\partial^5 C}{\partial x^5}\right)_i$$

$$\text{T.E} \;= -\frac{h^4}{5}\left(\frac{\partial^5 C}{\partial x^5}\right)_i$$

3.2.2. Fourth-Order Backward Difference Approximation of $\frac{\partial C}{\partial x}$

It is found by using a Taylor series (3.3). Start by expressing the value of C_{i-1}, C_{i-2}, C_{i-3} and C_{i-4} in terms of C_i:

$$C_{i-1} = C_i - h\left(\frac{\partial C}{\partial x}\right)_i + \frac{h^2}{2}\left(\frac{\partial^2 C}{\partial x^2}\right)_i - \frac{h^3}{6}\left(\frac{\partial^3 C}{\partial x^3}\right)_i + \frac{h^4}{24}\left(\frac{\partial^4 C}{\partial x^4}\right)_i - \frac{h^5}{120}\left(\frac{\partial^5 C}{\partial x^5}\right)_i + \cdots \tag{3.16}$$

$$C_{i-2} = C_i - 2h\left(\frac{\partial C}{\partial x}\right)_i + \frac{(2h)^2}{2}\left(\frac{\partial^2 C}{\partial x^2}\right)_i - \frac{(2h)^3}{6}\left(\frac{\partial^3 C}{\partial x^3}\right)_i + \frac{(2h)^4}{24}\left(\frac{\partial^4 C}{\partial x^4}\right)_i - \frac{(2h)^5}{120}\left(\frac{\partial^5 C}{\partial x^5}\right)_i + \cdots \tag{3.17}$$

$$C_{i-3} = C_i - 3h\left(\frac{\partial C}{\partial x}\right)_i + \frac{(3h)^2}{2}\left(\frac{\partial^2 C}{\partial x^2}\right)_i - \frac{(3h)^3}{6}\left(\frac{\partial^3 C}{\partial x^3}\right)_i + \frac{(3h)^4}{24}\left(\frac{\partial^4 C}{\partial x^4}\right)_i - \frac{(3h)^5}{120}\left(\frac{\partial^5 C}{\partial x^5}\right)_i + \cdots \tag{3.18}$$

$$C_{i-4} = C_i - 4h\left(\frac{\partial C}{\partial x}\right)_i + \frac{(4h)^2}{2}\left(\frac{\partial^2 C}{\partial x^2}\right)_i - \frac{(4h)^3}{6}\left(\frac{\partial^3 C}{\partial x^3}\right)_i + \frac{(4h)^4}{24}\left(\frac{\partial^4 C}{\partial x^4}\right)_i - \frac{(4h)^5}{120}\left(\frac{\partial^5 C}{\partial x^5}\right)_i + \cdots \tag{3.19}$$

As such, we again can express the first derivative by multiplying equations (3.16), (3.17), (3.18) and (3.19) by the coefficients β, γ, δ and θ respectively. Then, that taking the summation of these four equations, one obtains the following expression:

$$\begin{aligned} \beta\, C_{i-1} + \gamma\, C_{i-2} + \delta\ C_{i-3} + \ \theta\ C_{i-4} = {} & \frac{1}{h}(\theta + \delta + \gamma + \beta)\, C_i \\ & +(-4\theta - 3\delta - 2\gamma - \beta)\left(\frac{\partial C}{\partial x}\right)_i \\ & + \frac{h}{2}(16\theta + 9\delta + 4\gamma + \beta)\left(\frac{\partial^2 C}{\partial x^2}\right)_i \\ & + \frac{h^2}{6}(-64\theta - 27\delta - 8\gamma - \beta)\left(\frac{\partial^3 C}{\partial x^3}\right)_i \\ & + \frac{h^3}{24}(256\theta + 81\delta + 16\gamma - \beta)\left(\frac{\partial^4 C}{\partial x^4}\right)_i \\ & + \frac{h^4}{120}(-1024\theta - 243\delta - 32\gamma - \beta)\left(\frac{\partial^5 C}{\partial x^5}\right)_i \end{aligned} \tag{3.20}$$

At this stage; in order to satisfy the accurate fourth order in equation (3.20) we need to find the value of the coefficients β, γ, δ and θ such that the coefficient of $\left(\frac{\partial C}{\partial x}\right)_i$ must equal 1 and the coefficients of $\left(\frac{\partial^2 C}{\partial x^2}\right)_i$, $\left(\frac{\partial^3 C}{\partial x^3}\right)_i$ and $\left(\frac{\partial^4 C}{\partial x^4}\right)_i$ must be zeros and the coefficient of $\left(\frac{\partial^5 C}{\partial x^5}\right)_i$ should be not zero. We can call the coefficient of C_i as α such that $\alpha = \theta + \delta + \gamma + \beta$, thus we obtain the following linear equations to be solved:

E_1: $\theta + \delta + \gamma + \beta + \alpha = 0$

E_2: $-4\theta - 3\delta - 2\gamma - \beta = 1$

E_3: $16\theta + 9\delta + 4\gamma + \beta = 0$ (3.21)

E_4: $-64\theta - 27\delta - 8\gamma - \beta = 0$

E_5: $256\theta + 81\delta + 16\gamma + \beta = 0$

Truncation error (T.E) = $\frac{h^2}{120}(-1024\theta - 243\delta - 32\gamma - \beta)\left(\frac{\partial^5 C}{\partial x^5}\right)_i$ (3.22)

Multiplying the equations E2 and E4 by (-1), we obtain the system:

E_1: $\alpha + \beta + \gamma + \delta + \theta = 0$

E_2: $\beta + 2\gamma + 3\delta + 4\theta = -1$

E_3: $\beta + 4\gamma + 9\delta + 16\theta = 0$ (3.23)

E_4: $\beta + 8\gamma + 27\delta + 46\theta = 0$

E_5: $\beta + 16\gamma + 81\delta + 256\theta = 0$

The system of linear equation (3.23) is equivalent to the system of equations (3.9) except that the coefficients of equations E_2 and E_4 one multiplied by (-1). Then the solution of the system (3.23) is as follows:

$$\alpha = \frac{25}{12}, \beta = \frac{-48}{12}, \gamma = \frac{36}{12}, \delta = \frac{-16}{12} \text{ And } \theta = \frac{3}{12}$$

Substituting solutions into equations (3.20) and (3.22) gives the fourth order backward – difference approximation of $\frac{\partial C}{\partial x}$ as:

$$\left(\frac{\partial C}{\partial x}\right)_i = \frac{3C_{i-4} - 16C_{i-3} + 36C_{i-2} - 48C_{i-1} + 25C_i}{12h} \quad (3.24)$$

$\text{Truncation error} = O(h^4)$

$$= \frac{h^4}{120}\left(-1024 * \frac{3}{12} - 243 * \frac{-16}{12} - 32 * \frac{36}{72} + \frac{48}{12}\right)\left(\frac{\partial^5 C}{\partial x^5}\right)_i$$

$$T.E = -\frac{h^4}{5}\left(\frac{\partial^5 C}{\partial x^5}\right)_i \qquad (3.25)$$

3.2.3. Fourth-Order Central Difference Approximation of $\frac{\partial C}{\partial x}$

It is found by using a Taylor series (3.3). Start by expressing the values of C_{i-1}, C_{i-2},C_{i+1}, and C_{i+2} then multiplying the equations (3.4), (3.5), (3.16) and (3.17) by α, β, δ and θ respectively and collocating the summation of these equation we obtain the following expression:

$$\alpha C_{i-2} + \beta C_{i-1} + \delta C_{i+1} + \theta C_{i+2}$$
$$= \frac{1}{h}(\alpha + \beta + \delta + \theta)C_i + (-2\alpha - \beta + \delta + 2\theta)\left(\frac{\partial C}{\partial x}\right)_i$$
$$+ \frac{h}{2}(4\alpha + \beta + \delta + 4\theta)\left(\frac{\partial^2 C}{\partial x^2}\right)_i + \frac{h^2}{6}(-8\alpha - \beta - \delta + 8\theta)\left(\frac{\partial^3 C}{\partial x^3}\right)_i$$
$$+ \frac{h^3}{24}(16\alpha + \beta + \delta + 16\theta)\left(\frac{\partial^4 C}{\partial x^4}\right)_i$$
$$+ \frac{h^4}{120}(-32\alpha - \beta + \delta + 32\theta)\left(\frac{\partial^5 C}{\partial x^5}\right)_i \qquad (3.26)$$

At this stage; in order to satisfy the accurate fourth order in equation (3.26) we need to find the values of the coefficients β, γ, δ and θ such that the coefficient of $\left(\frac{\partial C}{\partial x}\right)_i$ must equal 1 and the coefficients of $\left(\frac{\partial^2 C}{\partial x^2}\right)_i$, $\left(\frac{\partial^3 C}{\partial x^3}\right)_i$ and $\left(\frac{\partial^4 C}{\partial x^4}\right)_i$ must be zeros and the coefficient of $\left(\frac{\partial^5 C}{\partial x^5}\right)_i$ should be not zero. We can call the coefficient of C_i as α such that $\gamma = \theta + \delta + \alpha + \beta$, thus we obtain the following linear equations to be solved:

$$E_1: \quad \alpha + \beta + \gamma + \delta + \theta = 0$$

$$E_2: \quad -2\alpha - \beta + 2\gamma + 2\theta = 1$$

$$E_3: \quad 4\alpha + \beta + 9\delta + 4\theta = 0 \tag{3.27}$$

$$E_4: \quad -8\alpha - \beta + \delta + 8\theta = 0$$

$$E_5: \quad 16\alpha + \beta + \delta + 16\theta = 0$$

$$\text{Truncation error} = \frac{h^4}{120}(-32\alpha - \beta + \delta + 32\theta)\left(\frac{\partial^5 C}{\partial x^2}\right)_i \tag{3.28}$$

The five equations (3.27) are solved for the unknown α,β,γ,δ and θ respectively. The first step to rearrange the equation E_1, resulting the system is:

$$E_1: \quad -\gamma + \alpha + \beta + \delta + \theta = 0$$

$$E_2: \quad -2\alpha - \beta + \delta + 2\theta = 1$$

$$E_3: \quad 4\alpha + \beta + \delta + 4\theta = 0 \tag{3.29}$$

$$E_4: \quad -8\alpha - \beta + \delta + 8\theta = 0$$

$$E_5: \quad 16\alpha + \beta + \delta + 16\theta = 0$$

The rest steps we can do the same procedures that previously be followed in, as resulting in the system:

$$E_1: \quad \gamma + \alpha + \beta + \delta + \theta = 0$$

$$E_2: \quad -2\alpha - \beta + \delta + 2\theta = 1 \tag{3.30}$$

$$E_3: \quad -\beta + 3\delta + 8\theta = 2$$

$$E_4: \quad 6\delta + 24\theta = 2$$

$$E_5: \quad 24\theta = -2$$

The system of equations (3.30) is now in reduced from and can easily be solved for the unknown by a backward-substation process:

$$\theta = -\frac{1}{12}, \delta = \frac{8}{12}, \beta = -\frac{8}{12}, \alpha = \frac{1}{12} \ , \gamma = 0$$

It can easily be verified that these values also satisfy the equations in (3.27).

Substituting solutions into equations (3.26) and (3.28) gives the fourth-order central-difference approximation of $\frac{\partial C}{\partial x}$ as following:

$$\left(\frac{\partial C}{\partial x}\right)_i = \frac{C_{i-2} - 8C_{i-1} + 8C_{i+1} - C_{i+1}}{12h} \tag{3.31}$$

And Truncation error $= O(h^4) = \frac{h^4}{120}\left(-32 * \frac{1}{12} + \frac{8}{12} + \frac{8}{12} + 32 * \frac{-1}{12}\right)\left(\frac{\partial^5 C}{\partial x^5}\right)_i$

$$T.E = -\frac{h^4}{30}\left(\frac{\partial^5 C}{\partial x^5}\right)_i \tag{3.32}$$

3.3. Fourth–Order Central-Difference Approximation of $\frac{\partial^2 C}{\partial x^2}$

It is found by using a Taylor series in (3.3). Start by substituting the value of C_{i-2}, C_{i-1}, $C_{i+1}$and C_{i+2} in (3.4), (3.5), (3.16) and (3.17) and multiplying them by α, β, δ and θ respectively and collocated the summation of these equation we obtain the following expression:

$$\begin{aligned}\alpha C_{i-2} + \beta C_{i-1} + \delta C_{i+1} + \beta C_{i+2} \\ = \frac{1}{h^2}(\alpha + \beta + \delta + \theta)C_i + \frac{1}{h}(-2\alpha - \beta + \delta + 2\theta)\left(\frac{\partial C}{\partial x}\right)_i \\ + \frac{1}{2}(4\alpha + \beta + \delta + 4\theta)\left(\frac{\partial^2 C}{\partial x^2}\right)_i + \frac{h}{6}(-8\alpha - \beta + \delta + 8\theta)\left(\frac{\partial^3 C}{\partial x^3}\right)_i \\ + \frac{h^2}{24}(16\alpha + \beta + \delta + 16\theta)\left(\frac{\partial^4 C}{\partial x^4}\right)_i \\ + \frac{h^3}{120}(-32\alpha - \beta + \delta + 32\theta)\left(\frac{\partial^5 C}{\partial x^5}\right)_i\end{aligned} \tag{3.33}$$

At this stage; in order to satisfy the accurate fourth order in equation (3.33) we need to find the value of the coefficientsβ, γ, δ and θ such that the coefficient of $\left(\frac{\partial^2 C}{\partial x^2}\right)_i$ must equal 1 and the coefficients of $\left(\frac{\partial C}{\partial x}\right)_i$, $\left(\frac{\partial^3 C}{\partial x^3}\right)_i$ and $\left(\frac{\partial^4 C}{\partial x^4}\right)_i$ must be zeros and the coefficient of $\left(\frac{\partial^5 C}{\partial x^5}\right)_i$ should be not zero, we can call the coefficient of C_i as α such that $\gamma = \theta + \delta + \alpha + \beta$, thus we obtain the following linear equations to be solved :

E_1: $\alpha + \beta - \gamma + \delta + \theta = 0$

E_2: $-2\alpha - \beta + \delta + 2\theta = 0$

E_3: $4\alpha + \beta + \delta + 4\theta = 2$ (3.34)

E_4: $-8\alpha - \beta + \delta + 8\theta = 0$

E_5: $16\alpha + \beta + \delta + 16\theta = 0$

Yielding,

$$T.E = \frac{h^3}{120}(-32\alpha - \beta + \delta + 32\theta)\left(\frac{\partial^5 C}{\partial x^5}\right)_i + \frac{h^4}{720}(64\alpha + \beta + \delta + 64\theta) \ldots \quad (3.35)$$

We follow the same procedure in previous sections to solve the system of linear equations (3.34), reduced from and can easily be solved for the unknown by a backward-substation process:

$$\theta = -\frac{1}{12}, \delta = \frac{16}{12}, \beta = \frac{16}{12}, \alpha = -\frac{1}{12}, \quad \gamma = -\frac{30}{12}$$

when these values are substituted in (3.34) gives:

The fourth-order central-difference approximation of $\frac{\partial^2 C}{\partial x^2}$ as following

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_i = \frac{-C_{i-2} + 16C_{i-1} - 30C_i + 16C_{i+1} - C_{i+2}}{12h^2} \quad (3.36)$$

With the truncation error:

$$\mathrm{T.E} = \frac{h^3}{120}(-32\alpha - \beta + \delta + 32\theta)\frac{\partial^5 C}{\partial x^5} + \frac{h^4}{720}(64\alpha - \beta + \delta + 64\theta)\frac{\partial^6 C}{\partial x^6}$$

$$\mathrm{T.E} = \frac{-h^4}{90}\frac{\partial^6 C}{\partial x^6} \tag{3.37}$$

3.4. Finite Difference Approximation

For illustrative purpose, in the previous section, we presented the derivation of backward, forward and central differences fourth order finite difference for first derivative and the derivation of central differences fourth order finite difference for second derivative. The similar procedure can be carried out for the other approximation of any order in a similar fashion. For the sake of brevity, we summarized them in Table 3.1, where one can see the approximations and the truncation error terms.

Table 3.1. The approximation and truncation errors of first and second derivative backward, forward and central differences for several order of accuracy

	Order	m	q	Approximation	Truncation error
1	First-order backward	1	2	$\frac{\partial C}{\partial x} \approx \frac{C_i - C_{i-1}}{h}$	$\frac{h}{2}\left(\frac{\partial^2 C}{\partial x^2}\right)_i$
2	First-order forward	1	2	$\frac{\partial C}{\partial x} \approx \frac{C_{i+1} - C_i}{h}$	$\frac{h}{2}\left(\frac{\partial^2 C}{\partial x^2}\right)_i$
3	Second-order central	1	3	$\frac{\partial C}{\partial x} \approx \frac{C_{i+1} - C_{i-1}}{2h}$	$\frac{h^2}{3}\left(\frac{\partial^3 C}{\partial x^3}\right)_i$
4	Second-order backward	1	3	$\frac{\partial C}{\partial x} \approx \frac{C_{i-2} - 4C_{i-1} + 3C_i}{2h}$	$\frac{-5h^2}{14}\left(\frac{\partial^3 C}{\partial x^3}\right)_i$
5	Second-order forward	1	3	$\frac{\partial C}{\partial x} \approx \frac{-3C_i + 4C_{i+1} - C_{i+2}}{2h}$	$\frac{-5h^2}{24}\left(\frac{\partial^3 C}{\partial x^3}\right)_i$
6	Third-order backward	1	4	$\frac{\partial C}{\partial x} \approx \frac{C_{i-2} - 6C_{i-1} + 3C_i + 2C_{i+1}}{6h}$	$\frac{-h^3}{12}\left(\frac{\partial^4 C}{\partial x^4}\right)_i$
7	Third-order forward	1	4	$\frac{\partial C}{\partial x} \approx \frac{-2C_{i-1} - 3C_i + 6C_{i+1} - C_{i+2}}{6h}$	$-\frac{h^3}{12}\left(\frac{\partial^4 C}{\partial x^4}\right)_i$
8	Fourth-order central	1	5	$\frac{\partial C}{\partial x} \approx \frac{C_{i-2} - 8C_{i-1} + 8C_{i+1} - C_{i+2}}{12h}$	$-\frac{h^4}{30}\left(\frac{\partial^5 C}{\partial x^5}\right)_i$
9	Fourth-order backward	1	5	$\frac{\partial C}{\partial x} \approx \frac{3C_{i-4} - 16C_{i-3} + 36C_{i-2} - 48C_{i-1} + 25C_i}{12h}$	$-\frac{h^4}{5}\left(\frac{\partial^5 C}{\partial x^5}\right)_i$
10	Fourth-order forward	1	5	$\frac{\partial C}{\partial x} \approx \frac{-25C_i + 48C_{i+1} - 36C_{i+2} + 16C_{i+3} - 3C_{i+4}}{12h}$	$-\frac{h^4}{5}\left(\frac{\partial^5 C}{\partial x^5}\right)_i$
11	Second-order central	2	3	$\frac{\partial^2 C}{\partial x^2} \approx \frac{C_{i+1} - 2C_i + C_{i-1}}{h^2}$	$\frac{h^2}{12}\left(\frac{\partial^4 C}{\partial x^4}\right)_i$
12	Fourth-order central	2	5	$\frac{\partial^2 C}{\partial x^2} \approx \frac{-C_{i-2} + 16C_{i-1} - 30C_i + 16C_{i+1} - C_{i+2}}{12h^2}$	$\frac{-h^4}{90}\left(\frac{\partial^6 C}{\partial x^6}\right)_i$
13	Third-order forward	2	5	$\frac{\partial^2 C}{\partial x^2} \approx \frac{35C_i - 104C_{i+1} + 114C_{i+2} - 56C_{i+3} + 11C_{i+4}}{12h^2}$	$\frac{5\,h^3}{36}\left(\frac{\partial^5 C}{\partial x^5}\right)_i$
14	Third-order backward	2	5	$\frac{\partial^2 \mathrm{C}}{\partial \mathrm{x}^2} \approx \frac{-11\mathrm{C}_{\mathrm{i-4}} + 56\mathrm{C}_{\mathrm{i-3}} - 114\mathrm{C}_{\mathrm{i-2}} + 104\mathrm{C}_{\mathrm{i-1}} - 35\mathrm{C}_{\mathrm{i}}}{12\mathrm{h}^2}$	$\frac{5\,h^3}{36}\left(\frac{\partial^5 C}{\partial x^5}\right)_i$

CHAPTER 4

A NUMERICAL APPROXIMATION TO CDE

The following notation is used with j, i for the time and space, respectively (see Figure 4.1.)

$C_i^j = C(t_j, x_i)$

$C_i^{j+1} = C(t_j + k, x_i)$

$C_{i+1}^j = C(t_j, x_i + h)$

$C_{i-1}^j = C(t_j, x_i - h)$

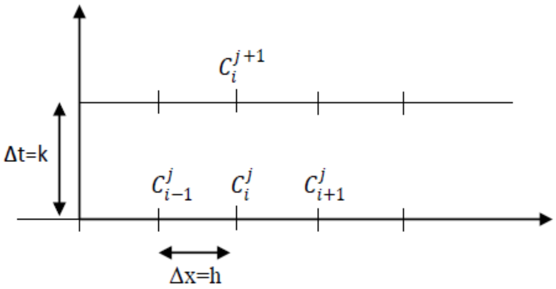


Figure 4.1. Numerical grid in one dimension

A numerical approximation to C.D.E:

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} \tag{4.1}$$

can be obtained by replacing the derivatives by the following approximations

$$\left(\frac{\partial C}{\partial t}\right)_i^j + U\left(\frac{\partial C}{\partial x}\right)_i^j = D\left(\frac{\partial^2 C}{\partial x^2}\right)_i^j \tag{4.2}$$

Depending upon the order and method approximation to first and second derivatives we presented 10 different cases of approximation to C.D.E. method in the following sections.

4.1. Second-Order Central Difference Approximation of $\frac{\partial C}{\partial x}$ and $\frac{\partial^2 C}{\partial x^2}$ (FTC2S).

$$\left(\frac{\partial C}{\partial t}\right)_i^j = \frac{C_i^{j+1} - C_i^j}{k} + O(k)$$

$$\left(\frac{\partial C}{\partial x}\right)_i^j = \frac{C_{i+1}^j - C_{i-1}^j}{2h} + O(h^2)$$

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_i^j = \frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{h^2} + O(h^2)$$

Substituting these approximations into (4.1) gives:

$$\frac{C_i^{j+1} - C_i^j}{k} + U\frac{C_{i+1}^j - C_{i-1}^j}{2h} = D\frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{h^2} + O(k, h^2)$$

Solving for the new value and dropping the error terms yields

$$C_i^{j+1} = C_i^j - \frac{Uk}{2h}\left(C_{i+1}^j - C_{i-1}^j\right) + \frac{Dk}{h^2}\left(C_{i+1}^j - 2C_i^j + C_{i-1}^j\right) + O(k, h^2)$$

Thus, given *C* at one time (or time level), *C* at the next time level is given by:

$$C_i^{j+1} = C_i^j - \frac{Uk}{2h}\left(C_{i+1}^j - C_{i-1}^j\right) + \frac{Dk}{h^2}\left(C_{i+1}^j - 2C_i^j + C_{i-1}^j\right) + O(k, h^2)$$

General difference approximation then becomes:

$$C_i^{j+1} = \left(\frac{Uk}{2h} + \frac{Dk}{h^2}\right)C_{i-1}^j + \left(1 - \frac{2Dk}{h^2}\right)C_i^j + \left(\frac{DK}{h^2} - \frac{Uk}{2h}\right)C_{i+1}^j \qquad (4.3)$$

4.2. Fourth-Order Central Difference Approximation of $\frac{\partial C}{\partial x}$ and $\frac{\partial^2 C}{\partial x^2}$ (FTC4S).

$$\left(\frac{\partial C}{\partial x}\right)_i^j = \frac{C_{i-2}^j - 8C_{i-1}^j + 8C_{i+1}^j - C_{i+2}^j}{12h} + O(h^4)$$

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_i^j = \frac{-C_{i-2}^j + 16C_{i-1}^j - 30C_i^j + 16C_{i+1}^j - C_{i+2}^j}{12h^2} + O(h^4)$$

Substituting these approximations into (4.1) gives:

$$\frac{C_i^{j+1} - C_i^j}{k} + U\frac{C_{i-2}^j - 8C_{i-1}^j + 8C_{i+1}^j - C_{i+2}^j}{12h} = D\frac{-C_{i-2}^j + 16C_{i-1}^j - 30C_i^j + 16C_{i+1}^j - C_{i+2}^j}{12h^2} + O(k, h^4)$$

Solving for the new value and dropping the error terms yields

$$C_i^{j+1} = C_i^j - \frac{Uk}{12h}\left(C_{i-2}^j - 8C_{i-1}^j + 8C_{i+1}^j - C_{i+2}^j\right) + \frac{Dk}{12h^2}\left(-C_{i-2}^j + 16C_{i-1}^j - 30C_i^j + 16C_{i+1}^j - C_{i+2}^j\right)$$

General difference approximation then becomes:

$$C_i^{j+1} = -\left(\frac{Uk}{12h} + \frac{Dk}{12h^2}\right)C_{i-2}^j + \left(\frac{8Uk}{12h} + \frac{16Dk}{12h^2}\right)C_{i-1}^j + \left(1 - \frac{30Dk}{12h^2}\right)C_i^j + \left(\frac{16Dk}{12h^2} - \frac{8Uk}{12h}\right)C_{i+1}^j + \left(\frac{Uk}{12h} - \frac{Dk}{12h^2}\right)C_{i+2}^j \qquad (4.4)$$

4.3. Third-Order Forward Difference Approximation of $\frac{\partial C}{\partial x}$ and $\frac{\partial^2 C}{\partial x^2}$ (FTF3S).

$$\left(\frac{\partial C}{\partial x}\right)_i^j = \frac{-2C_{i-1}^j - 3C_i^j + 6C_{i+1}^j - C_{i+2}^j}{6h} + O(h^3)$$

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_i^j = \frac{35C_i^j - 104C_{i+1}^j + 114C_{i+2}^j - 56C_{i+3}^j + 11C_{i+4}^j}{12h^2} + O(h^3)$$

Substituting these approximations into (4.1) gives:

$$\frac{C_i^{j+1} - C_i^j}{k} + \frac{U}{6h}\left(-2C_{i-1}^j - 3C_i^j + 6C_{i+1}^j - C_{i+2}^j\right)$$
$$= \frac{D}{12h^2}\left(35C_i^j - 104C_{i+1}^j + 114C_{i+2}^j - 56C_{i+3}^j + 11C_{i+4}^j\right) + O(k, h^3)$$

Solving for the new value and dropping the error terms yields

$$C_i^{j+1} = C_i^j - \frac{Uk}{6h}\left(-2C_{i-1}^j - 3C_i^j + 6C_{i+1}^j - C_{i+2}^j\right)$$
$$+ \frac{Dk}{12h^2}\left(35C_i^j - 104C_{i+1}^j + 114C_{i+2}^j - 56C_{i+3}^j + 11C_{i+4}^j\right)$$

General difference approximation then becomes:

$$C_i^{j+1} = \frac{2Uk}{6h}C_{i-1}^j + \left(1 + \frac{3Uk}{6h} + \frac{35Dk}{12h^2}\right)C_i^j - \left(\frac{6Uk}{6h} + \frac{104Dk}{12h^2}\right)C_{i+1}^j$$
$$+ \left(\frac{Uk}{6h} + \frac{114Dk}{12h^2}\right)C_{i+2}^i - \frac{56Dk}{12h^2}C_{i+3}^j + \frac{11Dk}{12h^2}C_{i+4}^j \qquad (4.5)$$

4.4. Third-Order Backward Difference Approximation of $\frac{\partial C}{\partial x}$ and $\frac{\partial^2 C}{\partial x^2}$ (FTB3S).

$$\left(\frac{\partial C}{\partial x}\right)_i^j = \frac{C_{i-2}^j - 6C_{i-1}^j + 3C_i^j + 2C_{i+1}^j}{6h} + O(h^3)$$

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_i^j = \frac{-11C_{i-4}^j + 56C_{i-3}^j - 114C_{i-2}^j + 104C_{i-1}^j - 35C_i^j}{12h^2} + O(h^3)$$

Substituting these approximations into (4.1) gives:

$$\frac{C_i^{j+1} - C_i^j}{k} + \frac{U}{6h}\left(C_{i-2}^j - 6C_{i-1}^j + 3C_i^j + 2C_{i+1}^j\right)$$
$$= \frac{D}{12h^2}(-11C_{i-4}^j + 56C_{i-3}^j - 114C_{i-2}^j + 104C_{i-1}^j - 35C_i^j) + O(k, h^3)$$

Solving for the new value and dropping the error terms yields

$$C_i^{j+1} = C_i^j - \frac{Uk}{6h}\left(C_{i-2}^j - 6C_{i-1}^j + 3C_i^j + 2C_{i+1}^j\right)$$
$$+ \frac{Dk}{12h^2}\left(-11C_{i-4}^j + 56C_{i-3}^j - 114C_{i-2}^j + 104C_{i-1}^j - 35C_i^j\right)$$

General difference approximation then:

$$C_i^{j+1} = -\frac{11Dk}{12h^2}C_{i-4}^j + \frac{56Dk}{12h^2}C_{i-3}^j - \left(\frac{Uk}{6h} + \frac{114Dk}{12h^2}\right)C_{i-2}^j + \left(\frac{6Uk}{6h} + \frac{104Dk}{12h^2}\right)C_{i-1}^j$$
$$+ \left(1 - \frac{3Uk}{6h} - \frac{35Dk}{12h^2}\right)C_i^j - \frac{2Uk}{6h}C_{i+1}^j \qquad (4.6)$$

4.5. Second-Order Central Difference Approximation of $\frac{\partial C}{\partial x}$ and Third-Order Forward Difference Approximation of $\frac{\partial^2 C}{\partial x^2}$ (FTC2F3S).

$$\left(\frac{\partial C}{\partial x}\right)_i^j = \frac{C_{i+1}^j - C_{i-1}^j}{2h} + O(h^2)$$

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_i^j = \frac{35C_i^j - 104C_{i+1}^j + 114C_{i+2}^j - 56C_{i+3}^j + 11C_{i+4}^j}{12h^2} + O(h^3)$$

Substituting these approximations into (4.1) gives:

$$\frac{C_i^{j+1} - C_i^i}{k} + U\frac{C_{i+1}^j - C_{i-1}^j}{2h} = D\,\frac{35C_i^j - 104C_{i+1}^j + 114C_{i+2}^j - 56C_{i+3}^j + 11C_{i+4}^j}{12h^2} + O(k, h^2)$$

Solving for the new value and dropping the error terms yields

$$C_i^{j+1} = C_i^j - \frac{Uk}{2h}\left(C_{i+1}^j - C_{i-1}^j\right) + \frac{Dk}{12h^2}\left(35C_i^j - 104C_{i+1}^j + 114C_{i+2}^j - 56C_{i+3}^j + 11C_{i+4}^j\right)$$

General difference approximation then becomes:

$$C_i^{j+1} = \frac{Uk}{2h}C_{i-1}^j + \left(1 + \frac{35Dk}{12h^2}\right)C_i^j - \left(\frac{104Dk}{12h^2} + \frac{Uk}{2h}\right)C_{i+1}^j + \frac{114Dk}{12h^2}C_{i+2}^j - \frac{56Dk}{12h^2}C_{i+3}^j + \frac{11Dk}{12h^2}C_{i+4}^j \tag{4.7}$$

4.6. Second-Order Central Difference Approximation of $\frac{\partial C}{\partial x}$ and Fourth-Order Central Difference Approximation of $\frac{\partial^2 C}{\partial x^2}$ (FTC2C4S).

$$\left(\frac{\partial C}{\partial x}\right)_i^j = \frac{C_{i+1}^j - C_{i-1}^j}{2h} + O(h^2)$$

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_i^j = \frac{-C_{i-2}^j + 16C_{i-1}^j - 30C_i^j + 16C_{i+1}^j - C_{i+2}^j}{12h^2} + O(h^4)$$

Substituting these approximations into (4.1) gives:

$$\frac{C_i^{j+1} - C_i^j}{k} + U\frac{C_{i+1}^j - C_{i-1}^j}{2h} = D\frac{-C_{i-2}^j + 16C_{i-1}^j - 30C_i^j + 16C_{i+1}^j - C_{i+2}^j}{12h^2} + O(k, h^2)$$

Solving for the new value and dropping the error terms yields

$$C_i^{j+1} = C_i^j - \frac{Uk}{2h}\left(C_{i+1}^j - C_{i-1}^j\right) + \frac{Dk}{12h^2}\left(-C_{i-2}^j + 16C_{i-1}^j - 30C_i^j + 16C_{i+1}^j - C_{i+2}^j\right)$$

General difference approximation is:

$$C_i^{j+1} = -\frac{Dk}{12h^2}C_{i-2}^j + \left(\frac{Uk}{2h} + \frac{16Dk}{12h^2}\right)C_{i-1}^j + \left(1 - \frac{30Dk}{12h^2}\right)C_i^j + \left(\frac{16Dk}{12h^2} - \frac{Uk}{2h}\right)C_{i+1}^j - \frac{Dk}{12h^2}C_{i+2}^j \qquad (4.8)$$

4.7. Third-Order Forward Difference Approximation of $\frac{\partial C}{\partial x}$ and Fourth-Order Central Difference Approximation of $\frac{\partial^2 C}{\partial x^2}$ (FTF3C4S)

$$\left(\frac{\partial C}{\partial x}\right)_i^j = \frac{-2C_{i-1}^j - 3C_i^j + 6C_{i+1}^j - C_{i+2}^j}{6h} + O(h^3)$$

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_i^j = \frac{-C_{i-2}^j + 16C_{i-1}^j - 30C_i^j + 16C_{i+1}^j - C_{i+2}^j}{12h^2} + O(h^4)$$

Substituting these approximations into (4.1) gives:

$$\frac{C_i^{j+1} - C_i^j}{k} + U\frac{-2C_{i-1}^j - 3C_i^j + 6C_{i+1}^j - C_{i+2}^j}{6h} = D\frac{-C_{i-2}^j + 16C_{i-1}^j - 30C_i^j + 16C_{i+1}^j - C_{i+2}^j}{12h^2}$$

Solving for the new value and dropping the error terms yields

$$C_i^{j+1} = C_i^j - \frac{Uk}{6h}\left(-2C_{i-1}^j - 3C_i^j + 6C_{i+1}^j - C_{i+2}^j\right) + \frac{Dk}{12h^2}\left(-C_{i-2}^j + 16C_{i-1}^j - 30C_i^j + 16C_{i+1}^j - C_{i+2}^j\right) + O(k, h^3)$$

General difference approximation becomes in compact form as:

$$C_i^{j+1} = -\frac{Dk}{12h^2}C_{i-2}^j + \left(\frac{2Uk}{6h} + \frac{16Dk}{12h^2}\right)C_{i-1}^j + \left(1 + \frac{3Uk}{6h} - \frac{30Dk}{12h^2}\right)C_i^j + \left(\frac{16Dk}{12h^2} - \frac{6Uk}{6h}\right)C_{i+1}^j + \left(\frac{Uk}{6h} - \frac{Dk}{12h^2}\right)C_{i+2}^j \quad (4.9)$$

4.8. Third-Order Forward Difference Approximation of $\frac{\partial C}{\partial x}$ and Second-Order Central Difference Approximation of $\frac{\partial^2 C}{\partial x^2}$ (FTF3C2S).

$$\left(\frac{\partial C}{\partial x}\right)_i^j = \frac{-2C_{i-1}^j - 3C_i^j + 6C_{i+1}^j - C_{i+2}^j}{6h} + O(h^3)$$

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_i^j = \frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{h^2} + O(h^2)$$

Substituting these approximations into (4.1) gives:

$$\frac{C_i^{j+1} - C_i^j}{k} + U\frac{-2C_{i-1}^j - 3C_i^j + 6C_{i+1}^j - C_{i+2}^j}{6h} = D\frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{h^2}$$

Solving for the new value and dropping the error terms yields

$$C_i^{j+1} = C_i^j - \frac{Uk}{6h}\left(-2C_{i-1}^j - 3C_i^j + 6C_{i+1}^j - C_{i+2}^j\right) + \frac{Dk}{h^2}\left(C_{i+1}^j - 2C_i^j + C_{i-1}^j\right) + O(k, h^2)$$

General difference approximation becomes:

$$C_i^{j+1} = \left(\frac{2Uk}{6h} + \frac{Dk}{h^2}\right)C_{i-1}^j + \left(1 - \frac{2Dk}{h^2} + \frac{3Uk}{6h}\right)C_i^j + \left(\frac{Dk}{h^2} - \frac{6Uk}{6h}\right)C_{i+1}^j + \frac{Uk}{6h}C_{i+2}^j \qquad (4.10)$$

4.9. Fourth-Order Forward Difference Approximation of $\frac{\partial C}{\partial x}$ and Third-Order Forward Difference Approximation of $\frac{\partial^2 C}{\partial x^2}$ (FTC4F3S).

$$\left(\frac{\partial C}{\partial x}\right)_i^j = \frac{C_{i-2}^j - 8C_{i-1}^j + 8C_{i+1}^j - C_{i+2}^j}{12\text{h}} + O(h^4)$$

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_i^j = \frac{35C_i^j - 104C_{i+1}^j + 114C_{i+2}^j - 56C_{i+3}^j + 11C_{i+4}^j}{12\text{h}^2} + O(h^3)$$

Substituting these approximations into (4.1) gives:

$$\frac{\text{C}_\text{i}^{\text{j}+1} - \text{C}_\text{i}^\text{j}}{\text{k}} + \text{U}\frac{C_{i-2}^j - 8C_{i-1}^j + 8C_{i+1}^j - C_{i+2}^j}{12\text{h}} = \text{D}\frac{35C_i^j - 104C_{i+1}^j + 114C_{i+2}^j - 56C_{i+3}^j + 11C_{i+4}^j}{12\text{h}^2}$$

Solving for the new value and dropping the error terms yields

$$C_i^{j+1} = C_i^j - \frac{Uk}{12h}\left(C_{i-2}^j - 8C_{i-1}^j + 8C_{i+1}^j - C_{i+2}^j\right) + \frac{Dk}{12h^2}\left(35C_i^j - 104C_{i+1}^j + 114C_{i+2}^j - 56C_{i+3}^j + 11C_{i+4}^j\right) + O(k, h^3)$$

General difference approximation:

$$C_i^{j+1} = \frac{-Uk}{12h}C_{i-2}^j + \frac{8Uk}{12h}C_{i-1}^j + \left(1 + \frac{35Dk}{12h^2}\right)C_i^j + \left(\frac{104Dk}{12h^2} - \frac{8Uk}{12h}\right)C_{i+1}^j + \left(\frac{Uk}{12h} + \frac{114Dk}{12h^2}\right)C_{i+2}^j - \frac{56Uk}{12h}C_{i+3}^j + \frac{11Dk}{12h^2}C_{i+4}^j \quad (4.11)$$

4.10. Fourth-Order Central Difference Approximation of $\frac{\partial C}{\partial x}$ and Second-Order Central Difference Approximation of $\frac{\partial^2 C}{\partial x^2}$ (FTC4C2S).

$$\left(\frac{\partial C}{\partial x}\right)_i^j = \frac{C_{i-2}^j - 8C_{i-1}^j + 8C_{i+1}^j - C_{i+2}^j}{12h} + O(h^4)$$

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_i^j = \frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{h^2} + O(h^2)$$

Substituting these approximations into (4.1) gives:

$$\frac{C_i^{j+1} - C_i^j}{k} + U\frac{C_{i-2}^j - 8C_{i-1}^j + 8C_{i+1}^j - C_{i+2}^j}{12h} = D\frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{h^2}$$

Solving for the new value and dropping the error terms yields

$$C_i^{j+1} = C_i^j - \tfrac{Uk}{12h}\left(C_{i-2}^j - 8C_{i-1}^j + 8C_{i+1}^j - C_{i+2}^j\right) + \tfrac{Dk}{h^2}\left(C_{i+1}^j - 2C_i^j + C_{i-1}^j\right) + O(k, h^2)$$

General difference approximation in a compact form is:

$$C_i^{j+1} = -\frac{Uk}{12h}C_{i-2}^j + \left(\frac{Dk}{h^2} + \frac{8Uk}{12h}\right)C_{i-1}^j + \left(1 - \frac{2Dk}{h^2}\right)C_i^j + \left(\frac{Dk}{h^2} - \frac{8Uk}{12h}\right)C_{i+1}^j + \frac{Uk}{12h}C_{i+2}^j \qquad (4.12)$$

CHAPTER 5

NUMERICAL ILLUSTRATIONS

To demonstrate the applicability of the previous methods, we have applied it to some model problems of the convection-diffusion equation with the initial and boundary conditions whose numerical results are presented and compared with the exact solutions. The differences between the computed solutions and the exact solutions are shown in tables for next two examples. To test the performance of the proposed method, L_2 and L_∞ error norms are used as follows:

$$L_2 = \sqrt{\sum_{i=0}^{i=N} |C_i^{exact} - C_i^{numerical}|^2} \tag{5.1}$$

and

$$L_\infty = \max\left|C_i^{exact} - C_i^{numerical}\right| \tag{5.2}$$

An important non-dimensional parameter in numerical analysis is the Courant (Cr) number. This parameter gives the fractional distance relative to the grid spacing travelled due to advection in a single time step, $Cr = u\,\Delta t/\Delta x$. It is possible to show using a Fourier error analysis that for a forward difference in time approximation (i.e. explicit), no matter what approximation is used for the spatial derivatives, that the transport equation is stable for values of the $Cr \leq 1$. This stability constraint for explicit transport equations states that one cannot advent the concentration more than one grid cell in a single time step (Sari et al, 2010).

The Peclet number is another important non-dimensional parameter which compares the characteristic time for dispersion and diffusion given a length scale with the characteristic time for advection. In numerical analysis, one normally refers to a grid Peclet number $Pe = u\,\Delta x/\mathrm{D}$, where u is the velocity of water flow and the characteristic length scale is given by the grid spacing Δx. The literature suggests that for stable solution $Pe \leq 5$. More details on the effects of the Courant and Peclet numbers on the results can be found in Steefel and MacQuarrie (1996)

5.1. Example 1:

Flow velocity and diffusion coefficient are taken to be u = 0.01 m/s and D = 0.002 m^2/s in this experiment. Let the length of the channel be L = 100m. For this example, the Pe number is accepted to be ≤ 5 that leads Δx to be not greater than 1. Accordingly, to satisfy $Cr \leq 1$, Δt must not be more than 100 s. Exact solution of the current problem is (Szymkiewicz, 1993):

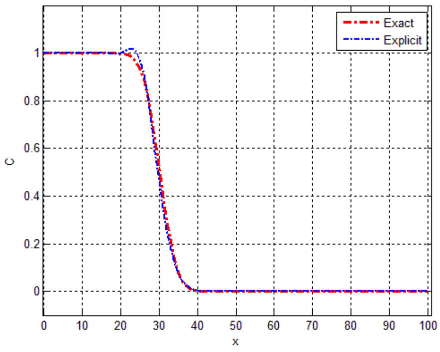
$$C(x,t) = \frac{1}{2} erfc\left(\frac{x-ut}{\sqrt{2Dt}}\right) + \frac{1}{2} exp\left(\frac{ux}{D}\right) erfc\left(\frac{x+ut}{\sqrt{2Dt}}\right) \tag{5.3}$$

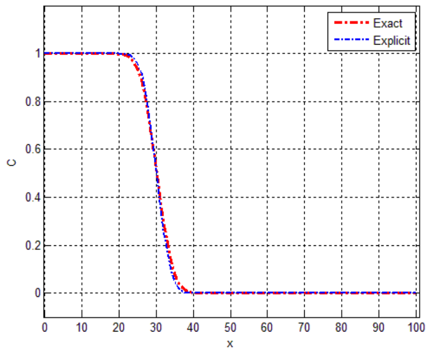
At the boundaries the following conditions are used:

$$C(0,t) = 1 \ , \qquad -D\left(\frac{\partial c}{\partial x}\right)(L,t) = 0 \tag{5.4}$$

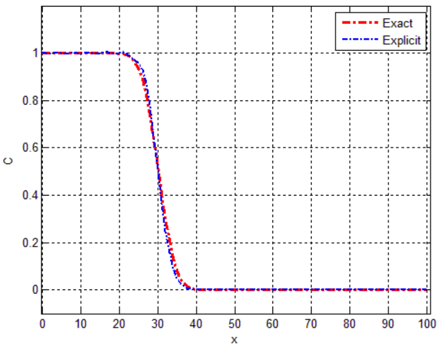
Initial condition can be deduced from the exact solution. Comparison between the numerical solutions and the exact solution is given in Table 5.1. The exact results were calculated in MATLAB. In Table 5.1, the solutions were produced by FTC2S, FTC2C4S, FTF3C4S, FTC4C2S and FTC4S schemes for space step Δx=1 and time step Δt=10 s. Note that the schemes give stable results but are not close enough to the exact solution (see Figures 5.1 and 5.2).

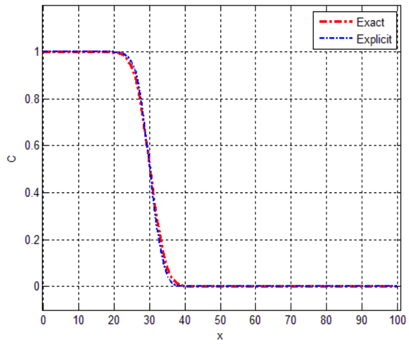
The calculations were repeated for different time step Δt = 1, 0.5 and 0.1s and space step Δx = 1, 0.5, 0.1 and the corresponding maximum errors obtained from these computations are presented in Tables 5.2 and 5.3.





(a) FTC2S (b) FTC24S





(c) FTF3C4 (d) FTC42S

Figure 5.1. Comparison of the analytical solution and the numerical solution obtained by (a)FTC2S, (b) FTC24S, (c) FTF3C4S and (d) FTC42S schemes for $\Delta t = 10$ and $\Delta x = 1$ at time=3000s

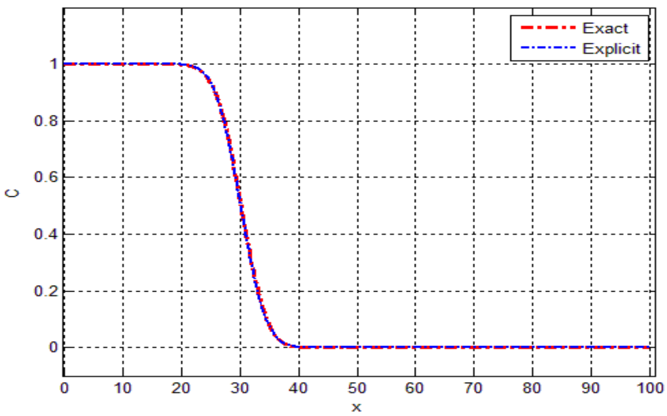


Figure 5.2. Comparison of the analytical solution and the numerical solution obtained by FTC4S scheme for $\Delta t = 10$ and $\Delta x = 1$ at time=3000s

Table 5.1. Comparison between numerical solutions of different schemes and the exact solution for Δx = h = 1 m and Δt = k = 10 s at Time=3000 s.

X	**FTC2S**	**FTC2C4S**	**FTF3C4S**	**FTC4C2S**	**FTC4S**	**Exact**
0	1	1	1	1	1	1
10	1.000042793	0.999997699	0.99511773	0.99999934	1.000000042	0.999999998
20	1.000124237	1.001640527	0.99988434	0.99931768	0.999436030	0.998480283
30	0.464220777	0.466014337	0.50475789	0.51218883	0.513069832	0.522956922
40	0.004574256	0.004335654	0.00114622	7.11264e-05	0.000253283	0.002251550
50	1.445295e-06	9.782067e-07	1.38096e-08	1.05051e-09	3.078858e-08	4.87825e-09
60	3.082604e-11	9.582876e-12	1.75836e-15	8.97263e-14	2.576221e-13	3.14712e-18
70	6.919535e-17	5.200627e-18	1.23081e-24	2.39140e-19	1.994503e-18	5.360089e-31
80	2.171451e-23	1.433724e-25	1.56591e-34	1.63797e-25	3.758043e-24	2.310465e-47
90	1.156595e-30	6.402280e-35	4.19556e-44	6.06539e-32	1.636997e-29	2.472812e-67
100	7.683836e-38	1.408349e-44	5.44279e-53	6.62012e-38	3.328681e-35	6.504858e-91

As shown in Tables 5.2 and 5.3, the FTC4S scheme provided the less error among others. Thus, it gave better results and closer to the exact solution. The results of the FTC2S, FTC2C4S, FTF3C4S, FTC4C2S schemes for Δt = 1s are seen to be acceptable level. Comparison of the exact solution and the numerical solution obtained with FTC4S scheme for Δx = 0.1 m and Δt = 0.1 s is shown in Figure 5.3. As can be seen in this figure; there is an excellent agreement between FTC4S and exact solutions.

Table 5.2. Error calculated by L_∞ norm for various Δt, Δx values at Time = 3000 s.

Δt	**Δx**	**L_∞ of FTC2S**	**L_∞ of FTC2C4S**	**L_∞ of FTF3C4S**	**L_∞ of FTC4C2S**	**L_∞ of FTC4S**
1	1	0.0441423	0.0434360	0.0142497	0.0064126	0.0050347
1	0.5	0.01254143	0.0123152	0.0049283	0.0041731	0.0037178
1	0.1	0.0037939	0.0037749	0.0038313	0.0038400	0.0038226
0.5	1	0.0439290	0.0432437	0.0124733	0.0054143	0.0045548
0.5	0.5	0.01214416	0.0119480	0.0030549	0.0023013	0.0018181
0.5	0.1	0.00190392	0.001884	0.0019073	0.0019158	0.0018988
0.1	1	0.04376306	0.043094	0.0112973	0.0048095	0.0043552
0.1	0.5	0.01184982	0.0116813	0.0016765	0.0009370	0.0004940
0.1	0.1	0.00059969	0.0005845	0.0003861	0.0003945	**0.0003777**

Table 5.3. Error calculated by L_2 norm for various Δt, Δx values at Time = 3000 s

Δt	Δx	L_2 of FTC2S	L_2 of FTC2C4S	L_2 of FTF3C4S	L_2 of FTC4C2S	L_2 of FTC4S
1	1	0.098786	0.097027	0.0324829	0.01462199	0.01178481
1	0.5	0.037651	0.0369527	0.0164043	0.01431268	0.01302495
1	0.1	0.029159	0.0290429	0.0293775	0.02943430	0.02932083
0.5	1	0.098260	0.0966612	0.0285396	0.01159430	0.00952232
0.5	0.5	0.036322	0.0358264	0.0099588	0.00778993	0.00649151
0.5	0.1	0.014621	0.0145065	0.0146476	0.01470347	0.01459202
0.1	1	0.097988	0.0965160	0.0256848	0.01012930	0.00909709
0.1	0.5	0.036077	0.0357542	0.0052152	0.00290268	0.00162710
0.1	0.1	0.004143	0.0040543	0.0029627	0.00301864	0.00290756

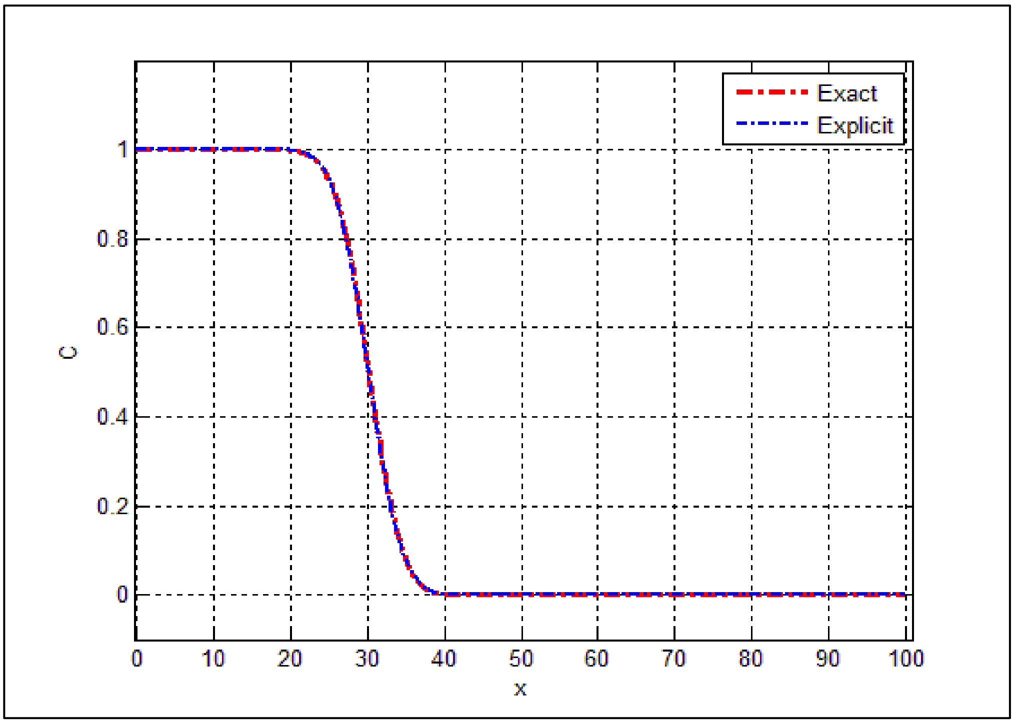


Figure 5.3. Comparison of the analytical solution and the numerical solution obtained by FTC4S scheme for Δt =0.1 and Δx=0.1 at time=3000s

5.2. Example 2:

A problem for which the exact solution is known is used to test the methods described for solving the advection–diffusion equation. These techniques are applied to solve equation (1.1) with g_0, g_1 and $f(x)$ known and C unknown (Dehghan, 2004). Consider the initial and boundary conditions as following:

$$f(x) = exp\left(-\frac{(x+0.5)^2}{0.00125}\right) \tag{5.5}$$

$$g_0(0,t) = \frac{0.025}{\sqrt{(0.025)^2+0.02t}}\ exp\left(-\frac{(0.5-t)^2}{(0.00125+0.04\ t)}\right) \tag{5.6}$$

$$g_1(1,t) = \frac{0.025}{\sqrt{(0.025)^2+0.02t}}\ exp\left(-\frac{(1.5-t)^2}{(0.00125+0.04\ t)}\right) \tag{5.7}$$

With D=0.01 and u=1, for which the exact solution is:

$$C(x,t) = \frac{0.025}{\sqrt{(0.025)^2+0.02t}}\ exp\left(-\frac{(x+0.5-t)^2}{(0.00125+0.04\ t)}\right) \tag{5.8}$$

In this example Pe number is also accepted to be ≤ 5 that leads Δx to be not greater than 0.05. To satisfy the the condition $Cr \leq 1$, Δt must not be more than 0.05 s. The results obtained for $C(x,t)$ computed at time, t=1 s for Δt = 0.008 and Δx = 0.05, using the FTC2S, FTC2C4S, FTF3C4S, FTC4C2S and FTC4S techniques are shown in Table 5.4 and Figures 5.4 and 5.5.

As seen, the results are acceptable but not at a desired level. Therefore, tests were carried out for different values of the Courant number Cr. For each value of Cr, three values of Δt were used, namely Δt =0.001, 0.002 and 0.004. For the three tests for each Cr were chosen to force Δx =0.01, 0.02, 0.04 and 0.05.

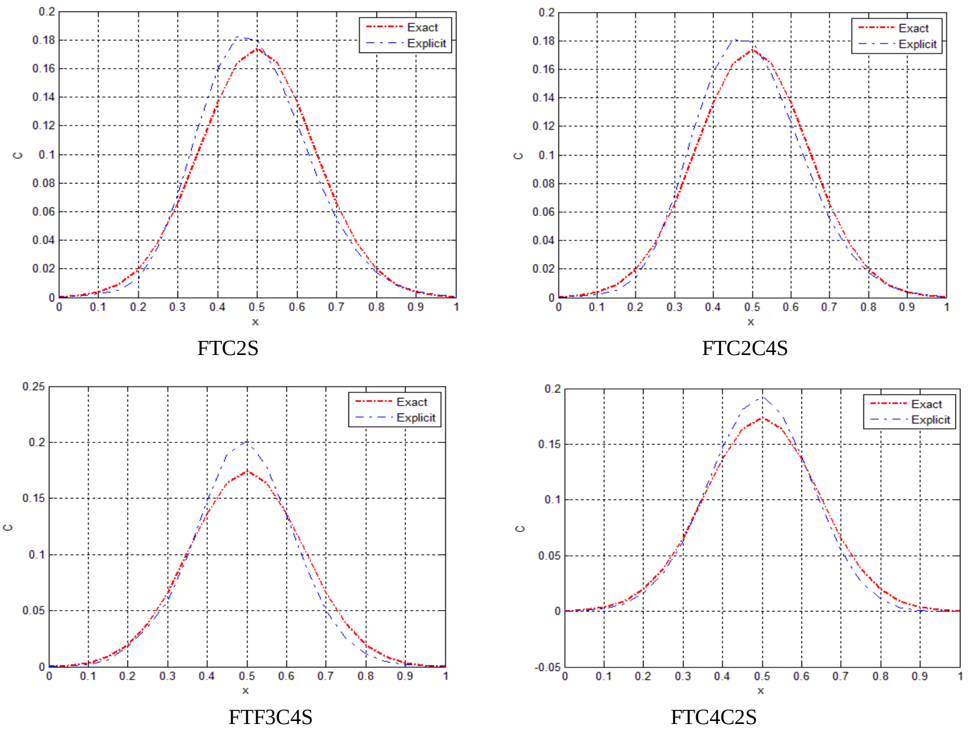


Figure 5.4. Comparison of the analytical solution and the numerical solution obtained by FTC2S, FTC2C4S, FTF3C4S and FTC4C2S schemes for Δt =0.008 and Δx=0.05 at time=1s

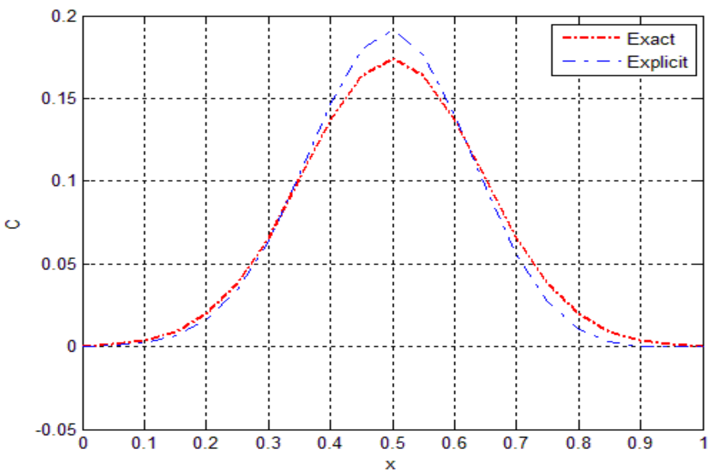


Figure 5.5. Comparison of the analytical solution and the numerical solution obtained by FTC4S schemes for Δt = 0.008 and Δx = 0.05 at time=1 s

Table 5.4. Comparison between numerical solutions of different schemes and the exact solution for Δx= h = 0.05 m and Δt= k = 0.008 s at Time= 1 s.

x	FTC2S	FTC2C4S	FTF3C4S	FTC4C2S	FTC4S	Exact
0	0.000406	0.0004061	0.0004061	0.0004061	0.0004061	0.0004061
0.1	0.002361	0.0021607	0.0020033	0.0024914	0.0024716	0.0035992
0.2	0.013213	0.0137380	0.0179764	0.0163945	0.0163713	0.0196423
0.3	0.071859	0.0723070	0.0589178	0.0629977	0.0636372	0.0660099
0.4	0.159839	0.1584572	0.1477484	0.1467381	0.1464142	0.1366028
0.5	0.179882	0.1794202	0.2013436	0.1928833	0.1913374	0.1740777
0.6	0.121636	0.1224944	0.1349935	0.1392791	0.1398626	0.1366028
0.7	0.054770	0.0552682	0.0502551	0.0545550	0.0556842	0.0660099
0.8	0.017536	0.0174647	0.0114197	0.0106773	0.0106042	0.0196423
0.9	0.004162	0.0040118	0.0015620	0.0006354	0.0003194	0.0035992
1	0.0004061	0.0004061	0.0004061	0.0004061	0.0004061	0.0004061

Table 5.5. Error calculated by L_2 norm for various Cr and Δx =0.01 values at Time = 1s

	Cr	L_2 of FTC2S	L_2 of FTC2C4S	L_2 of FTF3C4S	L_2 of FTC4C2S	L_2 of FTC4S
1	0.1	0.0091819	0.009706195	0.00987037	0.0098713	0.00899398
2	0.2	0.0188940	0.019764724	0.01993810	0.01993919	0.01870624
3	0.4	0.0398658	0.040991924	0.04118870	0.04118923	0.03966196

Table 5.6. Error calculated by L_∞ norm for various Cr and Δx = 0.01 values at Time = 1s

	Cr	L_∞ of FTC2S	L_∞ of FTC2C4S	L_∞ of FTF3C4S	L_∞ of FTC4C2S	L_∞ of FTC4S
1	0.1	0.0020302	0.00214636	0.00219392	0.00219392	0.0019806
2	0.2	0.0041794	0.00437941	0.00443064	0.00443064	0.0041267
3	0.4	0.0088727	0.00912411	0.00918114	0.00918114	0.0088134

As seen, FTC4S produces comparable less error. The performances of the schemes are in an acceptable range. Tables 5.5 and 5.6, present the error measures for different Cr and Δt conditions. FTC4S produces less L_2 and L_∞ error values. Figure 5.6 shows the simulation for the case Cr = 0.1 and Δt = 0.001 at time t = 1s for FTC4S scheme. As seen, the method captures the exact solution.

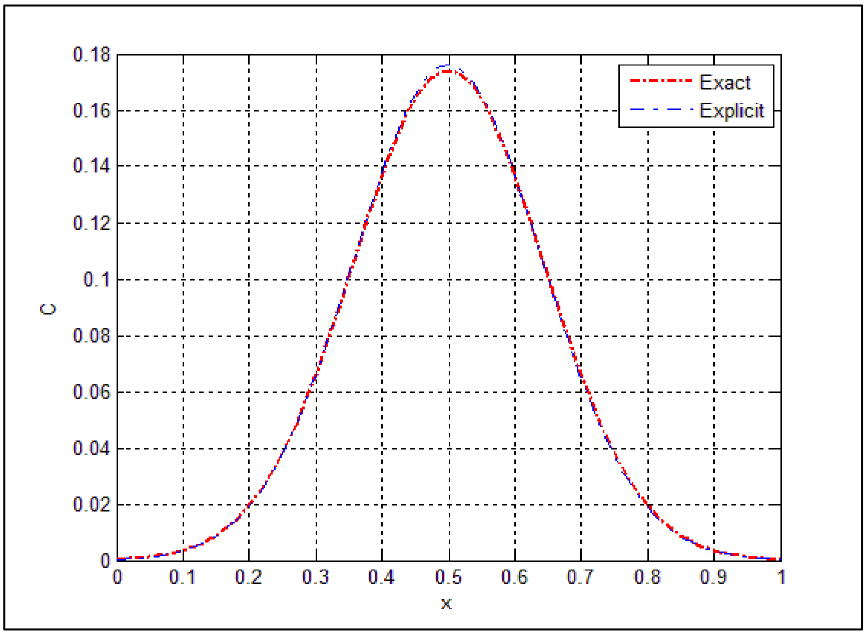


Figure 5.6. Comparison of the analytical solution and the numerical solution obtained by FTC4S schemes for Cr = 0.1 such that Δt = 0.001 and Δx = 0.01 at time t =1s

Table 5.7. summarizes the errors calculated by the two norms (L_2 and L_∞) for Δt = 0.001, 0.002, 0.004 and 0.008, Δx = 0.02,0.04 and 0.05 at simulation time of 1 s. As seen, all the methods perform comparable well though FTC4S produces less error.

Table 5.7 Error calculated by L_2 and L_∞ norms for various Δt =0.001, 0.002, 0.004 and 0.008 and Δx =0.02, 0.04 and 0.08 values at Time = 1s

Δx	**Δt**	**FTC2S**		**FTC2C4S**		**FTF3C4S**		**FTC4C2S**		**FTC4S**	
		L_2	L_∞	L_2	L_∞	L_2	L_∞	L_2	L_∞	L_2	L_∞
0.02	0.001	0.0098124	0.0029526	0.0093719	0.0028319	0.007693	0.0024688	0.007199	0.00228	0.0067309	0.002087
0.02	0.002	0.0141507	0.0044640	0.0135983	0.0042712	0.014814	0.0046974	0.014312	0.00449	0.0138264	0.004295
0.02	0.004	0.0271584	0.0086223	0.0265540	0.0083820	0.029916	0.0094862	0.029359	0.00926	0.0288158	0.009042
0.02	0.008	0.0591869	0.0189910	0.0584499	0.0186640	0.063927	0.0205089	0.063196	0.02019	0.0624836	0.019877
0.04	0.001	0.0252148	0.0108313	0.0244634	0.0104743	0.010338	0.0047912	0.006040	0.00280	0.0049409	0.002291
0.04	0.002	0.0254406	0.0104099	0.0244509	0.0100218	0.014789	0.0070882	0.010210	0.00459	0.0089310	0.003872
0.04	0.004	0.0285049	0.0126602	0.0270933	0.0120222	0.025266	0.0119898	0.020296	0.00907	0.0188789	0.008254
0.04	0.008	0.0430993	0.0201471	0.0411493	0.0190288	0.050126	0.0234914	0.043763	0.01942	0.0419663	0.018357
0.05	0.001	0.0345378	0.0158988	0.0335427	0.0153800	0.014815	0.0079030	0.007834	0.00402	0.0069836	0.003635
0.05	0.002	0.0345316	0.0156590	0.0333261	0.0151025	0.018353	0.0100535	0.010084	0.00515	0.0086786	0.004507
0.05	0.004	0.0359904	0.0166343	0.0343565	0.0155533	0.027312	0.0146826	0.017710	0.00894	0.0159116	0.007897
0.05	0.008	0.0448554	0.0232361	0.0424777	0.0218544	0.050081	0.0272659	0.037549	0.01881	0.0352611	0.017260

CHAPTER 6

CONCLUSIONS

In this study, several numerical schemes were applied to the one-dimensional convection–diffusion equation. The proposed numerical schemes solved this equation quite satisfactorily. The explicit finite difference schemes are very simple to implement and economical to use. They are very efficient and they need less time step than the other finite difference methods. A comparison with the different schemes for the numerical solution of the advection–diffusion problem shows that the FTC4S finite difference methods, even though they have extended range of stability, use large central processor times. The explicit finite difference FTC4S scheme is very easy to implement for similar higher dimensional problems, but it may be more difficult when dealing with the FTC2S, FTC2C4S, FTF3C4S and FTC4C2S schemes. When comparing the explicit finite difference techniques described in this study, it was found that the most accurate method is the fourth-order explicit formula FTC4S scheme. This scheme like other explicit schemes can be used to take advantage on vector or parallel computers. For each of the finite difference schemes investigated the modified equivalent partial differential equation is employed which permits the order of accuracy of the numerical methods to be determined. The performance of the method for the considered problems was tested by computing L_∞ and L_2 error norms. Also from the truncation error of the modified equivalent equation, it is possible to eliminate the dominant error terms associated with the finite-difference equations that contain free parameters (weights), thus leading to more accurate methods.

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