Improved averaging-based finite-difference schemes for the convection-diffusion equation

By

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I dedicate this thesis to my late parents (Md. Modabbir Ali & Sufia Akhtar), my husband Mahamudul Hashan

And

To my little prince Arham Hasan.

Abstract

Convection and diffusion have significant effect on reservoir flow systems. To represent the reservoir properly, these effects are encountered in models of reservoir engineering. Many researchers have worked on the convection-diffusion equations. Barakat and Clark considered a diffusion equation in 1966 and proposed a new explicit finite-difference scheme which gives a better result with less error using an averaging of two lower-order schemes. Bokhari and Islam extended this work to solve convection-diffusion equations and claimed to get the accuracy of $O(\Delta t^4)$. In the present study, we analyse the Barakat and Clark Scheme numerically and provide details of the truncation error analysis and stability by Von Neumann analysis. The Bokhari-Islam Scheme is also studied here. After the analysis, it is found that the claim of Bokhari and Islam, to get the accuracy of $O(\Delta t^4)$, is not valid. Two new numerical schemes, Generalised Barakat-Clark and Upwind Barakat-Clark are proposed with better accuracy.

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D	Diffusion Coefficient
U	Convection Coefficient
Nr	Number of Grid blocks
Nt	Number of time steps
t	Time
r, x	Space
n	Time level
γ	Amplification Factor
P	Pressure
i	Number of grid
ϵ	Error
c	Variable representing species temperature for heat transfer, and concentration for mass transfer
v	Field velocity
R	Sources or sinks
∇	Gradient
$\nabla .$	Divergence

Chapter 1 Introduction

Reservoir simulation is one of the most used tools in reservoir engineering, which predicts the future performance of oil and gas reservoirs (Ertekin et al. 2001; Chen 2007; Lie and Mallison 2013; Deb et al. 2017). Flexibility, availability, accuracy over a wide range of operating conditions, and reliability have made reservoir simulation an accepted technology. Reservoir simulation is also done for finding ways of enhancing and optimizing recovery. Improved numerical methods, increased capacity and speed of computers, low computing cost, and the capability of modelling diverse oil and gas reservoirs have given numerical reservoir simulation a wide acceptance in the petroleum industry (Mustafiz and Islam 2008; Islam et al. 2010).

Reservoir simulation is done by analyzing a physical or mathematical model of a reservoir. Physical modelling may be done at a laboratory scale, while mathematical modelling leads to partial differential equations along with appropriate boundary conditions. Such mathematical models adequately describe the processes taking place in a reservoir, for example, mass transfer, fluid flow through porous media, convection, and diffusion. Mathematical models are usually solved numerically. The first step of numerical solution is discretization, which leads to systems of linear and nonlinear algebraic equations. The systems of equations are solved to predict reservoir performance accurately. Numerical methods have an advantage of dealing with very complex reservoir conditions.

Use of improved and efficient numerical methods in reservoir engineering plays an important role in recovery. It is important to account for all processes near a well when modelling a reservoir. There are two methods of mass transfer through fluid flow in the reservoir. One is diffusion and the other is convection. Diffusion is an intermolecular phenomenon, where mass transfer happens due to relative activity of each molecule, while convection is a major mode of mass transfer due to bulk motion of phase. Convection-diffusion equations describe physical phenomena where particles, energy, or other physical quantities are transferred inside a physical system due to both diffusion and convection. The general equation is (Socolofsky and Jirka 2005, Stocker 2011).

$$\frac{\delta c}{\delta t} = \nabla.(D\nabla c) - \nabla.(\mathrm{vc}) + \mathrm{R} \tag{1.1}$$

Here, c is the variable representing species temperature for heat transfer, and concentration for mass transfer; v is the field velocity (field that the quantity is moving around); R represents sources or sinks; ∇ and $\nabla.$ represents gradient and divergence respectively; the term $\nabla.(D\nabla c)$ describes diffusion; and the term $-\nabla.(\mathrm{vc})$ describes convection.

Concentration gradients causes diffusion in mass transport of a dissolved species or in a gas mixture; and the convection (bulk fluid motion) contributes to the flux of chemical species. Thus, the combined effect of convection and diffusion is considered while solving problems describing flows by convection-diffusion equation.

To solve the convection-diffusion equation numerical methods are preferred over analytical methods (Huang et al., 2008; Kaya, 2010; Ding and Jiang, 2013). Because, the analytical solutions are time-consuming and sometimes it is not possible to solve for a complex flow system. On the other hand, the numerical solutions can solve complex systems with acceptable error of approximations within a short time compared to analytical solution (Morton and Mayers, 2005).

1.1 Basis of the research

Near injection wells, both convection and diffusion have vital effects on the fluid flow. Thus, it is necessary to account for both convection and diffusion processes in modelling any recovery process.

Many researchers have studied both diffusion and convection-diffusion equations using different numerical differentiation techniques (Guymon et.al., 1970; Dehghan, 2004; Roos et.al., 2008; Zhuang et.al., 2009; Shen et.al., 2011; Liu et.al., 2013; and many more). In 1966, Barakat and Clark proposed a numerical solution algorithm for the diffusion equation (Barakat and Clark 1966) which was expanded later by others. Barakat and Clark proposed an explicit-finite difference procedure to solve the diffusion equation based on an averaging of two low-order schemes to reach a high-order scheme. Their proposed method has the advantage of unconditional stability along with simplicity.

Later, many researchers (Kettleborough, 1972; Welty, 1974; Evans and Abdullah, 1983, 1985; Evans, 1985; Bogetti and Gillespie,1992; Gupta et.al., 1997; Xu and Lavernia, 1999; Michaud, 2000; Aboudheir et.al., 2003; Belhaj et.al., 2003; and many more) have worked with Barakat and Clark scheme. In 2005, Bokhari and Islam proposed a scheme for convection-diffusion equations based on the Barakat and Clark scheme (Bokhari and Islam 2005). They used a central difference approximation in time along with aspects of the Barakat and Clark scheme, and claim to get fourth-order accuracy in time. The claim to get fourth-order accuracy makes the Bokhari and Islam scheme eye-catching. However, there were no detailed steps shown for the analysis of the method proposed by Barakat and Clark, nor by Bokhari and Islam.

Though there are many fourth-order time integration schemes (Cullen and Davies, 1991; Ascher et.al., 1995; Wesseling, 1996; Chawla et.al. 2000; Donea et.al., 2000; Li and Tang, 2001; Bijl et.al., 2002; Wicker and Skamarock, 2002; Appadu et.al., 2016; Sengupta et.al., 2017; Fu et.al., 2018; Ge et.al., 2018; and many more), the lack of evidence in support of their claim of Bokhari-Islam and the advantages of accuracy with simplicity of Barakat-Clark Scheme influenced the present study to deal with Barakat-Clark and Bokhar-Islam Scheme. The focuses of this thesis are:

- To provide detailed steps of the Barakat-Clark and Bokhari-Islam schemes
- Check the validity of the claim of Bokhari and Islam regarding accuracy in time, and
- Propose two improved averaging-based finite difference schemes.

For doing the analysis:

- A one-dimensional convection-diffusion equation with Dirichlet boundary conditions is considered.
- All schemes are validated using an analytical solution where the pressure is defined as a known function of space and time.
- Numerical solutions of the 1-D convection-diffusion equations are compared with this analytical solution to calculate exact error values.

In Chapter 2, the background of the research and the analytical solution considered here are provided. Chapter 3 presents the detailed analysis of the centred difference explicit scheme and the centred difference implicit scheme for the one-dimensional convection-diffusion equation. Chapter 4 provides the detailed analysis of error and stability and numerical validation of the Barakat-Clark Scheme. The error and stability analysis with numerical validation of the Bokhari-Islam Scheme is provided in Chapter 5. One of the proposed schemes, the Generalised Barakat-Clark Scheme, is discussed in Chapter 6. The second proposed scheme, the Upwind Barakat-Clark Scheme, is analysed and validated in Chapter 7. Finally, Chapter 8 presents the comparison of the different schemes and potential future research.

Chapter 2 Background

2.1 Finite difference method

The finite difference method (FDM) is a numerical procedure for finding approximate solutions to partial differential equations (PDEs). In this technique, the physical domain is represented by a set of discrete nodes. An FDM proceeds by replacing the derivative terms of a PDE by finite-difference approximations (FDAs).

In discretization, the spatial and temporal domains are represented by a finite number of nodes, specified by the user. Discretization can be two-dimensional (e.g. one dimension in space and one dimension in time or two dimensions in space), three-dimensional (e.g. two dimensions in space and one dimension in time), and four-dimensional (e.g. three dimensions in space and one dimension in time). Figure 2.1 represents discretization of a two-dimensional space-time domain. The spacing between two adjacent nodes of the space and time domains are defined as the spatial step size (Δr) and time step size (Δt), respectively. Δr and Δt can be uniform or non-uniform throughout the domain.

An FDA approximates a derivative of a function at a point r using its values at points in the neighborhood of r (Figure 2.2). For an FDM, such an approximation is made at all points of a space domain and all time steps. This gives an approximation of the PDE as a system of equations using the FDA to replace all derivatives in the PDE. The finite difference solution comes from solving this system of equations. Two of the most important parameters for the accuracy of an FDM are the spacing between the nodes and the specific formula used for the approximations.

The true derivative, $f'(r)$, of a function $f(r)$ at point r is the value of the slope of the tangent line drawn at that point. In an FDM, the derivative at point r is approximated from the value of the slope of the secant line between point r and/or neighboring points. The approximated derivative generally becomes closer to the true derivative as the neighborhood points come closer to point r. This implies that the resolution and the accuracy are increased with a decrease in spacing between the nodes. But there is a risk of increase in round-off error with increasing numbers of nodes (Gautschi, 2012).

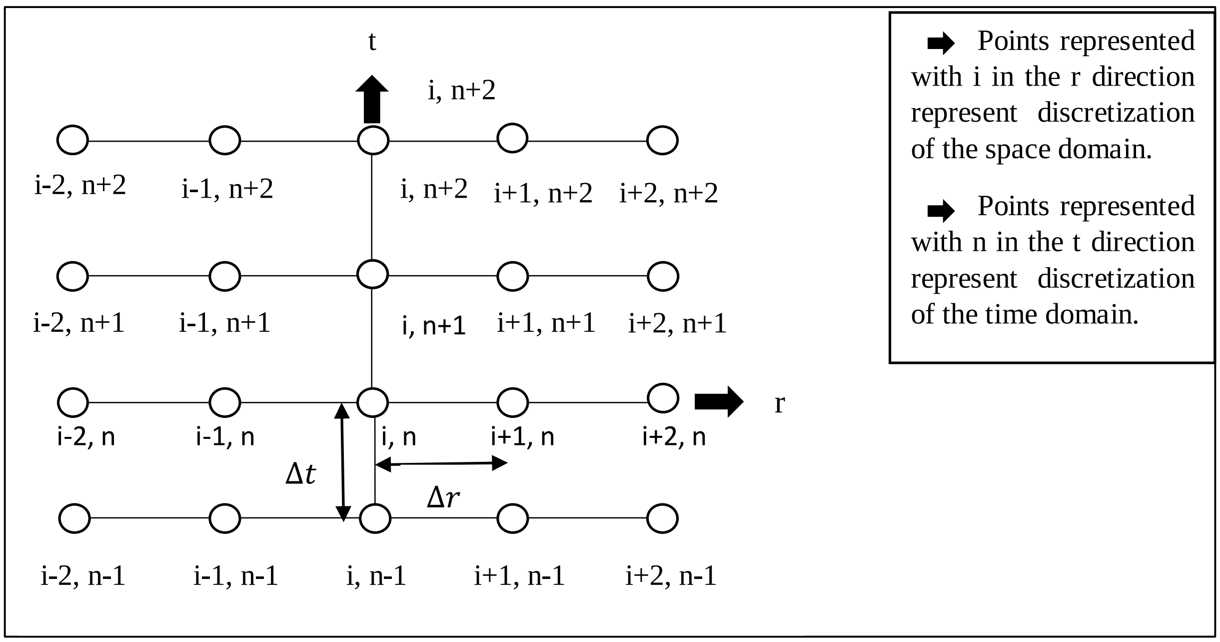


Figure 2.1: Two-Dimensional discretization

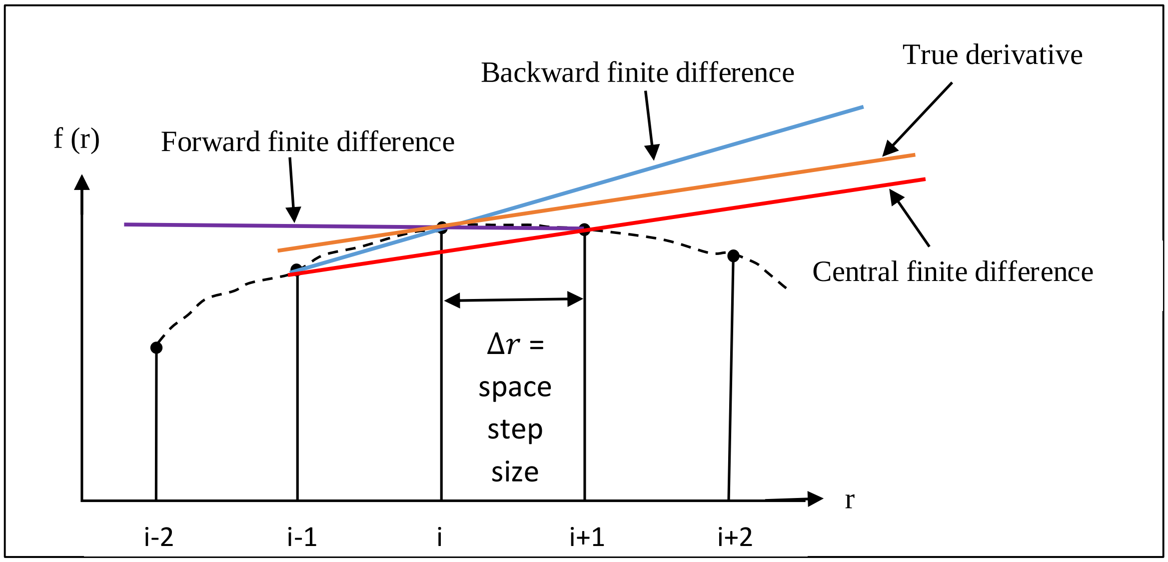


Figure 2.2: FDM Approximations of first derivative of f(r) at point i.

2.2 Some approaches to solve convection-diffusion equation using FDM

Convection-diffusion equations have significant application in heat transfer (Isenberg and Gutfinger, 1973), fluid dynamics (Kumar, 1983), and mass transfer (Guvanasen and Volker, 1983). Thus, convection-diffusion equations play a vital role in reservoir simulation. Many researchers have solved convection-diffusion equations using various techniques. Analytical solution techniques are strongly influenced by the initial and boundary conditions, and complex geometry often makes these approaches intractable. On the other hand, numerical methods are free from such limitations. In spite of having analytical solutions for the convection-diffusion equation in many settings (Fry et al., 1993; Zoppou and Knight, 1997; Lin and Ball, 1998; Jiang et al., 2012; Eli and Gyuk, 2015; Samani et al., 2018; among many), generally researchers are more inclined to use numerical methods (Zhao and Valliappan, 1994; Huang et al., 2008; Kaya, 2010; Ding and

Jiang, 2013; Ali and Malik, 2014; Karakoç et al., 2014; Kaya and Gharehbaghi, 2014; Nazir et al., 2016; Korkmaza and Dag˘, 2016; Askari and Adibi, 2017; among many) because of the advantages of numerical solutions (i.e, less time, acceptable error, and ability to solve complex systems) over analytical.

Many numerical methods are used to solve convection-diffusion equations. Some of the methods which are mentioned in this study are given below.

Forward Time Centered Space (FTCS), a fully explicit finite difference method, is used for solving heat equation and parabolic partial differential equations (Anderson et.al., 2016). It is based on the Forward Euler method in time and central difference in space. FTCS method is computationally inexpensive and easy to solve numerically (Anderson, 1995).

Backward Time Centered Space (BTCS), a fully implicit finite difference method, steeped backward in time using increments of time interval and centered difference in space (Ames, 1965; Anderson, 1995). The fully implicit scheme is unconditionally stable.

The explicit centered difference method is an explicit second order method which approximates the solution of the second order differential equation.

Implicit Centered Difference Method is an implicit second order method which approximates the solution of the second order differential equation.

Upwind Scheme solves hyperbolic partial differential equations by numerically simulating the direction of propagation of information in a flow field (Courant et.al., 1953). It gives numerically stable results for convection dominated flows (Abbott and Basco, 1989). The upwind differencing scheme is used in computational fluid dynamics for solving convection-diffusion equations (Versteeg and Malalasekera, 2007).

Since the 1990’s, the Lattice Boltzmann Method (LBM) has been used with high attention for fluid flow simulation (Higuera et al. 1989; Chen et al. 1991; Chen et al. 1992). To solve diffusion and convection-diffusion equations, LBM can also be applied as shown by Moriyama and Inamuro (1983), Kang (2003), Ginzburg (2005), and Stiebler et al. (2008). Gebäck and Heintz (2013) applied LBM for convection-diffusion equation considering Neumann boundary conditions, finding second-order convergence both theoretically and numerically. In addition, for solving one-dimensional time-dependent convection-diffusion equations with Neumann boundary conditions, Kereyu and Gofe (2016) considered the Forward Time Centered Space (FTCS) and Backward Time Centered Space (BTCS) schemes. They found first order convergence for both methods regardless of the actual order of the spatial dimension.

For the solution of the diffusion equation and time dependent transport equation, different numerical methods have been suggested by Crank and Nicolson (1947), and Peaceman and Rachford (1955). Barakat and Clark (1966) proposed an unconditionally stable explicit finite difference scheme to solve the nonhomogeneous, multidimensional diffusion equation. Aboudheir et al. (1999) numerically solved the convection-diffusion equation and showed that the accuracy of the DuFort-Frankel scheme was the highest of the schemes in their study, but it is not unconditionally stable as urged in literature. In addition, they found the Barakat- Clark scheme to be more accurate compared to the fully implicit scheme. Later, Bokhari and Islam (2005) applied the same technique proposed by Barakat and Clark (1966) to solve nonhomogeneous, multidimensional convection-diffusion equations to get the overall accuracy in time of the order of Δt^4, but they did not provide any evidence supporting their claim.

Spline interpolation techniques (a form of interpolation using piecewise polynomials) were used to solve convection equations by Pepper et al. (1979) and Okmoto et al. (1998). Later, Thongmoon and McKibbin (2006) applied spline interpolation techniques to convection-diffusion equations and compared with two finite-difference methods. They used FTCS and the Crank-Nicolson methods for solving convection-diffusion equations and found that these FDM give more accurate point-wise solutions than the spline technique.

The one-dimensional convection-diffusion equation was solved by Appadu (2013) using three numerical methods. He used the Lax-Wendroff scheme, the Crank-Nicolson Scheme, and the Nonstandard Finite Difference scheme (NSFD) (Mickens, 1991). After numerical investigation, he found that the Lax-Wendroff and the NSDF methods give better approximations than the Crank-Nicolson scheme for the same space and time step sizes.

The convection-diffusion equation on unstructured grids is solved by Pereira et al. (2013). They used a first-order upwind and high-order flux-limiter schemes and applied the methods to a model of the Guaíba River in Brazil. They found good agreement between the model and observed data and, for all scenarios, the first-order upwind scheme is more diffusive than the high-order flux-limiter scheme.

The one-dimensional convection-diffusion equation is solved by Savović and Djordjevich (2012) using an explicit finite difference method considering semi-infinite media with variable coefficients. They solved the equation for three different dispersion problems. First, they considered solute dispersion along steady flow in an inhomogeneous medium. Secondly, temporally dependent solute dispersion along steady flow in a homogeneous medium. Thirdly, solute dispersion along temporally dependent unsteady flow in a homogenous medium. Finally, they compared their results with analytical solutions reported in the literature. Through their numerical investigation, they showed that for solving one-dimensional convection-diffusion equation with variable coefficient in semi-infinite media, the explicit finite difference method is accurate and effective.

Gharehbaghi (2016) and Gharehbaghi et al. (2017) also solved the time-dependent one-dimensional convection-diffusion equation with variable coefficients in semi-infinite media. They used differential quadrature methods in both explicit and implicit conditions. Finally, they compared their results with analytical solutions presented in the literature and found that the differential quadrature methods are robust, efficient and reliable. Also they found that the predictions of the explicit forms are less accurate than those of the implicit form.

FDM is used by many researchers to solve one-dimensional convection-diffusion equations, giving high accuracy compared with analytical solutions. The following table gives an overview of some of the work done on convection-diffusion equation.

Table 2.1 Some of the works done on convection-diffusion equation

Author(s)	Method(s) /approach(es)	Applied for	Remark(s)
Higuera et al. 1989; Chen et al. 1991; Chen et al. 1992; Moriyama and Inamuro, 1983; Kang, 2003; Ginzburg, 2005; Stiebler et al., 2008; Gebäck and Heintz, 2013	Lattice Boltzmann Method (LBM)	Convection-diffusion	Considering Neumann boundary conditions, found second-order convergence both theoretically and numerically.
Kereyu and Gofe, 2016	Forward Time Centered Space (FTCS) and Backward Time Centered Space (BTCS) schemes.	Convection-diffusion	Found first order convergence for both methods regardless of the actual order of the spatial dimension
Barakat and Clark, 1966	Explicit finite difference scheme	Diffusion	Unconditionally stable
Aboudheir et al. 1999	Followed DuFort-Frankel scheme	Convection-diffusion	Found highest accuracy of the studied schemes.

Bokhari and Islam, 2005	Followed Barakat and Clark scheme	Convection-diffusion	Claimed to get fourth order accuracy.
Pepper et al., 1979; Okmoto et al., 1998	Spline interpolation techniques	Convection	FDM gives better results.
Thongmoon and McKibbin, 2006	Spline interpolation techniques	Convection-diffusion	FDM gives better results.
Mickens, 1991; Appadu, 2013	Lax-Wendroff scheme, the Crank-Nicolson Scheme, and the Nonstandard Finite Difference scheme (NSFD)	Convection-diffusion	Found that the Lax-Wendroff and the NSDF methods give better approximations than the Crank-Nicolson scheme
Pereira et al. (2013).	First-order upwind and high-order flux-limiter schemes	Convection-diffusion equation on unstructured grids	Found that the first-order upwind scheme is more diffusive than the high-order flux-limiter scheme.
Savović and Djordjevich, 2012	Explicit finite difference method considering semi-	Convection-diffusion	Showed that the explicit finite

	infinite media with variable coefficients		difference method is accurate and effective.
Gharehbaghi, 2016); Gharehbaghi et al., 2017	differential quadrature methods in both explicit and implicit conditions for variable coefficients in semi-infinite media.	Convection-diffusion	Found that the differential quadrature methods are robust, efficient and reliable.
Shukla et.al., 2011	Finite difference method (FDM), Finite element method (FEM)	Convection-dominated diffusion	Found that the finite difference method or finite element method does not work well.
Sun and Zhang, 2004; Ma and Ge, 2010	Richardson extrapolation technique and an operator interpolation scheme	Convection-diffusion	Found sixth order compact finite difference discretization strategy for coarse grain.
Wang and Zhang, 2010; Ge et.al., 2013	Multiscale multigrid method	Convection-diffusion	Sixth-order explicit compact finite difference scheme was presented

Samarskii et.al., 1993; Hu and Argyropoulos, 1996; Voller, 1997; Teskeredžić et.al., 2002; Feng and Chang, 2008	Stefan approximation and Boussinesq approximation	Convection-diffusion	Did numerical simulation of convection/diffusion phase change processes.
Li, 1983	Based on the method of operator splitting	Convection-diffusion	For miscible displacement processes. This method is superior to the conventional finite difference methods
Nove and Tan, 1988; Spotz and Cary, 1995	Weighted modified equation method.	Convection-diffusion	A computationally fast third-order semi-implicit five-point finite difference method is proposed with large stability region and better accuracy.

Hariharan and Kannan, 2010; Jiwari, 2012	Wavelet transform or wavelet analysis.	Convection-diffusion	Developed an accurate and efficient Haar transform or Haar wavelet method which is found to be simple, flexible, fast, and convenient.
Wen-gia, 2003	Followed Saul'yev type difference scheme and the Alternating Segment Crank-Nicolson (ASC-N) method	Convection-diffusion	A new discrete approximation to the convection term was proposed and found that ASC-N method is unconditionally stable.
Jinfu and Fengli, 1998; Wen-qia, 2003; Feng and Tian, 2006	AGE methods	Convection-diffusion	Unconditionally stable with the property of parallelism.
Ismail and Elbarbary, 1999; Ismail and Rabboh, 2004	Implicit method	Convection-diffusion	Showed that the method is highly accurate, fast and with good results whatever the exact solution is

			too large *i.e.*, the absolute error still very small.
Evans and Abdullah, 1985; Evans, 1985; Noye and Tan, 1988;	Explicit method	Convection-diffusion	The formulas are asymmetric and can be used to develop group explicit method.
Tian and Yu, 2011; Zhang and Zhang, 2013	The fourth-order compact exponential difference formula	Convection-diffusion	High-order exponential (HOE) scheme is developed which is highly accurate.
Mihaila and Mihaila, 2002; Temsah, 2009	The method of El-Gendi	Convection-diffusion	Numerical solutions with interface points are provided for linear and non-linear convection-diffusion equation. The solutions maintain good accuracy.

Tan and Shu, 2010; Lu et.al., 2016	Inverse Lax–Wendroff procedure considering numerical boundary conditions	Convection-diffusion	A careful combination of the boundary treatments is designed which is stable.
Chen et.al. 2014; Bai and Feng, 2017	Variational multiscale method (VMS)	Convection-dominated convection–diffusion equations	Stabilized projection based method is proposed which is better than VMS for some examples.
Gelu et.al., 2017; Bisheh-Niasar et.al., 2018	Finite difference approximations.	Reaction–diffusion	Sixth-order compact finite difference method is presented which approximates the exact solution very well.

The present study focuses on the approach presented by Barakat and Clark (1966) and adapted by Bokhari and Islam (2005) to solve the one-dimensional time-dependent convection-diffusion equation.

2.3 Numerical Error

Numerical methods do not provide the exact solution to a differential equation. Two kinds of errors are introduced while computing the approximate solution– round-off error and truncation error. These two errors together form the total error in an approximation (Figure 2.3).

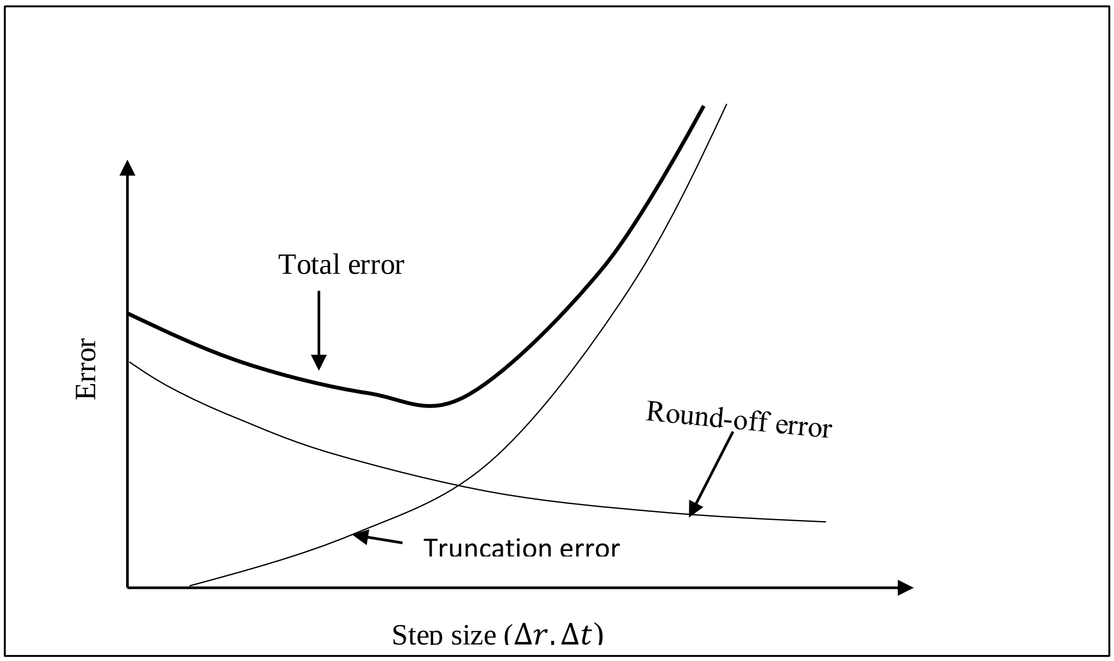


Figure 2.3: Change of error with step size (modified from Gautschi, 2012; Hoffman and Frankel, 2001).

2.3.1 Truncation error

Truncation error occurs in numerical analysis and scientific computing due to use of approximate mathematical procedures, i.e., the use of finite sums instead of infinite sums in solving a numerical problem. For example, truncation error occurs in approximating a sine function using the first two terms ($\text{Sin x} = x - \frac{x^3}{3!}$) instead of using an infinite number of terms of the Taylor series expansion ($\text{Sin}\, x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots$). The truncation error of a finite-difference approximation of a time-dependent partial differential equation can be written by using the two-dimensional version of Taylor's Theorem for gridpoint i at time level n, $T_i^n = \frac{1}{\Delta t}\{(AP^{n+1})_i - (BP^n)_i\}$, where P^n and P^{n+1} represent the solution at time levels n and n+1 respectively and the operators A and B will be explained later. The truncation error is dependent on the numerical method used in solving a mathematical problem (Hoffman and Frankel, 2001).

In numerical differentiation, the truncation error depends on the step size ($\Delta r, \Delta t$) and the specific finite-difference formulas used in approximating the derivatives. The truncation error can be reduced by reducing the step size or by using a higher-order formula. Numerical methods used in solving differential equations consist of different steps. It is essential to find the accuracy of a numerical solution as only approximate solutions can be obtained using numerical methods (Epperson, 2013).

2.3.2 Round-off error

Round-off error is defined as the difference between the approximate value of a number used in calculation and its precise (exact) value (Pegg and Weisstein, 2017; Clapham and Nicholson, 2009). Round-off error is introduced due to the technique of storing the numbers and performing the numerical computation by computer. A finite number of bits are used to store the real numbers in computer. When the mantissa of the real numbers is longer than the available bits then the real numbers are shortened to be stored. This shortening procedure is done by two ways– chopping and rounding. Chopping removes the extra digits that cannot be stored, whereas rounding operation rounds the last digit that can be stored. The round-off error is introduced by these chopping and rounding actions.

Many researchers studied the significance of round-off error. For example, Qin and Liao (2017) studied the impact of round-off error on the reliability of numerical simulations of chaotic dynamic systems; Bellhouse (2015) investigated the effect of round-off error using the historical tables produced by Simon Stevin (1959) and, McCullough and Vinod (1999) showed the consequence of round-off error on Vancouver stock exchange index. Several true incidences can be found in different references that also states about the significance of round-off error. Destruction of the Ariane 5 rocket launched from the European Space Agency on June 4, 1996 (Huizinga and Kolawa, 2007) and killing of 28 people in American soldier's barrack due to failure of the Patriot missile defence system used in Gulf War (Skeel, 1992) are the true extreme occurrences that happened due to round-off error.

The round-off error can be increased by three factors– (i) existence of error in initial steps of computation, (ii) increase in the magnitude of the involved numbers, and (iii) subtraction of identical numbers from each other (Weisstein, 2017; Hoffman and Frankel, 2001). Huizinga and Kolawa (2007) categorized the main reasons of round-off error into four groups. Detailed root causes of round-off error and action plans that need to be executed to minimise the round-off error (as described by Huizinga and Kolawa, 2007), are shown in Table 2.2.

Table 2.2: Main causes of round-off error and action plans that need to be executed to reduce the round-off error.

Root causes of round-off error	Action plans to minimise the round-off error
1. Lack of expertise in programming. 2. Inadequate test methods. 3. Ineffective development techniques. 4. Low precision.	1. Key programmers need to be trained in math and programming courses. 2. Precision should be minimum 64 bit. 3. Consultation needs to be done with an expert who has expertise in numerical analysis and coding. 4. Stability and accumulative errors should be checked while running the code for extended period. 5. Interval arithmetic math technique can be used to check the error. 6. Floating-point error analysis must be performed.

2.4 Stability

The concept of numerical stability of a finite-difference scheme is closely related with the numerical error of the scheme. A scheme is said to be stable if the errors made in earlier stages of the computation do not propagate into increasing errors in the later stages of the calculation. The prime requirement of a stable scheme is that the local error made in one step of the computation should not be increased by further calculation. The effect of an error should remain constant or reduce with time by further computation.

2.4.1 Procedure of von Neumann stability analysis

The explicit scheme for the one dimensional heat equation (parabolic partial differential equation) is considered here (Equation (2.1)) to illustrate the technique of von Neumann stability analysis. Equation (2.2) is the discretized form of Equation (2.1), using a central difference approximation in space (r direction) and forward difference approximation in time (t direction).

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \tag{2.1}$$

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta r)^2} + O(\Delta t, \Delta r^2) \tag{2.2}$$

Here, α is the thermal diffusivity. Let T_i^n be a solution of the explicit scheme for the one-dimensional heat equation (Equation (2.2)), and let a perturbation, $T_i^n + \epsilon_i^n$, satisfy the same scheme. Thus,

$$\frac{(T_i^{n+1} + \epsilon_i^{n+1}) - (T_i^n + \epsilon_i^n)}{\Delta t} = \alpha \frac{(T_{i+1}^n + \epsilon_{i+1}^n) - 2(T_i^n + \epsilon_i^n) + (T_{i-1}^n + \epsilon_{i-1}^n)}{(\Delta r)^2} \tag{2.3}$$

The definition of T_i^n implies that

$$\frac{\epsilon_i^{n+1} - \epsilon_i^n}{\Delta t} = \alpha \frac{\epsilon_{i+1}^n - 2\epsilon_i^n + \epsilon_{i-1}^n}{(\Delta r)^2} \tag{2.4}$$

Expanding the error, ϵ_i^n, using Fourier series gives

$$\epsilon_i^n = \sum_k \gamma_k^n \exp(\bar{\imath} k r_i) \tag{2.5}$$

Where $\bar{\imath} = \sqrt{-1}$, k= wave number.

To simplify the analysis, it is assumed that the solution has only one term.

$$\epsilon_i^n = \gamma^n \exp(\bar{\imath} k i \Delta r) \tag{2.6}$$

Substituting this into Equation (2.4) gives

$$\frac{(\gamma^{n+1} - \gamma^n)\exp(\bar{\imath} k \Delta r i)}{\Delta t} = \alpha \frac{\gamma^n \exp(\bar{\imath} k \Delta r) - 2\gamma^n + \gamma^n \exp(-\bar{\imath} k \Delta r)}{\Delta r^2} \exp(\bar{\imath} k \Delta r i) \tag{2.7}$$

$$\gamma^{n+1} = \alpha \frac{\Delta t}{\Delta r^2} [2\cos(k\Delta r) - 2]\gamma^n \tag{2.8}$$

$$\gamma = 1 - \alpha \frac{4\Delta t}{\Delta r^2} Sin^2\left(\frac{k\Delta r}{2}\right) \tag{2.9}$$

The von Neumann criteria for stability is fulfilled if

$$|1 - \alpha \frac{4\Delta t}{\Delta r^2} Sin^2\left(\frac{k\Delta r}{2}\right)| \leq 1 \tag{2.10}$$

The term $\alpha \frac{4\Delta t}{\Delta r^2} Sin^2\left(\frac{k\Delta r}{2}\right)$ is always positive.

Noting that $Sin^2\left(\frac{k\Delta r}{2}\right) \leq 1$, to satisfy Equation (2.10), we require $\alpha \frac{4\Delta t}{\Delta r^2} Sin^2\left(\frac{k\Delta r}{2}\right) \leq 2$, which is guaranteed if

$$\alpha \frac{\Delta t}{\Delta r^2} \leq \frac{1}{2} \tag{2.11}$$

Equation (2.11) gives the stability requirement for one-dimensional heat equation. For a given value of Δr^2, the value of Δt must be small enough to satisfy the equation.

2.5 Analytical solution for 1-D convection-diffusion equation

The 1-D convection-diffusion equation with Dirichlet boundary condition is given below:

$$\frac{\partial \mathrm{P}}{\partial t} = \mathrm{D}\frac{\partial^2 \mathrm{P}}{\partial \mathrm{x}^2} + \mathrm{U}\frac{\partial \mathrm{P}}{\partial \mathrm{x}}; \qquad (2.12)$$

The factorized function $\mathrm{P(x,t) = X(x)T(t)}$ is a solution to the 1-D convection-diffusion equation, if and only if

$$\mathrm{X(x)T'}(t) = \mathrm{DX''(x)T(t) + UX'(x)T(t)} \qquad (2.13)$$

Rearranging terms, we have

$$\frac{\mathrm{T'}(t)}{\mathrm{T}(t)} = \mathrm{D}\frac{\mathrm{X"(x)}}{\mathrm{X(x)}} + \mathrm{U}\frac{\mathrm{X'(x)}}{X(x)} = \lambda, \quad \text{where } \lambda \text{ is a constant.} \qquad (2.14)$$

Separating variables and separately considering time and space, we have

$\mathrm{T'(t) = \lambda T(t)}$, which gives

$$T(t) = e^{\lambda t} \qquad (2.15)$$

Similarly, for the spatial terms, we get

$$\mathrm{DX"(x) + UX'(x) - \lambda X(x) = 0} \qquad (2.16)$$

Here, $X(x) = c_1 e^{s_1 x} + c_2 e^{s_2 x}; \quad X(0) = X(1) = 0$ (2.17)

Substituting e^{sx} into Equation (2.16) gives

$$\mathrm{D}s^2 + Us - \lambda = 0 \tag{2.18}$$

$$\text{So, } s = \pm\sqrt{\frac{U^2}{4D^2} + \frac{\lambda}{D}} - \frac{U}{2D} \tag{2.19}$$

Thus, $s_1 = \sqrt{\frac{U^2}{4D^2} + \frac{\lambda}{D}} - \frac{U}{2D}$ and $s_2 = -\sqrt{\frac{U^2}{4D^2} + \frac{\lambda}{D}} - \frac{U}{2D}$

Applying $X(0) = 0$, Equation (2.17) gives $c_1 = -c_2$

$$\text{So } X(x) = c_1(e^{s_1 x} - e^{s_2 x}) \tag{2.20}$$

For $\frac{U^2}{4D^2} + \frac{\lambda}{D} < 0$, Equation (2.20) becomes

$$c_1(e^{s_1 x} - e^{s_2 x}) = c_1\left(e^{-\frac{U}{2D}x}\left(e^{i\sqrt{-\frac{U^2}{4D^2} - \frac{\lambda}{D}}\,x} - e^{-i\sqrt{-\frac{U^2}{4D^2} - \frac{\lambda}{D}}\,x}\right)\right) \tag{2.21}$$

$$\text{Or, } c_1(e^{s_1 x} - e^{s_2 x}) = c_1 2i\, e^{-\frac{U}{2D}x} \sin\left(\sqrt{-\frac{U^2}{4D^2} - \frac{\lambda}{D}}\; x\right) \tag{2.22}$$

Now applying $X(1) = 0$, Equation (2.22) gives

$$c_1(e^{s_1} - e^{s_2}) = c_1 2i\, e^{-\frac{U}{2D}} \sin\left(\sqrt{-\frac{U^2}{4D^2} - \frac{\lambda}{D}}\right) = 0 \tag{2.23}$$

So, $\sqrt{-\frac{U^2}{4D^2} - \frac{\lambda}{D}} = n\pi$ and, after simplification, we get

$$\lambda = -\left(\frac{U^2}{4D} + Dn^2\pi^2\right) \tag{2.24}$$

By putting the value of λ in Equations (2.15) and (2.23), we get

$$T(t) = e^{-\left(\frac{U^2}{4D}+Dn^2\pi^2\right)t} \text{ and } X(x) = c_1\, e^{-\frac{U}{2D}x} \sin(n\pi x) \tag{2.25}$$

Thus, we can write

$$\mathrm{P(x,t)} = \sum_{n=1}^{\infty} c_n e^{-((\frac{U^2}{4D}+Dn^2\pi^2)t}\, e^{-\frac{Ux}{2D}} \sin(n\pi x) \tag{2.26}$$

For the initial condition at $t = 0$, we get

$$\sum_{n=1}^{\infty} c_n \sin(n\pi x) = P_0(x)e^{\frac{Ux}{2D}} \tag{2.27}$$

Let $P_0 = x(1-x)$. Then, Equation (2.27) can be written as

$$e^{\frac{Ux}{2D}} * x(1-x) = \sum_{n=1}^{\infty} c_n \sin(n\pi x) \tag{2.28}$$

By using Fourier series and orthogonal functions, we can write

$$e^{\frac{Ux}{2D}} * x(1-x)\sin(m\pi x) = \sum_{n=1}^{\infty} c_n \sin(n\pi x)\sin(m\pi x) \tag{2.29}$$

If $n \neq m$, $\int \sin(n\pi x)\sin(m\pi x)\, dx = 0$, so, we get

$$c_n = \frac{\int_0^1 e^{\frac{Ux}{2D}} * x(1-x)\sin(n\pi x)dx}{\int_0^1 sin^2(n\pi x)dx} \tag{2.30}$$

$$\Rightarrow c_n = -\frac{16D^3\pi n}{(4\pi^2D^2n^2+U^2)^3}[(-8\pi^2D^3n^2 + 4\pi^2D^2n^2U + 6DU^2 + U^3) +$$

$$e^{\frac{U}{2D}}(-1)^n(8\pi^2D^3n^2 + 4\pi^2D^2n^2U - 6DU^2 + U^3)]/(\tfrac{1}{2}) \tag{2.31}$$

Thus, the analytical solution for the 1-D convection-diffusion equation with initial condition $x(1-x)$ becomes

$$P(x,t) = \sum_{n=1}^{\infty}\left(-\frac{32D^3\pi n}{(4\pi^2D^2n^2+U^2)^3}\left[(-8\pi^2D^3n^2 + 4\pi^2D^2n^2U + 6DU^2 + U^3) + e^{\frac{U}{2D}}(-1)^n(8\pi^2D^3n^2 + 4\pi^2D^2n^2U - 6DU^2 + U^3)\right]\right) e^{-\left(\frac{U^2}{4D}+Dn^2\pi^2\right)t}\, e^{-\frac{Ux}{2D}}\, Sin\,(n\pi x)$$

(2.32)

The following graph is found when the analytical solution is plotted for $t = 1, D = 1,$ $U = 1.$

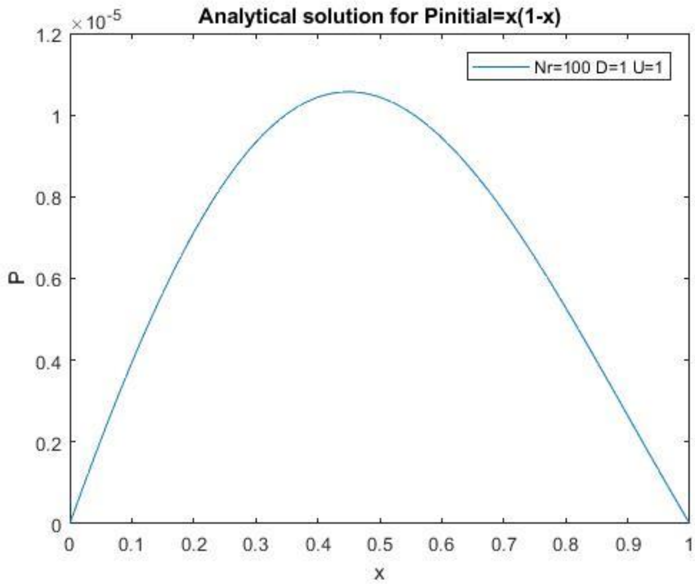


Figure 2.4: Analytical solution for $P_{initial}$=x(1-x)

The above analytical solution is used to calculate true errors of finite difference schemes. The truncation error analysis provides the idea of error propagation and the true errors give the actual error occurring in the scheme. The stability analysis gives the stability condition for which the schemes are stable.

Chapter 3 Centered-Difference Explicit and Implicit Schemes

3.1 Centered-Difference Explicit Scheme

The Centered-difference explicit method calculates the values of the finite difference approximation at the next time step from the values of the approximation at the current time. The explicit scheme has low cost per step and is easy to program.

However, the stability of the explicit scheme requires smaller time step sizes to avoid divergence. The Centered-difference explicit finite-difference scheme for the convection-diffusion equation is

$$\frac{P_i^{n+1}-P_i^n}{\Delta t} = D\,\frac{P_{i+1}^n-2P_i^n+P_{i-1}^n}{(\Delta r)^2} + U\,\frac{P_{i+1}^n-P_{i-1}^n}{2\Delta r} \tag{3.1}$$

3.1.1 Error Analysis of Centered-Difference Explicit Scheme

Using the Taylor series expansion, the truncation error for the explicit scheme is determined.

Denote $\frac{\partial P}{\partial x}(t_n, r_{i+1}) = \frac{\partial P_{i+1}^n}{\partial x}$, with similar notation for other partial derivatives evaluated at $(t_{n,} r_i)$.

For the first derivative, we get

$$\frac{\partial {\mathrm{P}_\mathrm{i}}^n}{\partial \mathrm{x}} = \frac{\mathrm{P}_{i+1}^n-\mathrm{P}_{i-1}^n}{2\Delta \mathrm{r}} + \mathrm{O}(\Delta \mathrm{r}^2) \tag{3.2}$$

For the second derivative,

$$\frac{\partial^2 P_i}{\partial x^2} = \frac{P_{i+1}^n - 2P_i^n + P_{i-1}^n}{(\Delta r)^2} + O(\Delta r^2) \tag{3.3}$$

For time derivative,

$$\frac{\partial P_i^n}{\partial t} = \frac{P_i^{n+1} - P_i^n}{\Delta t} + O(\Delta t) \tag{3.4}$$

From Equations (3.2), (3.3) and (3.4), we get,

$$\frac{\mathrm{P_i^{n+1} - P_i^n}}{\Delta \mathrm{t}} + \mathrm{O}(\Delta \mathrm{t}) = \mathrm{D}\,\frac{\mathrm{P}_{i+1}^n - 2\mathrm{P}_i^n + \mathrm{P}_{i-1}^n}{(\Delta \mathrm{r})^2} + \mathrm{U}\,\frac{\mathrm{P}_{i+1}^n - \mathrm{P}_{i-1}^n}{2\Delta \mathrm{r}} + \mathrm{O}(\Delta \mathrm{r}^2) \tag{3.5}$$

Therefore, the truncation error for this scheme is given by $\mathrm{O}(\Delta \mathrm{r}^2) + O(\Delta t)$ (3.6)

3.1.2 Stability analysis for the Centered-Difference Explicit Scheme

To find the stability criterion for the centered-difference explicit scheme applied to the convection-diffusion equation, we use Von Neumann analysis.

Let P_i^n be a solution of the explicit scheme, and consider a perturbation (deviation), $P_i^n + \epsilon_i^n$, that satisfies the same scheme.

$$\frac{(P_i^{n+1} + \epsilon_i^{n+1}) - (P_i^n + \epsilon_i^n)}{\Delta t} = D\,\frac{(P_{i+1}^n + \epsilon_{i+1}^n) - 2(P_i^n + \epsilon_i^n) + (P_{i-1}^n + \epsilon_{i-1}^n)}{(\Delta r)^2} + U\,\frac{(P_{i+1}^n + \epsilon_{i+1}^n) - (P_{i-1}^n + \epsilon_{i-1}^n)}{2\Delta r} \tag{3.7}$$

Using the definition of P_i^n, we see that

$$\frac{\epsilon_i^{n+1} - \epsilon_i^n}{\Delta t} = D\,\frac{\epsilon_{i+1}^n - 2\epsilon_i^n + \epsilon_{i-1}^n}{(\Delta r)^2} + U\,\frac{\epsilon_{i+1}^n - \epsilon_{i-1}^n}{2\Delta r} \tag{3.8}$$

We expand the error ϵ_i^n using Fourier series. For simplification, we consider that the error has one term and let $\theta = k\Delta r$.

$$\epsilon_i^n = \gamma^n \exp(\bar{\imath}ki\Delta r) = \gamma^n \exp(\bar{\imath}i\theta) \tag{3.9}$$

Thus, Equation (3.8) becomes

$$\frac{(\gamma^{n+1}-\gamma^n)}{\Delta t}\exp(\bar{\imath}\theta i) = D\frac{\gamma^n \exp(\bar{\imath}\theta)-2\gamma^n+\gamma^n \exp(-\bar{\imath}\theta)}{\Delta r^2}\exp(\bar{\imath}\theta i) + U\frac{\gamma^n \exp(\bar{\imath}\theta)-\gamma^n \exp(-\bar{\imath}\theta)}{2\Delta r}\exp(\bar{\imath}\theta i) \tag{3.10}$$

$$\Rightarrow \gamma = D\frac{\Delta t}{\Delta r^2}[2\cos(\theta)-2] + U\frac{\Delta t}{\Delta r}[\bar{\imath}\sin(\theta)] + 1 \tag{3.11}$$

The explicit scheme will be stable if

$$|1 + D\frac{\Delta t}{\Delta r^2}[2\cos(\theta)-2] + U\frac{\Delta t}{\Delta r}\bar{\imath}\sin(\theta)| \leq 1, \text{ for all } \theta,\ 0 \leq \theta \leq 2n\pi \tag{3.12}$$

$$(1 + D\frac{\Delta t}{\Delta r^2}[2\cos\theta - 2])^2 + (U\frac{\Delta t}{\Delta r}\sin\theta)^2 \leq 1 \tag{3.13}$$

Defining $\alpha = \frac{D\Delta t}{\Delta r^2}$ and $\beta = \frac{U\Delta t}{\Delta r}$, we get

$$\left(1 + \alpha(2cos\theta - 2)\right)^2 + (\beta sin\theta)^2 \leq 1 \tag{3.14}$$

Note that $(2cos\theta - 2) \leq 0$ and $0 \leq sin\theta \leq 1$

Thus, the stability of this scheme depends on the values of α and β. A few conditions for which the scheme is stable are given below.

Let $x = cos\theta$, so that $-1 \leq x \leq 1$

The stability condition in (3.4) can be rewritten as

$$f(x) = (1 + 2\alpha(x-1))^2 + \beta^2(1 - x^2) \leq 1$$

Note that $\mathrm{f}(1) = 1$ and $\mathrm{f}(-1) = (1 - 4\alpha)^2$ which requires $0 \le \alpha \le \frac{1}{2}$

If both f(1) and f(-1) are bounded by 1, and f(x) has only a minimum value, then the condition will be satisfied.

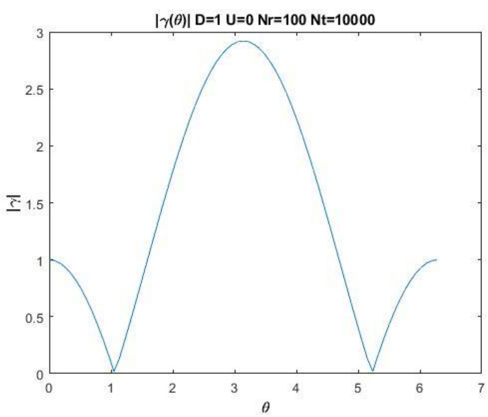
By rewriting f(x) in a quadratic form to find the value of its vertex, we get,

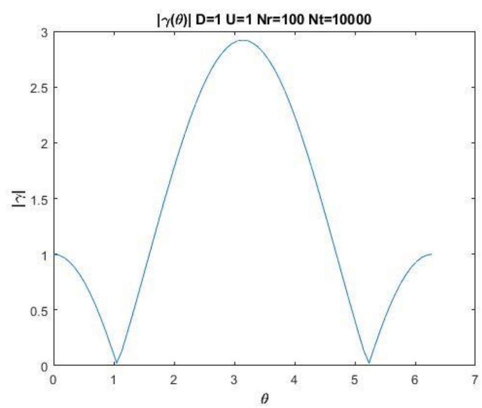
$$f(x) = x^2(4\alpha^2 - \beta^2) + x(2\alpha - 8) + (1 - 2\alpha + \beta^2)$$

Ensuring $(4\alpha^2 - \beta^2) > 0$, f(x) has a minimum value when $|2\alpha| > |\beta|$. Thus, the scheme is guaranteed to be stable if $0 \le \alpha \le \frac{1}{2}$ and $|\beta| < |2\alpha|$.

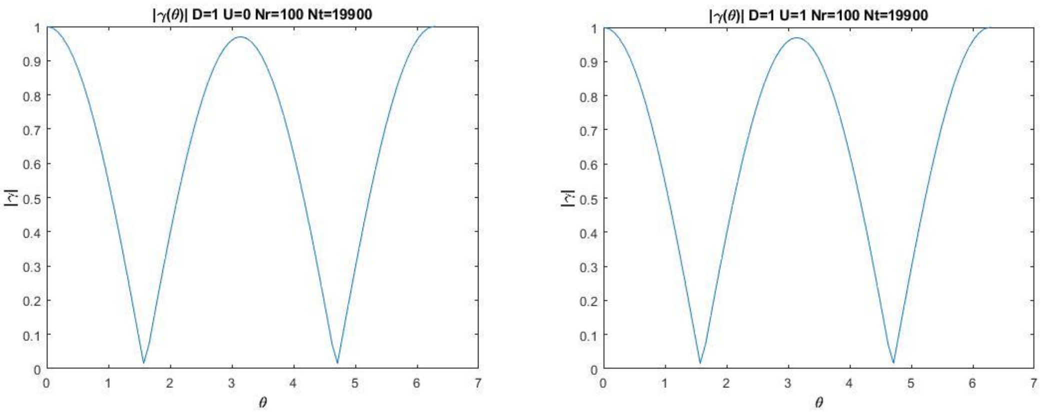
The following values are used for demonstrating the stability of the explicit scheme,

$\mathrm{D} = 1, \mathrm{U} = 0{,}1, \ \mathrm{Nr} = 100$

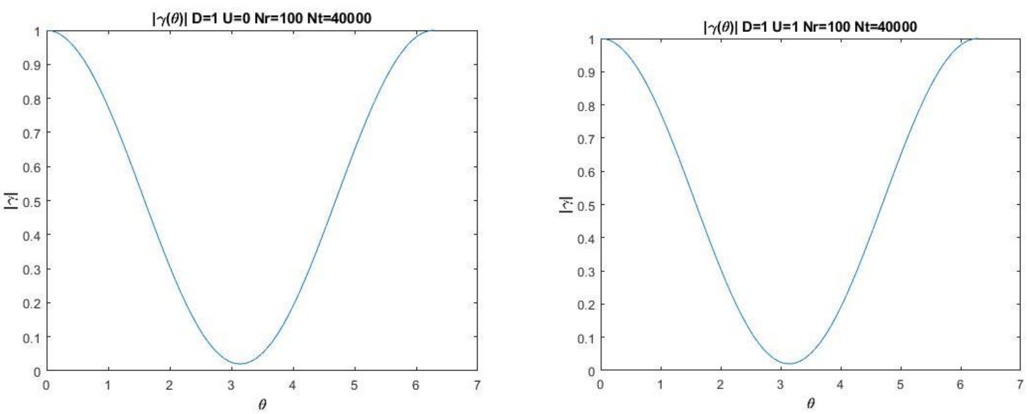




(a) For $\mathrm{Nt} = 10{,}000$



(b) For $\mathrm{Nt} = 19{,}900$



(c) For $\mathrm{Nt} = 40{,}000$

Figure 3.1: Stability analysis of Centered-Difference Explicit Scheme

After few trials, it is found that the explicit scheme is stable when $\mathrm{Nt} = 19900$ or higher.

Because, for $\mathrm{Nt} = 10000$, $\alpha = 1$, which violates the condition $0 \le \alpha \le \frac{1}{2}$.

For $\mathrm{Nt} = 19{,}900$, $\alpha = 0.5$ and for $\mathrm{Nt} = 40{,}000$, $\alpha = 0.25$, which follows the condition.

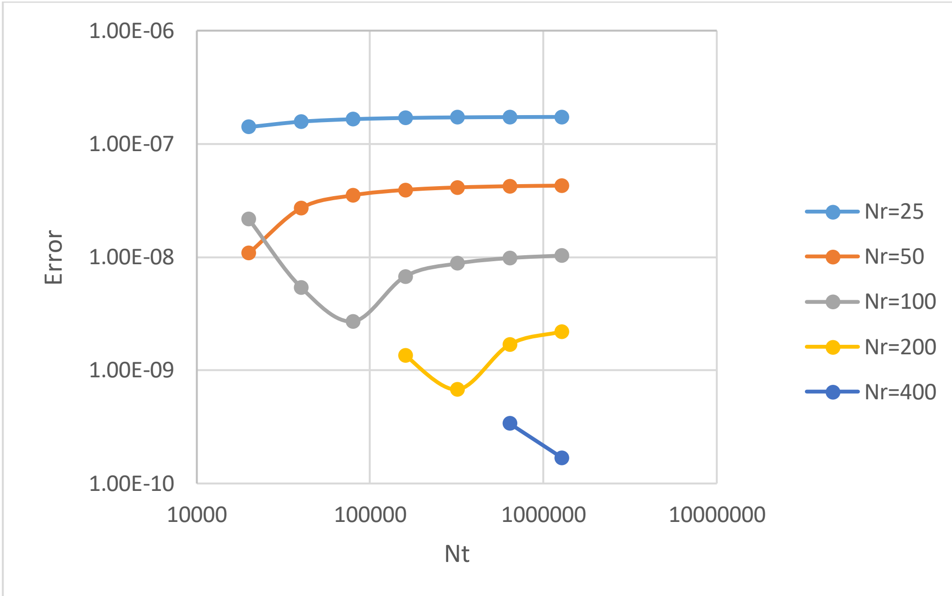
3.1.3 Numerical Validation

Numerical simulation is done for this scheme using MATLAB. Some of the data found after simulation are given below

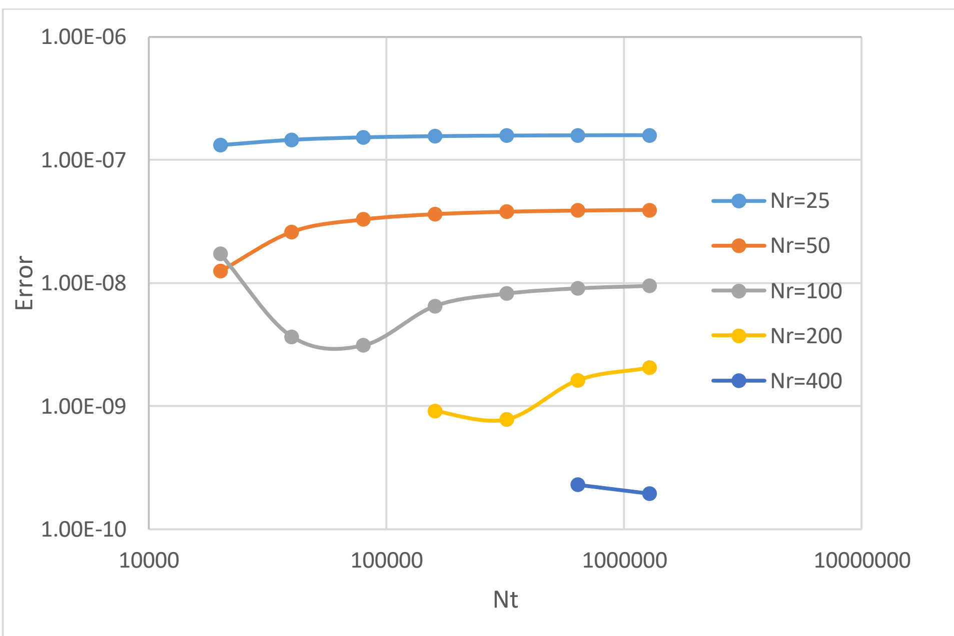
Table 3.1: Error values for Centered-Difference Explicit Scheme for different numbers of time steps (Nt) and numbers of grid blocks (Nr)

Nr	Nt	Error (D=1,U=0)	Error (D=1,U=1)
25	20000	1.41E-07	1.32E-07
50	80000	3.53E-08	3.28E-08
100	20000	2.17E-08	1.72E-08
200	80000	5.42E-09	4.30E-09
400	320000	1.35E-09	1.07E-09

If we increase Nr by a factor of two and Nt by a factor of four, we see that the error will be decreased by factor of four, as expected from the truncation error analysis.



(a) U=0



(b) U=1

Figure 3.2: Error values for Centered-Difference Explicit Scheme

Figure 3.2 represents the error values for the centered-difference explicit scheme for both $U = 0$ and $U = 1$. From the above graphs, it is clear that explicit scheme is giving less error with higher values of Nr. If an Error value of 1.00E-09 is desired, $\mathrm{Nr} = 200$ and $\mathrm{Nt} = 320000$ gives the most stable result with maximum time step.

3.2 Centered-Difference Implicit Scheme

The Centered-difference implicit method calculates the values of the finite difference approximation at the next time step from the values of the approximation at the current time and future time. The implicit scheme has a high cost per step and can be difficult to program. But, the stability of the implicit scheme is unconditional and it can deal with larger time step sizes.

The Centered-difference implicit finite-difference scheme for the convection-diffusion equation is

$$\frac{P_i^{n+1}-P_i^n}{\Delta t} = D\,\frac{P_{i+1}^{n+1}-2P_i^{n+1}+P_{i-1}^{n+1}}{(\Delta r)^2} + U\,\frac{P_{i+1}^{n+1}-P_{i-1}^{n+1}}{2\Delta r} \tag{3.15}$$

3.2.1 Truncation Error Analysis of Centered-Difference Implicit scheme

Using the Taylor series expansion, the truncation error for the implicit scheme is determined as

$$\frac{P_i^{n+1}-P_i^n}{\Delta t} + O(\Delta t) = D\,\frac{P_{i+1}^{n+1}-2P_i^{n+1}+P_{i-1}^{n+1}}{(\Delta r)^2} + U\,\frac{P_{i+1}^{n+1}-P_{i-1}^{n+1}}{2\Delta r} + O(\Delta r^2) \tag{3.16}$$

Therefore, the truncation error for this scheme is given by $O(\Delta r^2) + O(\Delta t)$ (3.17)

3.2.2 Stability analysis for Centered-Difference Implicit scheme

To find the stability criterion for the centered-difference implicit scheme applied to the convection-diffusion equation, we use Von Neumann analysis.

Let P_i^n be a solution of the centered-difference implicit scheme, and consider a perturbation (deviation), $P_i^n + \epsilon_i^n$, that satisfies the same scheme.

$$\frac{(P_i^{n+1}+\epsilon_i^{n+1})-(P_i^n+\epsilon_i^n)}{\Delta t} = D\frac{(P_{i+1}^{n+1}+\epsilon_{i+1}^{n+1})-2(P_i^{n+1}+\epsilon_i^{n+1})+(P_{i-1}^{n+1}+\epsilon_{i-1}^{n+1})}{(\Delta r)^2} + U\frac{(P_{i+1}^{n+1}+\epsilon_{i+1}^{n+1})-(P_{i-1}^{n+1}+\epsilon_{i-1}^{n+1})}{2\Delta r} \quad (3.18)$$

Using the definition of P_i^n, we see that

$$\frac{\epsilon_i^{n+1}-\epsilon_i^n}{\Delta t} = D\frac{\epsilon_{i+1}^{n+1}-2\epsilon_i^{n+1}+\epsilon_{i-1}^{n+1}}{(\Delta r)^2} + U\frac{\epsilon_{i+1}^{n+}-\epsilon_{i-1}^{n+1}}{2\Delta r} \quad (3.19)$$

We expand the error ϵ_i^n using Fourier series. For simplification, we consider that the error Equation has one term and let $\theta = k\Delta r$.

$$\epsilon_i^n = \gamma^n \exp(\bar{\imath}ki\Delta r) = \gamma^n \exp(\bar{\imath}i\theta) \quad (3.20)$$

Thus, Equation (3.19) becomes

$$\frac{(\gamma^{n+1}-\gamma^n)}{\Delta t}\exp(\bar{\imath}\theta i) = D\frac{\gamma^{n+1}\exp(\bar{\imath}\theta)-2\gamma^{n+1}+\gamma^{n+1}\exp(-\bar{\imath}\theta)}{(\Delta r)^2}\exp(\bar{\imath}\theta i) +$$

$$U\frac{\gamma^{n+1}\exp(\bar{\imath}\theta)-\gamma^{n+1}\exp(-\bar{\imath}\theta)}{2\Delta r}\exp(\bar{\imath}\theta i) \quad (3.21)$$

$$\Rightarrow \gamma = \frac{1}{1-\frac{D\Delta t}{(\Delta r)^2}[2\cos(\theta)-2]-\frac{U\Delta t}{2\Delta r}[2\bar{\imath}\sin(\theta)]} \quad (3.22)$$

The implicit scheme will be stable if

$$\left|\frac{1}{1-\frac{D\Delta t}{(\Delta r)^2}[2\cos\theta-2]-\frac{U\Delta t}{2\Delta r}[2\bar{\imath}\sin\theta]}\right| \leq 1, \text{ for all } \theta, 0 \leq \theta \leq 2\pi \qquad (3.23)$$

$$\Rightarrow \frac{1}{[1-\frac{D\Delta t}{(\Delta r)^2}[2cos\theta-2]]^2+[\frac{U\Delta t}{\Delta r}sin\theta]^2} \leq 1 \qquad (3.24)$$

As $(2cos\theta - 2) \leq 0$ and $0 \leq sin\theta \leq 1$, the denominator of Equation (3.24) is always bigger than 1. Therefore, the centered-difference implicit scheme for the convection-diffusion equation is stable without any conditions.

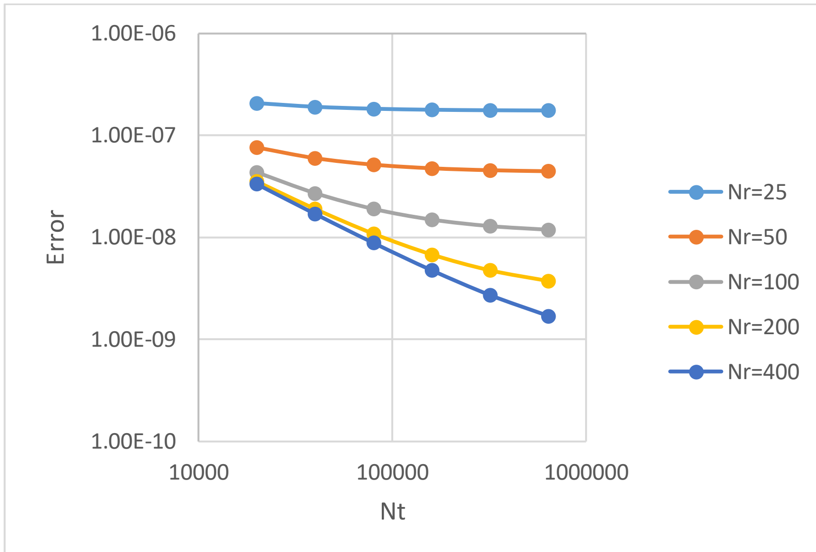
3.2.3 Numerical Validation

Numerical simulation is done for the centered-difference implicit scheme using MATLAB. Some of the data found after simulation are given below.

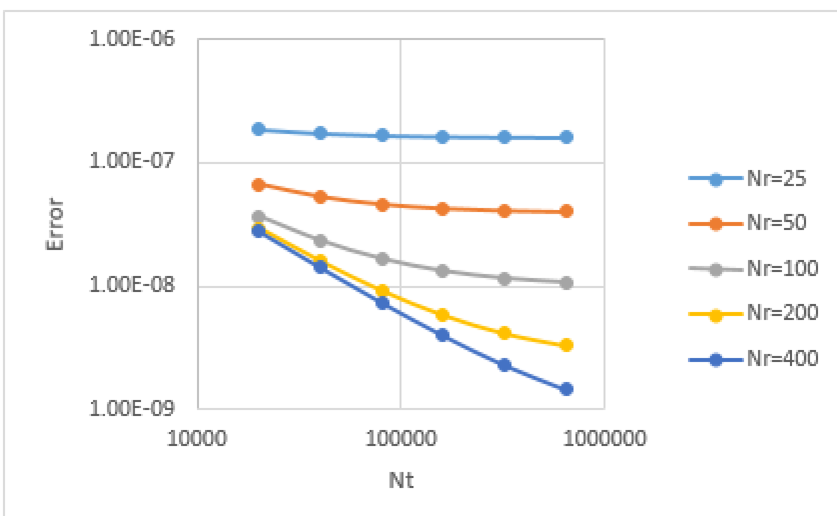
Table 3.2: Error values for Centered-Difference Implicit Scheme for different numbers of time steps (Nt) and numbers of grid blocks (Nr)

Nr	Nt	Error (D=1,U=0)	Error (D=1,U=1)
25	20000	2.07E-07	1.86E-07
50	80000	5.15E-08	4.63E-08
100	320000	1.29E-08	1.16E-08
200	80000	1.08E-08	9.24E-09
400	320000	2.71E-09	2.31E-09

If we increase Nr by a factor of two and Nt by a factor of four, the error is decreased by roughly factor of four, as expected from the truncation error analysis.



(a) U=0



(b) U=1

Figure 3.3: Error values for Centered-Difference Implicit Scheme

Figure 3.3 represents the error values for the centered-difference implicit scheme for both $U = 0$ and $U = 1$. From the graphs, it is clear that the implicit scheme gives less error with higher Nr and higher Nt.

Chapter 4 Barakat-Clark Scheme

In 1966, Barakat and Clark proposed an unconditionally stable method to solve the general nonhomogeneous, multidimensional diffusion equation. While analyzing time-dependent convective phenomena, the authors faced a problem in selecting an appropriate numerical method. As seen above, the centered-difference explicit scheme, which requires less time, has a time step restriction for stability. In contrast, the centered-difference implicit scheme, which allows a larger time step, requires more time to solve the discrete equations. Barakat and Clark proposed a new explicit finite difference method, which has no severe limitation on the time-step size. They applied their proposed method to the diffusion equation. Barakat and Clark proposed two schemes, similar in design but meant to be complimentary, for the diffusion equation and claimed that the average of the solutions to these two discretizations provides a better approximation than either scheme by itself. Barakat and Clark solved the two-dimensional diffusion equation, but did not present detailed steps of error and stability analysis. Here, we apply the method proposed by Barakat and Clark to the one dimensional diffusion equation and present detailed steps of error and stability analysis of the Barakat-Clark scheme. We also provide numerical validation of the scheme in this setting.

The Barakat-Clark scheme for solving the one-dimensional diffusion equation is

Scheme Q: $$\frac{Q_i^{n+1}-Q_i^n}{\Delta t} = D\,\frac{Q_{i+1}^n-Q_i^n-Q_i^{n+1}+Q_{i-1}^{n+1}}{\Delta r^2} \tag{4.1}$$

Scheme S: $$\frac{S_i^{n+1}-S_i^n}{\Delta t} = D\,\frac{S_{i+1}^{n+1}-S_i^{n+1}-S_i^n+S_{i-1}^n}{\Delta r^2} \tag{4.2}$$

Average of the solutions: $P_i^{n+1} = \frac{1}{2}(Q_i^{n+1} + S_i^{n+1})$

4.1 Truncation Error Analysis of the Barakat-Clark Scheme

Using the two-dimensional form of Taylor's theorem, the truncation error analysis of the Barakat-Clark Scheme is given here.

First, the theorem is applied to the discretization given in Equation (4.1).

Let $(AP^{n+1})_i = P_i^{n+1} + \frac{D\Delta t}{\Delta r^2}(P_i^{n+1} - P_{i-1}^{n+1})$ and $(BP^n)_i = P_i^n + \frac{D\Delta t}{\Delta r^2}(P_{i+1}^n - P_i^n)$

Now,

$$(AP^{n+1})_i = P_i^{n+1} + \frac{D\Delta t}{\Delta r^2}(P_i^{n+1} - P_{i-1}^{n+1}) = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{D\Delta t}{\Delta r^2}(P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r - \frac{\partial P_i^n}{\partial t}\Delta t - \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} - \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}) \tag{4.3}$$

$$\Rightarrow P_i^{n+1} + \frac{D\Delta t}{\Delta r^2}(P_i^{n+1} - P_{i-1}^{n+1}) = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + D(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} - \frac{\partial^2 P_i^n}{\partial r}\frac{\Delta t}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{1}{\Delta r}\frac{\Delta t^2}{1!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta t\,\Delta r}{3!} - \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{1}{2!}\frac{\Delta t^2}{1!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{1}{\Delta r}\frac{\Delta t^3}{2!} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2 \Delta t}{4!} - \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{1}{2!}\frac{\Delta t^3}{2!} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r}{3!}\frac{\Delta t^2}{1!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{1}{\Delta r}\frac{\Delta t^4}{3!}) \tag{4.4}$$

Similarly,

$$(BP^n)_i = P_i^n + \frac{D\Delta t}{\Delta r^2}(P_{i+1}^n - P_i^n) = P_i^n + \frac{D\Delta t}{\Delta r^2}(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} - P_i^n) \tag{4.5}$$

$$\Rightarrow P_i^n + \frac{D\Delta t}{\Delta r^2}(P_{i+1}^n - P_i^n) = P_i^n + D(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r\Delta t}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2\Delta t}{4!}) \quad (4.6)$$

The truncation error for gridblock i at time level n is given by

$$T_i^n = \frac{1}{\Delta t}\{(AP^{n+1})_i - (BP^n)_i\} \quad (4.7)$$

$$\Rightarrow T_i^n = \frac{1}{\Delta t}(P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + D(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} - \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} +$$

$$\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{1}{\Delta r}\frac{\Delta t^2}{1!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta t\,\Delta r}{3!} - \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{1}{2!}\frac{\Delta t^2}{1!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{1}{\Delta r}\frac{\Delta t^3}{2!} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2\Delta t}{4!} - \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{1}{2!}\frac{\Delta t^3}{2!} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r}{3!}\frac{\Delta t^2}{1!} +$$

$$\frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{1}{\Delta r}\frac{\Delta t^4}{3!}) - P_i^n - D(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r\Delta t}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2\Delta t}{4!})) \quad (4.8)$$

$$T_i^n = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} + D(\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{1}{\Delta r}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{1}{\Delta r}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{1}{2!}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} +$$

$$\frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{1}{\Delta r}\frac{\Delta t^3}{3!}) \quad (4.9)$$

Thus the truncation error for the first equation of Barakat-Clark Scheme is

$$T_i^n = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + D\left(\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{2\Delta r} - \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12}\right) + O(\Delta t^3) + O(\Delta r^4) +$$

$$O(\Delta t\Delta r) + O(\frac{\Delta t^2}{\Delta r}) \quad (4.10)$$

Now, Taylor's theorem is applied to the second equation of the Barakat-Clark Scheme.

Let $(CP^{n+1})_i = P_i^{n+1} - \frac{D\Delta t}{\Delta r^2}(P_{i+1}^{n+1} - P_i^{n+1})$ and $(DP^n)_i = P_i^n - \frac{D\Delta t}{\Delta r^2}(P_{i-1}^n - P_i^n)$

As above,

$$(CP^{n+1})_i = P_i^{n+1} - \frac{D\Delta t}{\Delta r^2}(P_{i+1}^{n+1} - P_i^{n+1}) = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} -$$

$$\frac{D\Delta t}{\Delta r^2}(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} +$$

$$\frac{\partial^3 P_i^n}{\partial r^2 \partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r \partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2 \partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^3 \partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r \partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!} - P_i^n - \frac{\partial P_i^n}{\partial t}\Delta t - \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!}) \quad (4.11)$$

$$\Rightarrow (CP^{n+1})_i = P_i^{n+1} - \frac{D\Delta t}{\Delta r^2}(P_{i+1}^{n+1} - P_i^{n+1}) = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - D(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} + \frac{\partial^2 P_i^n}{\partial r \partial t}\frac{1}{\Delta r}\frac{\Delta t^2}{1!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r \Delta t}{3!} + \frac{\partial^3 P_i^n}{\partial r^2 \partial t}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial r \partial t^2}\frac{1}{\Delta r}\frac{\Delta t^3}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2 \Delta t}{4!} + \frac{\partial^4 P_i^n}{\partial r^2 \partial t^2}\frac{1}{2!}\frac{\Delta t^3}{2!} + \frac{\partial^4 P_i^n}{\partial r^3 \partial t}\frac{\Delta r}{3!}\frac{\Delta t^2}{1!} + \frac{\partial^4 P_i^n}{\partial r \partial t^3}\frac{1}{\Delta r}\frac{\Delta t^4}{3!}) \quad (4.12)$$

And,

$$(DP^n)_i = P_i^n + \frac{D\Delta t}{\Delta r^2}(P_{i-1}^n - P_i^n) = P_i^n + \frac{D\Delta t}{\Delta r^2}(P_i^n - \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} - P_i^n) \quad (4.13)$$

$$\Rightarrow P_i^n + \frac{D\Delta t}{\Delta r^2}(P_{i-1}^n - P_i^n) = P_i^n - D(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} - \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r \Delta t}{3!} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2 \Delta t}{4!}) \quad (4.14)$$

The truncation error at gridpoint i and time step n is given by

$$T_i'^n = \frac{1}{\Delta t}\{(CP^{n+1})_i - (DP^n)_i\} \quad (4.15)$$

$$\Rightarrow T_i'^n = \frac{1}{\Delta t}(P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - D(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} + \frac{\partial^2 P_i^n}{\partial r \partial t}\frac{1}{\Delta r}\frac{\Delta t^2}{1!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r \Delta t}{3!} + \frac{\partial^3 P_i^n}{\partial r^2 \partial t}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial r \partial t^2}\frac{1}{\Delta r}\frac{\Delta t^3}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2 \Delta t}{4!} + \frac{\partial^4 P_i^n}{\partial r^2 \partial t^2}\frac{1}{2!}\frac{\Delta t^3}{2!} + \frac{\partial^4 P_i^n}{\partial r^3 \partial t}\frac{\Delta r}{3!}\frac{\Delta t^2}{1!} + \frac{\partial^4 P_i^n}{\partial r \partial t^3}\frac{1}{\Delta r}\frac{\Delta t^4}{3!}) - P_i^n + D(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} - \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r \Delta t}{3!} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2 \Delta t}{4!})) \quad (4.16)$$

$$\Rightarrow T_i'^n = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} - D(\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{1}{\Delta r}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r\Delta t}{3!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{1}{\Delta r}\frac{\Delta t^3}{3!}) \quad (4.17)$$

The truncation error for the second equation of the Barakat-Clark Scheme is

$$T_i'^n = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} - D\left(\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4}\right) + O(\Delta t^3) + O(\Delta r^3) + O(\Delta t\Delta r) + O(\frac{\Delta t^2}{\Delta r}) \quad (4.18)$$

Now, if we do the average of errors of the two equations of the Barakat-Clark Scheme, we get

$$\frac{T_i^n + T_i'^n}{2} = \frac{1}{2}(\frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} + D\left(\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{1}{\Delta r}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{1}{\Delta r}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{1}{2!}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{1}{\Delta r}\frac{\Delta t^3}{3!}\right) + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} - D(\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{1}{\Delta r}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r\Delta t}{3!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{1}{\Delta r}\frac{\Delta t^3}{3!})) \quad (4.19)$$

After simplification

$$\frac{T_i^n + T_i'^n}{2} = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} - D(\frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4}) \quad (4.20)$$

The truncation error for the averaged solutions of the Barakat-Clark Scheme becomes

$$\frac{T_i^n + T_i'^n}{2} = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} - D\left(\frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4}\right) + O(\Delta t^3) + O(\Delta r^3) \quad (4.21)$$

Thus, the Barakat-Clark Scheme is second-order accurate in both time and space. This proves the claim that the Barakat-Clark Scheme gets higher accuracy by averaging the two equations of the scheme.

4.2 Stability Analysis of the Barakat-Clark Scheme

Using Von-Neumann Analysis, Equation (4.25) is found to express the stability condition associated with Equation (4.1).

$$\frac{\gamma^{n+1}-\gamma^{n}}{\Delta t} = D\,\frac{\gamma^{n}\exp(\bar{\imath}\theta)-\gamma^{n}-\gamma^{n+1}+\gamma^{n+1}\exp(-\bar{\imath}\theta)}{(\Delta r)^2} \tag{4.22}$$

$$\Rightarrow \gamma^{n+1}[1-\frac{D\Delta t}{(\Delta r)^2}(\cos(\theta)-\bar{\imath}\sin(\theta)-1) = \gamma^{n}[1+\frac{D\Delta t}{(\Delta r)^2}(\cos(\theta)+\bar{\imath}\sin(\theta)-1) \tag{4.23}$$

$$\Rightarrow \gamma[1-\frac{D\Delta t}{h^2}\Big(\cos\theta-\bar{\imath}\sin\theta)+\frac{D\Delta t}{(\Delta r)^2}\Big] = 1+\frac{D\Delta t}{(\Delta r)^2}(\cos\theta+\bar{\imath}\sin\theta)-\frac{D\Delta t}{(\Delta r)^2} \tag{4.24}$$

$$\Rightarrow \gamma = \frac{1+\left(\frac{D\Delta t}{(\Delta r)^2}\right)(\cos\theta+\bar{\imath}\sin\theta)-\frac{D\Delta t}{(\Delta r)^2}}{1-\left(\frac{D\Delta t}{(\Delta r)^2}\right)(\cos\theta-\bar{\imath}\sin\theta)+\frac{D\Delta t}{(\Delta r)^2}} \tag{4.25}$$

Let $\alpha = \frac{D\Delta t}{(\Delta r)^2}$. Rewriting Equation (4.25) gives

$$\gamma = \frac{1+\alpha e^{i\theta}-\alpha}{1-\alpha e^{-i\theta}+\alpha} \tag{4.26}$$

$$\text{Or, } |\gamma|^2 = \frac{1+\alpha\left(e^{i\theta}+e^{-i\theta}-2\right)+\alpha^2\left(e^{i\theta}-1\right)\left(e^{-i\theta}-1\right)}{1+\alpha\left(2-e^{-i\theta}-e^{i\theta}\right)+\alpha^2\left(1-e^{i\theta}\right)\left(1-e^{-i\theta}\right)} = \frac{1+(\alpha^2-\alpha)(2-2cos\theta)}{1+(\alpha^2+\alpha)(2-2cos\theta)} \tag{4.27}$$

The minima of $(\alpha^2-\alpha)$ is $-\frac{1}{4}$; and $0 \le 2-2cos\theta \le 4$; hence, $0 \le 1+(\alpha^2-\alpha)(2-2cos\theta) \le 1$

For any value of α, $\alpha^2+\alpha \ge \alpha^2-\alpha$

$1+(\alpha^2-\alpha)(2-2cos\theta) \le 1+(\alpha^2+\alpha)(2-2cos\theta)$ leaving $|\gamma| \le 1$

So, from Equation (4.27) we can say that $|\gamma| \le 1$

Equation (4.31) is found to express the stability condition associated with Equation (4.2).

$$\frac{\gamma'^{n+1}-\gamma'^{n}}{\Delta t} = D\,\frac{\gamma'^{n+1}\exp(\bar{\imath}\theta)-\gamma'^{n+1}-\gamma'^{n}+\gamma'^{n}\exp(-\bar{\imath}\theta)}{(\Delta r)^2} \tag{4.28}$$

$$\Rightarrow \gamma'^{n+1}[1-\frac{D\Delta t}{(\Delta r)^2}(\cos\theta+\bar{\imath}\sin\theta-1)] = \gamma'^{n}[1+\frac{D\Delta t}{(\Delta r)^2}(\cos\theta-\bar{\imath}\sin\theta-1)] \tag{4.29}$$

$$\Rightarrow \gamma'[1-\left(\frac{D\Delta t}{(\Delta r)^2}\right)\left(\cos\theta+\bar{\imath}\sin\theta\right)+\frac{D\Delta t}{(\Delta r)^2}\Big] = 1+\left(\frac{D\Delta t}{(\Delta r)^2}\right)(\cos\theta-\bar{\imath}\sin\theta)-\frac{D\Delta t}{(\Delta r)^2} \tag{4.30}$$

$$\Rightarrow \gamma' = \frac{1+\left(\frac{D\Delta t}{(\Delta r)^2}\right)(\cos\theta-\bar{\imath}\sin\theta)-\frac{D\Delta t}{(\Delta r)^2}}{1-\left(\frac{D\Delta t}{(\Delta r)^2}\right)(\cos\theta+\bar{\imath}\sin\theta)+\frac{D\Delta t}{(\Delta r)^2}} \tag{4.31}$$

Similarly, we can write,

$$\gamma' = \frac{1+\alpha e^{-i\theta}-\alpha}{1-\alpha e^{i\theta}+\alpha} \tag{4.32}$$

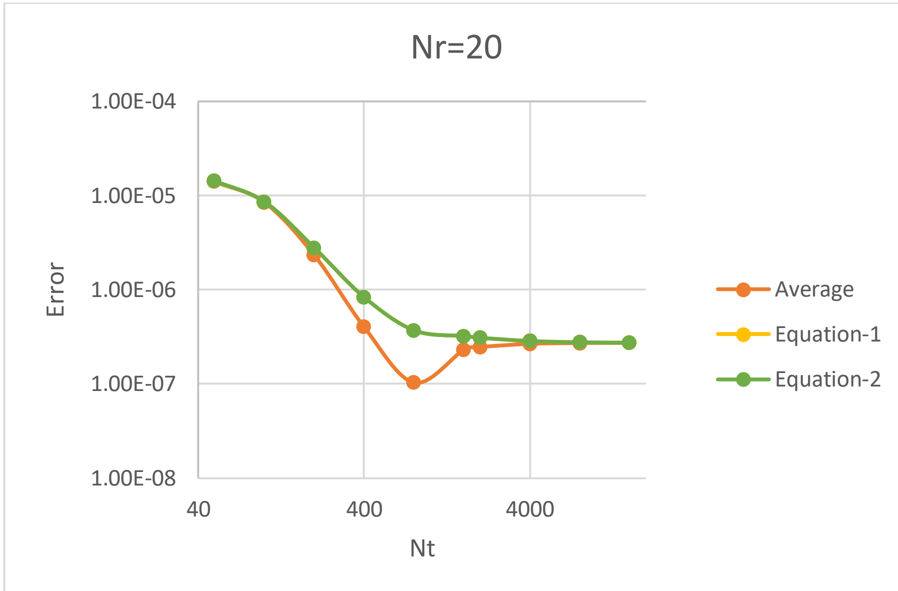
Or, $|\gamma'|^2 = \frac{1+\alpha\left(e^{i\theta}+e^{-i\theta}-2\right)+\alpha^2\left(e^{i\theta}-1\right)\left(e^{-i\theta}-1\right)}{1+\alpha\left(2-e^{-i\theta}-e^{i\theta}\right)+\alpha^2\left(1-e^{i\theta}\right)\left(1-e^{-i\theta}\right)} = \frac{1+(\alpha^2-\alpha)(2-2cos\theta)}{1+(\alpha^2+\alpha)(2-2cos\theta)}$

So, $|\gamma'| \leq 1$ as before.

Thus, the Barakat-Clark Scheme is unconditionally stable.

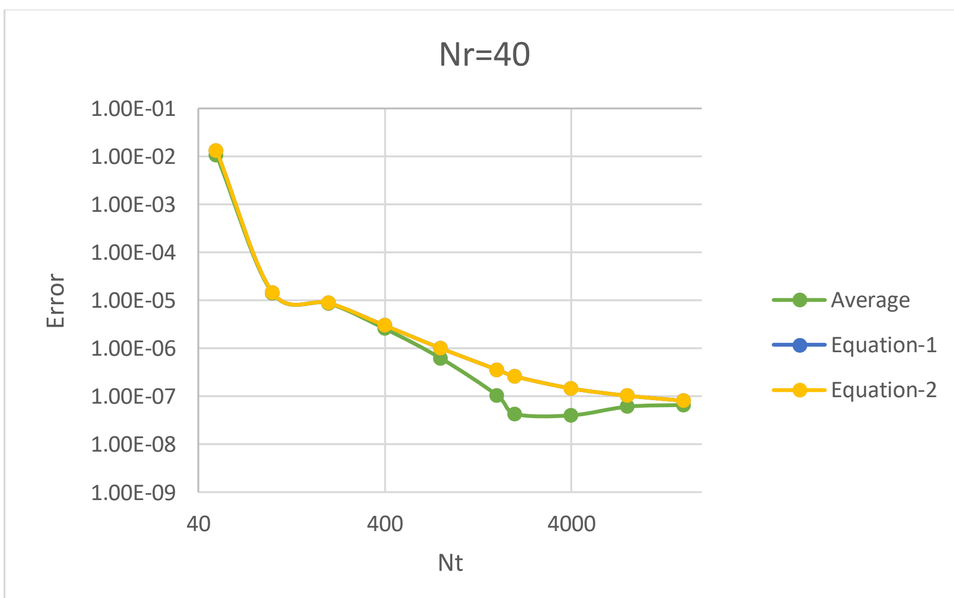
4.3 Numerical Validation

Numerical simulation is done for the Barakat-Clark scheme using MATLAB. The following data are found from this simulation for D=1. The error values are given in Appendix-1.



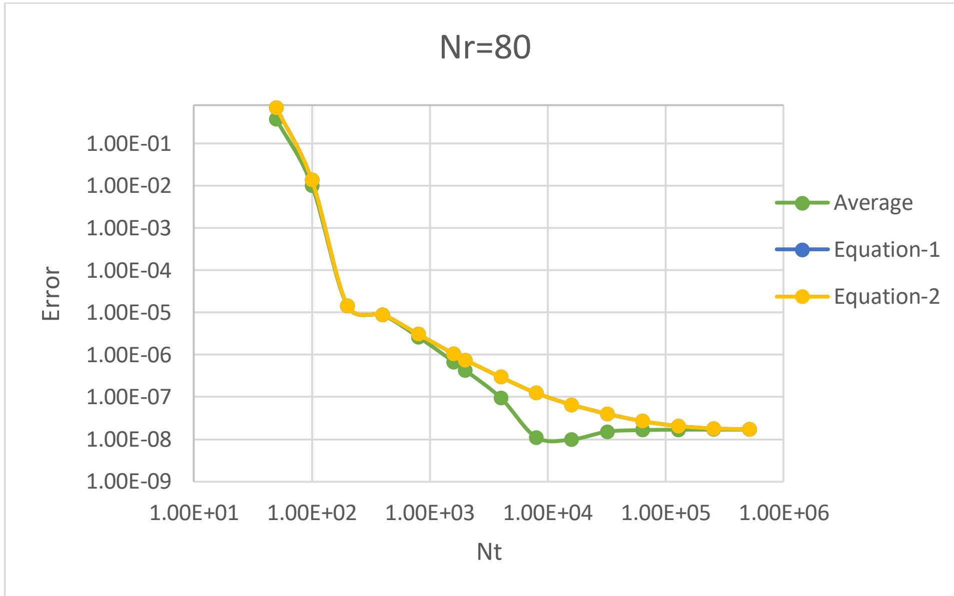
Nr=20
1.00E-04
1.00E-05
1.00E-06
1.00E-07
1.00E-08
Error
40
400
4000
Nt
Average
Equation-1
Equation-2

(a) Nr = 20

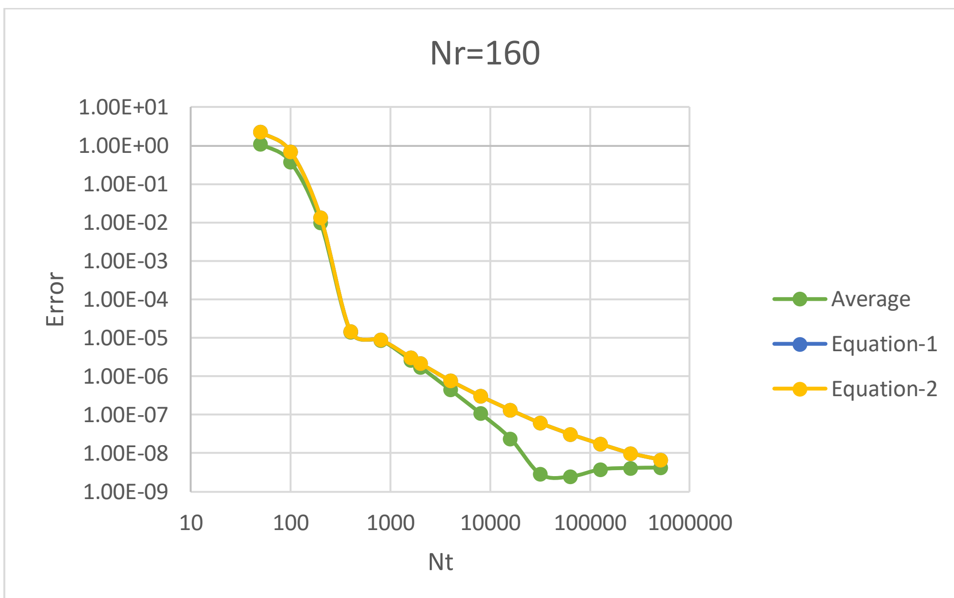


Nr=40
1.00E-01
1.00E-02
1.00E-03
1.00E-04
1.00E-05
1.00E-06
1.00E-07
1.00E-08
1.00E-09
Error
40
400
4000
Nt
Average
Equation-1
Equation-2

(b) Nr = 40



(c) Nr= 80



14

(d) Nr = 160

Figure 4.1: Error values for the Barakat-Clark Scheme

First of all, comparing the minimal values attached, it is seen that, for Nr = 40, the minimum average error is approximately 4e-8 at Nt = 4000; for Nr = 80, the minimum average error is approximately 1e-8 at Nt = 16000; and for Nr = 160, the minimum average error is approximately 2.5e-9 at Nt = 64000. So, we clearly see the $(\Delta r)^2$ behaviour of the final truncation error terms in Equation (4.21).

Fixing Nr = 160, comparing errors for $2000 \leq Nt \leq 16000$, we see the $(\Delta t)^2$ behaviour also from Equation (4.21).

Finally, comparing the error for the average to that for either of the two schemes, we see the "extra" cancellation, with the two schemes reporting larger errors than the average does, and with that error growing for a fixed Nt and increasing Nr (decreasing Δr). For example, if we consider Nt = 16000, for Nr = 160, the Equation (4.1) error is 1.32e-7, while for Nr = 80, it is 6.56e-8. This is in accordance with the $\frac{1}{\Delta r}$ factor in the truncation error analysis of the individual schemes.

Chapter 5 Bokhari-Islam Scheme

To solve the convection-diffusion equation by finite difference schemes, Bokhari and Islam proposed a new scheme extending the Barakat and Clark scheme. For the time term, they used a central difference model, which gives accuracy of Δt^2 inherently, aiming to get overall accuracy of Δt^4. Bokahri and Islam claimed to get the desired accuracy but did not provide any details.

In the present study, we analyse the Bokhari and Islam scheme for the one-dimensional convection-diffusion equation and provide detailed error analysis for that scheme. Bokhari and Islam also did not do a stability analysis for their proposed scheme, which is done in this study. We also provide numerical validation of the scheme in the following setting.

The Bokhari-Islam scheme for solving the one-dimensional convection-diffusion equation is: Scheme A: $\frac{A_i^{n+1}-A_i^{n-1}}{2\Delta t} = D\,\frac{A_{i+1}^{n}-A_i^{n}-A_i^{n+1}+A_{i-1}^{n+1}}{\Delta r^2} + U\,\frac{A_{i+1}^{n}-A_{i-1}^{n}}{2\Delta r}$ (5.1)

Scheme B: $\frac{B_i^{n+1}-B_i^{n-1}}{2\Delta t} = D\,\frac{B_{i+1}^{n+1}-B_i^{n+1}-B_i^{n}+B_{i-1}^{n}}{\Delta r^2} + U\,\frac{B_{i+1}^{n}-B_{i-1}^{n}}{2\Delta r}$ (5.2)

Average of the solutions, $\mathrm{P_i^{n+1}} = \frac{1}{2}(\mathrm{A_i^{n+1}} + \mathrm{B_i^{n+1}})$

As it is a three-step scheme, additional initial conditions are required. Here, we use the analytical solution to provide the exact value of $\mathrm{P_i^2}$ a time Δt, eliminating any possible error entering the solution scheme from using a low-order approximation here.

5.1 Truncation Error Analysis of Bokhari-Islam Scheme

Using the two-dimensional form of Taylor's theorem, the truncation error analysis of the Bokhari-Islam Scheme is given here.

First, the theorem is applied to the discretization given in Equation (5.1).

Let $P_i^{n+1} - P_i^{n-1} - \frac{2D\Delta t}{\Delta r^2}(P_{i-1}^{n+1} - P_i^{n+1}) = (AP^{n+1})_i$ and $\frac{2D\Delta t}{\Delta r^2}(P_{i+1}^{n} - P_i^{n}) + \frac{U\Delta t}{\Delta r}(P_{i+1}^{n} - P_{i-1}^{n}) = (BP^{n})_i$

Now,

$$(AP^{n+1})_i = P_i^{n+1} - P_i^{n-1} - \frac{2D\Delta t}{\Delta r^2}(P_{i-1}^{n+1} - P_i^{n+1}) = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t - \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{2D\Delta t}{\Delta r^2}\Big(P_i^n - \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} - \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!} - P_i^n - \frac{\partial P_i^n}{\partial t}\Delta t - \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!}\Big) \tag{5.3}$$

$$\Rightarrow (AP^{n+1})_i = \frac{\partial P_i^n}{\partial t}2\Delta t + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3} + 2D\Big(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} - \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t^2}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r\Delta t}{3!} - \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^3}{2\,\Delta r} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2\Delta t}{4!} - \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^3}{4} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^4}{6\,\Delta r}\Big) \tag{5.4}$$

Similarly,

$$(BP^n)_i = \frac{2D\Delta t}{\Delta r^2}(P_{i+1}^n - P_i^n) + \frac{U\Delta t}{\Delta r}(P_{i+1}^n - P_{i-1}^n) = \frac{2D\Delta t}{\Delta r^2}\left(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} - P_i^n\right) + \frac{U\Delta t}{\Delta r}\left(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} - P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r - \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}\right) \quad (5.5)$$

$$\Rightarrow (BP^n)_i = 2D\left(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r\Delta t}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2\Delta t}{4!}\right) + U\left(\frac{\partial P_i^n}{\partial r}2\Delta t + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2\Delta t}{3}\right) \quad (5.6)$$

The truncation error at gridpoint i and time step n is given by

$$T_i^n = \frac{1}{\Delta t}\{(AP^{n+1})_i - (BP^n)_i\} \quad (5.7)$$

$$\Rightarrow T_i^n = \frac{1}{\Delta t}\{\frac{\partial P_i^n}{\partial t}2\Delta t + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3} + 2D\left(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} - \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t^2}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r\Delta t}{3!} - \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^3}{2\,\Delta r} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2\Delta t}{4!} - \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^3}{4} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^4}{6\,\Delta r}\right) - 2D\left(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r\Delta t}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2\Delta t}{4!}\right) - U\left(\frac{\partial P_i^n}{\partial r}2\Delta t + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2\Delta t}{3}\right) \quad (5.8)$$

$$\Rightarrow T_i^n = 2\frac{\partial P_i^n}{\partial t} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3} + D(-2\frac{\partial^2 P_i^n}{\partial r^2} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{2\,\Delta t}{\Delta r} - \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\Delta t + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{\Delta r} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{6} - \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{2} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r\Delta t}{3} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^3}{3\,\Delta r}) - U\left(2\frac{\partial P_i^n}{\partial r} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3}\right) \quad (5.9)$$

Applying $2\frac{\partial P_i^n}{\partial t} - 2D\frac{\partial^2 P_i^n}{\partial r^2} - 2U\frac{\partial P_i^n}{\partial r} = 0$ in Equation (5.9) gives

$$T_i^n = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3} + D(\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{2\,\Delta t}{\Delta r} - \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\Delta t + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{\Delta r} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{6} - \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{2} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r\Delta t}{3} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^3}{3\,\Delta r}) - U\left(\frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3}\right) \quad (5.10)$$

Thus the truncation error for the first equation of Bokhari-Islam scheme becomes

$$T_i^n = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3} + D\left(\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{2\,\Delta t}{\Delta r} - \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\Delta t - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{6} - \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{2}\right) - U\left(\frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3}\right) + O(\Delta t^3) + O(\Delta r\Delta t) + O\left(\frac{\Delta t^2}{\Delta r}\right) + O(\Delta r^3)$$

We now apply Taylor's theorem to the second equation of the Bokhari-Islam Scheme

Let $P_i^{n+1} - P_i^{n-1} - \frac{2D\Delta t}{\Delta r^2}(P_{i+1}^{n+1} - P_i^{n+1}) = (CP^{n+1})_i$ and $\frac{2D\Delta t}{\Delta r^2}(P_{i-1}^n - P_i^n) + \frac{U\Delta t}{\Delta r}(P_{i+1}^n - P_{i-1}^n) = (DP^n)_i$

Now,

$$(CP^{n+1})_i = P_i^{n+1} - P_i^{n-1} - \frac{2D\Delta t}{\Delta r^2}(P_{i+1}^{n+1} - P_i^{n+1}) = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t - \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{2D\Delta t}{\Delta r^2}(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!} - P_i^n - \frac{\partial P_i^n}{\partial t}\Delta t - \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!}) \tag{5.11}$$

$$\Rightarrow (CP^{n+1})_i = \frac{\partial P_i^n}{\partial t}2\Delta t + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3} - 2D(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t^2}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r\Delta t}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^3}{2\,\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2\Delta t}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^3}{4} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r}{3!}\frac{\Delta t^2}{1!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^4}{6\,\Delta r}) \tag{5.12}$$

Similarly,

$$(DP^n)_i = \frac{2D\Delta t}{\Delta r^2}(P_{i-1}^n - P_i^n) + \frac{U\Delta t}{\Delta r}(P_{i+1}^n - P_{i-1}^n) = \frac{2D\Delta t}{\Delta r^2}\left(P_i^n - \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} - P_i^n\right) + \frac{U\Delta t}{\Delta r}\left(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} - P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r - \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}\right) \tag{5.13}$$

$$\Rightarrow (DP^n)_i = 2D\left(-\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r\Delta t}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2\Delta t}{4!}\right) + U(\frac{\partial P_i^n}{\partial r}2\Delta t + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2\Delta t}{3}) \tag{5.14}$$

The truncation error at gridpoint i and time step n is given by

$$T_i'^n = \frac{1}{\Delta t}\{(CP^{n+1})_i - (DP^n)_i\} \tag{5.15}$$

$$\Rightarrow T_i'^n = \frac{1}{\Delta t}\{(CP^{n+1})_i - (DP^n)_i\} = \frac{1}{\Delta t}\{\frac{\partial P_i^n}{\partial t}2\Delta t + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3} - 2D\left(\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t^2}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r\Delta t}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^3}{2\,\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2\Delta t}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^3}{4} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r}{3!}\frac{\Delta t^2}{1!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^4}{6\,\Delta r}\right) - 2D\left(-\frac{\partial P_i^n}{\partial r}\frac{\Delta t}{\Delta r} + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta t}{2!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r\Delta t}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2\Delta t}{4!}\right) - U\left(\frac{\partial P_i^n}{\partial r}2\Delta t + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2\Delta t}{3}\right)\} \tag{5.16}$$

$$\Rightarrow T_i'^n = 2\frac{\partial P_i^n}{\partial t} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3} - D\left(2\frac{\partial^2 P_i^n}{\partial r^2} + 2\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\Delta t + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{6} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{2} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r\,\Delta t}{3} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^3}{3\,\Delta r}\right) - U(2\frac{\partial P_i^n}{\partial r} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3}) \tag{5.17}$$

Applying $2\frac{\partial P_i^n}{\partial t} - 2D\frac{\partial^2 P_i^n}{\partial r^2} - 2U\frac{\partial P_i^n}{\partial r} = 0$ in Equation (5.17) gives

$$\Rightarrow T_i'^n = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3} - D\left(2\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\Delta t + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{6} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{2} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r\,\Delta t}{3} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^3}{3\,\Delta r}\right) - U(\frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3}) \tag{5.18}$$

Thus the truncation error for the second equation of Bokhari-Islam scheme becomes

$$T_i'^n = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3} - D\left(\frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\Delta t + 2\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{6} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{2}\right) - U\left(\frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3}\right) + O(\Delta t^3) + O(\Delta r^3) + O\left(\frac{\Delta t^2}{\Delta r}\right) + O(\Delta t\Delta r)$$

Now, if we average the truncation errors of the two equations for the Bokhari-Islam Scheme, we get

$$\frac{T_i^n + T_i'^n}{2} = \frac{1}{2}[\frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3} + D(\frac{\partial^2 P_i^n}{\partial r\partial t}\frac{2\,\Delta t}{\Delta r} - \frac{\partial^3 P_i^n}{\partial r^2\partial t}\Delta t + \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta t^2}{\Delta r} - \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{6} - \frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\frac{\Delta t^2}{2} + \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r\Delta t}{3} + \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta t^3}{3\,\Delta r}) - U\left(\frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3}\right) + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3} - D\left(2\frac{\partial^2 P_i^n}{\partial r\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r^2\partial t}\Delta t + \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta t^2}{\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{6} + \frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\frac{\Delta t^2}{2} + \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r\,\Delta t}{3} + \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta t^3}{3\,\Delta r}\right) - U(\frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3})] \tag{5.19}$$

So, after simplifications, the truncation Error for the Bokhari-Islam Scheme becomes,

$$\frac{T_i^n + T_i'^n}{2} = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3} - D\left(\frac{\partial^3 P_i^n}{\partial r^2\partial t}\Delta t + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{6} + \frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\frac{\Delta t^2}{2}\right) - U\frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3} + O(\Delta r^3) + O(\Delta t^3) + O(\Delta r\Delta t) \tag{5.20}$$

The truncation error in space for both convection and diffusion terms is $(\Delta r)^2$, which is similar to the Barakat-Clark scheme. However, the truncation error in time is less than $(\Delta t)^2$due to presence of the mixed term $\frac{\partial^3 P_i^n}{\partial r^2 \partial t}\Delta t$. According to our analysis the scheme has $O(\Delta t)$ accuracy, not $O(\Delta t^4)$. Bokhari-Isalm claim that their scheme is more accurate in time than the Barakat-Clark scheme.

5.2 Stability Analysis of Bokhari-Islam Scheme

Using Von-Neumann Analysis, Equation (5.23) is found to express the stability condition associated with Equation (5.1).

$$\frac{\gamma^{n+1}-\gamma^{n-1}}{2\Delta t} = D\,\frac{\gamma^n \exp(\bar{\iota}\theta)-\gamma^n-\gamma^{n+1}+\gamma^{n+1}\exp(-\bar{\iota}\theta)}{(\Delta r)^2} + U\,\frac{\gamma^n\, exp(\bar{\iota}\theta)-\gamma^n \exp(-\bar{\iota}\theta)}{2\Delta r} \tag{5.21}$$

$$\Rightarrow \gamma^{n+1}\left[1+\frac{2D\Delta t}{(\Delta r)^2}\{1-\cos(\theta)+\bar{\iota}\sin(\theta)\}\right] = \gamma^{n-1}+\gamma^n[\frac{2D\Delta t}{(\Delta r)^2}\{cos(\theta)+\bar{\iota}\,sin(\theta)-1\}+\frac{2\bar{\iota}U\Delta t}{\Delta r}\sin(\theta)] \tag{5.22}$$

$$\Rightarrow \gamma = \frac{\frac{2D\Delta t}{(\Delta r)^2}(cos\theta+\bar{\iota}sin\theta-1)+\frac{2\bar{\iota}U\Delta t}{\Delta r}sin\theta \pm \sqrt{\left(\frac{2D\Delta t}{(\Delta r)^2}(cos\theta+\bar{\iota}sin\theta-1)+\frac{2\bar{\iota}U\Delta t}{\Delta r}sin\theta\right)^2+4\{1+\frac{2D\Delta t}{\Delta r^2}(1-cos\theta+\bar{\iota}sin\theta)\}}}{2\left\{1+\frac{2D\Delta t}{(\Delta r)^2}(1-cos\theta+\bar{\iota}sin\theta)\right\}} \tag{5.23}$$

Using Von-Neumann Analysis, Equation (5.26) is found for Equation (5.2).

$$\frac{\gamma'^{n+1}-\gamma'^{n-1}}{2\Delta t} = D\,\frac{\gamma'^{n+1}\exp(\bar{\iota}\theta)-\gamma'^{n+1}-\gamma'^{n}+\gamma'^{n}\exp(-\bar{\iota}\theta)}{(\Delta r)^2} + U\,\frac{\gamma'^n\, exp(\bar{\iota}\theta)-\gamma'^n \exp(-\bar{\iota}\theta)}{2\Delta r} \tag{5.24}$$

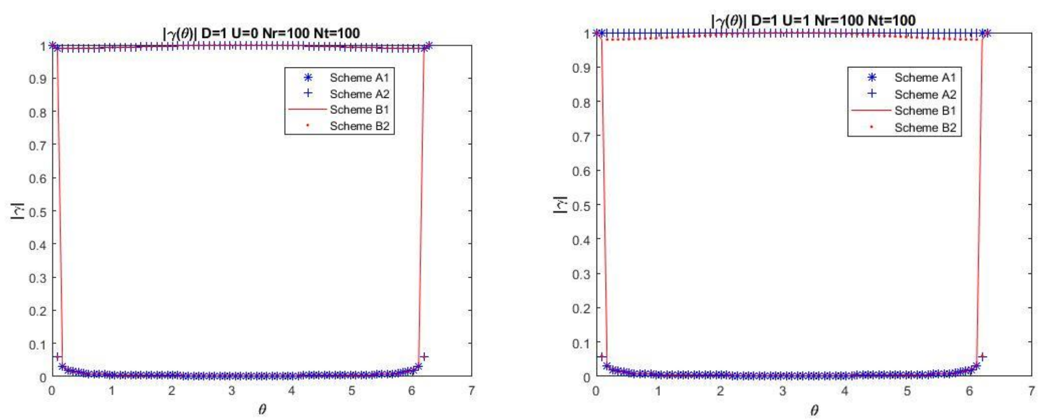
$$\Rightarrow \gamma'^{n+1}\left[1-\frac{2D\Delta t}{(\Delta r)^2}(\cos(\theta)+\bar{\imath}\sin(\theta)-1)\right]=\gamma'^{n-1}+\gamma'^{n}\left[\frac{2D\Delta t}{(\Delta r)^2}(\cos(\theta)-\bar{\imath}\sin(\theta)-1)+\frac{2\bar{\imath}U\Delta t}{\Delta r}\sin(\theta)\right] \quad (5.25)$$

$$\gamma'=\frac{\frac{2D\Delta t}{(\Delta r)^2}(cos\theta-\bar{\imath}sin\theta-1)+\frac{2\bar{\imath}U\Delta t}{\Delta r}sin\theta\pm\sqrt{\left(\frac{2D\Delta t}{(\Delta r)^2}(cos\theta-\bar{\imath}sin\theta-1)+\frac{2\bar{\imath}U\Delta t}{\Delta r}sin\theta\right)^2+4\{1-\frac{2D\Delta t}{(\Delta r)^2}(cos\theta+\bar{\imath}sin\theta-1)\}}}{2\{1-\frac{2D\Delta t}{(\Delta r)^2}(cos\theta+\bar{\imath}sin\theta-1)\}}$$

(5.26)

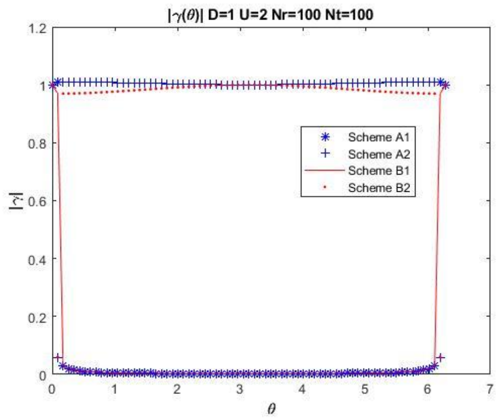
The Bokahri-Islam Scheme will be stable if both $|\gamma| \leq 1$ and $|\gamma'| \leq 1$.

For exploring the stability analysis, the following data are used, Nr=100, Nt=200, D=1, U=0,1,2,4,6,10

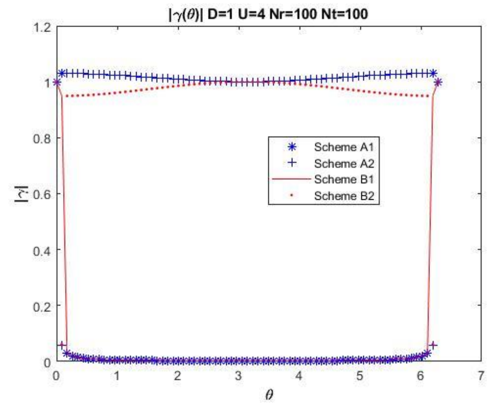


(a) U=0

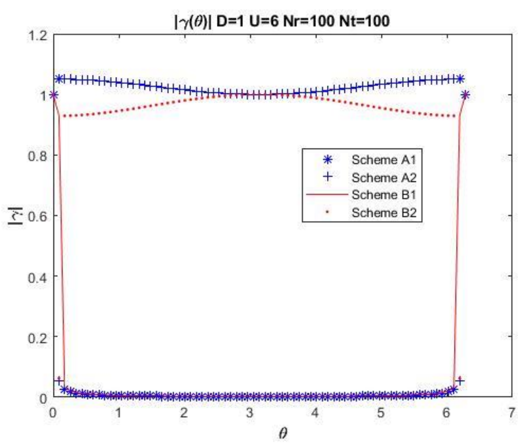
(b) U=1



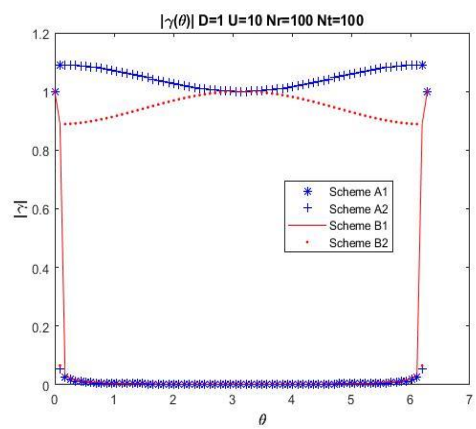
(c) U=2



(d) U= 4



(e) U=6



(f) U= 10

Figure 5.1: Stability analysis of the Bokhari-Islam Scheme

Here, A1 and A2 are the roots of Equation (5.22) and, B1 and B2 are the roots of Equation (5.25).

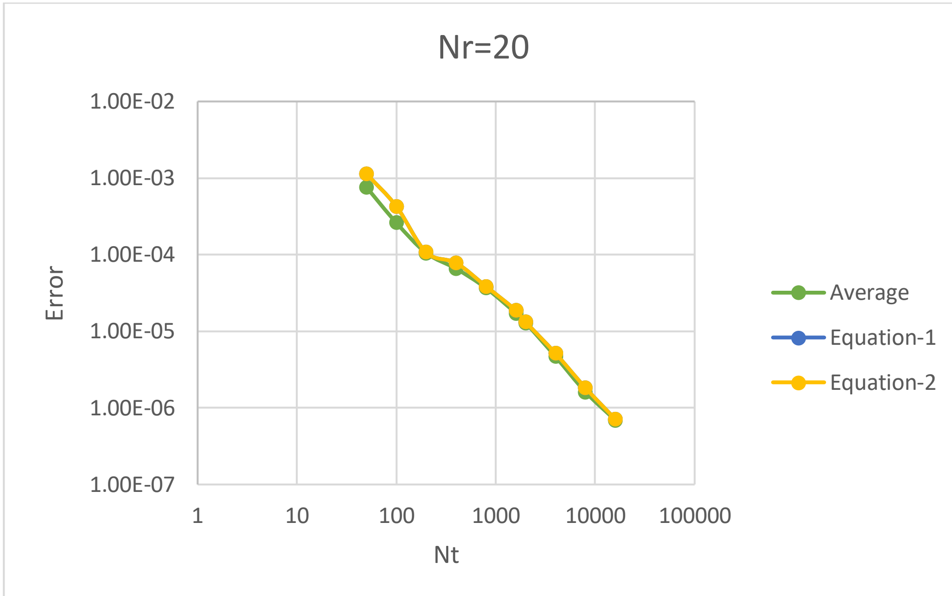
Table 5.1: Maximum values of $|\gamma|$ and $|\gamma'|$ for different values of U

U	$\|\gamma\|$		$\|\gamma'\|$	
	Scheme A1	Scheme A2	Scheme B1	Scheme B2
0	1	1	1	1
1	1	1	1	1
2	1.0099	1.0100	1	1
4	1.0300	1.0302	1	1
6	1.0502	1.0503	1	1
10	1.0904	1.0907	1	1

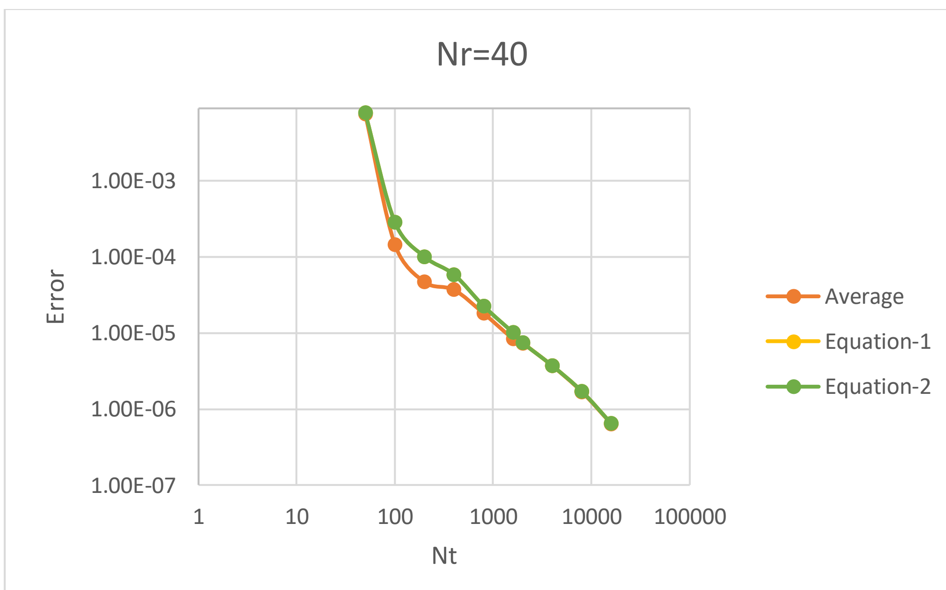
The stability analysis suggests that the Bokhari and Islam scheme is stable under certain conditions and it becomes unstable when U increases for the same values of D, Nr, and Nt.

5.3 Numerical Validation

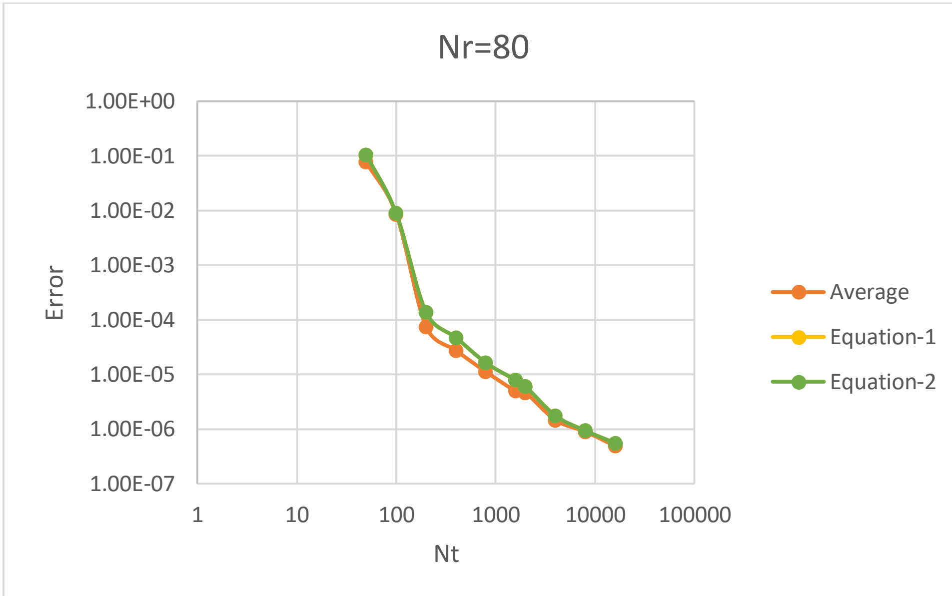
Numerical simulation is done for the Bokhari-Islam Scheme using MATLAB. Some of the data found after simulation are given below. The error values are given in Appendix-2.


Nr=20
1.00E-02
1.00E-03
1.00E-04
1.00E-05
1.00E-06
1.00E-07
Error
1
10
100
1000
10000
100000
Nt
Average
Equation-1
Equation-2

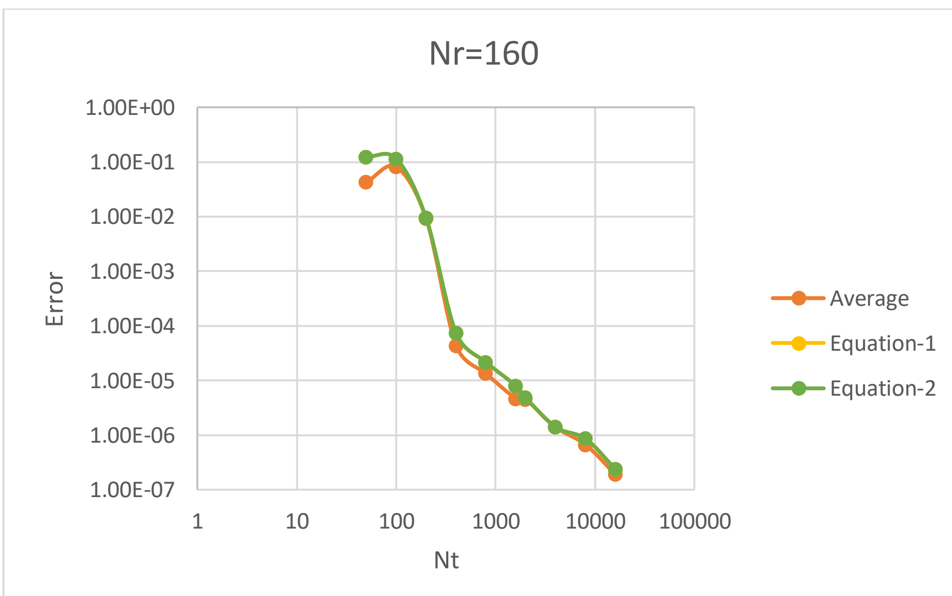
(a) Nr=20


Nr=40
1.00E-03
1.00E-04
1.00E-05
1.00E-06
1.00E-07
Error
1
10
100
1000
10000
100000
Nt
Average
Equation-1
Equation-2

(b) Nr=40



(c) Nr = 80



(d) Nr = 160

Figure 5.2: Error values of the Bokhari-Islam Scheme

From the above graphs, it is seen that the average of the two equations gives less error than Equations (5.1) and (5.2) do alone. Particularly, when Nt is smaller, the cancellation of errors is most noticeable.

If we simulate the Bokhari-Islam Scheme with U=0, it will give the approximations only for diffusion like Barakat-Clark Scheme. The graphical comparison of Barakat-Clark and Bokhari-Islam scheme is given below.

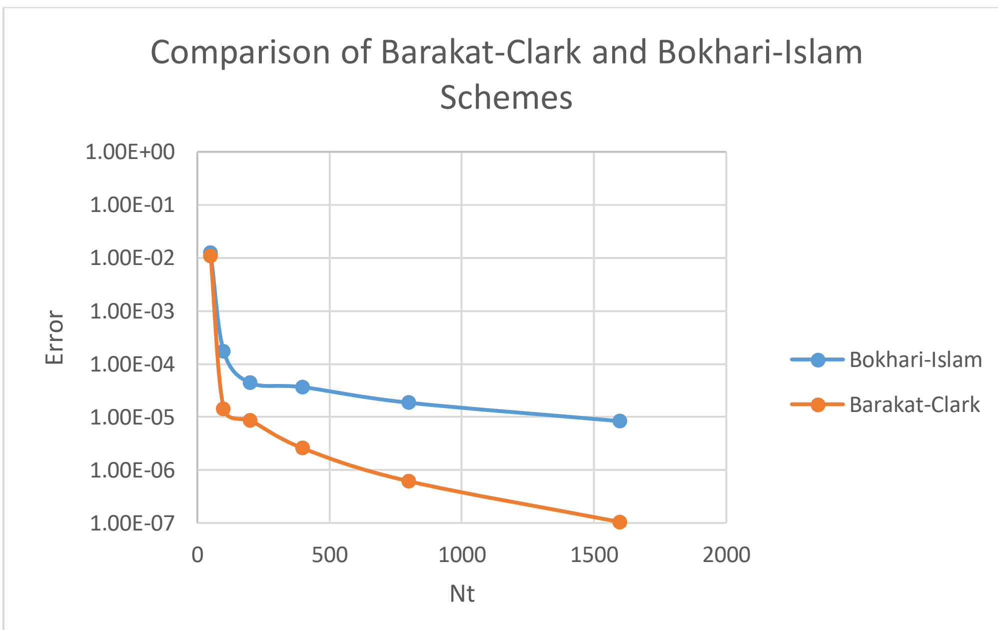


Figure 5.3: Comparison of Barakat-Clark and Bokhari-Islam

These numerical results demonstrate that the accuracy in time for the Bokhari-Isalm scheme is less than the Barakat-Clark scheme. Hence, Bokhari-Islam decreased the time accuracy from the Barakat-Clark scheme rather than increasing it.

Chapter 6 Generalised Barakat-Clark Scheme

Here, we propose an improved finite difference scheme to solve the convection-diffusion equation. The convective term is incorporated in the Barakat-Clark scheme to generalise the scheme for both convection and diffusion. In this chapter, the convection term is discretized in the same way as in the Bokhari-Islam Scheme, and we kept the time derivative term of the Barakat-Clark scheme to improve the Bokhari-Islam scheme. For the proposed scheme, truncation error analysis and stability analysis are done along with numerical validation.

The Generalised Barakat-Clark scheme for solving the 1-D convection-diffusion equation is

Scheme E: $$\frac{E_i^{n+1}-E_i^n}{\Delta t} = D\,\frac{E_{i+1}^n-E_i^n-E_i^{n+1}+E_{i-1}^{n+1}}{\Delta r^2} + U\,\frac{E_{i+1}^n-E_{i-1}^{n+1}}{2\Delta r} \quad (6.1)$$

Scheme F: $$\frac{F_i^{n+1}-F_i^n}{\Delta t} = D\,\frac{F_{i+1}^{n+1}-F_i^{n+1}-F_i^n+F_{i-1}^n}{\Delta r^2} + U\,\frac{F_{i+1}^n-F_{i-1}^{n+1}}{2\Delta r} \quad (6.2)$$

Averaging of the solutions, $\mathrm{P}_\mathrm{i}^{\mathrm{n+1}} = \frac{1}{2}(\mathrm{E}_\mathrm{i}^{\mathrm{n+1}} + \mathrm{F}_\mathrm{i}^{\mathrm{n+1}})$

6.1 Truncation Error Analysis of the Generalised Barakat-Clark Scheme

Using the two-dimensional form of Taylor's theorem, the truncation error analysis of the Generalised Barakat-Clark Scheme is given here.

First, the theorem is applied to the discretization given in Equation (6.1) and following steps are found.

Let $(AP^{n+1})_i = P_i^{n+1} - \frac{D\Delta t}{\Delta r^2}(P_{i-1}^{n+1} - P_i^{n+1}) + \frac{U\Delta t}{2\,\Delta r}P_{i-1}^{n+1}$ and $(BP^n)_i = P_i^n + \frac{D\Delta t}{\Delta r^2}(P_{i+1}^n - P_i^n) + \frac{U\Delta t}{2\,\Delta r}P_{i+1}^n$

Now,

$$(AP^{n+1})_i = P_i^{n+1} - \frac{D\Delta t}{\Delta r^2}(P_{i-1}^{n+1} - P_i^{n+1}) + \frac{U\Delta t}{2\,\Delta r}P_{i-1}^{n+1} = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{D\Delta t}{\Delta r^2}\Big(P_i^n - \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} - \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!} - P_i^n - \frac{\partial P_i^n}{\partial t}\Delta t - \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!}\Big) + \frac{U\Delta t}{2\,\Delta r}(P_i^n - \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} - \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!})\,) \tag{6.3}$$

$$(AP^{n+1})_i = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{D\Delta t}{\Delta r^2}\Big(-\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} - \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}\Big) + \frac{U\Delta t}{2\,\Delta r}(P_i^n - \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} - \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}) \tag{6.4}$$

Similarly,

$$(BP^n)_i = P_i^n + \frac{D\Delta t}{\Delta r^2}(P_{i+1}^n - P_i^n) + \frac{U\Delta t}{2\,\Delta r}P_{i+1}^n = P_i^n + \frac{D\Delta t}{\Delta r^2}\Big(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} - P_i^n\Big) + \frac{U\Delta t}{2\,\Delta r}(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}) \tag{6.5}$$

$$(BP^n)_i = P_i^n + \frac{D\Delta t}{\Delta r^2}\Big(\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}\Big) + \frac{U\Delta t}{2\,\Delta r}(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}) \tag{6.6}$$

The truncation error at gridpoint i and time step n is given by

$$T_i^n = \frac{1}{\Delta t}\{(AP^{n+1})_i - (BP^n)_i\} \tag{6.7}$$

$$\Rightarrow T_i^n = \frac{1}{\Delta t}\Big[\Big\{P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{D\Delta t}{\Delta r^2}\Big(-\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} - \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}\Big) + \frac{U\Delta t}{2\,\Delta r}\Big(P_i^n - \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} - \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}\Big)\Big\} - \Big\{P_i^n + \frac{D\Delta t}{\Delta r^2}\Big(\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}\Big) + \frac{U\Delta t}{2\,\Delta r}\Big(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}\Big)\Big\}\Big] \tag{6.8}$$

$$\Rightarrow T_i^n = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} - D\Big(-\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t}{\Delta r} - \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{2\,\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4} - \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r\,\Delta t}{6} - \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^3}{6\,\Delta r}\Big) - U\Big(-\frac{\partial P_i^n}{\partial t}\frac{\Delta t}{2\,\Delta r} - \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{4\,\Delta r} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{6} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{12\,\Delta r} - \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r\,\Delta t}{4} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{4} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{48\,\Delta r} - \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r\,\Delta t^2}{8} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^2\,\Delta t}{12} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^3}{12}\Big) \tag{6.9}$$

The truncation error for the first equation of Generalised Barakat-Clark scheme becomes

$$T_i^n = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} - D\Big(-\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4}\Big) - U\Big(-\frac{\partial P_i^n}{\partial t}\frac{\Delta t}{2\,\Delta r} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{6} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{4}\Big) + O(\Delta t^3) + O(\Delta r^3) + O(\Delta r\Delta t) + O\Big(\frac{\Delta t^2}{\Delta r}\Big)$$

We now apply Taylor's theorem to the second equation of the Generalised Barakat-Clark scheme.

Let $P_i^{n+1} - \frac{D\Delta t}{\Delta r^2}(P_{i+1}^{n+1} - P_i^{n+1}) - \frac{U\Delta t}{2\,\Delta r}P_{i+1}^{n+1} = (CP^{n+1})_i$ and $P_i^n + \frac{D\Delta t}{\Delta r^2}(P_{i-1}^n - P_i^n) - \frac{U\Delta t}{2\,\Delta r}P_{i-1}^n = (DP^n)_i$

Now,

$$(CP^{n+1})_i = P_i^{n+1} - \frac{D\Delta t}{\Delta r^2}(P_{i+1}^{n+1} - P_i^{n+1}) - \frac{U\Delta t}{2\,\Delta r}P_{i+1}^{n+1} = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{D\Delta t}{\Delta r^2}\left(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!} - P_i^n - \frac{\partial P_i^n}{\partial t}\Delta t - \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!}\right) - \frac{U\Delta t}{2\,\Delta r}\left(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}\right) \tag{6.10}$$

$$\Rightarrow (CP^{n+1})_i = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{D\Delta t}{\Delta r^2}\left(\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}\right) - \frac{U\Delta t}{2\,\Delta r}\left(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}\right) \tag{6.11}$$

Similarly,

$$(DP^n)_i = P_i^n + \frac{D\Delta t}{\Delta r^2}(P_{i-1}^n - P_i^n) - \frac{U\Delta t}{2\,\Delta r}P_{i-1}^n = P_i^n + \frac{D\Delta t}{\Delta r^2}\left(P_i^n - \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} - P_i^n\right) - \frac{U\Delta t}{2\,\Delta r}(P_i^n - \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}) \quad (6.12)$$

$$\Rightarrow (DP^n)_i = P_i^n + \frac{D\Delta t}{\Delta r^2}\left(-\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}\right) - \frac{U\Delta t}{2\,\Delta r}(P_i^n - \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}) \quad (6.13)$$

The truncation error for gridblock i at time level n is given by

$$T_i'^n = \frac{1}{\Delta t}\{(CP^{n+1})_i - (DP^n)_i\} \quad (6.14)$$

$$\Rightarrow T_i'^n = \frac{1}{\Delta t}[P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{D\Delta t}{\Delta r^2}\left(\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}\right) - \frac{U\Delta t}{2\,\Delta r}\left(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}\right) - P_i^n - \frac{D\Delta t}{\Delta r^2}\left(-\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}\right) + \frac{U\Delta t}{2\,\Delta r}(P_i^n - \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}) \quad (6.15)$$

$$\Rightarrow T_i'^n = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} - D(\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{2\,\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r\,\Delta t}{6} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^3}{6\,\Delta r}) - U(\frac{\partial P_i^n}{\partial t}\frac{\Delta t}{2\Delta r} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{4\Delta r} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{6} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{12\Delta r} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r\,\Delta t}{4} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{4} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{48\,\Delta r} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r\,\Delta t^2}{8} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^2\,\Delta t}{12} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^3}{12}) \quad (6.16)$$

The truncation error for the first equation of Generalised Barakat-Clark scheme becomes

$$T_i'^n = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} - D\left(\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12}\right) - U\left(\frac{\partial P_i^n}{\partial t}\frac{\Delta t}{2\Delta r} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{6} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{4}\right) +$$

$$O(\Delta t^3) + O(\Delta r^3) + O(\Delta r \Delta t) + O(\frac{\Delta t^2}{\Delta r})$$

The truncation error for the first Generalised Barakat-Clark scheme is the average of T_i^n and $T_i'^n$. Therefore,

$$\frac{T_i^n + T_i'^n}{2} = \frac{1}{2}\Big[\frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} - D\left(-\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t}{\Delta r} - \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{2\,\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4} -\right.$$

$$\left.\frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r\,\Delta t}{6} - \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^3}{6\,\Delta r}\right) - U\left(-\frac{\partial P_i^n}{\partial t}\frac{\Delta t}{2\,\Delta r} - \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{4\,\Delta r} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{6} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{12\,\Delta r} - \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r\,\Delta t}{4} +\right.$$

$$\left.\frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{4} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{48\,\Delta r} - \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r\,\Delta t^2}{8} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^2\,\Delta t}{12} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^3}{12}\right) + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} -$$

$$D\left(\frac{\partial^2 P_i^n}{\partial r\,\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{2\,\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4} + \frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r\,\Delta t}{6} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^3}{6\,\Delta r}\right) - U\left(\frac{\partial P_i^n}{\partial t}\frac{\Delta t}{2\Delta r} +\right.$$

$$\frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{4\Delta r} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{6} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{12\Delta r} + \frac{\partial^3 P_i^n}{\partial r^2\,\partial t}\frac{\Delta r\,\Delta t}{4} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{4} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{48\,\Delta r} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta r\,\Delta t^2}{8} +$$

$$\left.\frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^2\,\Delta t}{12} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^3}{12}\right)\Big] \qquad (6.17)$$

$$\frac{T_i^n + T_i'^n}{2} = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} - D\left(\frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4}\right) - U\left(\frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{6} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{4} +\right.$$

$$\left.\frac{\partial^4 P_i^n}{\partial r^3\,\partial t}\frac{\Delta r^2\,\Delta t}{12} + \frac{\partial^4 P_i^n}{\partial r\,\partial t^3}\frac{\Delta t^3}{12}\right) \qquad (6.18)$$

So, after simplifications, the truncation error for the Generalised Barakat-Clark Scheme becomes,

$$\frac{T_i^n + T_i'^n}{2} = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} - D(\frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\,\partial t^2}\frac{\Delta t^2}{4}) - U\left(\frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{6} + \frac{\partial^3 P_i^n}{\partial r\,\partial t^2}\frac{\Delta t^2}{4}\right) + O(\Delta r^3) +$$

$$O(\Delta t^3) + O(\Delta r^2 \Delta t) \qquad (6.19)$$

Thus, the Generalised Barakat-Clark Scheme is second order accurate in both time and space. That proves that the proposed scheme is similarly accurate to the Barakat-Clark scheme for convection-diffusion equations.

6.2 Stability Analysis of the Generalised Barakat-Clark Scheme

Using Von-Neumann Analysis, Equation (6.23) is found for Equation (6.1).

$$\frac{\gamma^{n+1}-\gamma^{n}}{\Delta t} = D\,\frac{\gamma^{n}\exp(\bar{\imath}\theta)-\gamma^{n}-\gamma^{n+1}+\gamma^{n+1}\exp(-\bar{\imath}\theta)}{(\Delta r)^2} + U\,\frac{\gamma^{n}\,exp(\bar{\imath}\theta)-\gamma^{n+1}\exp(-\bar{\imath}\theta)}{2\Delta r} \tag{6.20}$$

$$\Rightarrow \gamma^{n+1}[1-\frac{D\Delta t}{(\Delta r)^2}(\cos\theta-\bar{\imath}\sin\theta-1)+\frac{U\Delta t}{2\Delta r}(\cos\theta-\bar{\imath}\sin\theta)] = \gamma^{n}[1+\frac{D\Delta t}{(\Delta r)^2}(\cos\theta+\bar{\imath}\sin\theta-1)+\frac{U\Delta t}{2\Delta r}(\cos\theta+\bar{\imath}\sin\theta)] \tag{6.21}$$

$$\Rightarrow \gamma[1-\frac{D\Delta t}{(\Delta r)^2}(\cos\theta-\bar{\imath}\sin\theta)+\frac{D\Delta t}{(\Delta r)^2}+\frac{U\Delta t}{2\Delta r}(\cos\theta-\bar{\imath}\sin\theta)] = 1+\frac{D\Delta t}{(\Delta r)^2}(\cos\theta+\bar{\imath}\sin\theta)-\frac{D\Delta t}{(\Delta r)^2}+\frac{U\Delta t}{2(\Delta r)}(\cos\theta+\bar{\imath}\sin\theta)] \tag{6.22}$$

$$\Rightarrow \gamma = \frac{1+\left(\frac{D\Delta t}{(\Delta r)^2}+\frac{U\Delta t}{2\Delta r}\right)(cos\theta+\bar{\imath}sin\theta)-\frac{D\Delta t}{(\Delta r)^2}}{1-\left(\frac{D\Delta t}{(\Delta r)^2}-\frac{U\Delta t}{2\Delta r}\right)(cos\theta-\bar{\imath}sin\theta)+\frac{D\Delta t}{(\Delta r)^2}} \tag{6.23}$$

Using Von-Neumann Analysis, Equation (6.27) is found for Equation (6.2).

$$\frac{\gamma'^{n+1}-\gamma'^{n}}{\Delta t} = D\,\frac{\gamma'^{n+1}\exp(\bar{\imath}\theta)-\gamma'^{n+1}-\gamma'^{n}+\gamma'^{n}\exp(-\bar{\imath}\theta)}{(\Delta r)^2} + U\,\frac{\gamma'^{n+1}\,exp(\bar{\imath}\theta)-\gamma'^{n}\exp(-\bar{\imath}\theta)}{2\Delta r} \tag{6.24}$$

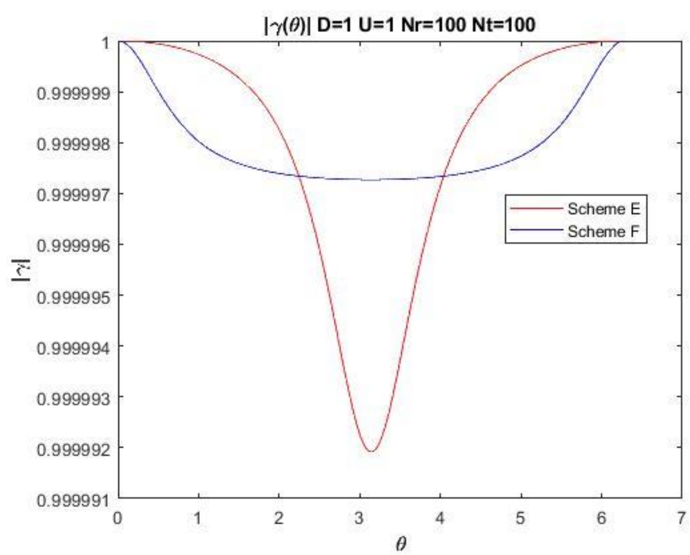
$$\Rightarrow \gamma'^{n+1}[1-\frac{D\Delta t}{(\Delta r)^2}(\cos\theta+\bar{\imath}\sin\theta-1)-\frac{U\Delta t}{2\Delta r}(\cos\theta+\bar{\imath}\sin\theta)] = \gamma'^{n}[1+\frac{D\Delta t}{(\Delta r)^2}(\cos\theta-\bar{\imath}\sin\theta-1)-\frac{U\Delta t}{2\Delta r}(\cos\theta-\bar{\imath}\sin\theta)] \tag{6.25}$$

$$\Rightarrow \gamma'[1 - \left(\frac{D\Delta t}{(\Delta r)^2} + \frac{U\Delta t}{2\Delta r}\right)\left(\cos\theta + \bar{\iota}\sin\theta\right) + \frac{D\Delta t}{(\Delta r)^2}] = 1 + \left(\frac{D\Delta t}{(\Delta r)^2} - \frac{U\Delta t}{2\Delta r}\right)(\cos\theta - \bar{\iota}\sin\theta) - \frac{D\Delta t}{(\Delta r)^2} \quad (6.26)$$

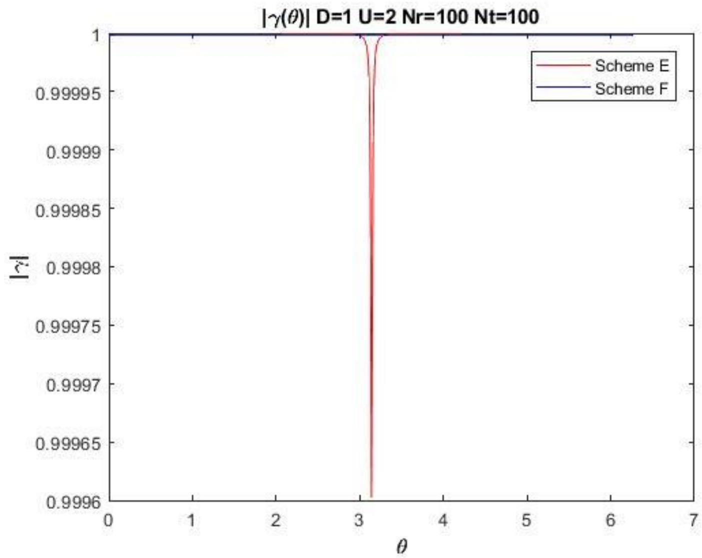
$$\gamma' = \frac{1+\left(\frac{D\Delta t}{(\Delta r)^2}-\frac{U\Delta t}{2(\Delta r)}\right)(cos\theta-\bar{\iota}sin\theta)-\frac{D\Delta t}{(\Delta r)^2}}{1-\left(\frac{D\Delta t}{(\Delta r)^2}+\frac{U\Delta t}{2\Delta r}\right)(cos\theta+\bar{\iota}sin\theta)+\frac{D\Delta t}{(\Delta r)^2}} \quad (6.27)$$

The Generalised Barakat-Clark Scheme will be stable if $|\gamma| \leq 1$ and $|\gamma'| \leq 1$.

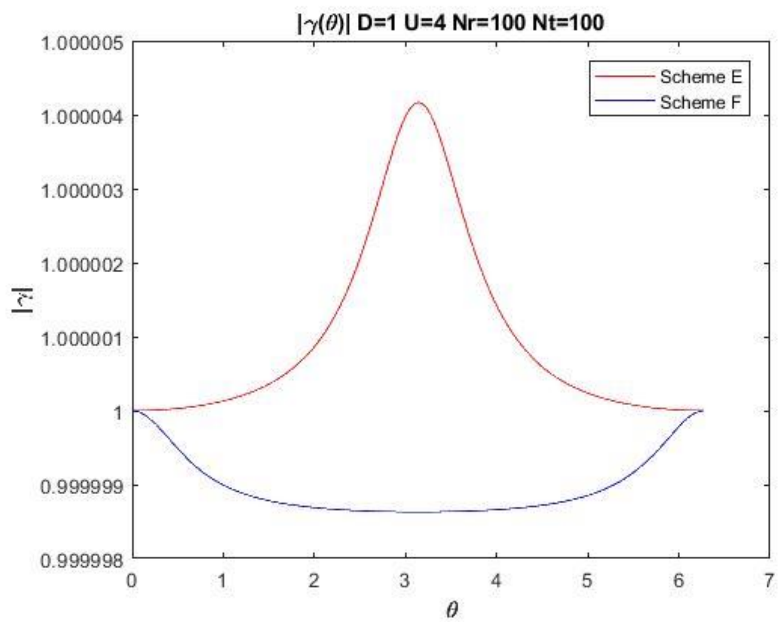
For exploing the stability analysis, the following data are used, $\mathrm{D} = 1, \mathrm{Nr} = 100, \mathrm{Nt} = 100, \mathrm{U} = 1, 2\ 4$



a) For U=1



b) For U=2



c) For U= 4

Figure 6.1: Stability analysis of the Generalised Barakat-Clark Scheme

Let $\alpha = \frac{D\Delta t}{(\Delta r)^2}, \beta = \frac{U\Delta t}{2\Delta r}$. At $\theta = \pi, sin\theta = 0, cos\theta = 1$, so

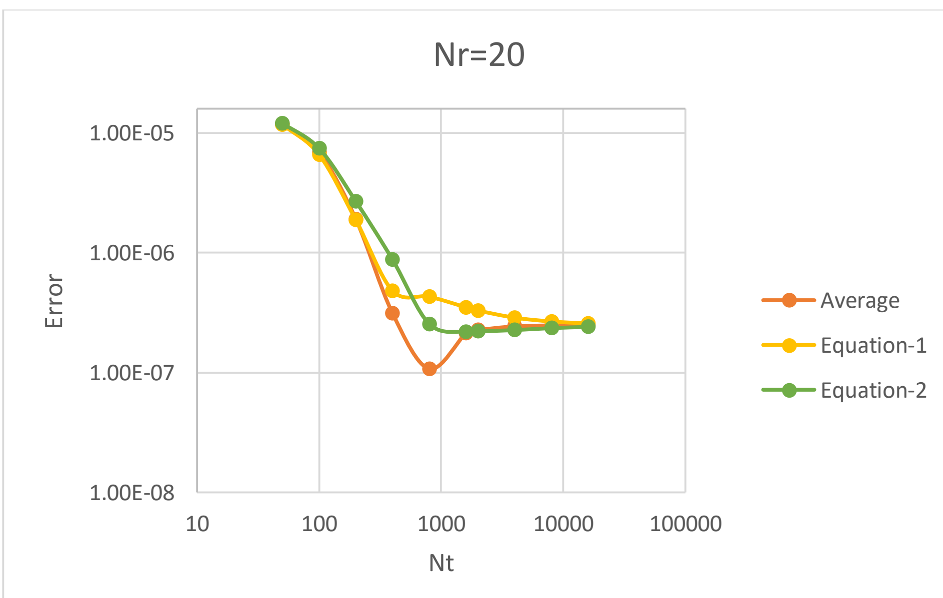
$$\gamma = \frac{1+(\alpha+\beta)(-1)-\alpha}{1-(\alpha-\beta)(-1)+\alpha} = \frac{1-2\alpha-\beta}{1+2\alpha-\beta} = -\left(\frac{2\alpha+\beta-1}{2\alpha-\beta+1}\right) \qquad \text{if } \beta > 1, |\gamma(\pi)| > 1$$

The scheme becomes unstable for $\beta > 1$ *and* any value of α .

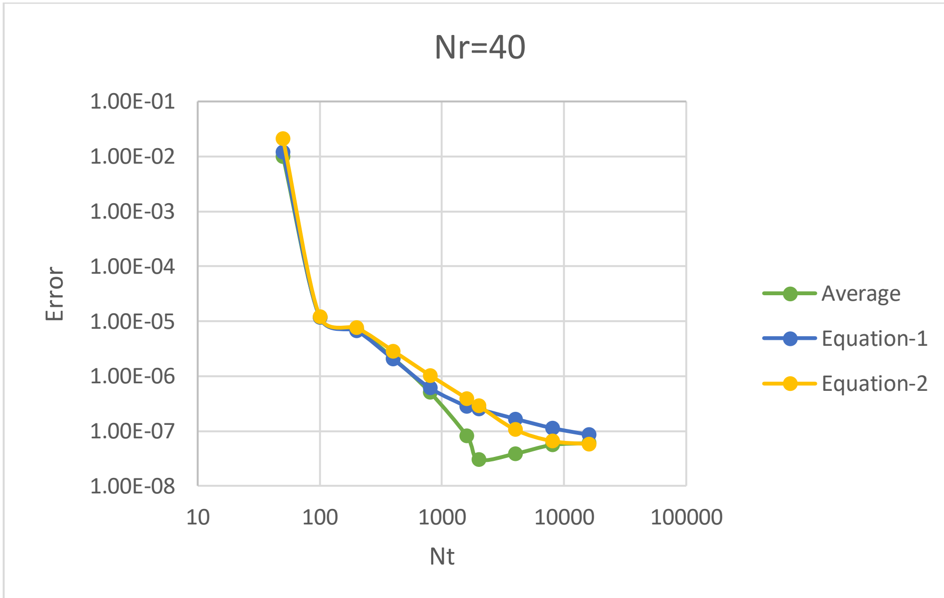
The stability analysis suggests that the Generalised Barakat-Clark Scheme is conditionally stable and it becomes unstable with increasing U for the same values of D, Nr, and Nt.

6.3 Numerical Validation

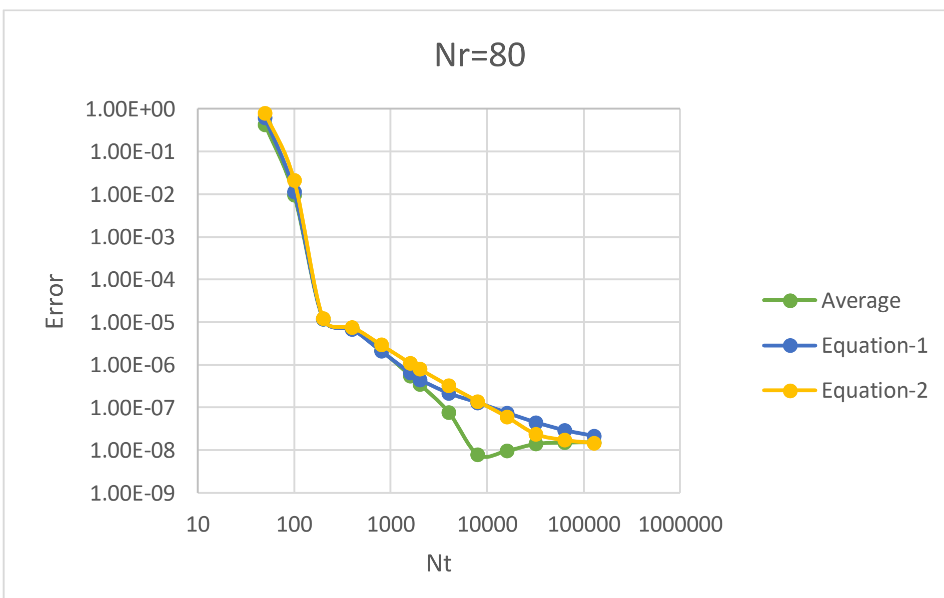
Numerical simulation is done for the Generalised Barakat-Clark scheme using MATLAB. The following data are found from this simulation for D=1 U=1. The error values are given in Appendix-3.



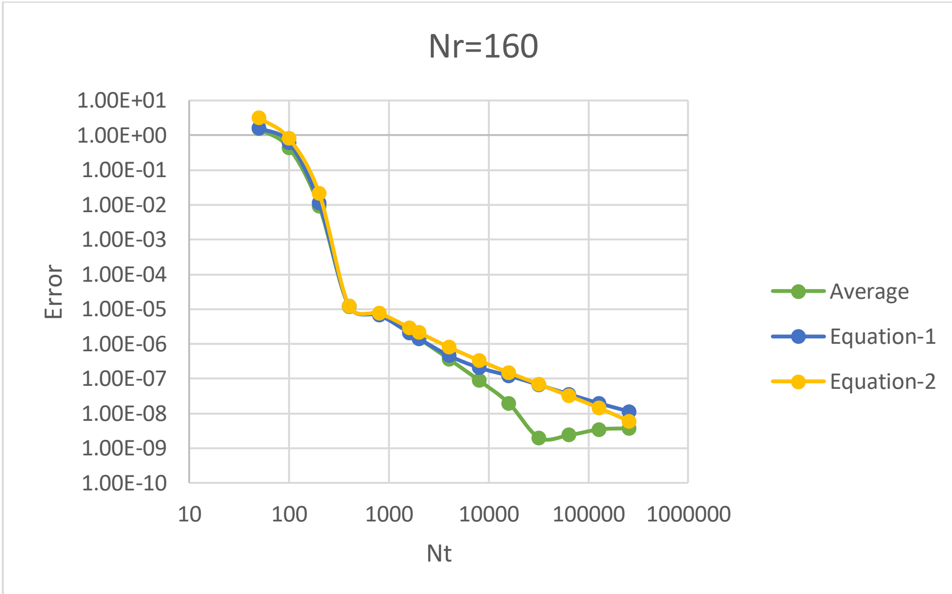
(a) Nr = 20


Nr=40
1.00E-01
1.00E-02
1.00E-03
1.00E-04
1.00E-05
1.00E-06
1.00E-07
1.00E-08
Error
10
100
1000
10000
100000
Nt
Average
Equation-1
Equation-2

(b) Nr = 40


Nr=80
1.00E+00
1.00E-01
1.00E-02
1.00E-03
1.00E-04
1.00E-05
1.00E-06
1.00E-07
1.00E-08
1.00E-09
Error
10
100
1000
10000
100000
1000000
Nt
Average
Equation-1
Equation-2

(c) Nr = 80



(d) Nr=160

Figure 6.2: Error analysis of Generalised Barakat-Clark Scheme

If Equations (6.1) and (6.2) are considered as individual schemes, the accuracy of individual Generalised Barakat-Clark scheme for both time and space are less than $O(\Delta t)^2$and O $(\Delta r)^2$, respectively. After averaging, the accuracy of the generalised Barakat-Clark scheme is $O(\Delta t)^2$and $O(\Delta r)^2$, respectively. The accuracy here for space is like the Bokhari-Islam scheme. But the accuracy for time is higher than the Bokhari-Islam scheme. So, this scheme can be seen to be an improved version of the Bokhari-Islam scheme.

Chapter 7 Upwind Barakat-Clark Scheme

Near an injection well, the convection current may dominate over diffusion. To incorporate strong convection flows, upwind differencing schemes are used. Here, we also propose another scheme incorporating the second-order upwind discretization for the convection term in the Barakat and Clark scheme. As Barakat and Clark described their proposed equation based on direction, an upwind scheme is a good candidate for the convection term, because upwind schemes follow the direction of propagation of information in a flow.

The Upwind Barakat-Clark scheme for solving the 1-D convection-diffusion equation is

$$\text{Scheme G: } \frac{G_i^{n+1}-G_i^n}{\Delta t} = D\,\frac{G_{i+1}^n-G_i^n-G_i^{n+1}+G_{i-1}^{n+1}}{\Delta r^2} + U\,\frac{3G_i^n-4G_{i-1}^{n+1}+G_{i-2}^{n+1}}{2\Delta r} \qquad (7.1)$$

$$\text{Scheme H: } \frac{H_i^{n+1}-H_i^n}{\Delta t} = D\,\frac{H_{i+1}^{n+1}-H_i^{n+1}-H_i^n+H_{i-1}^n}{\Delta r^2} + U\,\frac{3H_i^{n+1}-4H_{i-1}^n+H_{i-2}^n}{2\Delta r} \qquad (7.2)$$

Averaging of the solutions, $P_i^{n+1} = \frac{1}{2}(G_i^{n+1} + H_i^{n+1})$

While computing the solution near the left-hand end point, the first-order upwind discretization is used to avoid requiring values for the gridblocks G_{i-2} and H_{i-2}, as it is not possible to get these values when $i-2$ is negative (and the corresponding grid block is outside of the domain).

7.1 Truncation Error Analysis of Upwind Barakat-Clark Scheme

Using the two-dimensional form of Taylor's theorem, the truncation error analysis of the Upwind Barakat-Clark Scheme is given here.

First, the theorem is applied to the discretization given in Equation (7.1)

Let $(AP^{n+1})_i = P_i^{n+1} - \frac{D\Delta t}{\Delta r^2}(P_{i-1}^{n+1} - P_i^{n+1}) - \frac{U\Delta t}{2\,\Delta r}(P_{i-2}^{n+1} - 4P_{i-1}^{n+1})$ and

$(BP^n)_i = P_i^n + \frac{D\Delta t}{\Delta r^2}(P_{i+1}^n - P_i^n) + \frac{U\Delta t}{2\,\Delta r}3P_i^n$

Now, $(AP^{n+1})_i = P_i^{n+1} - \frac{D\Delta t}{\Delta r^2}(P_{i-1}^{n+1} - P_i^{n+1}) - \frac{U\Delta t}{2\,\Delta r}(P_{i-2}^{n+1} - 4P_{i-1}^{n+1}) = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t +$

$$\frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{D\Delta t}{\Delta r^2}(P_i^n - \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} -$$

$$\frac{\partial^2 P_i^n}{\partial r\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} +$$

$$\frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} - \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!} - P_i^n - \frac{\partial P_i^n}{\partial t}\Delta t - \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} -$$

$$\frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!}) - \frac{U\Delta t}{2\,\Delta r}(P_i^n - \frac{\partial P_i^n}{\partial r}2\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{4\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^2 P_i^n}{\partial r\partial t}\frac{2\Delta r}{1!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{8\Delta r^3}{3!} +$$

$$\frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\partial t}\frac{4\Delta r^2}{2!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{2\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{2\Delta r^4}{3} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{24} + \frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\Delta r^2\Delta t^2 -$$

$$\frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{4\Delta r^3\Delta t}{3} - \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta r\Delta t^3}{3} - 4(P_i^n - \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^2 P_i^n}{\partial r\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} -$$

$$\frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} -$$

$$\frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} - \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!})) \qquad (7.3)$$

$\Rightarrow (AP^{n+1})_i = P_i^{n+1} - \frac{D\Delta t}{\Delta r^2}(P_{i-1}^{n+1} - P_i^{n+1}) - \frac{U\Delta t}{2\,\Delta r}(P_{i-2}^{n+1} - 4P_{i-1}^{n+1}) = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t +$

$$\frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{D\Delta t}{\Delta r^2}(-\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^2 P_i^n}{\partial r\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} +$$

$$\frac{\partial^3 P_i^n}{\partial r^2\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} - \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}) -$$

$$\frac{U\Delta t}{2\,\Delta r}(-3P_i^n + \frac{\partial P_i^n}{\partial r}2\Delta r - 3\frac{\partial P_i^n}{\partial t}\Delta t - \frac{\partial^2 P_i^n}{\partial t^2}\frac{3\Delta t^2}{2} + \frac{\partial^2 P_i^n}{\partial r\partial t}2\Delta r\Delta t - \frac{\partial^3 P_i^n}{\partial r^3}\frac{2\Delta r^3}{3} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{2} + \frac{\partial^3 P_i^n}{\partial r\partial t^2}\Delta t^2\Delta r + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{2} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{8} - \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{2\Delta r^3\Delta t}{3} + \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta r\Delta t^3}{3}) \quad (7.4)$$

Similarly,

$$(BP^n)_i = P_i^n + \frac{D\Delta t}{\Delta r^2}(P_{i+1}^n - P_i^n) + \frac{U\Delta t}{2\,\Delta r}3P_i^n = P_i^n + \frac{D\Delta t}{\Delta r^2}\left(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} - P_i^n\right) + \frac{U\Delta t}{2\,\Delta r}3P_i^n \quad (7.5)$$

$$\Rightarrow (BP^n)_i = P_i^n + \frac{D\Delta t}{\Delta r^2}\left(\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}\right) + \frac{U\Delta t}{2\,\Delta r}3P_i^n \quad (7.6)$$

The truncation error at gridpoint i and time step n is given by

$$\mathrm{T_i^n} = \frac{1}{\Delta \mathrm{t}}\{(\mathrm{AP^{n+1}})_\mathrm{i} - (\mathrm{BP^n})_\mathrm{i}\} \quad (7.7)$$

$$\Rightarrow \mathrm{T_i^n} = \frac{1}{\Delta t}\{P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{D\Delta t}{\Delta r^2}\Big(-\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^2 P_i^n}{\partial r\partial t}\frac{\Delta r}{1!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} - \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} - \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} - \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}\Big) - \frac{U\Delta t}{2\,\Delta r}(-3P_i^n + \frac{\partial P_i^n}{\partial r}2\Delta r - 3\frac{\partial P_i^n}{\partial t}\Delta t - \frac{\partial^2 P_i^n}{\partial t^2}\frac{3\Delta t^2}{2} + \frac{\partial^2 P_i^n}{\partial r\partial t}2\Delta r\Delta t - \frac{\partial^3 P_i^n}{\partial r^3}\frac{2\Delta r^3}{3} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{2} + \frac{\partial^3 P_i^n}{\partial r\partial t^2}\Delta t^2\Delta r + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{2} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{8} - \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{2\Delta r^3\Delta t}{3} + \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta r\Delta t^3}{3}) - P_i^n - \frac{D\Delta t}{\Delta r^2}\left(\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!}\right) - \frac{U\Delta t}{2\,\Delta r}3P_i^n\} \quad (7.8)$$

$$\Rightarrow \mathrm{T_i^n} = \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} - \mathrm{D}\left(-\frac{\partial^2 P_i^n}{\partial r\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r^2\partial t}\frac{\Delta t}{2} - \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta t^2}{2\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\frac{\Delta t^2}{4} - \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r\Delta t}{6} - \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta t^3}{6\Delta r}\right) - \mathrm{U}(-\frac{\partial P_i^n}{\partial t}\frac{3\Delta t}{2\,\Delta r} - \frac{\partial^2 P_i^n}{\partial t^2}\frac{3\Delta t^2}{4\,\Delta r} + \frac{\partial^2 P_i^n}{\partial r\partial t}\Delta t - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{4\,\Delta r} + \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta t^2}{2} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^3}{4} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{16\Delta r} - \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r^2\Delta t}{3} + \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta t^3}{6}) \tag{7.9}$$

The truncation error for the first equation of Upwind Barakat-Clark scheme becomes

$$T_i^n = \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t}{2!} - D\left(-\frac{\partial^2 P_i^n}{\partial r\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r^2\partial t}\frac{\Delta t}{2} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12}\right) - U\left(-\frac{\partial P_i^n}{\partial t}\frac{3\Delta t}{2\Delta r} + \frac{\partial^2 P_i^n}{\partial r\partial t}\Delta t - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3}\right) + O(\Delta t^2) + O(\Delta r^3) + O(\Delta r\Delta t) + O(\frac{\Delta t^2}{\Delta r})$$

We apply Taylor's theorem to the second Equation of the Upwind Barakat-Clark Scheme.

Let $(CP^{n+1})_i = P_i^{n+1} - \frac{D\Delta t}{\Delta r^2}(P_{i+1}^{n+1} - P_i^{n+1}) - \frac{U\Delta t}{2\,\Delta r}(3P_i^{n+1})$ and $(DP^n)_i = P_i^n + \frac{D\Delta t}{\Delta r^2}(P_{i-1}^n - P_i^n) + \frac{U\Delta t}{2\,\Delta r}(P_{i-2}^n - 4P_{i-1}^n)$

Now,

$$(CP^{n+1})_i = P_i^{n+1} - \frac{D\Delta t}{\Delta r^2}(P_{i+1}^{n+1} - P_i^{n+1}) - \frac{U\Delta t}{2\,\Delta r}(3P_i^{n+1}) = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{D\Delta t}{\Delta r^2}\left(P_i^n + \frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^2 P_i^n}{\partial r\partial t}\Delta r\Delta t + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!} - P_i^n - \frac{\partial P_i^n}{\partial t}\Delta t - \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!}\right) - \frac{U\Delta t}{2\,\Delta r}(3P_i^n + 3\frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{3\,\Delta t^2}{2} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{2} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{8}) \tag{7.10}$$

$$\Rightarrow (CP^{n+1})_i = P_i^{n+1} - \frac{D\Delta t}{\Delta r^2}(P_{i+1}^{n+1} - P_i^{n+1}) - \frac{U\Delta t}{2\,\Delta r}(3P_i^{n+1}) = P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{D\Delta t}{\Delta r^2}\left(\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial r \partial t}\Delta r\Delta t + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2 \partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r \partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2 \partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^3 \partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r \partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}\right) - \frac{U\Delta t}{2\,\Delta r}(3P_i^n + 3\frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{3\,\Delta t^2}{2} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{2} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{8}) \tag{7.11}$$

Similarly,

$$(\mathrm{DP^n})_\mathrm{i} = \mathrm{P_i^n} + \frac{\mathrm{D\Delta t}}{\mathrm{\Delta r^2}}(\mathrm{P_{i-1}^n} - \mathrm{P_i^n}) + \frac{\mathrm{U\Delta t}}{2\,\mathrm{\Delta r}}(\mathrm{P_{i-2}^n} - 4\mathrm{P_{i-1}^n}) = \mathrm{P_i^n} + \frac{\mathrm{D\Delta t}}{\mathrm{\Delta r^2}}(\mathrm{P_i^n} - \frac{\partial \mathrm{P_i^n}}{\partial \mathrm{r}}\Delta\mathrm{r} + \frac{\partial^2 \mathrm{P_i^n}}{\partial \mathrm{r^2}}\frac{\Delta\mathrm{r^2}}{2!} - \frac{\partial^3 \mathrm{P_i^n}}{\partial \mathrm{r^3}}\frac{\Delta\mathrm{r^3}}{3!} + \frac{\partial^4 \mathrm{P_i^n}}{\partial \mathrm{r^4}}\frac{\Delta\mathrm{r^4}}{4!} - \mathrm{P_i^n}) + \frac{\mathrm{U\Delta t}}{2\,\mathrm{\Delta r}}(\mathrm{P_i^n} - \frac{\partial \mathrm{P_i^n}}{\partial \mathrm{r}}2\Delta\mathrm{r} + \frac{\partial^2 \mathrm{P_i^n}}{\partial \mathrm{r^2}}2\Delta\mathrm{r^2} - \frac{\partial^3 \mathrm{P_i^n}}{\partial \mathrm{r^3}}\frac{4\Delta\mathrm{r^3}}{3} + \frac{\partial^4 \mathrm{P_i^n}}{\partial \mathrm{r^4}}\frac{2\Delta\mathrm{r^4}}{3} - 4\mathrm{P_i^n} + \frac{\partial \mathrm{P_i^n}}{\partial \mathrm{r}}4\Delta\mathrm{r} - \frac{\partial^2 \mathrm{P_i^n}}{\partial \mathrm{r^2}}2\,\Delta\mathrm{r^2} + \frac{\partial^3 \mathrm{P_i^n}}{\partial \mathrm{r^3}}\frac{2\,\Delta\mathrm{r^3}}{3} - \frac{\partial^4 \mathrm{P_i^n}}{\partial \mathrm{r^4}}\frac{\Delta\mathrm{r^4}}{6}) \tag{7.12}$$

$$\Rightarrow (DP^n)_i = P_i^n + \frac{D\Delta t}{\Delta r^2}(-\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 \mathrm{P_i^n}}{\partial \mathrm{r^4}}\frac{\Delta\mathrm{r^4}}{4!}) + \frac{U\Delta t}{2\,\Delta r}(-3P_i^n + \frac{\partial P_i^n}{\partial r}2\Delta r - \frac{\partial^3 P_i^n}{\partial r^3}\frac{2\,\Delta r^3}{3} + \frac{\partial^4 \mathrm{P_i^n}}{\partial \mathrm{r^4}}\frac{\Delta\mathrm{r^4}}{2}) \tag{7.13}$$

The truncation error at gridpoint i and time step n is given by

$$\mathrm{T_i'^n} = \frac{1}{\Delta\mathrm{t}}\{(\mathrm{CP^{n+1}})_\mathrm{i} - (\mathrm{DP^n})_\mathrm{i}\} \tag{7.14}$$

$$\Rightarrow \mathrm{T_i'^n} = \frac{1}{\Delta t}[P_i^n + \frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{D\Delta t}{\Delta r^2}\left(\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} + \frac{\partial^2 P_i^n}{\partial r \partial t}\Delta r\Delta t + \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^3 P_i^n}{\partial r^2 \partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r \partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{4!} + \frac{\partial^4 P_i^n}{\partial r^2 \partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^3 \partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r \partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}\right) - \frac{U\Delta t}{2\,\Delta r}\left(3P_i^n + 3\frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{3\,\Delta t^2}{2} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{2} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{8}\right) -$$

$$P_i^n - \frac{D\Delta t}{\Delta r^2}\left(-\frac{\partial P_i^n}{\partial r}\Delta r + \frac{\partial^2 P_i^n}{\partial r^2}\frac{\Delta r^2}{2!} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^3}{3!} + \frac{\partial^4 \mathrm{P_i^n}}{\partial \mathrm{r}^4}\frac{\Delta \mathrm{r}^4}{4!}\right) - \frac{U\Delta t}{2\,\Delta r}(-3P_i^n + \frac{\partial P_i^n}{\partial r}2\Delta r - \frac{\partial^3 P_i^n}{\partial r^3}\frac{2\,\Delta r^3}{3} + \frac{\partial^4 \mathrm{P_i^n}}{\partial \mathrm{r}^4}\frac{\Delta \mathrm{r}^4}{2}) \tag{7.15}$$

$$\Rightarrow \mathrm{T_i'^n} = \frac{1}{\Delta t}[\frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t^2}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{4!} - \frac{D\Delta t}{\Delta r^2}\left(\frac{\partial^2 P_i^n}{\partial r\partial t}\Delta r\Delta t + \frac{\partial^3 P_i^n}{\partial r^2\partial t}\frac{\Delta r^2}{2!}\frac{\Delta t}{1!} + \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta r}{1!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^4}{12} + \frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\frac{\Delta r^2}{2!}\frac{\Delta t^2}{2!} + \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r^3}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta r}{1!}\frac{\Delta t^3}{3!}\right) - \frac{U\Delta t}{2\,\Delta r}\left(3\frac{\partial P_i^n}{\partial t}\Delta t + \frac{\partial^2 P_i^n}{\partial t^2}\frac{3\,\Delta t^2}{2} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{2} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{8} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{2\,\Delta r^3}{3} + \frac{\partial^4 \mathrm{P_i^n}}{\partial \mathrm{r}^4}\frac{\Delta \mathrm{r}^4}{2}\right)] \tag{7.16}$$

$$\Rightarrow \mathrm{T_i'^n} = \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} - D\left(\frac{\partial^2 P_i^n}{\partial r\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r^2\partial t}\frac{\Delta t}{2!} + \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta t^2}{2\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\frac{\Delta t^2}{4} + \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta t^3}{3!\Delta r}\right) - U\left(3\frac{\partial P_i^n}{\partial t}\frac{\Delta t}{2\,\Delta r} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{3\,\Delta t^2}{4\Delta r} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{4\Delta r} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{16\Delta r} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3} + \frac{\partial^4 \mathrm{P_i^n}}{\partial \mathrm{r}^4}\frac{\Delta \mathrm{r}^3}{4}\right) \tag{7.17}$$

The truncation error for the second equation of Upwind Barakat-Clark scheme becomes

$$T_i'^n = \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t}{2!} - D\left(\frac{\partial^2 P_i^n}{\partial r\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r^2\partial t}\frac{\Delta t}{2} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12}\right) - U\left(3\frac{\partial P_i^n}{\partial t}\frac{\Delta t}{2\,\Delta r} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3}\right) + O(\Delta t^2) + O(\Delta r^3) + O(\Delta t\Delta r) + O\left(\frac{\Delta t^2}{\Delta r}\right)$$

The truncation error for the Upwind Barakat-Clark scheme is the average of T_i^n and $T_i'^n$.

Therefore,

$$\frac{T_i^n + T_i'^n}{2} = \frac{1}{2}\{\frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} - \mathrm{D}\left(-\frac{\partial^2 P_i^n}{\partial r\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r^2\partial t}\frac{\Delta t}{2} - \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta t^2}{2\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\frac{\Delta t^2}{4} - \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r\Delta t}{6} - \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta t^3}{6\Delta r}\right) - \mathrm{U}\left(-\frac{\partial P_i^n}{\partial t}\frac{3\Delta t}{2\,\Delta r} - \frac{\partial^2 P_i^n}{\partial t^2}\frac{3\Delta t^2}{4\,\Delta r} + \frac{\partial^2 P_i^n}{\partial r\partial t}\Delta t - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3} - \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{4\,\Delta r} + \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta t^2}{2} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^3}{4} - \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{16\Delta r} - \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r^2\Delta t}{3} + \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta t^3}{6}\right) + \frac{\partial^2 P_i^n}{\partial t^2}\frac{\Delta t}{2!} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} - D\left(\frac{\partial^2 P_i^n}{\partial r\partial t}\frac{\Delta t}{\Delta r} + \frac{\partial^3 P_i^n}{\partial r^2\partial t}\frac{\Delta t}{2!} + \frac{\partial^3 P_i^n}{\partial r\partial t^2}\frac{\Delta t^2}{2\Delta r} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2\partial t^2}\frac{\Delta t^2}{4} + \frac{\partial^4 P_i^n}{\partial r^3\partial t}\frac{\Delta r}{3!}\frac{\Delta t}{1!} + \frac{\partial^4 P_i^n}{\partial r\partial t^3}\frac{\Delta t^3}{3!\Delta r}\right) - U\left(3\frac{\partial P_i^n}{\partial t}\frac{\Delta t}{2\,\Delta r} + \frac{\partial^2 P_i^n}{\partial t^2}\frac{3\,\Delta t^2}{4\Delta r} + \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^3}{4\Delta r} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^4}{16\Delta r} - \frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3} + \frac{\partial^4 \mathrm{P_i^n}}{\partial \mathrm{r}^4}\frac{\Delta \mathrm{r}^3}{4}\right)\} \tag{7.18}$$

$$\Rightarrow \frac{T_i^n + T_i'^n}{2} = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} + \frac{\partial^4 P_i^n}{\partial t^4}\frac{\Delta t^3}{4!} - \mathrm{D}\left(\frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2 \partial t^2}\frac{\Delta t^2}{4}\right) - \mathrm{U}\left(-\frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3} + \frac{\partial^3 P_i^n}{\partial r \partial t^2}\frac{\Delta t^2}{4} + \frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^3}{4} - \frac{\partial^4 P_i^n}{\partial r^3 \partial t}\frac{\Delta r^2 \Delta t}{6} + \frac{\partial^4 P_i^n}{\partial r \partial t^3}\frac{\Delta t^3}{12}\right) \quad (7.19)$$

So, the truncation Error for the Upwind Barakat-Clark Scheme becomes,

$$\Rightarrow \frac{T_i^n + T_i'^n}{2} = \frac{\partial^3 P_i^n}{\partial t^3}\frac{\Delta t^2}{3!} - D\left(\frac{\partial^4 P_i^n}{\partial r^4}\frac{\Delta r^2}{12} + \frac{\partial^4 P_i^n}{\partial r^2 \partial t^2}\frac{\Delta t^2}{4}\right) - U\left(-\frac{\partial^3 P_i^n}{\partial r^3}\frac{\Delta r^2}{3} + \frac{\partial^3 P_i^n}{\partial r \partial t^2}\frac{\Delta t^2}{2}\right) + O(\Delta t^3) + O(\Delta r^3) + O(\Delta r \Delta t)$$

7.2 Stability Analysis of Upwind Barakat-Clark Scheme

Using Von-Neumann Analysis, Equation (7.23) is found to express the stability condition associated with Equation (7.1).

$$\frac{\gamma^{n+1} - \gamma^n}{\Delta t} = D\,\frac{\gamma^n \exp(\bar{\imath}\theta) - \gamma^n - \gamma^{n+1} + \gamma^{n+1}\exp(-\bar{\imath}\theta)}{(\Delta r)^2} + U\,\frac{3\gamma^n - 4\gamma^{n+1}\, exp(-\bar{\imath}\theta) + \gamma^{n+1}\exp(-2\bar{\imath}\theta)}{2\Delta r} \quad (7.20)$$

$$\Rightarrow \gamma^{n+1}\left[1 - \frac{D\Delta t}{(\Delta r)^2}(\cos\theta - \bar{\imath}\sin\theta - 1) - \frac{U\Delta t}{2\Delta r}((\cos 2\theta - \bar{\imath}\sin 2\theta) - 4(\cos\theta - \bar{\imath}\sin\theta))\right] = \gamma^n\left[1 + \frac{D\Delta t}{(\Delta r)^2}(\cos\theta + \bar{\imath}\sin\theta - 1) + \frac{3U\Delta t}{2\Delta r}\right] \quad (7.21)$$

$$\gamma = \frac{1 + \frac{D\Delta t}{(\Delta r)^2}(cos\theta + \bar{\imath}sin\theta - 1) + \frac{3U\Delta t}{2\Delta r}}{1 - \frac{D\Delta t}{(\Delta r)^2}(cos\theta - \bar{\imath}sin\theta - 1) - \frac{U\Delta t}{2\Delta r}((cos2\theta - \bar{\imath}sin2\theta) - 4(cos\theta - \bar{\imath}sin\theta))} \quad (7.22)$$

Let $\alpha = \frac{D\Delta t}{(\Delta r)^2}$ and $\beta = \frac{U\Delta t}{2\Delta r}$

$$\gamma = \frac{1 + \alpha(e^{i\theta} - 1) + 3\beta}{1 - \alpha(e^{-i\theta} - 1) - \beta(e^{-2i\theta} - 4e^{-i\theta})} \quad (7.23)$$

For $\theta = \pi$, $\gamma = \frac{1 + \alpha(-2) + 3\beta}{1 - \alpha(-2) - \beta(1+4)} = \frac{1 - 2\alpha + 3\beta}{1 + 2\alpha - 5\beta} = -\left(\frac{2\alpha - 3\beta - 1}{2\alpha - 5\beta + 1}\right)$

Thus $\gamma > 1$, if $\beta > 1$.

Using Von-Neumann Analysis, Equation (7.27) is found to express the stability condition associated with Equation (7.2).

$$\frac{\gamma'^{n+1}-\gamma'^{n}}{\Delta t} = D\,\frac{\gamma'^{n+1}\exp(\bar{\imath}\theta)-\gamma'^{n+1}-\gamma'^{n}+\gamma'^{n}\exp(-\bar{\imath}\theta)}{(\Delta r)^2} + U\,\frac{3\gamma'^{n+1}-4\gamma'^{n}\,exp(-\bar{\imath}\theta)+\gamma'^{n}\exp(-2\bar{\imath}\theta)}{2\Delta r}$$

(7.24)

$$\Rightarrow \gamma'^{n+1}[1-\frac{D\Delta t}{(\Delta r)^2}\Big(\cos\theta+\bar{\imath}\sin\theta-1\Big)-\frac{3U\Delta t}{2\Delta r}\Big] = \gamma'^{n}[1+\frac{D\Delta t}{(\Delta r)^2}(\cos\theta-\bar{\imath}\sin\theta-1)+$$

$$\frac{U\Delta t}{2\Delta r}(\,(\cos 2\theta-\bar{\imath}\sin 2\theta)-4(\cos\theta-\bar{\imath}\sin\theta))] \quad (7.25)$$

$$\gamma' = \frac{1+\frac{D\Delta t}{(\Delta r)^2}(cos\theta-\bar{\imath}sin\theta-1)+\frac{U\Delta t}{2\Delta r}((cos2\theta-\bar{\imath}sin2\theta)-4(cos\theta-\bar{\imath}sin\theta))}{1-\frac{D\Delta t}{(\Delta r)^2}(cos\theta+\bar{\imath}sin\theta-1)-\frac{3U\Delta t}{2\Delta r}} \quad (7.26)$$

Similarly, $\gamma' = \frac{1+\alpha\left(e^{-i\theta}-1\right)+\beta(e^{-2i\theta}-4e^{-i\theta})}{1-\alpha\left(e^{i\theta}-1\right)-3\beta}$ (7.27)

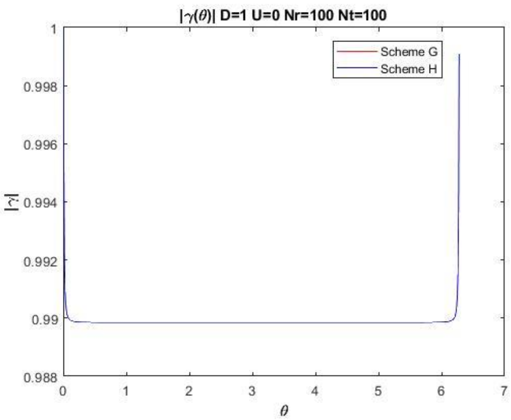
For $\theta = \pi$, $\gamma' = \frac{1+\alpha(-2)+\beta(1+4)}{1-\alpha(-2)-3\beta} = \frac{1-2\alpha+5\beta}{1+2\alpha-3\beta} = -\left(\frac{2\alpha-5\beta-1}{2\alpha-3\beta+1}\right)$

Thus $\gamma' > 1$ if $\beta \geq 1$.

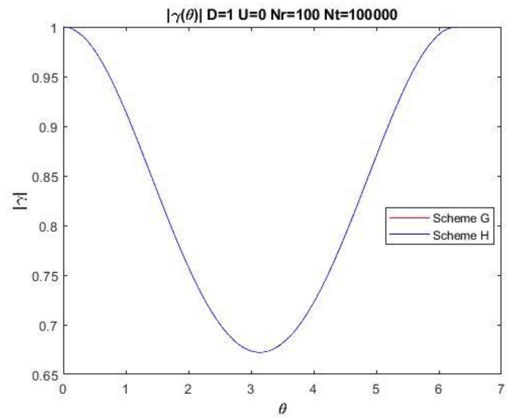
The Upwind Barakat-Clark Scheme will be stable if both $|\gamma| \leq 1$ and $|\gamma'| \leq 1$. But the scheme becomes unstable if $\beta > 1$, indicating the scheme is, at best, conditionally stable.

To explore the stability analysis, the following data are used, $\mathrm{D} = 1, \mathrm{Nr} = 100$,

$\mathrm{Nt} = 100$ and 100000, $\mathrm{U} = 0{,}1{,}2$

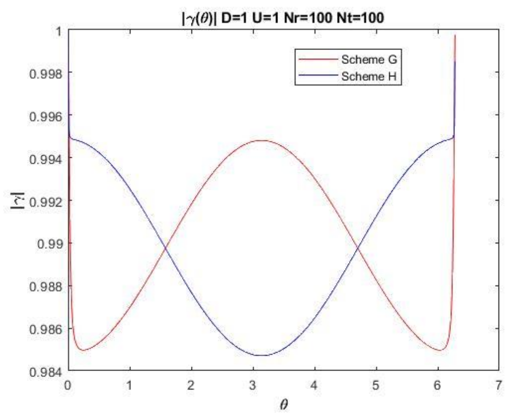


Nt=100, $\beta = 0$

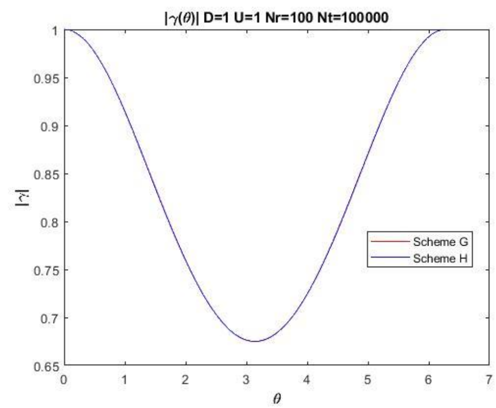


Nt=100000, $\beta = 0$

a) For U=0

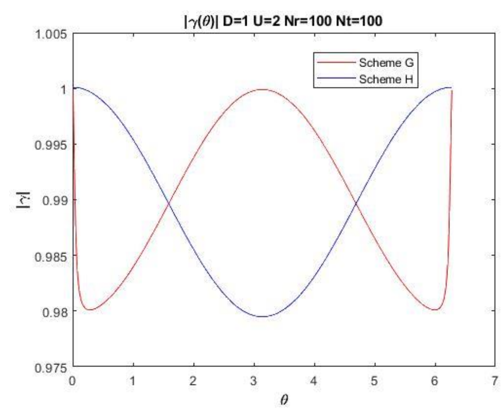


Nt=100, $\beta = 0.5$

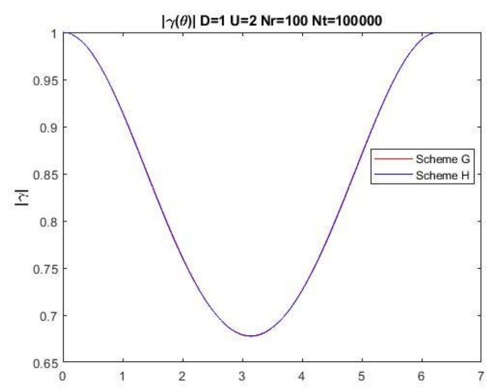


Nt=100000, $\beta = 0.0005$

b) For U=1

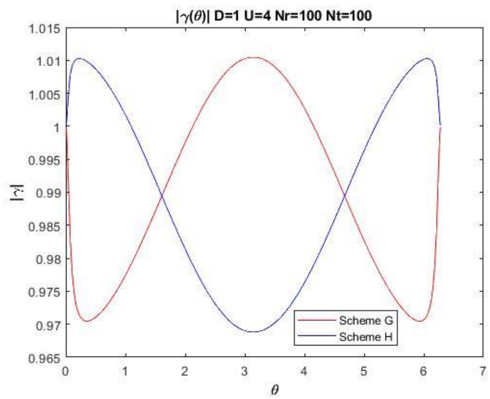


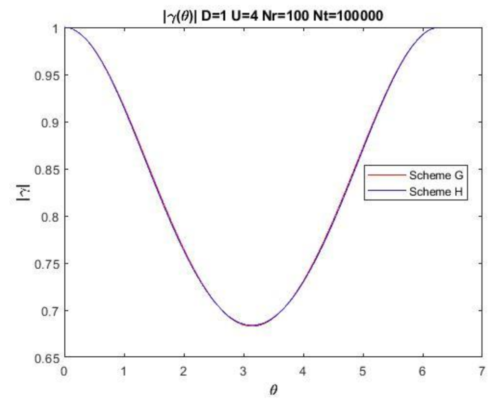
Nt=100, $\beta = 1$



Nt=100000, $\beta = 0.001$

d) For U=2





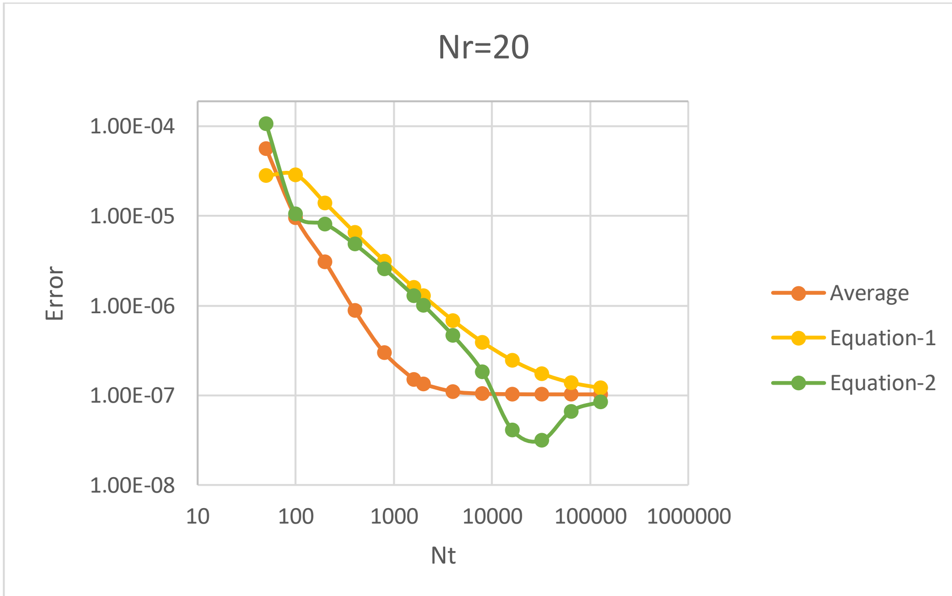
Nt=100, $\beta = 2$ Nt=100000, $\beta = 0.002$

e) For U=4

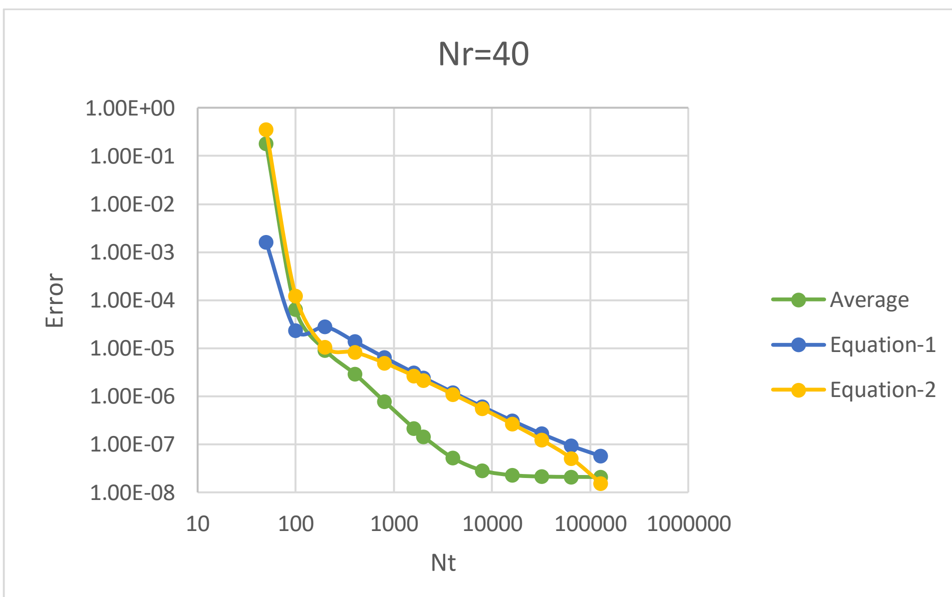
Figure 7.1: Stability analysis of Upwind Barakat-Clark Scheme

7.3 Numerical Validation

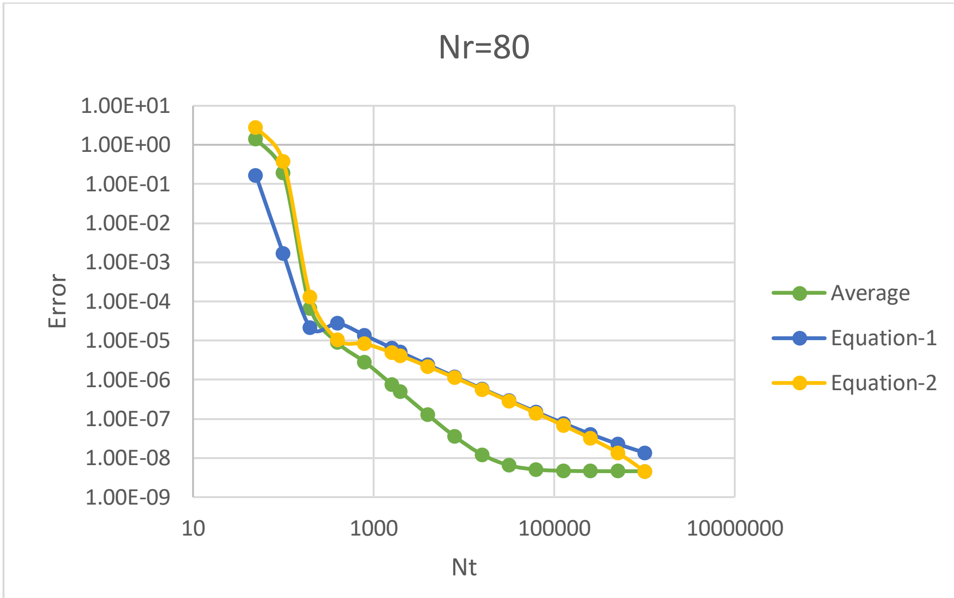
Numerical simulation is done for the Barakat-Clark scheme using MATLAB. The following data are found from this simulation for D=1 U=1. . The error values are given in Appendix-4.


Nr=20
1.00E-04
1.00E-05
1.00E-06
1.00E-07
1.00E-08
Error
10
100
1000
10000
100000
1000000
Nt
Average
Equation-1
Equation-2

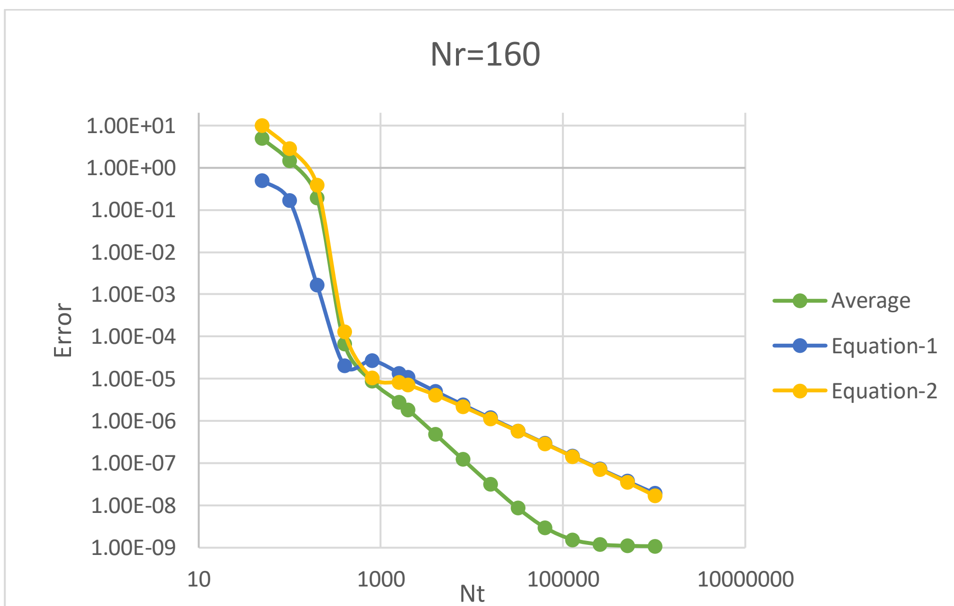
(a) Nr = 20


Nr=40
1.00E+00
1.00E-01
1.00E-02
1.00E-03
1.00E-04
1.00E-05
1.00E-06
1.00E-07
1.00E-08
Error
10
100
1000
10000
100000
1000000
Nt
Average
Equation-1
Equation-2

(b) Nr = 40



(c) Nr = 80



(d) Nr = 160

Figure 7.2: Error values of the Upwind Barakat-Clark Scheme

From the above graphs, it is seen that the average of the two equations gives much less error than the individual equations. If we consider the error values for fixed Nt and different Nr, we see that the error reduces like $(\Delta r)^2$. Again, if we consider the error values for fixed Nr and different Nt, we see that the error reduces like $(\Delta t)^2$. Thus, the accuracy of this Upwind Barakat-Clark scheme for both time and space are $O\,(\Delta t^2)$ and $O\,(\Delta r^2)$, respectively. The accuracy here for both time and space is like the Generalized Barakat-Clark scheme. Though the Upwind Discretization for the convection term was done to improve stability restrictions, it did not improve the stability. However, the Upwind Barakat-Clark scheme is observed to give more accurate results than the Generalised Barakat-Clark scheme. So, this scheme appears to be an improved version of the Generalized Barakat-Clark scheme.

Chapter 8 Conclusion

8.1 Comparison of different schemes

The summary of the numerical analysis of different schemes is as follows.

Table 8.1: Summary of different schemes

Schemes	**Equation(s)**	**Error (space, time)**	**Remarks**
Explicit	$\frac{P_i^{n+1}-P_i^n}{\Delta t} = D\frac{P_{i+1}^n-2P_i^n+P_{i-1}^n}{(\Delta r)^2} + U\frac{P_{i+1}^n-P_{i-1}^n}{2\Delta r}$	$O(\Delta r^2), O(\Delta t)$	Conditionally Stable
analyticalImplicit	$\frac{P_i^{n+1}-P_i^n}{\Delta t} = D\frac{P_{i+1}^{n+1}-2P_i^{n+1}+P_{i-1}^{n+1}}{(\Delta r)^2} + U\frac{P_{i+1}^{n+1}-P_{i-1}^{n+1}}{2\Delta r}$	$O(\Delta r^2), O(\Delta t)$	Unconditionally Stable
Barakat-Clark	$\frac{Q_i^{n+1}-Q_i^n}{\Delta t} = D\frac{Q_{i+1}^n-Q_i^n-Q_i^{n+1}+Q_{i-1}^{n+1}}{\Delta r^2}$ $\frac{S_i^{n+1}-S_i^n}{\Delta t} = D\frac{S_{i+1}^{n+1}-S_i^{n+1}-S_i^n+S_{i-1}^n}{\Delta r^2}$ Average of the solutions: $P_i^{n+1} = \frac{1}{2}(Q_i^{n+1} + S_i^{n+1})$	$O(\Delta r^2), O(\Delta t^2)$	Average of two Equations gives better result. Unconditionally stable.

Bokhari-Islam	$\frac{A_i^{n+1}-A_i^{n-1}}{2\Delta t} = D\frac{A_{i+1}^{n}-A_i^{n}-A_i^{n+1}+A_{i-1}^{n+1}}{\Delta r^2} + U\frac{A_{i+1}^{n}-A_{i-1}^{n}}{2\Delta r}$ $\frac{B_i^{n+1}-B_i^{n-1}}{2\Delta t} = D\frac{B_{i+1}^{n+1}-B_i^{n+1}-B_i^{n}+B_{i-1}^{n}}{\Delta r^2} + U\frac{B_{i+1}^{n}-B_{i-1}^{n}}{2\Delta r}$ Average of the solutions, $P_i^{n+1} = \frac{1}{2}(A_i^{n+1} + B_i^{n+1})$	$O(\Delta r^2), O(\Delta t^2)$	Less accurate in time than the claimed accuracy. Conditionally stable.
Generalised Barakat-Clark	$\frac{E_i^{n+1}-E_i^{n}}{\Delta t} = D\frac{E_{i+1}^{n}-E_i^{n}-E_i^{n+1}+E_{i-1}^{n+1}}{\Delta r^2} + U\frac{E_{i+1}^{n}-E_{i-1}^{n+1}}{2\Delta r}$ $\frac{F_i^{n+1}-F_i^{n}}{\Delta t} = D\frac{F_{i+1}^{n+1}-F_i^{n+1}-F_i^{n}+F_{i-1}^{n}}{\Delta r^2} + U\frac{F_{i+1}^{n}-F_{i-1}^{n+1}}{2\Delta r}$ Averaging of the solutions, $P_i^{n+1} = \frac{1}{2}(E_i^{n+1} + F_i^{n+1})$	$O(\Delta r^2), O(\Delta t^2)$	Similarly accurate as the Barakat-Clark Scheme after including the convection term. Conditionally stable.

Upwind Barakat-Clark	$\frac{G_i^{n+1}-G_i^n}{\Delta t} = D\frac{G_{i+1}^n-G_i^n-G_i^{n+1}+G_{i-1}^{n+1}}{\Delta r^2} + U\frac{3G_i^n-4G_{i-1}^{n+1}+G_{i-2}^{n+1}}{2\Delta r}$ $\frac{H_i^{n+1}-H_i^n}{\Delta t} = D\frac{H_{i+1}^{n+1}-H_i^{n+1}-H_i^n+H_{i-1}^n}{\Delta r^2} + U\frac{3H_i^{n+1}-4H_{i-1}^n+H_{i-2}^n}{2\Delta r}$ Averaging of the solutions, $\mathrm{P}_i^{n+1} = \frac{1}{2}(\mathrm{G}_i^{n+1} + \mathrm{H}_i^{n+1})$	$O(\Delta r^2), O(\Delta t^2)$	Same accuracy as Barakat-Clark, but observed to give less error than Generalised Barakat-Clark scheme. Conditionally stable.

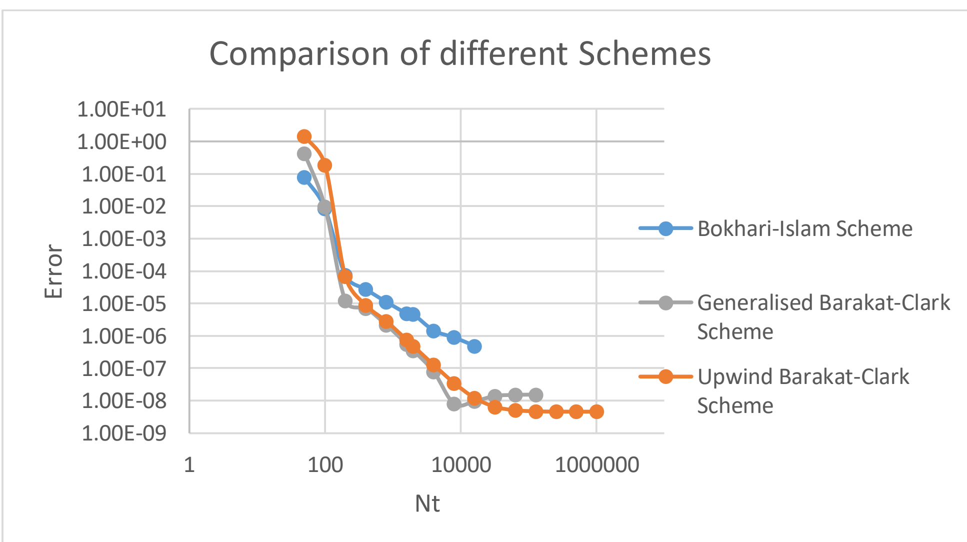


Figure 8.1: Comparison of different schemes

Figure 8.1 shows that the Generalised Barakat-Clark scheme gives less error than the Bokhari-Islam Scheme and that the Upwind Barakat-Clark Scheme gives less error than the Generalised Barakat-Clark Scheme.

After analyzing these different schemes, it can be concluded that some schemes give better results as they are expected to do. In this thesis, we have shown that the Barakat-Clark Scheme gives less error after averaging the solutions from the two equations. Further, the Bokhari-Islam Scheme fails to achieve the claim that it gets better accuracy than the Barakat-Clark Scheme. Our first proposed scheme, the Generalised Barakat-Clark Scheme, gives similarly accurate results for convection-diffusion equations as the Barakat-Clark gives for diffusion equations, but is only conditionally stable. The second proposed scheme, the Upwind Barakat-Clark Scheme gives better accuracy than the Generalised Barakat-Clark Scheme and is also conditionally stable.

8.2 Concluding Remarks

The results of our numerical investigation are influenced by the choice of Nr and Nt. In general, we observe that the Barakat-Clark scheme is most suitable for solving diffusion equations, with unconditional stability. On the contrary, the Bokahri-Islam scheme claimed to be suitable and accurate for convection-diffusion equations, but fails to fulfill this claim. The Bokhari-Islam scheme is first-order accurate in time, instead of fourth-order accurate, as was claimed. In addition, between two proposed schemes, the Upwind Barakat-Clark scheme appears to give more accurate results than the Generalised Barakat-Clark scheme with similar stability. Thus, we can conclude that the Upwind Barakat-Clark scheme is the best method among all analyzed methods for solving the one-dimensional convection-diffusion equation.

8.3 Potential Future Research

As convection-diffusion is a very important factor for Reservoir engineering, it is really necessary to account for effects of both convection and diffusion in fluid flow when designing plans for reservoir engineering. Thus, the following recommendations are made based on the present study.

This study is done for the 1-D convection-diffusion equations. Multidimensional analysis of this study will be worthy for improving or developing better methods applied to reservoir engineering. Secondly, nonlinearity of convection and diffusion is not considered here. So, inclusion of nonlinearity in the discussed schemes will give more precise results. Finally, case studies on different fields will establish the validity of the proposed and discussed schemes.

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APPENDIX 1

Table 4.1: Error values for Barakat-Clark Scheme for different numbers of time steps (Nt) and numbers of grid blocks (Nr)

Nr	Nt	Average	Equation 5.1	Equation 5.2
20	50	1.41E-05	1.43E-05	1.43E-05
	100	8.48E-06	8.63E-06	8.63E-06
	200	2.34E-06	2.80E-06	2.80E-06
	400	4.03E-07	8.34E-07	8.34E-07
	800	1.03E-07	3.71E-07	3.71E-07
	1600	2.31E-07	3.23E-07	3.23E-07
	2000	2.46E-07	3.09E-07	3.09E-07
	4000	2.67E-07	2.85E-07	2.85E-07
	8000	2.72E-07	2.77E-07	2.77E-07
	16000	2.73E-07	2.74E-07	2.74E-07
40	50	1.07E-02	1.32E-02	1.32E-02
	100	1.42E-05	1.45E-05	1.45E-05
	200	8.66E-06	8.80E-06	8.80E-06
	400	2.57E-06	2.99E-06	2.99E-06
	800	6.18E-07	9.99E-07	9.99E-07
	1600	1.05E-07	3.59E-07	3.59E-07
	2000	4.30E-08	2.60E-07	2.60E-07
	4000	4.01E-08	1.46E-07	1.46E-07
	8000	6.09E-08	1.03E-07	1.03E-07
	16000	6.61E-08	8.11E-08	8.11E-08
80	50	3.74E-01	6.98E-01	6.98E-01
	100	1.02E-02	1.35E-02	1.35E-02
	200	1.43E-05	1.46E-05	1.46E-05
	400	8.72E-06	8.86E-06	8.86E-06

	800	2.64E-06	3.05E-06	3.05E-06
	1600	6.76E-07	1.04E-06	1.04E-06
	2000	4.28E-07	7.55E-07	7.55E-07
	4000	9.51E-08	2.96E-07	2.96E-07
	8000	1.11E-08	1.24E-07	1.24E-07
	16000	9.92E-09	6.56E-08	6.56E-08
	32000	1.52E-08	3.99E-08	3.99E-08
	64000	1.65E-08	2.67E-08	2.67E-08
	128000	1.68E-08	2.05E-08	2.05E-08
	256000	1.69E-08	1.80E-08	1.80E-08
	512000	1.69E-08	1.72E-08	1.72E-08
160	50	1.11E+00	2.27E+00	2.27E+00
	100	3.75E-01	7.02E-01	7.02E-01
	200	9.88E-03	1.37E-02	1.37E-02
	400	1.44E-05	1.46E-05	1.46E-05
	800	8.75E-06	8.89E-06	8.89E-06
	1600	2.66E-06	3.07E-06	3.07E-06
	2000	1.74E-06	2.16E-06	2.16E-06
	4000	4.44E-07	7.66E-07	7.66E-07
	8000	1.09E-07	3.05E-07	3.05E-07
	16000	2.40E-08	1.33E-07	1.33E-07
	32000	2.83E-09	6.05E-08	6.05E-08
	64000	2.47E-09	3.11E-08	3.11E-08
	128000	3.79E-09	1.73E-08	1.73E-08
	256000	4.13E-09	9.97E-09	9.97E-09

APPENDIX 2

Table 5.2: Error values for Bokhari-Islam Scheme for different numbers of time steps (Nt) and numbers of grid blocks (Nr)

Nr	Nt	Average	Equation 5.1	Equation 5.2
20	50	7.64E-04	1.14E-03	1.14E-03
	100	2.62E-04	4.29E-04	4.29E-04
	200	1.05E-04	1.07E-04	1.07E-04
	400	6.56E-05	7.79E-05	7.79E-05
	800	3.66E-05	3.86E-05	3.86E-05
	1600	1.72E-05	1.87E-05	1.87E-05
	2000	1.29E-05	1.32E-05	1.32E-05
	4000	4.66E-06	5.14E-06	5.14E-06
	8000	1.61E-06	1.82E-06	1.82E-06
	16000	6.88E-07	7.10E-07	7.10E-07
40	50	7.49E-03	7.76E-03	7.76E-03
	100	1.46E-04	2.86E-04	2.86E-04
	200	4.69E-05	1.01E-04	1.01E-04
	400	3.69E-05	5.86E-05	5.86E-05
	800	1.82E-05	2.27E-05	2.27E-05
	1600	8.37E-06	1.01E-05	1.01E-05
	2000	7.35E-06	7.43E-06	7.43E-06

	4000	3.71E-06	3.72E-06	3.72E-06
	8000	1.69E-06	1.72E-06	1.72E-06
	16000	6.39E-07	6.46E-07	6.46E-07
80	50	7.68E-02	1.04E-01	1.04E-01
	100	8.56E-03	8.85E-03	8.85E-03
	200	7.41E-05	1.36E-04	1.36E-04
	400	2.74E-05	4.71E-05	4.71E-05
	800	1.11E-05	1.63E-05	1.63E-05
	1600	4.94E-06	7.84E-06	7.84E-06
	2000	4.64E-06	6.05E-06	6.05E-06
	4000	1.46E-06	1.75E-06	1.75E-06
	8000	8.91E-07	9.29E-07	9.29E-07
	16000	4.89E-07	5.51E-07	5.51E-07
160	50	4.27E-02	1.24E-01	1.24E-01
	100	8.12E-02	1.15E-01	1.15E-01
	200	9.10E-03	9.37E-03	9.37E-03
	400	4.35E-05	7.36E-05	7.36E-05
	800	1.34E-05	2.16E-05	2.16E-05
	1600	4.65E-06	8.00E-06	8.00E-06

	2000	4.53E-06	4.87E-06	4.87E-06
	4000	1.40E-06	1.40E-06	1.40E-06
	8000	6.70E-07	8.61E-07	8.61E-07
	16000	1.91E-07	2.38E-07	2.38E-07

APPENDIX 3

Table 6.1: Error values for the Generalised Barakat-Clark Scheme for different numbers of time steps (Nt) and numbers of grid blocks (Nr) (D=1, U=1)

Nr	Nt	Average	Equation 6.1	Equation 6.2
20	50	1.19E-05	1.18E-05	1.21E-05
	100	6.92E-06	6.61E-06	7.46E-06
	200	1.92E-06	1.88E-06	2.69E-06
	400	3.13E-07	4.84E-07	8.78E-07
	800	1.08E-07	4.31E-07	2.55E-07
	1600	2.14E-07	3.51E-07	2.20E-07
	2000	2.27E-07	3.30E-07	2.21E-07
	4000	2.44E-07	2.88E-07	2.27E-07
	8000	2.48E-07	2.68E-07	2.36E-07
	16000	2.49E-07	2.57E-07	2.41E-07
40	50	1.01E-02	1.19E-02	2.11E-02
	100	1.19E-05	1.19E-05	1.22E-05
	200	7.07E-06	6.75E-06	7.60E-06
	400	2.12E-06	2.04E-06	2.88E-06
	800	5.08E-07	6.10E-07	1.04E-06
	1600	8.20E-08	2.82E-07	3.94E-07
	2000	3.04E-08	2.52E-07	2.89E-07

	4000	3.88E-08	1.67E-07	1.06E-07
	8000	5.61E-08	1.14E-07	6.59E-08
	16000	6.04E-08	8.58E-08	5.81E-08
80	50	4.29E-01	6.15E-01	8.02E-01
	100	9.60E-03	1.16E-02	2.16E-02
	200	1.19E-05	1.20E-05	1.22E-05
	400	7.12E-06	6.80E-06	7.65E-06
	800	2.18E-06	2.09E-06	2.94E-06
	1600	5.59E-07	6.45E-07	1.08E-06
	2000	3.54E-07	4.54E-07	7.98E-07
	4000	7.77E-08	2.17E-07	3.26E-07
	8000	7.90E-09	1.31E-07	1.41E-07
	16000	9.61E-09	7.55E-08	6.05E-08
	32000	1.40E-08	4.50E-08	2.39E-08
	64000	1.51E-08	2.93E-08	1.72E-08
	128000	1.53E-08	2.16E-08	1.47E-08
160	50	1.55E+00	1.63E+00	3.17E+00
	100	4.30E-01	6.18E-01	8.06E-01
	200	9.35E-03	1.14E-02	2.18E-02

	400	1.20E-05	1.21E-05	1.22E-05
	800	7.14E-06	6.81E-06	7.67E-06
	1600	2.20E-06	2.10E-06	2.95E-06
	2000	1.44E-06	1.43E-06	2.13E-06
	4000	3.68E-07	4.62E-07	8.10E-07
	8000	8.98E-08	2.09E-07	3.36E-07
	16000	1.96E-08	1.22E-07	1.50E-07
	32000	2.02E-09	6.66E-08	6.92E-08
	64000	2.39E-09	3.58E-08	3.21E-08
	128000	3.49E-09	1.97E-08	1.44E-08
	256000	3.76E-09	1.15E-08	6.04E-09

APPENDIX 4

Table 7.1: Error values for Upwind Barakat-Clark scheme for different number of time steps (Nt) and numbers of grid blocks (Nr) (D = 1,U = 1)

Nr	Nt	Average	Equation 7.1	Equation 7.2
20	50	5.67E-05	2.82E-05	1.07E-04
	100	9.67E-06	2.90E-05	1.05E-05
	200	3.07E-06	1.40E-05	8.17E-06
	400	8.82E-07	6.56E-06	4.86E-06
	800	3.00E-07	3.17E-06	2.59E-06
	1600	1.52E-07	1.59E-06	1.29E-06
	2000	1.34E-07	1.29E-06	1.02E-06
	4000	1.11E-07	6.88E-07	4.66E-07
	8000	1.05E-07	3.94E-07	1.84E-07
	16000	1.04E-07	2.48E-07	4.15E-08
	32000	1.03E-07	1.75E-07	3.16E-08
	64000	1.03E-07	1.39E-07	6.70E-08
	128000	1.03E-07	1.21E-07	8.51E-08
40	50	1.81E-01	1.63E-03	3.61E-01
	100	6.47E-05	2.36E-05	1.24E-04
	200	9.13E-06	2.79E-05	1.05E-05
	400	2.91E-06	1.37E-05	8.25E-06
	800	7.82E-07	6.42E-06	4.95E-06

	1600	2.14E-07	3.07E-06	2.66E-06
	2000	1.44E-07	2.43E-06	2.16E-06
	4000	5.15E-08	1.20E-06	1.10E-06
	8000	2.84E-08	6.03E-07	5.47E-07
	16000	2.27E-08	3.10E-07	2.65E-07
	32000	2.12E-08	1.65E-07	1.23E-07
	64000	2.09E-08	9.27E-08	5.11E-08
	128000	2.08E-08	5.67E-08	1.54E-08
80	50	1.42E+00	1.63E-01	2.82E+00
	100	1.89E-01	1.66E-03	3.77E-01
	200	6.66E-05	2.14E-05	1.29E-04
	400	8.85E-06	2.73E-05	1.05E-05
	800	2.83E-06	1.36E-05	8.27E-06
	1600	7.53E-07	6.38E-06	4.97E-06
	2000	4.87E-07	5.01E-06	4.10E-06
	4000	1.26E-07	2.41E-06	2.17E-06
	8000	3.50E-08	1.18E-06	1.11E-06
	16000	1.21E-08	5.86E-07	5.62E-07
	32000	6.44E-09	2.93E-07	2.81E-07
	64000	5.03E-09	1.49E-07	1.39E-07

	128000	4.68E-09	7.64E-08	6.71E-08
	256000	4.60E-09	4.05E-08	3.13E-08
	512000	4.57E-09	2.25E-08	1.34E-08
	1024000	4.57E-09	1.35E-08	4.47E-09
160	50	4.92E+00	4.99E-01	9.95E+00
	100	1.44E+00	1.64E-01	2.86E+00
	200	1.94E-01	1.68E-03	3.86E-01
	400	6.71E-05	2.02E-05	1.30E-04
	800	8.70E-06	2.70E-05	1.05E-05
	1600	2.80E-06	1.35E-05	8.28E-06
	2000	1.84E-06	1.06E-05	7.16E-06
	4000	4.78E-07	5.00E-06	4.10E-06
	8000	1.21E-07	2.40E-06	2.18E-06
	16000	3.12E-08	1.18E-06	1.12E-06
	32000	8.59E-09	5.82E-07	5.65E-07
	64000	2.93E-09	2.90E-07	2.84E-07
	128000	1.53E-09	1.45E-07	1.42E-07
	256000	1.18E-09	7.29E-08	7.05E-08
	512000	1.09E-09	3.69E-08	3.48E-08
	1024000	1.07E-09	1.90E-08	1.69E-08