An-Najah National University
Faculty of Graduate Studies

NUMERICAL ANALYSIS OF 2D REACTION-DIFFUSION EQUATIONS: TECHNIQUES AND APPLICATION

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Dedication

This work is dedicated to my husband Ahmad for his continuous support and encouragement. I also dedicate this work to my family, especially my mother Alham, my father Ekrema, my brothers Yosef and Yaser, and my sisters Yasmeen and Kadega, for their constant support throughout my academic journey.

I also dedicate this work to my friends who made this academic journey easier, and to the souls of my grandfather and grandmother, as well as the martyrs in Palestine and Gaza, whose resilience and sacrifice continue to inspire strength and perseverance.

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Finally, I extend my thanks to my university and all those who contributed directly or indirectly to the completion of this work.

Declaration

I, the undersigned, declare that I submitted the thesis entitled:

NUMERICAL ANALYSIS OF 2D REACTION-DIFFUSION EQUATIONS: TECHNIQUES AND APPLICATION

I declare that the work provided in this thesis, unless otherwise referenced, is the researcher's own work, and has not been submitted elsewhere for any other degree or qualification.

Student's Name: ____ **Abeer Ekrema Yosef Amer**________

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Date: _________21/5/2026_________________

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Abstract

This study focuses on the reaction-diffusion process inside a two dimensional (2D) simple microfluidic channel. The material initially concentrated at the middle of the channel and was affected by diffusion and a first-order decay reaction. This work aims to investigate the numerical methods to solve 2D reaction-diffusion systems. We employ the Finite Difference Method (FDM) and Finite Volume Method (FVM) to solve the governing equations. The simulations are implemented in Python language, in order to compare the accuracy of the methods in relation with the analytical solution. The results revealed that FDM and FVM are in good agreement and suitable with the analytical solution and indicated that FVM is more practical due to efficiency and maintains lower max error and L2 norm values in the case of coarse grids, while the efficiency of the FDM is evident when the mesh is finer. The study concludes that FVM is a better choice for simulating reaction-diffusion problems where we have complex geometry or coarse mesh, while FDM is better for fine mesh or regular geometry.

Keywords: Finite Volume Method, Finite Difference Method, Reaction-Diffusion Equation, Microfluidic, Boundary and Initial Conditions, Partial Differential Equation.

Chapter One

Introduction

Reaction-diffusion systems, described by partial differential equations (PDEs), govern countless phenomena in physics, chemistry, and biology where interacting species both react and spread spatially. In two dimensions (2D), these systems appear in wide range of applications, from pattern formation in animal coats to the spread of chemical reactions on surfaces.

From here, a field emerged Microfluidics was in 1990 by A.Manz [18], he described this field by used the name Micro Total Analysis Systems(MTAS). This field has had previous research that began in the year 1980 with different names such as "micro fluid" or "micro-liquid flows". But the research paper for P.Gravesen represented a turning point and spread after 1993 [12], and he used the word Microfluidics, which was appropriate because it accurately represents fluid manipulations at the microscopic level.

The Microfluidics is a scientific field that is concerned with the study of fluid flow and behavior within channels dimensions are extremely small ranging from micrometer to nanometer [29]. More explicitly, it is the science of analyzing, moving, and directing fluids within small networks of channels as we see in figure (1.1).

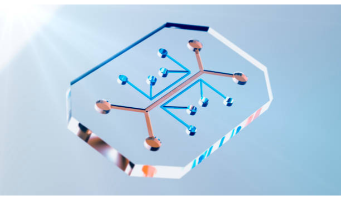


Figure 1.1: *Microfluidic device*

The most prominent components of microfluidics systems: Microchannels to control lengths and shapes as needed, valves to control corridors, reservoirs to store fluids before or after the experiment, and sensors to contribute to detecting interactions or changes within the system. The most famous processes that happening inside microfluidic systems: fluid flow, mixing, chemical reaction, diffusion, separation and filtration. We will be interested in this work in chemical reaction and diffusion.

Interaction and diffusion processes are described by Reaction-Diffusion Equation [20] which are a physical and mathematical models that play a crucial role in modeling chemical, physical, and biological phenomena, that are used to describe how concentrations of one or more substances change over time and space as a result of chemical reaction and the movement of materials from one place to another [1], Which there described mathematically by (PDEs) [7].The reaction-diffusion systems have popular examples involve the Gierer-Meinhardt model[10], the Gray-Scott model [13], the Schnakenberg model [27].

The processes of reaction is interaction between two or more substances within channels, by transformation or change in materials due to chemical or physical processes, it can reduce or increase concentrations so that materials can be consumed or produced. This concept is followed by several types: linear reaction term represents growth or decay or nonlinear reaction term like logistic reaction, single or multi-species reaction terms for more than one variable like Activator-Inhibitor systems in turing patterns[8]. While the diffusion term focus on in the movement of molecules from high concentration regions to low concentration without mechanical intervention, it is caused by the random movement of molecules, the Ficks Law used to describe the diffusion [3]. Its classified as linear (Constant-Coefficient) diffusion , or nonlinear (variable) diffusion, fractional diffusion and it common in anomalous diffusion, and multi-species diffusion or cross-diffusion for systems with multiple variables. Its importance appears in transporting drugs, mixing solutions, and distributing substances within cells.

Analytical solution to the resulted partial differential equation (PDEs) are often impossible, requiring numerical analysis. It is a type of applied mathematics concerned with built and development of algorithms designed to use numerical approximation to solve mathematical problems that it cannot easily find exact solutions for it or that we can never be found [30]. Previous studies discussed the reaction-diffusion equation with various dimensions from 1D to 3D with various kinds of reaction and diffusion for single or multiple variables and finding analytical solutions if it possible and numerical methods.

In 2001, Pao [23] presented nonlinear reaction-diffusion equations and study the case of nonlocal boundary conditions, using the numerical algorithm FDM and the method of lower and upper solutions, investigated the time-dependent and the steady-state systems by using monotone iterative method, the numerical result for steady-state and time-dependent solution compared with analytical solution and there compatible.

In 2003, Baroud et al. [2] investigate the reaction-diffusion equations in two dimension and compared with experimental measurements, the results was compatible and good agreement.

In 2009, Phongthanapanich [26]used the finite volume element method by employing the concepts of finite volume and finite element method to analyze unsteady scalar reaction-diffusion problems in two dimensions, the numerical result was stable and presents a accurate solution.

In 2018, March [19] developed the finite volume method and used second order accuracy in space to solve multilayer diffusion equation, the results demonstrated a good argument. In the same year, Zhang [35] focus on the reaction-diffusion equation in multi-dimensional domain, he performed compact finite difference method(CFDM) for discretizations in space and compact implicit integration factor method(CIIF) for discretizations in time, the numerical result show the reliability and efficiency of the scheme.

In 2020, Selmer [28] used FDM and FVM for Mass Transport Model , he examine the euclidean and maximum norm errors for two numerical methods, the FVM showed a higher overall accuracy, more efficient and preferable than FDM.

In 2021, Jalghaf [15] developed a new 2-stage explicit unconditionally positive finite difference scheme(UPFD) to solution the reaction-diffusion-advection equation, using two term of reaction linear and proportional. he conclude that the method is stable.

In 2022, Kanokwarun [24] investigated advection-diffusion-reaction equations in water pollution problems in 1D and 2D, then presented comparison between two numerical methods FVM and FDM with implicit forward time central space FTCS scheme with analytical solution, the results is a strong agreement.

In 2023, Heidari et al.[14] studied the reaction-diffusion equation and used numerical method a spectral collocation algorithm by used interpolating polynomial, the approximation results converge to the exact results and efficiency precisely when increases the number of collocation points.

In 2024, Nyaupane et al.[21] compared the analytical and numerical solutions in fluid flow applications. The FDM and FVM were investigated and they found that the FVM method gives more accurate solutions.

In this work we will investigate the reaction diffusion phenomena in a simple microfluidic system with a constant diffusion and linear reaction term. Finite Difference Methods (FDM) and Finite Volume Methods (FVM) will be introduced and will be used to solve the govern PDEs. Their results will be analyzed and compared.

We will present the governing equation in the beginning mathematically and physically then begin with explain the mathematical concepts related to governing equation from initial and boundary condition passing through the classification of differential equation to arrives the concept of PDE and analytical solution then find the analytical solution of governing equation.

we will demonstrate the numerical analysis specifically in two methods FVM and FDM beginning from definition ,grid discretizations and solving governing equation by these methods.

Applying algorithms and finding the two errors L2 error and max error to decide which one is more accurate and effective by comparing the results in tables and images, we will get the result by using the python language.

Chapter Two

Mathematical Formulation of 2D Reaction-Diffusion Equations

2.1 Reaction-Diffusion Equations

Reaction-diffusion equations are a class of partial differential equations (PDEs) that describe the relation between chemical reactions and diffusion processes [32]. In two dimensions, the general form of a single-component reaction-diffusion equation is given by:

$$\frac{\partial u}{\partial t} = D\nabla^2 u + f(u) \tag{2.1}$$

Where u is the concentration of the material, D is the diffusion coefficient, t is the time and $f(u)$ is the reaction term.

This system describes how the material u reacts and diffuses in both time and space. In equation (2.1), the diffusion term ($D\nabla^2 u$) describes the change of concentration due to the diffusion processes and the reaction term ($f(u)$) describes the change of concentration due to chemical reactions. Depending on the specific application the reaction term can take different forms such as constant, linear and non-linear forms.

In this work, a simple microfluidic system will be considered. With a 2D microfluidic channel where a chemical component is mid-channel injection, and over time the concentration of the material diffuses in both directions symmetrically with a first-order decay reaction. In this system we assume there is no advection and the change of concentration is only due to diffusion and reaction. Then, the system can be described using the following equation:

$$\frac{\partial u}{\partial t} = D\nabla^2 u - \alpha u \tag{2.2}$$

Where the linear reaction term ($-\alpha u$) describes how the material u decays with time proportionally to its concentration with respect to the positive α.

2.2 Boundary and Initial Conditions

In the filed of differential equations , the analytical solution for (2.2) is usually not unique [9], the field of initial and boundary conditions play decisive role to specify the unique solution for analytical solution , hence appear the importance of initial and boundary conditions.

Initial conditions are specialized in determining the values of the function or the derivative at the initial time, for PDE the highest-order time derivative is determine the number of initial conditions for example if the equation has 1st order time we need one initial condition but if the equation 2nd-order time it needs two initial conditions and so on [22]. The boundary conditions deal with the boundary domain by specifying function or derivatives values at domain. The most common boundary conditions:

- **Dirichlet Boundary Condition (called Fixed Boundary Conditions**): first type of boundary condition and is refers to the exact solution along the boundary it is require for elliptic and parabolic equations [31]. example for Dirichlet BC is determination the temperature at inlets and outlets of the rod in 1D is $T(0,t) = 0$,$T(l,t) = 10$ and also to the example if the temperature of rod is $T(0,t) = T(l,t) = 0$ that is a called homogeneous conditions [30].
- **Neumann boundary condition**: second type of boundary condition, is associated with rate of change of the solution perpendicular to the boundary it is require for elliptic and parabolic equations [31]. For example, the condition on the domain take the form $\frac{du}{dn}(x) = f(x)$ where n denotes the normal derivative to the boundary, and f is a given scalar function.
- **Robin boundary condition (called convective Boundary Condition)**: third type of boundary condition, many name for it, convective BC from their application in heat transfer problems or impedance BC from their application in electromagnetic problems. The condition is a weighted combination of Dirichlet and Neumann BC which is a specification of a linear combination of the values of its derivative on the boundary of the domain and the values of a function $c_0 y + c_1 \frac{dy}{dn} = f$, It appears widely in the solution Sturm-Liouville problems.

In this work, as we describe mid-channel injection, We will adopt the initial conditions for length L:

$$u(x,y,0) = sin(\frac{\pi x}{L})sin(\frac{\pi y}{L}) \tag{2.3}$$

And using Dirichlet BC to describe that the concentration is zero on the four sides:

$$u(x,0,t) = 0, u(x,L,t) = 0 \tag{2.4}$$

$$u(0,y,t) = 0, u(L,y,t) = 0 \tag{2.5}$$

2.3 Analytical Solution

To clarify how we can solve the equation (2.2) analytically, we need to clarify the concept of the differential equation. Therefore, a differential equation is an equation that involves the unknown function and its derivatives, the classification of differential equation:

- **Classification by type:** We have two type for differential equation for a function, based on number of independent variable. if the equation have just one independent variable then its named ordinary differential equation (ODE), but if the equation have more than one independent variable then its named partial differential equation (PDE). clearly, the second type is had more challenge and complex to find solution.
- **Classification by degree and order:** The exponent of the highest derivative in the differential equation represents the degree of differential equation. While the highest derivative contained in the differential equation denotes the order of differential equation. For example $(\frac{d^2y}{dx^2})^3 + 5y + (\frac{dy}{dx})^2 = 0$ is of degree 3, which denote the highest derivative is multiplied three times by itself and it ordinary differential equations of second order. In other words, which mean the function is differentiated two times.
- **Classification as linear or non linear differential equation:** The linear differential equation refers to the unknown function like u and its derivatives appear only to the first power. In other words, the degree is one and its not multiplied together. The general form of linear differential equation is[11]:

$$a_n(x)\frac{d^n u}{dx^n} + a_{n-1}(x)\frac{d^{n-1}u}{dx^{n-1}} + \ldots + a_1(x)\frac{du}{dx} + a_0(x)u = g(x)$$

The differential equation is said to be non-linear if the unknown function and its derivatives is multiplied together which mean the power is greater than one or inside function appear $sin(y)$ or $cos(y)$ or e^y and so on.

In particular, We will talk about standard texts the linear second-order differential equation and classification of PDEs into elliptic, parabolic, and hyperbolic equations is given of the form [31]:

$$au_{yy} + 2bu_{yx} + cu_{xx} + eu_y + du_x + fu = g.$$

Where the classification is determined by the sign of the discriminant

$$\begin{aligned} ac - b^2 \quad & > 0 \longrightarrow hyperbolic \\ & = 0 \longrightarrow parabolic \\ & < 0 \longrightarrow elliptic \end{aligned}$$

Specifically, our equation (2.2) falls under a parabolic equation in particular time-dependent problems, these equations describe different types of phenomena and need different techniques for their solution both analytically and numerically.

The analytical solution method we can use for ODE and PDE is different because ODEs have one independent variable but PDEs more than one independent variable. separation of variables, Fourier transform, method of characteristics, Green function and traveling wave for solving PDEs.

Therefore, we will use the separation of variables to solving the PDE equation (2.2). Firstly, we assume that u(x,y,t) can be written as a product of three other functions, where two depend on the space x and y respectively with the time t. Such as, we make the formula

$$u(x,y,t) = X(x)Y(y)T(t) \tag{2.6}$$

After that, substituting (2.6) into (2.2), we obtain

$$XY\frac{dT}{dt} = DT(Y\frac{d^2X}{dx^2} + X\frac{d^2Y}{dy^2}) - \alpha YXT$$

Which we rewrite by divide by X Y T and separating x , y and t

$$\frac{1}{T}\frac{dT}{dt} = D(\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2}) - \alpha$$

Therefore, both sides of this equation are independent of both y,x and t and equal to a constant. Furthermore, the right hand side is independent of t and the left hand side of this equation is independent of x and y. assuming $-\mu$ as the separation constant , we got

$$D(\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2}) = -\mu \tag{2.7}$$

$$\frac{1}{T}\frac{dT}{dt} = -\mu - \alpha$$

Then, the following become

$$\frac{dT}{dt} = (-\mu - \alpha)T$$

And we obtain the three ordinary differential equations , the first

$$\frac{dT}{dt} + (\mu + \alpha)T = 0$$

Whereas ,The second and third extracted from the formula (2.7)

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} = \frac{-\mu}{D}$$

Thus, we have two ordinary differential equations because the left hand side equal to constant by assuming $\mu = (\beta^2 + \lambda^2)$ D then

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} = \frac{-(\beta^2 + \lambda^2)D}{D}$$

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} = -(\beta^2 + \lambda^2)$$

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} = -\beta^2 - \lambda^2$$

Solving for X, we have:

$$\frac{1}{X}\frac{d^2X}{dx^2} = -\beta^2$$

$$\frac{d^2X}{dx^2} + \beta^2 X = 0$$

Similarity to Y we obtain:

$$\frac{1}{Y}\frac{d^2Y}{dy^2} = -\lambda^2$$

Thus, The finally equation become

$$\frac{d^2Y}{dy^2} + \lambda^2 Y = 0$$

As we see, we arrived from the basic equation (2.2) to three main equations: the first dependent on the variable t, the second dependent on the variable x and the third dependent on the variable y.

We rearrange there in below and we will to solve there one by one in order, let us note together that the equation second and third is same way solution but their different by the variable while the first is need to another way to solution. But overall the equations is ODE with differently solution methods.

$$\begin{cases} \dfrac{dT}{dt} + (\mu+\alpha)T = 0 & (1) \\ \dfrac{d^2X}{dx^2} + \beta^2 X = 0 & (2) \\ \dfrac{d^2Y}{dy^2} + \lambda^2 Y = 0 & (3) \end{cases}$$

To solve the first ODE linear equation (1) we will using the integrating factor method which is specialized in 1st order linear ODE by multiplying the equation with the integrating factor to convert it to the derivative of the multiplication[4]. Multiplying both sides of the Eq(1) by the integrating factor I defined as

$$\begin{aligned} I &= e^{\int(\mu+\alpha)dt} \\ &= e^{(\mu+\alpha)t} \end{aligned}$$

Multiply Eq(1) by I we have

$$e^{(\mu+\alpha)t}\frac{dT}{dt}+e^{(\mu+\alpha)t}(\mu+\alpha)T=0$$

The left-hand side is the derivative of the multiplication of $\frac{d\ e^{(\mu+\alpha)t}\ T}{dt}$ so by integrating both sides we got the general solution for the first equation:

$$\int\frac{d\ e^{(\mu+\alpha)t}\ T}{dt}=\int 0$$
$$e^{(\mu+\alpha)t}\ T=0$$

$$T(t)=e^{-(\mu+\alpha)t} \tag{2.8}$$

Now, we will solve the second equation (2) which is called an ODE eigenvalue problem and it is a 2nd order linear homogeneous differential equation.

Certainly, the trivial solution X(x) = 0 is a solution, but nontrivial solutions exist only for values of β^2 with corresponding functions X(x) are referred to as eigenvalues and eigenfunctions of the differential equation, to solve this equation we will use the characteristic equation method which is a method for solving the linear higher order ODEs on condition constant coefficients.

Assume the solution is

$$X(x)=e^{rx}$$

Where r is a constant

$$\frac{d^2(e^{rx})}{dx^2}+\beta^2e^{rx}=0$$

After substituting into the equation(2) the characteristic equation become

$$r^2e^{rx}+\beta^2e^{rx}=0$$

$$e^{rx}(r^2+\beta^2)=0$$

Since $e^{rx} \neq 0$, so $(r^2+\beta^2=0)$,we are solving for r

$$r^2 = -\beta^2 \implies \sqrt{r^2} = \sqrt{-\beta^2} \implies r = \mp i\beta$$

The Case $\beta = 0$ leads to a trivial solution under homogeneous boundary conditions so its excluded.[5]

In the Case $\beta^2 > 0$ we substitute. $r = \pm i\beta x$

$$X(x) = e^{\pm i\beta x} = C_1 e^{i\beta x} + C_2 e^{-i\beta x}$$

Using the Euler formula $(e^{i\ \beta x} = cos\ \beta x + i\ sin\ \beta x)$ and $(e^{-i\ \beta x} = cos\ \beta x - i\ sin\ \beta x)$

$$X(x) = C_1(cos\ \beta x + i\ sin\ \beta x) + C_2(cos\ \beta x - i\ sin\ \beta x)$$

$$X(x) = C_1 cos\ \beta x + C_1 i\ sin\ \beta x + C_2 cos\ \beta x - C_2 i\ sin\ \beta x$$

$$X(x) = (C_1+C_2) cos\ (\beta x) + i(C_1-C_2)\ sin\ (\beta x)$$

This leads us to the general solution for the second equation(2)

$$X(x) = B_1\ cos\ (\beta x) + A_1\ sin\ (\beta x) \tag{2.9}$$

Where $B_1 = C_1 + C_2$ and $A_1 = C_1 - C_2$.

The finally equation (3) have the form:

$$\frac{d^2Y}{dy^2} + \lambda^2 Y = 0$$

By similarity, we can solving it by the characteristic equation method as we did in the previous equation, we will beginning with assuming the solution:

$$Y(y) = e^{ky}$$

Where k is a constant. After substituting into the equation(3) the characteristic equation become:

$$\frac{d^2(e^{ky})}{dy^2} + \lambda^2 e^{ky} = 0$$

$$k^2e^{ky} + \lambda^2e^{ky} = 0$$

$$e^{ky}(k^2 + \lambda^2) = 0$$

Since $e^{ky} \neq 0$, so ($k^2 + \lambda^2 = 0$), we are solving for k:

$$k^2 = -\lambda^2 \implies \sqrt{k^2} = \sqrt{-\lambda^2} \implies k = \mp i\lambda$$

The Case $\lambda = 0$ is excluded [5].

The Case $\lambda^2 > 0$ substituting k by $k = \pm i\lambda y$

$$Y(y) = e^{\pm i\lambda y} = C_3e^{i\lambda y} + C_4e^{-i\lambda y}$$

We will using the Euler formula ($e^{i\ \lambda y} = cos\ \lambda y + i\ sin\ \lambda y$) and ($e^{-i\ \lambda y} = cos\ \lambda y - i\ sin\ \lambda y$)

$$Y(y) = C_3(cos\ \lambda y + i\ sin\ \lambda y) + C_4(cos\ \lambda y - i\ sin\ \lambda y)$$

$$Y(y) = C_3cos\ \lambda y + C_3i\ sin\ \lambda y + C_4cos\ \lambda y - C_4i\ sin\ \lambda y$$

$$Y(y) = (C_3 + C_4)cos\ (\lambda y) + i(C_3 - C_4)\ sin\ (\lambda y)$$

The general solution is:

$$Y(y) = B_2\ cos\ (\lambda y) + A_2\ sin\ (\lambda y) \tag{2.10}$$

Where $B_2 = C_3 + C_4$ and $A_2 = C_3 - C_4$.

Now we want to transformation the general solution to a unique solution by substitution the conditions.

We will substitute the condition (2.4) into the EQ (2.10)

$$u(x,0,t) = 0 \implies X(x)Y(0)T(t) = 0 \implies Y(0) = 0$$

$$Y(0) = B_2\ cos\ (\lambda * 0) + A_2\ sin\ (\lambda * 0)$$

$$0 = B_2$$

$$\begin{aligned} u(x,L,t) = 0 \implies X(x)Y(L)T(t) = 0 \implies Y(L) = 0, B_2 = 0 \\ Y(L) = 0 * \; cos\ (\lambda * L) + A_2\ sin\ (\lambda * L) \\ 0 = A_2\ sin\ (\lambda * L) \end{aligned}$$

The value of $sin(\lambda L) = 0$ if $\lambda L = m\pi \implies \lambda = \frac{m\pi}{L}$ where m=1,2,3 .... so, the solution is:

$$Y_m(y) = A_m sin(\frac{m\pi y}{L}) \quad m = 1,2,3,..... \tag{2.11}$$

We will compensation the condition (2.5) into the EQ (2.9)

$$\begin{aligned} u(0,y,t) = 0 \implies X(0)Y(y)T(t) = 0 \implies X(0) = 0 \\ X(0) = B_1\ cos\ (\beta * 0) + A_1\ sin\ (\beta * 0) \\ 0 = B_1 \end{aligned}$$

$$\begin{aligned} u(L,y,t) = 0 \implies X(L)Y(y)T(t) = 0 \implies X(L) = 0, B_1 = 0 \\ X(L) = 0 * \; cos\ (\beta * L) + A_1\ sin\ (\beta * L) \\ 0 = A_1\ sin\ (\beta * L) \end{aligned}$$

The value of $sin(\beta L) = 0$ if $\beta L = n\pi \implies \beta = \frac{n\pi}{L}$ where n=1,2,3 .... so, the solution is:

$$X_n(x) = A_n sin(\frac{n\pi x}{L}) \qquad ,n = 1,2,3..... \tag{2.12}$$

In EQ(2.8) we will using the assumption $\mu = D(\beta^2 + \lambda^2)$ and the values of β and λ

$$\mu = D((\frac{n\pi}{L})^2 + (\frac{m\pi}{L})^2) \tag{2.13}$$

$$T(t) = e^{-(D((\frac{n\pi}{L})^2 + (\frac{m\pi}{L})^2) + \alpha)t} \tag{2.14}$$

Eventually, we want to substitute all solutions(2.12, 2.11, 2.14) in (2.6) to get to the solution which become

$$u(x,y,t) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} e^{[-D((\frac{n\pi}{L})^2 + (\frac{m\pi}{L})^2) - \alpha]t} (A_{n,m}\ sin\ (\frac{n\pi x}{L})\ sin\ (\frac{m\pi y}{L}))$$

When we add the initial condition to determine $A_{n,m}$, let take the condition u(x,y,0)=$sin(\frac{\pi x}{L})\ sin(\frac{\pi y}{L})$

$$u(x,y,0) = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} e^{[-D((\frac{n\pi}{L})^2+(\frac{m\pi}{L})^2)-\alpha]*0}(A_{n,m}\ sin\ (\frac{n\pi x}{L})\ sin\ (\frac{m\pi y}{L}))$$

$$sin(\frac{\pi x}{L})sin(\frac{\pi y}{L}) = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} A_{n,m}\ sin\ (\frac{n\pi x}{L})\ sin\ (\frac{m\pi y}{L})$$

This Leads to all coefficients $A_{n,m} = 0$ except $A_{1,1} = 1$

$$u(x,y,t) = e^{[-D((\frac{1*\pi}{L})^2+(\frac{1*\pi}{L})^2)-\alpha]*t}(A_{1,1}\ sin\ (\frac{1*\pi x}{L})\ sin\ (\frac{1*\pi y}{L}))$$

So, the final solution is

$$u(x,y,t) = e^{[-2D(\frac{\pi}{L})^2-\alpha]t}(\ sin\ (\frac{\pi x}{L})\ sin\ (\frac{\pi y}{L})) \tag{2.15}$$

Chapter Three

Numerical Analysis

In many applications such as mathematics, engineering, physics and computer science we are having trouble finding the exact solution or it is difficult or impossible to find it.

Consequently, there was a need to develop and analyze algorithms to find approximate solution for exact solution, which raize the importance of Numerical Analysis[16]. The main concepts we have in numerical analysis are direct and iterative methods, where direct computes the solution to a problem in a finite number of steps but iterative uses an initial guess successive approximations that converge to the exact solution.

Another concept is numerical stability, during the calculation to find the approximation the error does not grow to be much larger, this is related with the problem is well-conditioned which is meaning if small changes in the input lead to small changes in the output with good accuracy and efficiently. In contrast, instability means small errors in input leading to incorrect results .

In addition, to solve differential equations numerically, in ODEs we can use Runge-Kutta methods, Euler method and Multistep methods. But in PDEs we use the finite element method (FEM), finite difference method (FDM) and finite volume method (FVM), and there are many methods.

It is important to note that the equation (2.2) is PDEs so to find a numerical solution we can use any of the methods mentioned above, but in this research we focus on FDM and FVM and compare their results with the analytic solution.

3.1 Finite Difference Method

This method is called finite difference approximation, it is mainly based on replacing each of the derivatives in the differential equation with finite difference by creating a grid over the domain and then using values at discrete points to approximate the solution.

A three main classification of FDM: approximation, time integration and order of accuracy. The case of approximation have three types : the forward difference method is first order accurate and easy to implement but less precise, the backward difference method is first order accurate and stable, and the central difference method is second order accurate such that the average of forward and backward and more precise than forward and backward.

The case of time integration is divided into three types : the Explicit scheme is stability depends on time step size, the Implicit scheme is computationally expensive but unconditionally stable, and the Crank-Nicolson scheme is combination of implicit and explicit method and second order accurate in both space and time and is common for parabolic PDE.

Finally, The case of order of accuracy start from the first order scheme include forward and backward with less accurate and computationally cheaper to the second order scheme include central difference with balance accuracy and computational effort, and more and more to the higher order scheme by using Taylor series expansion, we can derive the backward, forward, and central difference formulas, along with many other finite difference formulas for approximating derivatives.

The advantages of Taylor series are used for finite difference formulas for approximating higher-order derivatives and it provides an estimate for the truncation error in the approximation [17].

3.1.1 Finite Difference Formulas of First Derivative

We have several formulas for approximating the first derivative at point x_i which based on the values of the points near x_i. First in one dimension, we assume that we have an interval [a,b], divide the interval into (n+1) by selecting an integer $n > 0$, equal sub-intervals where h=(b-a)/n+1 and the endpoints are the grid points $x_i = a + ih$, for i = 0,1,..., n+1.

Two-point forward difference formula for the first derivative : from Taylor series, we can approximate the value of a function at the point x_{i+1} from the value of the function and its derivatives at point x_i.

$$u(x_{i+1}) = u(x_i) + hu'(x_i) + \frac{1}{2!}h^2u''(x_i) + \frac{1}{3!}h^3u'''(x_i) + \frac{1}{4!}h^4u^{(4)}(x_i) + \dots \tag{3.1}$$

Where h = $x_{i+1} - x_i$, by using two term from Eq (3.1) it's can be rewritten as:

$$u(x_{i+1}) = u(x_i) + u'(x_i)h + O(h^2)$$

Solving for $u'(x_i)$ yields:

$$u'(x_i) = \frac{u(x_{i+1}) - u(x_i)}{h} + O(h) \tag{3.2}$$

If the second term on the right-hand side of Eq (3.2) is ignored, the approximate value of the derivative $u'(x_i)$ can be calculated[6].

Two-point backward difference formula for first derivative : from Taylor series, we can approximate the value of a function at the point x_{i-1} from the value of the function and its derivatives at point x_i.

$$u(x_{i-1}) = u(x_i) - hu'(x_i) + \frac{1}{2!}h^2u''(x_i) - \frac{1}{3!}h^3u'''(x_i) + \frac{1}{4!}h^4u^{(4)}(x_i) - \dots \tag{3.3}$$

Where h = $x_i - x_{i-1}$, by using two term from Eq (3.3) it's can be rewritten as:

$$u(x_{i-1}) = u(x_i) - u'(x_i)h + O(h^2)$$

Solving for $u'(x_i)$ yields:

$$u'(x_i) = \frac{u(x_i) - u(x_{i-1})}{h} + O(h) \tag{3.4}$$

If the second term on the right-hand side of Eq (3.4) is ignored, the approximation is called backward difference approximation.

Two-point central difference formula for first derivative : can be obtained through by using three terms in the Taylor series expansion, subtracting the Eq (3.3) from Eq (3.1) gives:

$$u(x_{i+1}) - u(x_{i-1}) = 2hu'(x_i) + \frac{2}{3!}(h)^3u'''(x_i) + \dots$$

Dividing by 2h

$$\frac{u(x_{i+1})-u(x_{i-1})}{2h} = u'(x_i)+\frac{1}{3!}h^2u'''(x_i)+\dots$$

$$u(x_i)' = \frac{u(x_{i+1})-u(x_{i-1})}{2h}+O(h^2)$$

If h is sufficiently small , we can neglecting the O term which introduces a truncation error, and it is of order of h^2. Thus, the Central Difference Approximation is given by

$$u(x_i)' \approx \frac{u(x_{i+1})-u(x_{i-1})}{2h} \tag{3.5}$$

So a comparison of Eqs (3.2) and (3.4) shows that in the forward and backward difference approximation the truncation error is of the order of h, while the Eq (3.5) is the central difference approximation the truncation error is of the order of h^2, This indicates that gives a more accurate approximation of the derivative. So the FDM of first derivative have three form :

$$u'(x_i) \approx \begin{cases} \frac{u(x_{i+1})-u(x_i)}{h} & \text{Forward difference} \\ \frac{u(x_i)-u(x_{i-1})}{h} & \text{Backward difference} \\ \frac{u(x_{i+1})-u(x_{i-1})}{2h} & \text{Central difference} \end{cases}$$

Most problems in science or engineering include a functions of several independent variables since reallife applications are either two or three-dimensional it's more than one dimensional, and in addition may be a function of time. For example, our equation (2.2), the concentration in an object is a function of time with two coordinates used to describe the domain u(x,y,t).

We can generalize the method of finite difference to include more than one independent variable. In two space dimensions, we consider a function of two independent variables u(x,y) by discretizations of the domain we put $y_j = jk$ and $x_i = ih$ and discrete grid with grid points and we consider the spacing between the points in each direction is constant such that $h = x_{i+1} - x_i$, $k = y_{i+1} - y_i$, To clarify further: see figure [3.1] which explain the grid and significantly the coordinate of point (x,y) and the point around it, while the figure [3.2] demonstrate the discretizations of the grid by i and j.

- $u(x,y) = u(ih, jk) = u_{i,j}$

- $u(x+h,y) = u(ih+h,y) = u((i+1)h,y) = u_{i+1,j}$
- $u(x-h,y) = u(ih-h,j) = u((i-1)h,j) = u_{i-1,j}$
- $u(x,y-k) = u(i,jk-k) = u(i,(j-1)k) = u_{i,j-1}$
- $u(x,y+k) = u(i,jk+k) = u(i,(j+1)k) = u_{i,j+1}$
- $u(x+2h,y+k) = u(ih+2h,jk+k) = u(h(i+2),(j+1)k) = u_{i+2,j+1}$

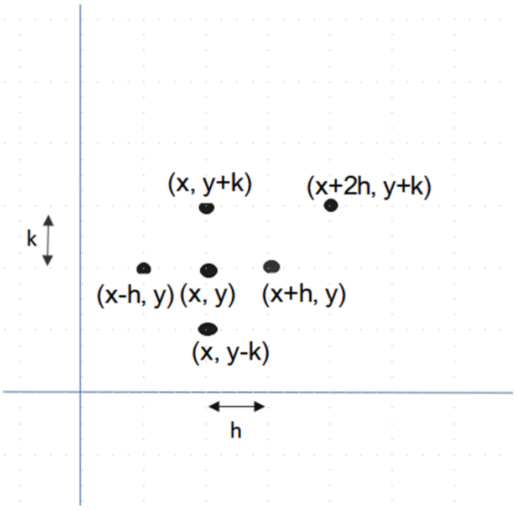


Figure 3.1: *Discretizations of the domain by x and y*

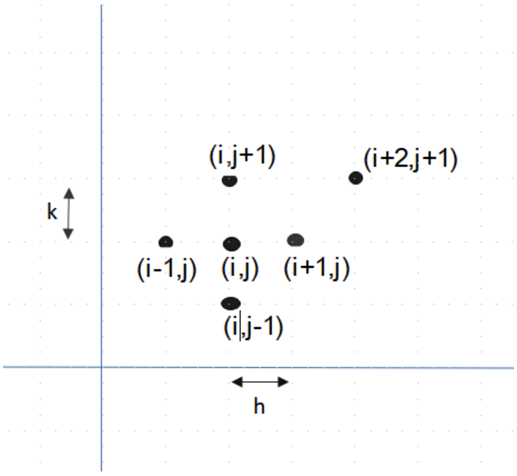


Figure 3.2: *Discretizations of the domain by i and j*

The method is mainly based on applied for one of the variables, while the other variables are kept constant, clarifying the approximation for the partial derivative at point (x_i, y_i) on two space dimensions with the two-point forward, the two-point backward and central difference formulas are

- $u_x = \frac{\partial u}{\partial x}$ where

$$u_x = \frac{\partial u}{\partial x} = \begin{cases} \frac{u_{i+1,j} - u_{i,j}}{h} & \textbf{forward difference} \\ \frac{u_{i,j} - u_{i-1,j}}{h} & \textbf{Backward difference} \\ \frac{u_{i+1,j} - u_{i-1,j}}{2h} & \textbf{Central difference} \end{cases}$$

- $u_y = \frac{\partial u}{\partial y}$ where

$$u_y = \frac{\partial u}{\partial y} = \begin{cases} \frac{u_{i,j+1} - u_{i,j}}{k} & \textbf{forward difference} \\ \frac{u_{i,j} - u_{i,j-1}}{k} & \textbf{Backward difference} \\ \frac{u_{i,j+1} - u_{i,j-1}}{2k} & \textbf{Central difference} \end{cases}$$

3.1.2 Finite Difference Formulas for the Second Derivative

The Combination of the forward differences and the backward differences is presented for approximating the second derivative at a point x_i, **Three-point central difference formula for the second derivative** in one dimension by adding Eq (3.1) and Eq (3.3) gives:

$$u(x_{i+1}) + u(x_i - 1) = 2u(x_i) + h^2 u''(x_i) + \frac{h^4}{4!} u^{(4)}(x_i) + \dots$$

An estimate for the second derivative yields:

$$u''(x_i) = \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2} + O(h^2) \tag{3.6}$$

While neglecting the O term which is introduces a truncation error of the order of h^2, the Eq (3.6) is the three-point central difference approximation. To generalize in two dimensions the formula become:

- $u_{xx} = \frac{\partial^2 u}{\partial x^2}$ where
$$u_{xx} = \frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2}$$
- $u_{yy} = \frac{\partial^2 u}{\partial y^2}$ where
$$u_{yy} = \frac{\partial^2 u}{\partial y^2} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2}$$

Now we want to related variations in space to variations in time by finite difference methods for time-dependent PDE, as mentioned previously, the time integration is divided into three types and here we want to use the forward difference scheme, which is an explicit FDM and depends on estimate time derivatives.

The method is represented by calculated the time step n and n+1, we will use the time step Δt where $u^n = u(t_n)$ the value at time step n, $u^{n+1} = u(t_n + \Delta t)$ the value at the next time step and Δt is the size of the time step , let $u^n_{i,j} \approx u(x_i, y_j, t_n)$ represent the numerical approximation at the point of the grid (x_i, y_j, t_n) and $u^{n+1}_{i,j} \approx u(x_i, y_j, t_{n+1})$ represent the numerical approximation at the point of the grid next time. Applying the forward difference method for time and the central difference method for space, this scheme is called the FTCS (Forward Time Central Space), the Eq (2.2) becomes:

$$\frac{u_{i,j}^{n+1}-u_{i,j}^{n}}{\Delta t}=D(\nabla^2 u_{i,j}^{n})-\alpha(u_{i,j}^{n}) \tag{3.7}$$

Where

$$\nabla^2 u_{i,j}^{n}=\frac{u_{i+1,j}^{n}-2u_{i,j}^{n}+u_{i-1,j}^{n}}{h^2}+\frac{u_{i,j+1}^{n}-2u_{i,j}^{n}+u_{i,j-1}^{n}}{k^2} \tag{3.8}$$

If we multiplication all limits of the equation (3.7) by Δt, implies

$$u_{i,j}^{n+1}-u_{i,j}^{n}=\Delta t*(D(\nabla^2 u_{i,j}^{n})-\alpha(u_{i,j}^{n}))$$

Then arrange the equation through time

$$\begin{aligned}u_{i,j}^{n+1}-u_{i,j}^{n}&=\Delta t(D(\nabla^2 u_{i,j}^{n})-\alpha(u_{i,j}^{n}))\\ u_{i,j}^{n+1}&=u_{i,j}^{n}+\Delta t(D(\nabla^2 u_{i,j}^{n})-\alpha(\ u_{i,j}^{n}))\end{aligned}$$

Then the following become:

$$u_{i,j}^{n+1}=u_{i,j}^{n}+\Delta t(D(\frac{u_{i+1,j}^{n}-2u_{i,j}^{n}+u_{i-1,j}^{n}}{h^2}+\frac{u_{i,j+1}^{n}-2u_{i,j}^{n}+u_{i,j-1}^{n}}{k^2})-\alpha(\ u_{i,j}^{n})) \tag{3.9}$$

3.2 Finite Volume Method

Numerical methods like FDM and FVM play an important role in solution the PDE that describes the engineering and physical problem. the FVM is common method because it is provides ability to handle irregular and complex computational domains [33], this is an advantage over (FDM), and it is also a depends on integration of the equation transport into finite volume control with applying the law of conservation of quantity, while the FDM dependent of differential governing equations by taylor expansions using approximation derivatives, also the FDM find the derivatives in one point exactly, whereas FVM show small volume (like cell) and formulate the change of rate of quantity inside the small volume and decide if there the change is enters or exits from the volume.

The beginning of the emergence of this method began in 1971 and was published in 1980 in a book (Numerical Heat Transfer And Fluid Flow)[25]. The method relied on conversion of mathematical differential equations to linear algebraic equations in order to solve it numerically.

The advantages of FVM beginning from preserve the physical quantities, for example mass, energy and concentration, and another advantage of the FVM technique is it more flexible with complex domain until irregular shape, because of that its widely used in engineering and chemical diffusion systems. We will now explain the steps of this method and in addition to applying it directly to our equation (2.2).

Step 1 Generation of the grid

We can generate of the grid by division of the domain into finite control volumes or small cells, and as we see in figure (3.3) we named the nodal point W, P, and E between A and B. A general nodal point is identified by P, it is bordered in the west side face the control volume boundaries w and to the east side it is bordered by the control volume boundaries e, the distances between the nodal point W and P, and between P and E are equal Δx, similarly to the distances between face w and e.

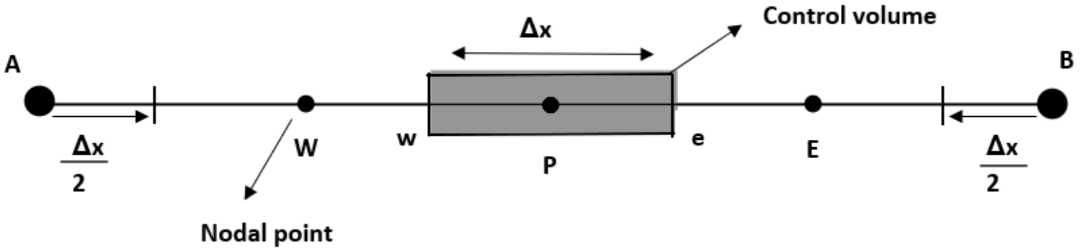


Figure 3.3: *One Dimensional Finite Volume Mesh*

In addition, the general grid node P we extended to a two-dimensional grid by adding neighbors north N and south S which each square represents a cell as we see in figure (3.4) we use the square shape for discretization of space and place the nodal in the center of each cell.

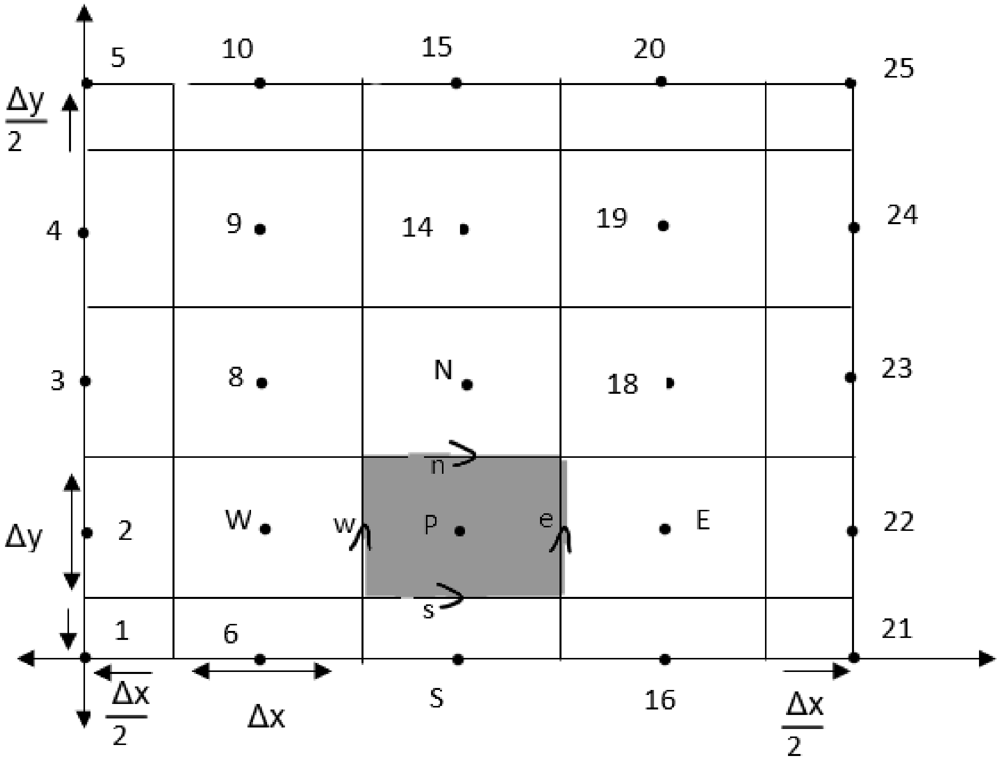


Figure 3.4: *Two dimensional finite volume mesh*

We also point out that we depend on applying the law of conservation of quantity (here concentration) the rate of change of quantity inside the cell is equal to the amount of material inside subtracted from the amount of material outside plus internal interaction [33].

Step 2 Discretizations The Equation

The idea behind this method is integrate the governing equations of fluid flow "here we consider the EQ(2.2) is a governing equations "over each control volume of the domain to yield a discrete equation at its nodal point P. For take integral over the control volume this gives:

$$\frac{\partial u}{\partial t}\,dV = D\nabla^2 u - \alpha u$$

$$\int_{Vp} \frac{\partial u}{\partial t}\,dV = \int_{Vp} D\nabla^2 u\,dV - \int_{Vp} \alpha u\,dV$$

$$\int_{Vp} \frac{\partial u}{\partial t}\, dV \approx \frac{u_p^{n+1} - u_p^n}{\Delta t} V_p$$

Where $V_p = \Delta x.\Delta y$ is the area (or volume in 2D) of the cell .

$$\int_{Vp} -\alpha u\, dV \approx -\alpha u_p^n \Delta x \Delta y$$

We used Gauss's divergence theorem to convert the volume integral of divergence into a surface integral[34]. Which is the physical meaning that is the flux of quantity out of small surface element, positive if the flux outside and negative if the flux inside. lets solve the diffusion term and put the expressions for the flux through control volume faces by using the approximations.

$$\begin{aligned}\int_{V_p} D\nabla^2 u\, dV &= \int_{V_p} D\nabla.(\nabla u)\, dV \\ &= \oint_{S_p} D(\nabla u).n\, dS\end{aligned}$$

We have four faces boundaries of the nodal P the west, east, south, north faces. To approximation the flux across the west face:

$$Flux_{\ w} \ = D.A_w.(\frac{\partial u}{\partial x})_w \approx D.\Delta y.\frac{u_W^n - u_P^n}{\Delta x}$$

$$Flux_{\ w} \ \approx D\frac{\Delta y}{\Delta x}(u_W^n - u_P^n)$$

Similarly to other faces:

$$\text{Flux across east face } = D\Delta y(\frac{\partial u}{\partial x})_e \approx D\frac{\Delta y}{\Delta x}(u_E^n - u_P^n)$$

$$\text{Flux across south face } = D\Delta x(\frac{\partial u}{\partial y})_s \approx D\frac{\Delta x}{\Delta y}(u_S^n - u_P^n)$$

$$\text{Flux across north face} = D\Delta x(\frac{\partial u}{\partial y})_n \approx D\frac{\Delta x}{\Delta y}(u_N^n - u_P^n)$$

$$\begin{aligned}\sum_{faces}\text{Fluxes} &= D\Delta y\frac{u_W^n - u_P^n}{\Delta x} + D\Delta y\frac{u_E^n - u_P^n}{\Delta x} + D\Delta x\frac{u_S^n - u_P^n}{\Delta y} + D\Delta x\frac{u_N^n - u_P^n}{\Delta y} \\ &= D\frac{\Delta y}{\Delta x}\left[u_W^n - u_P^n + u_E^n - u_P^n\right] + D\frac{\Delta x}{\Delta y}\left[u_S^n - u_P^n + u_N^n - u_P^n\right] \\ &= D\frac{\Delta y}{\Delta x}\left[u_W^n - 2u_P^n + u_E^n\right] + D\frac{\Delta x}{\Delta y}\left[u_S^n - 2u_P^n + u_N^n\right]\end{aligned}$$

After rearrangement of the equation, we obtain the following:

$$\frac{u_p^{n+1} - u_p^n}{\Delta t}V_p = \sum_{faces}\text{Fluxes} - \alpha u_p^n V_p$$

$$\frac{u_p^{n+1} - u_p^n}{\Delta t}\Delta x\Delta y = \sum_{faces}\text{Fluxes} - \alpha u_p^n \Delta x\Delta y$$

$$\frac{u_p^{n+1} - u_p^n}{\Delta t} = \frac{1}{\Delta x\Delta y}\left[\sum_{faces}\text{Fluxes}\right] - \alpha u_p^n$$

$$u_p^{n+1} - u_p^n = \Delta t\left(\frac{1}{\Delta x\Delta y}\left[\sum_{faces}\text{Fluxes}\right] - \alpha u_p^n\right)$$

$$u_p^{n+1} = u_p^n + \Delta t\left(\frac{1}{\Delta x\Delta y}\left[\sum_{faces}\text{Fluxes}\right] - \alpha u_p^n\right)$$

$$u_p^{n+1} = u_p^n + \Delta t\left(\frac{1}{\Delta x\Delta y}\left[D\frac{\Delta y}{\Delta x}\left[u_W^n - 2u_P^n + u_E^n\right] + D\frac{\Delta x}{\Delta y}\left[u_S^n - 2u_P^n + u_N^n\right]\right] - \alpha u_p^n\right)$$

$$u_p^{n+1} = u_p^n + \frac{\Delta t}{\Delta x\Delta y}\left[D\frac{\Delta y}{\Delta x}\left[u_W^n - 2u_P^n + u_E^n\right] + D\frac{\Delta x}{\Delta y}\left[u_S^n - 2u_P^n + u_N^n\right]\right] - \Delta t\alpha u_p^n$$

In the following, we consider the general form:

$$u_p^{n+1} = u_p^n + D\Delta t\left[\frac{u_W^n - 2u_P^n + u_E^n}{(\Delta x)^2} + \frac{u_S^n - 2u_P^n + u_N^n}{(\Delta y)^2}\right] - \Delta t\alpha u_p^n \tag{3.10}$$

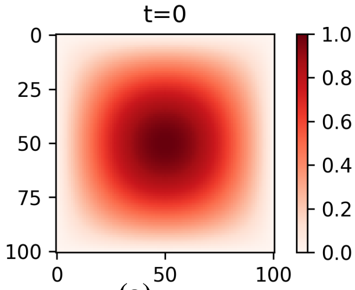
Chapter Four

Numerical Implementation and Comparison

This Chapter shows the solution for the Reaction-Diffusion equation includes two term exact and numerical results. We used two numerical methods FDM and FVM and comparison the results in order to decide if the numerical results closely matches with exact results, by calculate the absolute error, max error and L2 Norm.

4.1 Analytical and Numerical results

We implemented a simulation in Python that used Jupyter Notebook within Anaconda navigator environment to solve the equations(2.15, 3.9, 3.10), we had established values for the parameter: length of the square domain is $L = 1.0$, diffusion coefficient $D = 0.01$, linear decay rate is $\alpha = 0.1$, number of grid points in x-direction and y-direction is Nx=Ny=120 and $dt = (total\_time - 0)/(Nt - 1)$, where Nt=1000. And then we built and tested the code and got the following results at different time steps at total time t=0, 0.5 , 1 and 2.



(a)

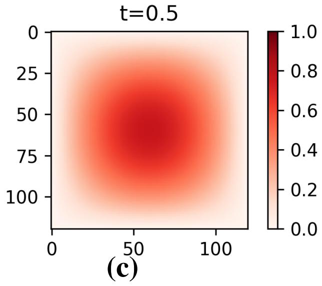
Exact solution

Figure 4.1: *The Exact results at total time t=0*

The first case at Figure (4.1): Observe that the concentration of material u before processes reacts and diffuses is higher in the middle of the mesh and lower in the edge of the mesh, because material u is injection into the middle channel.

(a) *Exact solution*

(b) *FDM solution*

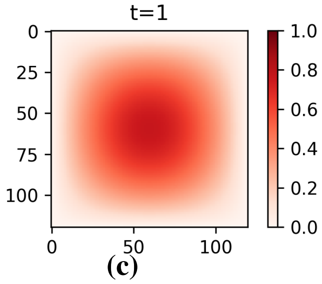


(c) *FVM solution*

Figure 4.2: *The Exact, FDM, and FVM results at total time t=0.5*

(a) *Exact solution*

(b) *FDM solution*



(c) *FVM solution*

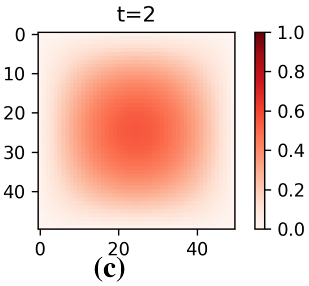
Figure 4.3: *The Exact, FDM, and FVM results at total time t=1*

Over time, The second and third case at Figure (4.2, 4.3): the concentration of material u is affected by reacts and diffuses in both space and time. As a result, the concentration is changing over time, decreasing in the middle of the grid and it is diffusion and distribute over space because of movement of molecules from high to low concentration area and this explain gradual change of concentration from middle to near boundaries.

While the reaction contributes to decay of the concentration over the domain and this is causes of sign of negative α. The numerical result from FD and FV reflecting good correspondence with analytical result, and observed that solution of FD and FV is free of oscillations across the domain.

(a) *Exact solution*

(b) *FDM solution*



(c) *FVM solution*

Figure 4.4: *The Exact, FDM, and FVM results at total time t=2*

The last case (total time t=2): figure (4.4) shows reduction of the peaks in the middle and distribution over the grid. In addition, the amount of concentration material u reduces the gradient comparison with the first time. The exact, FD and FV solution demonstrates a smooth solution and minor difference in the meddle of the computational domain. Now the following section discusses the error.

4.2 Absolute Error Between Exact Solution & Finite Difference Solution

The absolute error measures the absolute difference between numerical approximation and exact result, and its evaluated the accuracy of the numerical approximation , from here many parameters play a crucial role in the results, the most important parameter is the time step, as we say previously, we used the forward finite difference to approximation the derivative of time, which is conditionally stable. We used $N_t = 1000$ and dt=(total time-0)/(N_t-1). The figure below shows the absolute error of FDM at $N_x = N_y = 120$,

Figure 4.5: *Error at total time t= 0.5 and 1*

The Figure (4.5) illustrates the error between exact and finite difference solution at many time we using the Absolute Error = $|u_{\text{exact}} - u_{\text{approximation}}|$. As times change, at t=0.5 and t=1 observed the high value of the error in the middle of the computational domain and the sloping significant difference at the boundary. The figure also indicates that the value of error is very small which clarifies and explains a reason for strong agreement in the figure (4.1, 4.2, 4.3).

The parameters spatial discretizations $N_x \times N_y$ and time discretizations N_t influence the accuracy, convergence, stability and computational cost of the method. In the figures below show the calculated absolute error while varying the parameter Nt and fixing the value of $N_x \times N_y = 120 \times 120$, and fixed total time t =1.

Figure 4.6: *FD solution and Absolute error at $N_t = 500$ and total time t=1*

The size of the time steps $N_t = 500$ in figure (4.6) illustrates the oscillations and instability results, the CPU time for the speed measurement of the FDM simulation, total= 62.5 ms at $N_t = 500$.

Figure 4.7: *FD solution and Absolute error at $N_t = 1000$ and total time t=1*

The time step sizes $N_t = 1000$ in figure (4.7) illustrate the stability and convergence results, the CPU time for the speed measurement of the simulation of FDM, total= 78.1 ms at $N_t = 1000$, the CPU time increased as the time step sizes increased. The FD solution is close correspondence to the exact solution because the value of absolute error is very small.

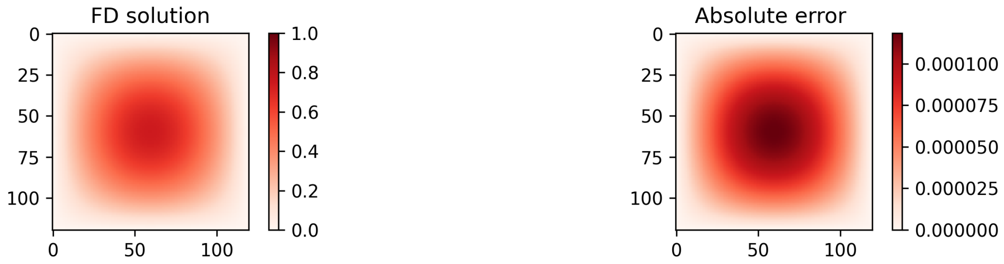


Figure 4.8: *FD solution and Absolute error at $N_t = 2000$ and total time t=1*

The time steps sizes $N_t = 2000$ in figure (4.8) illustrate the stability and convergence results, the CPU time for the speed measurement of the FDM simulation, total= 188 ms at $N_t = 2000$. The absolute error at $N_t = 2000$ is less than at $N_t = 1000$, which gives a more accurate solution but increases CPU time.

Figure (4.6, 4.7 , 4.8) demonstrates the effect of the time step sizes on the stability of the method. The large time step sizes of FDM leads to a stability solution and higher accuracy, while smaller time step sizes lead to oscillatory solutions. Although increasing of time step sizes improve accuracy, the computational time is affected by increasing.

4.3 Absolute Error Between Exact Solution & Finite Volume Solution

The precision and efficiency of FVM appear by evaluating the absolute difference between the FV approximation and the exact solution, we used $N_t = 1000$, $N_x = N_y = 120$ and dt=(total time-0)/(Nt-1). The figures below show the absolute error of FVM at total time t=0.5 and t=1.

Figure 4.9: *Absolute error of FVM*

Figures (4.9) demonstrate the error between exact and finite volume solutions when we used the Absolute Error = |u_exact - u_approximation|. At t=0.5 and t=1 we observed the high value of the error in the middle of the computational domain and the sloping significant difference at the boundary of the grid. The figure also indicates that the value of error is small which clarifies and explains the reason for the strong agreement in the figures (4.1, 4.2, 4.3).

The figures below explain the effect of N_t on accuracy, stability, convergence and computational cost of this method, fixing the values of space discretizations $N_x \times N_y = 120 \times 120$ and the total time t = 1.

Figure 4.10: *FV solution and Absolute error at* $N_t = 500$ *and total time t=1*

The time step sizes $N_t = 500$ in figure (4.10) illustrate the instability and oscillatory behavior results, the CPU time for the speed measurement of the simulation of FVM, total= 46.9 ms.

Figure 4.11: *FV solution and Absolute error at* $N_t = 1000$ *and total time t=1*

The time step sizes $N_t = 1000$ in figure (4.11) illustrate the stability and convergence behavior results, the CPU time for the speed measurement of the simulation of FVM, total= 93.8 ms. The increase in N_t gives a higher accuracy result, but requires more time to speed measurement of the simulation.

Figure 4.12: *FV solution and Absolute error at* $N_t = 2000$ *and total time t=1*

The time step sizes $N_t = 2000$ in figure (4.12) illustrate the stability and convergence behavior results, the CPU time for the speed measurement of the simulation of FVM, total= 250 ms, increasing N_t provide more accurate results but require more computational time.

The figures explain the effect of time step sizes on the stability and convergence of the method, the large time step sizes of FVM give to a higher accuracy and maintain stability, while smaller time step sizes lead to unbounded oscillatory solutions. And also increasing of time step sizes improve accuracy but increasing of computational time.

The results also indicate that the absolute errors of FDM and FVM pivoted or centered in the middle of the domain and decreased on the boundary of the domain.

The CPU times in $N_t = 1000$ and 2000 for FDM is less than FVM. In both cases, the CPU for the two methods is very small and nearly identical with a slight advantage for FDM. In the next section, we discuss the type of error specifically L∞ & L2 Norm for FD and FV solution.

4.4 L∞ & L2 Norm

The main categories of error: Pointwise Error in one point and Global Error in all field, from here appear the $L\infty$ & L2 Norm. The L∞ norm or Max Error measures the worst error in the domain which is local and indicates stability, the formula is $L_2 = \sqrt{\frac{1}{N}\sum_{i=1}^{N} e_{i,j}^2}$ whereas L2 Norm or Root Mean Square Error (RMSE) refers to average error in the domain and is sensitive for every point in the domain, it denotes general accuracy and rarely to be large and the formula is $L_\infty = \max|e_{i,j}|$ where $e_{i,j} = u_{i,j}^{\text{numerical}} - u_{i,j}^{\text{analytical}}$.

The table (4.1) demonstrates the relationship between the mesh discretizations and $L\infty$ & $L2$ Norm for FDM and FVM, the time step dt is fixed for all simulations to the mesh discretization error and is dependent on the a condition of dt= (total time -0)/ Nt-1 where Nt=2000 and take total time= 1 for all cases.

Table 4.1: *Quantitative Error Comparison*

Number of case	$N_x \times N_y$	Method	Max Error(L-inf)	L2 Norm(RMSE)
1	20×20	FDM	3.152460e-04	1.507700e-04
		FVM	2.831274e-04	1.424405e-04
2	50×50	FDM	3.375689e-05	1.655788e-05
		FVM	3.177155e-05	1.590147e-05
3	100×100	FDM	4.126707e-06	2.043235e-06
		FVM	4.371522e-06	2.186301e-06
4	150×150	FDM	1.099896e-05	5.463422e-06
		FVM	1.107115e-05	5.536182e-06
5	200×200	FDM	1.338611e-05	6.660007e-06
		FVM	1.341650e-05	6.708663e-06

In cases 1 and 2, denote the difference between L∞ and L2 for FDM and FVM at time t=1. The Max Error of FDM is larger than that of FVM, which leads to that FVM stable performance more than FDM under a low number of grid points. Although the L2 norm for FVM is smaller than for FDM, both methods yield acceptable results, but FVM is more overall accurate, this is due to the conservation of quantity.

When varying the parameter values Nx=Ny to equal 100 in case 3, the error indicates that the value of the max error for FDM is less than before in case 2, and the same error for FVM decreases compared to the value in case 2. Similarly, the comparison of L2 Norm with values in case 2, FDM and FVM decreases, this demonstrates that FDM and FVM improve as the mesh discretizations refinement.The value of L2 Norm and max error to the FDM is less than FVM with small difference, which means that FVM and FDM are in good agreement with slight difference.

The next case shows that the error at Nx=Ny= 150, the max error and L2 norm of FDM is less than the error values of FVM, indicating that FDM improved and gets good agreement better than FVM as the mesh discretizations increases.

When we increase the grid discretizations to Nx=Ny=200, the results show a significant reduction in both L2 norm and the max error in the FVM and FDM values, the FDM outperformed the FVM by a very slight margin. Consequently, FDM gives more efficient value and reliable results than FVM in this case.

The results of table (4.1) indicate that in case 3, the discretizations of the grid to Nx=Ny= 100 is the most favorable case for two methods compared to the other cases with a slight difference between FDM and FVM.

The small size taken of grid discretizations gives a small error to FVM compared to FDM because of conservative formulation. However, as the number of grid points is large, the grid becomes finer, and FDM gives more accurate compared to FVM. In real application, FVM is more widely used in real life problems because of the ability to coarse grids and complex problems, whereas FDM preferred under certain conditions regular geometry and structured grid to give higher accuracy.

In figure (4.13) explain the absolute error for FDM and FVM at $Nx \times Ny = 50$ and total

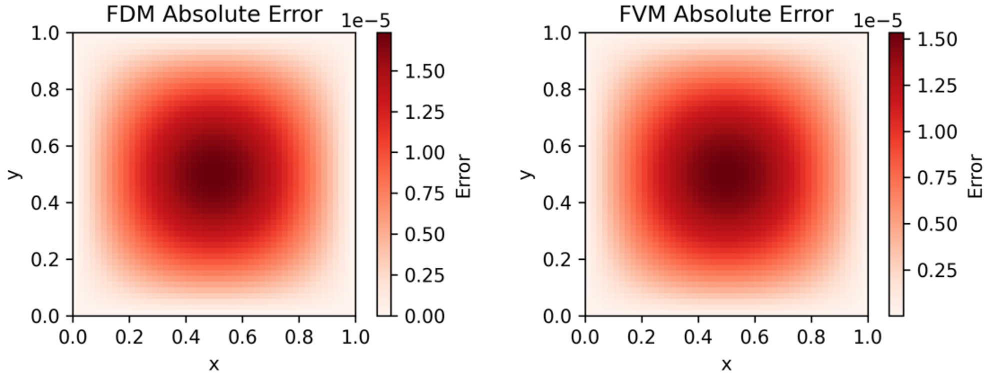


Figure 4.13: *Absolute Error for FDM and FVM*

time= 1, the absolute error is the difference between the approximate and exact solution at each grid point. The FVM absolute error indicates a higher value in the middle, while a lower value in the near boundaries similarly absolute error for FDM. The value of error is very small close to zero for two methods, the two methods show close and strong agreement so both methods are suitable for solving the governing equation (2.2).

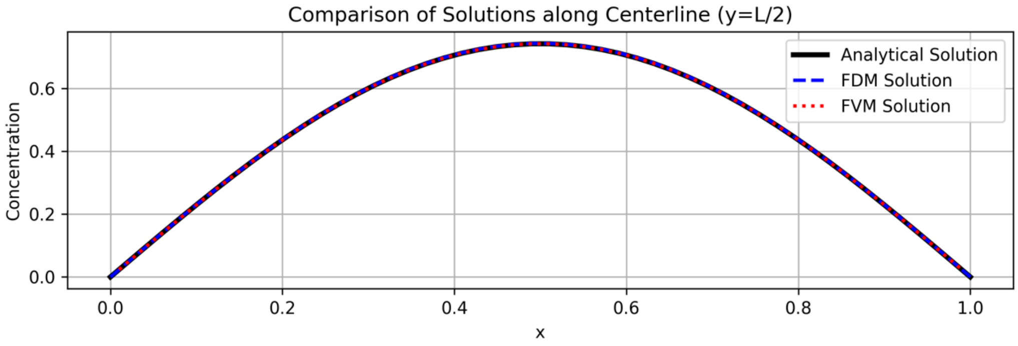


Figure 4.14: *Comparison of analytical, FDM and FVM solution along centerline*

In the figure (4.14) it take a cross-section includes analytical FDM and FVM solution and there is good correspondence and free of oscillations, the figure clearly supports the previous obtained result.

Chapter Five

Conclusion and Future prospects

5.1 Conclusion

This research focuses on studying the reaction-diffusion equation in two dimensions (2D) because of the important application in microfluidics filed, clarification behavior of material inside microfluidics channels. The analytical solution is usually difficult or impossible to find. So we used the numerical method finite difference method (FDM) and finite volume method (FVM). We performed a comparison between the numerical methods and exact solution, many parameters play a crucial role in the results, discretizations of space and time and the CPU time of the simulation, these parameters affected to error: Absolute Error, L2 Norm and Max Error. The results indicate that the FVM and FDM are stable, accuracy, efficiency and lower CPU time and error, but effectiveness of the FVM appear in practical situations with coarse grids. Overall, FVM and FDM agree well and provide a lower error. For structured grids and uniform shapes, FDM gives higher accuracy, while in real applications, complex geometries and coarse grids, FVM gives lower error and is more effective.

5.2 Future prospects

We are looking forward to experiencing applying the finite element method (FEM), and more than that, we can apply machine learning to solve the equation. Also, study the steady-state behavior of the reaction-diffusion equation to understand the solution after a long time. We are also looking forward to building a software application that aims to help researchers who do not have a mathematical and programming background. The application makes it easier for them to access the results. The app idea is to solve numerically to the reaction and diffusion equation maybe we can also add advection with using any method the researcher determines. Because there is no direct application that enables me to write the equation and determine the numerical solution method. As we know, there are applications and tools similar to this idea, such as: MATLAB and Python, and there needed to good knowledge of programming codes and the Python language, while COMSOL is able to solve the equation, but it does not offer the freedom to choose between numerical method.

List of Abbreviations

Abbreviations	**Meaning**
1D	One Dimension
2D	Two Dimension
BC	Boundary Condition
D	Diffusion Coefficient
α	Reaction Coefficient
∇^2	Laplacian
PDE	Partial differential equation
ODE	Ordinary differential equation
FDM	Finite Diference Method
FVM	Finite Volume Method
FEM	Finite Element Method
FTCS	Forward time central space
RMSE	Root Mean Square Error
CIIF	Compact Implicit Integration Factor
CFDM	Compact Finite Difference Method
UPFD	Unconditionally Positive Finite Difference
CPU	Central Processing Unit

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كلية الدراسات العليا

تحليل عددي لمعادلة التفاعل والانتشار ثنائية الأبعاد: التقنيات والتطبيقات

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قدمت هذه الرسالة استكمالاً لمتطلبات الحصول على درجة الماجستير في الرياضيات،
من كلية الدراسات العليا، في جامعة النجاح الوطنية، نابلس– فلسطين.

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الملخص

تتركز هذه الدراسة على عمليات التفاعل و الانتشار بداخل قناة الموائع الدقيقة في بعدين. تتمركز المادة في البداية في وسط القناة و تتاثر بوسطة الانتشار و تفاعل اضمحلال من الدرجة الأولى. هذا العمل يهدف الى استكشاف الطرق العددية لحل أنظمة التفاعل والانتشار ثنائية الأبعاد. قمنا بتوظيف طريقة الفروق المحدودة(FDM) و طريقة الحجم المحدود(FVM) لحل المعادلات الحاكمة. تم تنفيذ عمليات المحاكاة بواسطة لغة البايثون من اجل مقارنة دقة الطرق فيما يتعلق بالحل التحليلي. النتائج تكشف ان FDM و FVM متفقتان بشكل جيد و متناسبتان مع الحل التحليلي بالإشارة ايضا الى ان FVM اكثر عملية من حيث الفعالية و تحافظ على أقل Max Error و L2 Norm في حالة الشبكات الخشنة، بينما فعالية FDM تظهر في حالة الشبكة ادق. تختتم الدراسة بان FVM افضل خيار في حالة محاكاة مشاكل التفاعل والانتشار عندما تكون الشبكة معقدة او الشبكة خشنة، بينما FDM تكون افضل في حالة الشبكة الدقيقة أو الهندسة المنتظمة.

الكلمات المفتاحية : طريقة الفروق المحدودة ، طريقة الحجم المحدود، معادلة التفاعل و الانتشار، الموائع الدقيقة، الشروط الحدية والابتدائية، معادلة تفاضلية جزئية.