PATTERN FORMATION PROCESS WITH GRAY-SCOTT REACTION-DIFFUSION MODEL

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CERTIFICATION

This is to certify that this research work was carried out by Adedeji, Victor Tobiloba with matric number MTS/16/0173 under the supervision of Dr. K.M. Owolabi in the Department of Mathematical Sciences in partial fulfillment of the requirement of the award of Bachelor of Technology (B. Tech) in Industrial Mathematics of the Federal University of Technology, Akure, Ondo State, Nigeria.

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DEDICATION

I dedicate this project to God Almighty my creator, my strong pillar, my source of inspiration, wisdom, knowledge and understanding.

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ABSTRACT

Since Turing's pioneering work, the emergence of patterns in both animate and inanimate systems has been an intriguing research topic. In this project, we study the Gray-Scott reaction-diffusion model in a 2D spatial domain to uncover the spatiotemporal behaviour of chemical species U and V . The focus is on identifying the conditions for Turing instability and characterizing the Turing space where spatial patterns can develop. To explore the complex spatiotemporal behaviour of the Gray-Scott model, we employ the finite-difference method for numerical simulations The simulations reveal that the patterns formed by the model, including spots and stripes, resemble real-world phenomena.

TABLE OF CONTENTS

List of Figures

Chapter 1
INTRODUCTION

1.1 Background Information

A number of natural phenomena adhere to consistent patterns. One of such observation is the natural phenomenon which occurs in phyllotaxis. Phyllotaxis refers to the arrangement of leaves around a stem. It is obvious that different species of plants look very distinct, it has been observed that the formation of petals and branches is in accordance with Fibonacci sequence, a sequence of numbers with each subsequent number resulting from the sum of the last 2 preceding values.
The sequence looks like this: 0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, ...
Alan Turing became fascinated by the spontaneous formation of the phenomena of phyllotaxis this drive him to use mathematical equations to model biological processes.
Alan Turing coined the term "morphogen" when he published [1] "The Chemical Basis of Morphogensis" in 1952.
He presented a mathematical model that seeks to explain the formation of self-regulated patterns during the development of plants and animals. The term morphogenesis (which simply means the formation of the body's shape) is an abstraction of a molecule capable of inducing tissue differentiation later on.
His reaction-diffusion model demonstrates how patterns can form a new pattern from simple molecules. The concept of "morphogen" isn't strange to any molecular biologist because they are familiar with it. In Turing's sense, morphogens are essential for body patterning throughout the animal kingdom. Turing considered an idealized embryo beginning with a uniform concentration of morphogens, which have translational symmetry which results in loss as specific tissues emerge.
At the core of pattern formation is symmetry-breaking. Turing conjectured that the asymmetric of organisms originated from biological molecules. He presented an argument that utilized a mathematical technique which he created: he developed a nonlinear system by discontinuously introducing diffusion to an otherwise linear system at a specific instant, the homogeneous system without diffusion is stable but with diffusion, it, therefore, becomes unstable and forms spatial patterns.

The influence of Alan Turing's paper is difficult to overemphasize. It was a pivotal moment in the evolution of mathematics, as the discipline transitioned from emphasizing analytical methods to embracing computational mathematical techniques. His paper entails the first computer simulations of pattern formation in the presence of stochastic fluctuations.

1.2 Gray-Scott Reaction-Diffusion Model

[2]The Gray-Scott Reaction-diffusion model is a mathematical model which calculates the concentration of two substances at a given time based on the substances' diffusion, feed rate, removal rate, and reaction between the two. This simulation not only models the underlying process of a chemical reaction but can also result in patterns of the substances which are remarkably similar to patterns found in the real world.

$$U + 2V \rightarrow 3V \tag{1.1}$$

$$V \xrightarrow{k} P \tag{1.2}$$

The chemical system is composed of only two active chemical species U and V, along with a (virtual) inert product P. V is the species which catalyses its own replication through the conversion of the substrate U.

The reaction-diffusion system described above involves two generic chemical species U and V, whose concentration at a given point in space is referred to by variables u and v. They react with each other, and they diffuse through the medium. The concentration of U and V at any given location changes with time and can differ from that at other locations. There are two reactions which occur at different rates throughout the space according to the relative concentration at each point.

P is an inert product. It is assumed for simplicity that the reverse reactions do not occur. Because V appears on both sides of the first reaction, it acts as a catalyst for its own production.

The overall behaviour of the system is described by the following formula.

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + F(1-u), \tag{1.3}$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + uv^2 - (F+K)v. \tag{1.4}$$

The system may seem very difficult but it can be easily translated if we look closely. Both equations of the system have three terms. In the first equation 1.3, we call the 1st term as the diffusive term and the 2nd term as the reaction rate but the interesting case is the last one, the term $F(1-u)$ is the refill term for u and F is the feed rate. For 2nd equation 1.4, the term $(F+k)v$ has a diminishing term v without which the concentration of chemical V could increase without limit and k is the rate at which the reaction $v \rightarrow p$ takes place.

The constants D_u and D_v are the diffusion coefficients of U and V, respectively, and F is the dimensionless feed rate.

The dynamics take the shape of a system of non-linear parabolic PDE composed of 3 terms: a reaction function, a diffusion term and a flow process. The flow process regulates the inflow of species U in the system which prevents its exhaustion, as well as the elimination of inactivated V.

1.3 Differential Equation (DE)

Many of the laws underlying the behaviour of the natural world are relations involving rates at which things happen. When these relations are expressed in mathematical terms, the relations are equations and the rates are derivatives. Therefore, an equation containing one or more functions with its derivatives is **differential equations**.

A differential equation that describes some physical process is often called **mathematical model** of the process.

Direction Fields

Direction fields are valuable tools in studying the solutions of a differential equation of the form:

$$\frac{dy}{dt} = f(y,t) \tag{1.5}$$

Direction fields function as a graphical representation of the behaviour of the solution of a differential equation.

1.4 Classification of Differential Equation

Differential equations can be classified as either Ordinary (ODE) or Partial Differential Equation (PDE).

1.4.1 Ordinary Differential Equation (ODE)

An ordinary differential equation (ODE) is an equation that involves a function and its derivatives with respect to one independent variable only. Examples of ordinary differential equations are as follows:

$$\frac{d^2y}{dx^2} + 2\frac{dy}{dx} + 3y = 0$$
$$\frac{d^5y}{dx^5} + \frac{d^2y}{dx^2} + 3y = x$$

System of Differential Equation

Considering the number of functions in a DE, we can use the number of functions to classify a differential equation into systems of differential equations. If there are two or more unknown functions, then a system of differential equations is required.

$$\frac{dx}{dt} = ax - \alpha xy \tag{1.6}$$
$$\frac{dy}{dt} = -cy + \gamma xy \tag{1.7}$$

Order

The order of a differential equation is the order of the highest derivatives that appears in the equation.

$$y''' + ty' + 4y = 0 \tag{1.8}$$

The order of equation 1.8 is 3.

Degree

The degree of a differential equation is the power of the highest-order derivative that appears in the equation.

$$(y''')^3 + t(y')^2 + 4y = 0 \tag{1.9}$$

The degree of equation 1.9 is 3.

Linearity

An important classification of differential equations is whether they are linear or nonlinear. The ordinary differential equation in equation 1.10

$$F(t, y, y', ...y^{\mathrm{n}}) = 0 \tag{1.10}$$

is said to be linear if F is a linear function of the variables $y, y', ...y^{\mathrm{n}}$; The general linear ordinary differential equation of order n is:

$$a_0(t)y^{\mathrm{n}} + a_1(t)y^{\mathrm{n\text{-}1}} + ... + a^{\mathrm{n}}(t)y = g(t). \tag{1.11}$$

An equation that is not of the form 1.11 is not a linear equation e.g:

$$y''' + 2e^{"}y'' + yy'' = t^4 \tag{1.12}$$

1.12 is not linear because of the term yy' which is the product of the dependent variable y

Homogeneity

A differential equation $\frac{dy}{dt} + y = g(t)$, where $g(t) = 0$ is called homogeneous and non-homogeneous if $g(t) \neq 0$.

1.4.2 Partial Differential Equation (PDE)

Partial differential equations (PDEs) involve the rates of change with respect to continuous variables. They are mathematical equations that include two or more independent variables, an unknown function that depends on these variables, and partial derivatives of the unknown function with respect to the independent variables.
A simple PDE is written as

$$\frac{\partial u}{\partial x}(x, y) + \frac{\partial u}{\partial y}(x, y) = 0$$

Linear, Quasi-Linear And Non-Linear PDE

A first-order PDE for an unknown function $u(x, y)$ is said to be linear if it can be expressed in the form

$$a(x, y)\frac{\partial u}{\partial x} + b(x, y)\frac{\partial u}{\partial y} = c(x, y)$$

The PDE is said to be quasilinear if it can be expressed in the form

$$a(x,y,u(x,y))\frac{\partial u}{\partial x} + b(x,y,u(x,y))\frac{\partial u}{\partial y} = c(x,y,u(x,y))$$

Linearity And Non-Linearity Of PDE

A partial differential equation in the function u is said to be linear if it is at most of first degree in u and the derivatives of u. This means that the equation should not contain any term that involves powers or products of u and the derivatives of u.

$$x\frac{\partial u}{\partial x} + y\frac{\partial u}{\partial y} - 2u = 0$$

$$y\frac{\partial u}{\partial x} - x\frac{\partial u}{\partial y} = x$$

$$\frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial y} - u = 0$$

The above equations represent linear PDE.

On the other hand,

$$u\frac{\partial u}{\partial x} + y\frac{\partial u}{\partial y} - u^2 = xy$$

$$\frac{\partial^2 u}{\partial x^2} + x\frac{\partial u}{\partial y}\frac{\partial u}{\partial y} + yu = y$$

The above equations represent non-linear PDE

Semi-linear Equations

A first-order semilinear PDE has the form

$$a(x,y)\frac{\partial u}{\partial x} + b(x,y)\frac{\partial u}{\partial y} = c(x,y,u)$$

This equation is called semilinear because it is linear in the leading (highest-order) terms $\frac{\partial u}{\partial x}$ and $\frac{\partial u}{\partial y}$. However, it is not linear in u.

1.5 FINITE DIFFERENCE METHOD

The finite difference method (FDM) is a numerical technique used to approximate the solutions of partial differential equations. It has been widely used to solve a variety of problems, including linear and nonlinear problems, and time-independent and time-dependent problems. FDM can handle problems with different boundary shapes, various types of boundary conditions, and regions containing different materials.

Given that $f(x)$ is a function of an independent variable x, in elementary calculus, we study the change of $f(x)$ corresponding to any small change in x. This change may be constant in x and is denoted by $\partial x, \Delta x$ or dx. This change may be constant for all values of x or may vary for different values of x.

$\Delta f(x)$ is called the first derivative of $f(x)$ where Δ is known as an operator.

$$\Delta f(x) = f(x+h) - f(x) \qquad or$$

$$\Delta y_{(k)} = y_{k+1} - y_k \qquad \{k = 0, 1, 2, ...\}$$

1.5.1 Forward Difference

Let $f(x)$ be a function on an interval $f_{h+j} = f(x_{n+j}, h)$ for specific x_n, h and j are being the mesh interval, so we define forward difference as follows:

1. $\Delta f(x) = f(x+h) - f(x)$

2. $\Delta^2 f(x) = \Delta[\Delta f(x)]$
   $= \Delta[f(x+h) - f(x)]$

1.5.2 Backward Difference

This is the same as forward difference but this is where the succeeding term is taken from the preceding term. The first backward difference is denoted by $\nabla f(x)$ and defined by

$$\nabla f(x) = f(x) - f(x-h)$$

$$\nabla f(x) = f(x) - f(x-h)$$

$$\nabla f_k = f_k - f_{k-1}$$

The topic of differential equations is a wide one which can not be overemphasised in solving real-life problems. Mathematical models help us to understand the physical laws in many fields ranging from engineering to life sciences.

1.6 Basic Concepts and Definition of Terms

Pattern

Patterns are spatially heterogeneous solutions of U and V from the above systems of equation 1.3 and 1.4

Pattern formation process

Pattern formation process is considered the application of a mathematical model to explain or understand natural phenomena.

Diffusion-driven Instability or Turing Instability

Occurs when a steady state is stable in the absence of diffusion, and unsteady in the presence of diffusion.

Asymptotically stable

[16]Given a Jacobian matrix **J**, if all the eigenvalues of the jacobian matrix **J** are negative, or have negative real parts, then the critical point is said to be asymptotically stable.

Unstable

[16]Given a Jacobian matrix **J**, if at least one of the eigenvalues of the jacobian matrix **J** is positive or has positive real part, then the critical point is said to be unstable.

Stable (or neutrally stable)

[16]Each trajectory move about the critical point within a finite range of distance.

Hyperbolic point

[16]A hyperbolic equilibrium is characterized by having all eigenvalues of the Jacobian matrix with non-zero real parts. Such equilibria are considered to be structurally stable, as small perturbations of order do not significantly alter the phase portrait near the equilibria. Additionally, the local phase portrait of a hyperbolic equilibrium for a nonlinear system is equivalent to that of its linearization. This is known as the Hartman-Grobman theorem, which guarantees that the stability of the steady state

$$(\tilde{x}, \tilde{\tilde{y}})$$

for the nonlinear system is equivalent to the stability of the trivial steady state (0, 0) for the linearized system.

Non-Hyperbolic point:

[16]Given a Jacobian matrix **J**, if at least one eigenvalue of the Jacobian matrix is zero or has a zero real part, then the equilibrium is said to be non-hyperbolic. Non-hyperbolic equilibria are not robust means that the system is not structurally stable. Therefore, small perturbations can result in a local bifurcation of a non-hyperbolic equilibrium, that is, it can change stability, disappear, or split into many equilibria. Such equilibrium is referred to as bifurcation.

Bifurcation analysis

[16]Bifurcation analysis helps us to fully understand the models' dependence on parameter values.

Hopf bifurcation

[16]Hopf bifurcation occurs in systems of two or more dimensions when the system of non-linear equations is nonhyperbolic. In a differential equation, Hopf bifurcation will occur when the real part of a complex conjugate pair of eigenvalues, of the linearized flow at a fixed point switches from positive to negative or negative to positive that is when the eigenvalues become purely imaginary.

1.7 Motivation

This research work aims to explore spatial patterns that may involve the dynamics of pattern formation in biological processes. The specific objectives are to :

1.8 Aim and Objectives

The aim of this research work is to exploit spatial patterns that may involve the dynamics of pattern formation in biological processes. The specific objectives are to :

- Apply the Gray-Scott reaction-diffusion model to illustrate the dynamism of pattern formation considering 2 different species U and V.
- Perform computer simulation to generate numerical values that would be used to illustrate and interpret the model.

Chapter 2
LITERATURE REVIEW

2.1 Historical Development

[9]Self-organization is the natural phenomenon that is persistently usually obvious in the formation of spatiotemporal structures in systems composed of either few or many components. In fields such as physics, chemistry, and biology, self-organization has reportedly occurred in open systems which are driven away from thermal equilibrium. The process of self-organization which can also be referred to as the pattern formation process is found in various fields which include sociology, medicine, technology, and economy..

This process is also present in the animate world in which objects grow and acquire forms or functions without being augmented by humans. This is recognized in the animal kingdom which does not also neglect the human brain. There is a growing recognition that the human brain can be viewed as a self-organizing system because of the activities they engaged in such as economy and sociology.

This process can also be found in inanimate worlds such as planetary systems, galaxies, sands, and rocks.

[3]Most schemes for embryonic pattern formation are built around the notion of lateral inhibition. Models of this type arise in many settings, and all share some common characteristics. George et James examine a number of pattern formation models and then show how the process of lateral inhibition constrains the possible geometries that can arise. [5] Meinhardt . H (1990) The formation of a great variety of patterns on sea shells can be explained by employing reaction-diffusion equations, leading first to dynamic (dissipative) structures and subsequent solidification .

The study of complex population dynamics is nearly as old as population ecology. Lotka and Volterra independently developed a simple model of interacting species in the 1920s. The model was simple, but the predator-prey that was formed displayed neutrally stable cycles, and from that point on, the dynamic relationship between predators and prey has for quite some time been one of the predominant subjects in ecology and mathematical ecology which are due to its; universal existence importance.

Mathematical modelling plays an important role in the study of pattern formation. The prey-predator Lotka-Volterra equation model was used to model interactions, which describe the dynamics of biological systems in which two species i.e., the prey and predator interact. However, the presence of a diffusion mechanism changes the behaviour and nature of the whole model. It is now a reaction-diffusion system, which takes the form of non-linear partial differential equations and is very difficult to solve analytically. Thus, most researchers have turned to numerical simulations to study the behaviour of the system. The numerical simulations technique is used to study the rich spatiotemporal dynamical structure of the diffusive prey-predator model.
Not surprisingly, these models have found applications in describing a wide range of natural phenomena across various scales, from microbiological processes such as chemotaxis (the directed cellular movement based on concentration gradients), neural activity, tumour growth, wound healing, and animal pigmentation patterns, to population dynamics, such as ecological dispersal and invasions, as well as the spread of epidemics ([15]J. D. Murray). The formations of numerous patterns are observed i.e., spiral waves, patchy structures, spiral defect chaos and spatiotemporal chaos due to Turing instability in the model. These two-dimensional patterns are very beautiful and very interesting to be observed and interpreted accordingly from an ecological point of view.

2.2 Contemporary Researches

[19]Garvie (2007) and [20]Medvinsky et al. (2002). Studied the spatial-temporal dynamics in aquatic communities and discovered that the size of these patches has been related to the characters' length of observed plankton patterns in the ocean.
[10]Pan-Ping Liu et al. (2009) Investigate the pattern formation process of a spatially extended predator-prey model within a 2-dimensional space because of the complexity of solving the non-linear differential equation, they used Euler numerical solution to discover the spatial patterns including spotted, stripe and labyrinth patterns. Their research shows a moderate change in a single parameter of the system

$$\frac{\partial U}{\partial t} = (1-U)U - \frac{\beta UV}{U+V} + D^2V \tag{2.1}$$

$$\frac{\partial V}{\partial t} = \frac{\epsilon\beta UV}{U+V} - \mu V + D^2V \tag{2.2}$$

namely β can lead to dramatic changes in the qualitative dynamics of solutions. The Result shows that the ratio-dependent predator-prey model also represents rich spatial dynamics, which can be used for the study of the dynamic complexity of ecosystem or physical systems.

[11]Mohb et al.(2012) Used numerical simulation to study the spatiotemporal dynamical structures of the diffusive prey-predator model viz. Spiral waves have patchy structures, spiral defects, chaos and spatial-temporal chaos due to Turing instability. Amazing beautiful structures emerged due to the proper selection of model parameters and suitable initial conditions factor.

[14]Vagner Weide Rodrigues et al. (2019) Explored the spatiotemporal dynamics of a reaction-diffusion PDE model for the generalist predator-prey dynamics analyzed by Erbach and colleagues. Their findings revealed that movement can break the effect of hysteresis observed in the local dynamics which can have important implications for pest and species conservation

[17]Xinze Lian et al. (2013) Considered the effect of time delay and cross-diffusion on the dynamics of a modified Leslie-Gower predator-prey model incorporating a prey refuge. It was demonstrated that delayed feedback may generate Hopf and Turing instability under some conditions resulting in spatial patterns. The results indicated that time delay and cross-diffusion play important roles in pattern formation.

[18]John F. McLaughlin et al. Introduced a spatially heterogeneous environment to the Lotka-Volterra predator-prey diffusion model, which reveals that spatial pattern is amplified and the dynamics are stabilized by non-linear environmental heterogeneity and differential species mobility. The prey growth rate is amplified in the prey equilibrium distribution when predators diffuse and prey are sedentary. When both species diffuse rapidly, patterns in their distributions are homogenized.

[26]Mathematical biology models such as Fisher, Gray-Scott and auto-catalysis equations exist in non-linear form. They do not have closed-form solutions therefore, numerical methods have an important role to play in examining the behaviour of their solutions (Owolabi et al 2016).

[24]Kolawole Owolabi and Kailash C. Patidar investigated the numerical simulations of coupled one- dimensional Gray-Scott model for pulse splitting process, self-replicating patterns and unsteady oscillatory fronts associated with autocatalytic reaction-diffusion equations as well as homoclinic stripe patterns, self-replicating pulse and other chaotic dynamics in Gierer-Meinhardt equations. They solved the equation using a higher order exponential time differencing Runge-Kutta (ETDRK) scheme which was proposed by Cox and Matthews and was later presented as a result of instability in a modified form by Krogstad to solve stiff semi-linear problems. The

semi-linear problems were partitioned into two parts: a linear component, which encompasses the most rigid portion of the dynamic system, and a nonlinear component, which varies at a slower pace than the linear component.

Chapter 3
METHODOLOGY

To truly comprehend pattern formation, it is essential to study the spatial properties of reaction-diffusion equations. The gray-Scott system is a reaction-diffusion system. It models a process that consists of a reaction and diffusion and it is given below:

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u + F(u, v) \tag{3.1}$$
$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + G(u, v) \tag{3.2}$$

where $F(u, v)$ in 3.1 is equal to : $-uv^2 + F(1 - u)$

while $G(u, v)$ in 3.2 is equal to: $+uv^2 - (F + K)u$

therefore we have a new system:

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + F(1 - u) \tag{3.3}$$
$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + uv^2 - (F + K)v \tag{3.4}$$

Equation 3.3 describes how quickly the quantity U increases. The first term, $D_u \nabla^2 u$, represents the diffusion term, which indicates that the concentration of U will increase in proportion to the laplacian (∇) operator of u. When the neighbouring regions have a higher concentration of U, u will also increase. Conversely, when the surrounding regions have lower concentrations of U, $\nabla^2 u$ will be negative, and the diffusion term will become negative, causing u to decrease.

If we were to create an equation for u that included only the first term, it would be:

$$\frac{\partial u}{\partial t} = D_u \nabla^2 \tag{3.5}$$

where 3.5 is a diffusion-only system whic is also equivalent to the heat equation.

$$-uv^2 \tag{3.6}$$

3.6 Is the second term in 3.3. The first reaction described involves the consumption of one unit of U and two units of V. The rate at which this reaction takes place is proportional to the concentration of U multiplied by the square of the concentration of V. This is known as the reaction rate for the first reaction.

It also converts U into V: the increase in v is equal to the decrease in u (as shown by the $+uv^2$ in equation 3.4). The reaction terms do not contain any fixed constants, but the relative magnitudes of the other terms can be modified by adjusting the values of D_u, D_v, F, and k, as well as selecting an arbitrary time unit in the expression for ∂t.

$$\text{F(1-U)} \tag{3.7}$$

3.7, the third term in 3.3, is the replenishment term. The reaction process consumes U and produces V, meaning that the entire amount of chemical U will eventually be exhausted if there is no mechanism for replenishment. The term responsible for replenishing U specifies that u will increase at a rate proportional to the difference between its current concentration and 1. Therefore, even if the diffusion and reaction terms have no impact, the maximum value of u will be 1. The constant F represents the rate of replenishment and is referred to as the feed rate.

Comparing the two equations(3.3 and 3.4), the main difference between the two equations lies in the third term. In the u equation, the term is $F(1-u)$, which represents the rate of replenishment of U based on the difference between its current level and 1. On the other hand, the third term in the v equation is the diminishment term, which prevents the concentration of V from increasing without limit. This term is proportional to the concentration of V currently present, as well as the sum of two constants: F, which represents the permeability of the membrane to U, and k, which represents the difference between this rate and that for V. Although V could accumulate for a long time without interfering with further production of more V, it eventually diffuses out of the system through the same or a similar process as that which introduces the new supply of U.

3.1 Linear Stability Analysis

The linear stability analysis is performed to obtain the steady states of the model. The nature of the steady-state values is investigated for further analysis. Therefore, the steady-state values of the system will be obtained to aid the local stability analysis.

At stationary state the diffusive terms

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u \equiv 0$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v \equiv 0$$

therefore, equation (3.3 and 3.4) becomes

$$0 = -uv^2 + F(1-u) \tag{3.8}$$

$$0 = +uv^2 - (F+K)v \tag{3.9}$$

According to [20] Medvinsky et al.(2002) and [19] Garvie (2007), considering the local dynamics of the system is essential as this gives proper guidelines on the suitable choice of numerical parameter for simulation. Add 3.8 and 3.9 we have that:

$$-uv^2 + F(1-u) + uv^2 - (F+K)v = 0$$

F(1-u) - (F+K)v = 0

F(1-u) = (F+K)v

Divide both sides with $F + K$

$\frac{F}{F+K}(1-u) = v$

$$\text{Thus:} \quad v = \frac{F}{F+K}(1-u) \tag{3.10}$$

let $\gamma = \frac{F+K}{F}$

which also means that we can say $\frac{1}{\gamma} = \frac{F}{F+K}$

Therefore, sub $\frac{1}{\gamma}$ into 3.10, we have

$v = \frac{1}{\gamma}(1-u)$

Thus: 3.8 becomes

$$-u\frac{1-u^2}{\gamma} + F(1-u) = 0$$

$$-u\frac{(1-u)^2}{(\gamma)^2} + F(1-u) = 0$$

$$\frac{-u(1-u)^2 + F\gamma^2(1-u)}{\gamma^2} = 0$$

$$-u(1-u)^2 + F\gamma^2(1-u) = 0$$

$$-u(1-2u+u^2) + F\gamma^2(1-u) = 0$$

$$-u(1-u-u+u^2) + F\gamma^2(1-u) = 0$$

$$-u[1(1-u) - u(1-u)] + F\gamma^2(1-u) = 0$$

$$-u[(1-u)(1-u)] + F\gamma^2(1-u) = 0$$

$$-u[-(u-1)(1-u)] + F\gamma^2(1-u) = 0$$

$$u[(u-1)(1-u)] + F\gamma^2(1-u) = 0$$

$$(1-u)[u^2 - u + F\gamma^2] = 0 \tag{3.11}$$

Therefore, the equilibrium solution or steady-state values are the roots of the cubic equation 3.11 .

From 3.11 $1-u=0$

therefore we have $\quad u_0 = 1$

from 3.11 $u^2 - u + F\gamma^2 = 0$

the above equation is a quadratic equation, recall the quadratic formula: $-b \pm \frac{\sqrt{b^2-4ac}}{2a}$

$$a = 1, b = -1, c = F\gamma^2$$

$$u = \frac{(-1) \pm \sqrt{(-1)^2 - 4(1)(F\gamma^2)}}{2(1)}$$

$$u = \frac{1 \pm \sqrt{1 - 4F\gamma^2}}{2}$$

Thus

$$u_{1,2} = \frac{1}{2}(1 \pm \sqrt{1 - 4\gamma^2 F}) \tag{3.12}$$

Recall from 3.10 that $v = \frac{F}{F+K}(1-u)$, make u subject of the formula, thus:

$$v(F + K) = F(1 - u)$$

$$vF + vK = F - Fu$$

$$Fu = F - vF - vK$$

$$u = \frac{F - vF - vK}{F}$$

$$u = \frac{F}{F} - v(\frac{F + K}{F}) \tag{3.13}$$

Since $\gamma = \frac{F+K}{F}$, sub γ into 3.13 we have that

$$u = 1 - v\gamma \tag{3.14}$$

Sub 3.14 into 3.8

-(1-vγ)$v^2 + F[1 - (1 - v\gamma)] = 0$

$F(1 - 1 + v\gamma) = (1 - v\gamma)v^2$

$F(\gamma v) = v^2 - \gamma v^3$

$$\gamma v^3 - v^2 + F\gamma v = 0$$

$$v(\gamma v^2 - v + F\gamma) = 0 \tag{3.15}$$

from 3.15 $v_0 = 0$

or

$$\gamma v^2 - v + F\gamma = 0$$

recall the quadratic formula:

$$-b \pm \frac{\sqrt{b^2 - 4ac}}{2a}$$

where a = γ, b = -1, c = Fγ

thus we have:

$$v = \frac{-(-1) \mp \sqrt{(-1)^2 - 4(\gamma)F\gamma}}{2(\gamma)}$$

$$v = \frac{1 \mp \sqrt{1 - 4F\gamma^2}}{2(\gamma)}$$

$$v_{1,2} = \frac{1}{2\gamma} \mp \sqrt{1 - 4F\gamma^2} \tag{3.16}$$

We have the steady state values to be:

The trivial solution $(u_0, v_0) = (1, 0)$ and

$(u_{1,2}\, v_{1,2}) = (\frac{1}{2}(1 \pm \sqrt{1 - 4\gamma^2 F}), \frac{1}{2\gamma} \mp \sqrt{1 - 4F\gamma^2})$

The discriminant is 1-4$\gamma^2 F \geq= 0 \Leftrightarrow (F + K)^2 \leq \frac{F}{4}$. A saddle node-bifurcation occurs when

$$(\text{F+K})^2 = \frac{F}{4}$$

$$4F^2 + 8FK + 4K^2 - F = 0$$

$$4F^2 + (8K - 1)F + 4K^2 = 0 \tag{3.17}$$

The discriminant of 3.17 is $(8K - 1)^2 - 64K^2 = 1 - 16K^2$

Therefore, we

$$\frac{8K - 1 - \sqrt{(8K-1)^2 - 64k^2}}{8} < F < \frac{8K - 1 + \sqrt{(8K-1)^2 - 64k^2}}{8}$$

We proceed to obtain the Turing instability condition by analysing the stability of the obtained equilibrium points or steady state values.

3.1.1 Linear Stability Of The Homogeneous Non-linear System

To understand the dynamics of 3.3 and 3.4 in the homogeneous form, the R.H.S and the diffusive term becomes zero thus:

$$-uv^2 + F(1-u) = 0 \tag{3.18}$$

$$uv^2 - (F+K)v = 0 \tag{3.19}$$

Obtain the jacobian matrix of 3.18 and 3.19

$$\mathbf{A}_{u_i,v_i} = \begin{bmatrix} \frac{\partial h}{\partial u} & \frac{\partial h}{\partial v} \\ \\ \frac{\partial g}{\partial u} & \frac{\partial g}{\partial v} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ \\ a_{21} & a_{22} \end{bmatrix} \tag{3.20}$$

We check at the following two conditions for the stability of 3.20

3.2 Conditions For Turing Instability

Certain conditions need to be satisfied for turing instability to occur, the condition is stated below:

- If Trace of matrix A = $a_{11} + a_{22} < 0 \implies \mathbf{Tr}(A) < 0$
- If Determinant of matrix A = $a_{11}a_{22} - a_{12}a_{21} > 0 \implies \mathbf{det}(A) > 0$

To check for the stability of 3.20, we need to carry out the following calculations:

$$a_{11} = \frac{\partial}{\partial u}(-uv^2 + F(1-u))$$
$$a_{11} = -v^2 - F$$

$$a_{12} = \frac{\partial}{\partial v}(-uv^2 + F(1-u))$$
$$a_{12} = -2uv$$

$$a_{21} = \frac{\partial}{\partial u}(uv^2 - (F+K)v)$$
$$a_{21} = v^2$$

$$a_{22} = \frac{\partial}{\partial v}(uv^2 - (F + K)v)$$
$$a_{22} = 2uv - F - K$$

$$\mathbf{A}_{u_i,v_i} = \begin{bmatrix} -\mathrm{v}^2 - F & \text{-2uv} \\ \\ \mathrm{v}^2 & \text{2uv - F - K} \end{bmatrix} \tag{3.21}$$

Estimate 3.21 at steady state values $(u_0, v_0) = (1, 0)$

$$\mathbf{A}_{u_i,v_i} = \begin{bmatrix} \text{- F} & 0 \\ \\ 0 & \text{- F - K} \end{bmatrix} \tag{3.22}$$

The trace of the jacobian matrix 3.22 which is $\mathbf{Tr}(A_(u_0, v_0))$ is $-F - F - K$

The $\mathbf{Re}(\lambda_{1,2}) < 0$ and $\det(A_{1,0}) > 0$.

the eigen values of A at $u_0 = 1$ and $v_0 = 0$ respectively that is $A(u_0, v_0)$ is $\lambda_{1,2} = -F, -F - K$

Since the condition for Turing instability is satisfied, it implies that the steady-state values $u_0 = 1, v_0 = 0$ are linearly stable for the homogeneous equilibrium solution to the Gray-Scott reaction–diffusion system in equation 3.3 and 3.4 for all values of K and F.

To check for stability of the other steady state values $u_{1,2}$ in 3.12 and $v_{1,2}$ in 3.16, we need to estimate the jacobian matrix A in 3.21 at the steady states values of $u_{1,2}$ and $v_{1,2}$ and check for the turing instability conditions stated above in 3.2.

3.2.1 Instability With Diffusion

When we add the diffusive terms to the equation i.e (D_u and D_v are nonzero real numbers), we want it to be unstable.

Recall the systems of the equation in 3.3 which is now 3.23 and 3.4 which is now 3.24 let u_e and v_e be one of the steady-state solutions of the above equations in 3.23 and 3.24.

The equation 3.23 and 3.24 is additively perturbed by

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + F(1 - u) \tag{3.23}$$
$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + uv^2 - (F + K)v \tag{3.24}$$

$$\text{say} \quad u = u_e + \epsilon\tilde{u} \tag{3.25}$$

$$\text{and say} \quad v = v_e + \epsilon\tilde{v} \tag{3.26}$$

where ϵ is perturbation and $<< 1$

therefore, we apply the series expansion of the form:

$$u(x, y, t) = u_0 + \epsilon u_1(x, y, t) + O(\epsilon)$$
$$v(x, y, t) = v_0 + \epsilon v_1(x, y, t) + O(\epsilon)$$
$$\text{to 3.23 and 3.24}$$

Therefore substitute 3.25 into 3.23 and 3.26 into 3.24 and we have that:

$$\frac{\partial(u_e + \epsilon\tilde{u})}{\partial t} = D_u\nabla^2(u_e + \epsilon\tilde{u}) - (u_e + \epsilon\tilde{u})(v_e + \epsilon\tilde{v})^2 + F(1 - u_e - \epsilon\tilde{u}) \tag{3.27}$$
$$\frac{\partial(v_e + \epsilon\tilde{v})}{\partial t} = D_v\nabla^2(v_e + \epsilon\tilde{v}) + (u_e + \epsilon\tilde{u})(v_e + \epsilon\tilde{v})^2 + (F + K)(v_e + \epsilon\tilde{v}) \tag{3.28}$$

from 3.27 we have that

$$\frac{\partial\epsilon\tilde{u}}{\partial t} = D_u\nabla^2\epsilon\tilde{u} - (u_e + \epsilon\tilde{u})(v_e + \epsilon\tilde{v})^2 + F(1 - u_e - \epsilon\tilde{u}) \tag{3.29}$$
$$\frac{\partial\epsilon\tilde{u}}{\partial t} = D_u\nabla^2\epsilon\tilde{u} - (u_e + \epsilon\tilde{u})(v_e^2 + 2\epsilon\tilde{v}v_e + \epsilon^2\tilde{v}^2) + F(1 - u_e - \epsilon\tilde{u}) \tag{3.30}$$
$$\frac{\partial\epsilon\tilde{u}}{\partial t} = D_u\nabla^2\epsilon\tilde{u} - (u_ev_e^2 + 2\epsilon\tilde{v}v_eu_e + \epsilon^2\tilde{v}u_e + \epsilon\tilde{u}\tilde{v_e}^2 + 2\epsilon^2\tilde{u}\tilde{v}v_e + \epsilon^3\tilde{u}\tilde{v}^2) + F(1 - u_e - \epsilon\tilde{u}) \tag{3.31}$$
$$\frac{\partial\epsilon\tilde{u}}{\partial t} = D_u\nabla^2\epsilon\tilde{u} - (u_ev_e^2 + 2\epsilon\tilde{v}v_eu_e + \epsilon^2\tilde{v}u_e + \epsilon\tilde{u}\tilde{v_e}^2 + 2\epsilon^2\tilde{u}\tilde{v}v_e + \epsilon^3\tilde{u}\tilde{v}^2) + F - Fu_e - F\epsilon\tilde{u} \tag{3.32}$$

from 3.32 neglect the second-order expression in ϵ therefore, we obtain:

$$\frac{\partial\epsilon\tilde{u}}{\partial t} = D_u\nabla^2\epsilon\tilde{u} - (u_ev_e^2 + 2\epsilon\tilde{v}v_eu_e + \epsilon\tilde{u}v_e^2) + F - Fu_e - F\epsilon\tilde{u} \tag{3.33}$$
$$\frac{\partial\epsilon\tilde{u}}{\partial t} = D_u\nabla^2\epsilon\tilde{u} - (2\epsilon\tilde{v}v_eu_e + \epsilon\tilde{u}v_e^2 + F\epsilon\tilde{u}) + F - Fu_e - u_ev_e^2 \tag{3.34}$$
$$\epsilon\frac{\partial\tilde{u}}{\partial t} = \epsilon[D_u\nabla^2\tilde{u} - (2\tilde{v}v_eu_e + \tilde{u}v_e^2 + F\tilde{u})] + F - Fu_e - u_ev_e^2 \tag{3.35}$$
$$\epsilon\frac{\partial\tilde{u}}{\partial t} = \epsilon[D_u\nabla^2\tilde{u} - 2\tilde{v}v_eu_e - \tilde{u}v_e^2 - F\tilde{u}] + F - Fu_e - u_ev_e^2 \tag{3.36}$$

let $O(\epsilon) = F - Fu_e - u_ev_e^2$ in 3.36, therefore we have

$$\epsilon\frac{\partial\tilde{u}}{\partial t} = \epsilon[D_u\nabla^2\tilde{u} - 2\tilde{v}v_eu_e - \tilde{u}v_e^2 - F\tilde{u}] + O(\epsilon) \tag{3.37}$$
$$\frac{\partial\tilde{u}}{\partial t} = [D_u\nabla^2\tilde{u} - 2\tilde{v}v_eu_e - \tilde{u}v_e^2 - F\tilde{u}] + O(\epsilon) \tag{3.38}$$

Thus we have:

$$\frac{\partial \tilde{u}}{\partial t} = D_u \nabla^2 \tilde{u} - 2\tilde{v}v_e u_e - (v_e^2 + F)\tilde{u} + O(\epsilon) \tag{3.39}$$

Similarly, for equation 3.28, we have that:

$$\frac{\partial \epsilon\tilde{v}}{\partial t} = D_v \nabla^2 (\epsilon\tilde{v}) + (u_e + \epsilon\tilde{u})(v_e + \epsilon\tilde{v})^2 - F(v_e + \epsilon\tilde{v}) - K(v_e + \epsilon\tilde{v}) \tag{3.40}$$

$$\frac{\partial \epsilon\tilde{v}}{\partial t} = D_v \nabla^2 (\epsilon\tilde{v}) + (u_e + \epsilon\tilde{u})(v_e^2 + 2\epsilon\tilde{v}v_e + \epsilon^2\tilde{v}^2) - Fv_e - F\epsilon\tilde{v} - Kv_e - K\epsilon\tilde{v} \tag{3.41}$$

$$\frac{\partial \epsilon\tilde{v}}{\partial t} = D_v \nabla^2 (\epsilon\tilde{v}) + u_e v_e^2 + 2\epsilon\tilde{v}v_e u_e + \epsilon^2\tilde{v}^2 u_e + 2\epsilon^2\tilde{u}\tilde{v}v_e + \epsilon^3\tilde{v}^2\tilde{u} + \epsilon\tilde{u}v_e^2 - Fv_e - F\epsilon\tilde{v} - Kv_e - K\epsilon\tilde{v} \tag{3.42}$$

From 3.42 neglect all seconder order expression in $\epsilon therefore, we obtain:$

$$\frac{\partial \epsilon\tilde{v}}{\partial t} = D_v \nabla^2 (\epsilon\tilde{v}) + u_e v_e^2 + 2\epsilon\tilde{v}v_e u_e + \epsilon\tilde{u}v_e^2 - Fv_e - F\epsilon\tilde{v} - Kv_e - K\epsilon\tilde{v} \tag{3.43}$$

Factor out ϵ

$$\epsilon\frac{\partial \epsilon\tilde{v}}{\partial t} = \epsilon[D_v \nabla^2 \tilde{v} + 2\tilde{v}v_e u_e + \tilde{u}v_e^2 - F\tilde{v} - K\tilde{v}] + u_e v_e^2 - Fv_e - Kv_e \tag{3.44}$$

Let $O(\epsilon) = u_e v_e^2 - Fv_e - Kv_e$ in 3.44 thus:

$$\epsilon\frac{\partial \tilde{v}}{\partial t} = \epsilon[D_v \nabla^2 \tilde{v} + 2\tilde{v}v_e u_e + \tilde{u}v_e^2 - F\tilde{v} - K\tilde{v}] + O(\epsilon) \tag{3.45}$$

$$\frac{\partial \tilde{v}}{\partial t} = [D_v \nabla^2 \tilde{v} + 2\tilde{v}v_e u_e + \tilde{u}v_e^2 - F\tilde{v} - K\tilde{v}] + O(\epsilon) \tag{3.46}$$

$$\frac{\partial \tilde{v}}{\partial t} = D_v \nabla^2 \tilde{v} - (F + K - 2v_e u_e)\tilde{v} + \tilde{u}v_e^2 + O(\epsilon) \tag{3.47}$$

Therefore, putting equation 3.39 and 3.47 together, we have the following:

$$\frac{\partial \tilde{u}}{\partial t} = D_u \nabla^2 \tilde{u} - 2v_e u_e \tilde{v} - (v_e^2 + F)\tilde{u} + O(\epsilon) \tag{3.48}$$

$$\frac{\partial \tilde{v}}{\partial t} = D_v \nabla^2 \tilde{v} - (F + K - 2v_e u_e)\tilde{v} + v_e^2\tilde{u} + O(\epsilon) \tag{3.49}$$

Let

$$\tilde{u} = u_m e^{\alpha t} sin\lambda x \quad and \quad \tilde{v} = v_m e^{\alpha t} sin\lambda x \tag{3.50}$$

be amplitude equation on the perturbation. We substitute the above expression 3.50 into 3.48 and 3.49

$$\frac{\partial}{\partial t}(u_m e^{\alpha t} sin\lambda x) = D_u\nabla^2(u_m e^{\alpha t} sin\lambda x) - (v_e^2+F)u_m e^{\alpha t} sin\lambda x - 2(v_e u_e)v_m e^{\alpha t} sin\lambda x + O(\epsilon)$$

$$\frac{\partial}{\partial t}(v_m e^{\alpha t} sin\lambda x) = D_v\nabla^2(v_m e^{\alpha t} sin\lambda x) - (F+K-2v_e u_e)(v_m e^{\alpha t} sin\lambda x) + v_e^2(u_m e^{\alpha t} sin\lambda x) + O(\epsilon)$$

where $\nabla^2 = \dfrac{\partial^2}{\partial x} + \dfrac{\partial^2}{\partial y}$ therefore, we have the following result after differentiating.

$$\alpha u_m e^{\alpha t} sin\lambda x = -D_u(\lambda^2 u_m e^{\alpha t} sin\lambda x) - 2(v_e u_e)v_m e^{\alpha t} sinx\lambda x - (v_e^2+F)u_m e^{\alpha t} sin\lambda x$$

$$\alpha v_m e^{\alpha t} sin\lambda x = -D_v(\lambda^2 v_m e^{\alpha t} sin\lambda x) - (F+K-2v_e u_e)(v_m e^{\alpha t} sin\lambda x) + v_e^2(u_m e^{\alpha t} sin\lambda x)$$

Divide all through by the above systems by $e^{\alpha t} sin\lambda x$ and we have:

$$\alpha u_m = -D_u\lambda^2 u_m - 2(v_e u_e)v_m - (v_e^2+F)u_m \tag{3.51}$$

$$\alpha v_m = -D_v\lambda^2 v_m - (F+K-2v_e u_e)v_m + v_e^2 u_m \tag{3.52}$$

putting the above systems into a vectorial form:

$$\alpha \begin{bmatrix} u_m \\ v_m \end{bmatrix} = \begin{bmatrix} f_u & f_v \\ g_u & g_v \end{bmatrix} \begin{bmatrix} u_m \\ v_m \end{bmatrix}$$

where

$$\mathbf{J} = \begin{bmatrix} f_u & f_v \\ g_u & g_v \end{bmatrix}$$

is a Jacobian matrix. Where $f_u = \dfrac{\partial}{\partial u}F(u,v)$, $f_v = \dfrac{\partial}{\partial v}F(u,v)$, $g_u = \dfrac{\partial}{\partial u}G(u,v)$ and $g_v = \dfrac{\partial}{\partial v}G(u,v)$
Therefore we have the jacobian matrix is:

$$\mathbf{J} = \begin{bmatrix} -D_u\lambda^2 - v_e^2 - F & -2v_e u_e \\ v_e^2 & -D_u\lambda^2 + 2v_e u_e - F - K \end{bmatrix} \tag{3.53}$$

evaluate 3.53 at steady state $(u_0, v_0) = (1, 0)$ we have that:

$$\mathbf{J} = \begin{bmatrix} -D_u\lambda^2 - F & 0 \\ \\ 0 & -D_u\lambda^2 - F - K \end{bmatrix} \tag{3.54}$$

The Trace (J) in 3.54 is:

$$-D_u\lambda^2 - F - D_u\lambda^2 - F - K \tag{3.55}$$

$$-\lambda^2(D_u + D_v) - 2F - K \tag{3.56}$$

which implies that the trace of the jacobian 3.56 matrix is < 0 which $\implies$ *Negative*

Finding the determinant of J which is:

$$\mathbf{det}(J) = -D_u\lambda^2 - F(-D_u\lambda^2 - F - K)$$

$$\mathbf{det}(J) = D_u D_v\lambda^4 + D_u\lambda^2[F + K] + D_v\lambda^2 F + F(F + K)$$

$$\mathbf{det}(J) = D_u D_v\lambda^4 + \lambda^2[D_u(F + K) + D_v F] + F(F + K) \tag{3.57}$$

therefore 3.57 is Positive.

which means that the equilibrium point $(u_e, v_e) = (1, 0)$ is stable for parameters F, K, D_u, D_v of the reaction-diffusion model.

3.3 Finite Difference Discretization Of Gray-Scott in Two-Dimension

Using the following definition based on Taylor Series:

$$f(x + \Delta x) = f(x) + \frac{f'(x)\Delta x}{1!} + \frac{f'(x)(\Delta x)^2}{2!} + \frac{f'''(x)(\Delta x)^3}{3!} + \frac{f''''(x)(\Delta x)^4}{4!} + ...$$

Truncating the infinite power. So,

$$f(x+\Delta x) = f(x) + \frac{f'(x)\Delta x}{1!} + \frac{f''(x)(\Delta x)^2}{2!} + O(\Delta x)^3$$

$$f(x+\Delta x) - f(x) = \frac{f'(x)\Delta x}{1!} + \frac{f''(x)(\Delta x)^2}{2!} + O(\Delta x)^3$$

Divide through by Δx

$$\frac{f(x+\Delta x) - f(x)}{\Delta x} = \frac{f'(x)\Delta x}{\Delta x} + \frac{f''(x)(\Delta x)^2}{2\Delta x} + \frac{O(\Delta x)^3}{\Delta x}$$

$$\frac{f(x+\Delta x) - f(x)}{\Delta x} = f'(x) + \frac{f''(x)\Delta x}{2\Delta x} + O(\Delta x)^2$$

Since the error in the second term of the equation is proportional to Δx of the first power, the above equation can be written as

$$f'(x) = \frac{f(x+\Delta x) - f(x)}{\Delta x} \tag{3.58}$$

Second Order Taylor Series

$$f(x-\Delta x) = f(x) - f'(x)\Delta x + \frac{f''(x)(\Delta x)^2}{2!} + \frac{f'''(x)(\Delta x)^3}{3!} + O(\Delta x)^3 \tag{3.59}$$

$$f(x+\Delta x) = f(x) + f'(x)\Delta x + \frac{f''(x)(\Delta x)^2}{2!} + \frac{f'''(x)(\Delta x)^3}{3!} + O(\Delta x)^3 \tag{3.60}$$

Adding equation 3.59 and 3.60

$$f(x+\Delta x) + f(x-\Delta x) = 2f(x) + 2\frac{f''(x)(\Delta x)^2}{2!} + ...$$

$$f(x+\Delta x) + f(x-\Delta x) = 2f(x) + f''(x)(\Delta x)^2 \tag{3.61}$$

$$f(x+\Delta x) - 2f(x) + f(x-\Delta x) = f''(x)(\Delta x)^2 \tag{3.62}$$

Divide through 3.62 by $(\Delta x)^2$

$$\frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{(\Delta x)^2} = \frac{f''(x)(\Delta x)^2}{(\Delta x)^2}$$

$$f''(x) = \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{(\Delta x)^2} \tag{3.63}$$

Recall Gray-Scott equation

$$\begin{aligned} \frac{\partial u}{\partial t} &= D_u \nabla^2 u - uv^2 + F(1-u) \\ \frac{\partial v}{\partial t} &= D_v \nabla^2 v + uv^2 - (F+K)v \end{aligned} \tag{3.64}$$

Which is re-written as 3.65

$$\begin{aligned} \frac{\partial u}{\partial t} &= D_u \nabla^2 u - uv^2 + A(1-u) \\ \frac{\partial v}{\partial t} &= D_v \nabla^2 v + uv^2 - Bv \end{aligned} \tag{3.65}$$

Where $K = A$ and $F + K = B$

From 3.58 and 3.63, we can derive the coefficients of the Gray-Scott model. Hence

$$\frac{\partial u}{\partial t} = \frac{u_{i,j}^{n+1} - u_{i,j}^{n}}{\Delta t} \tag{3.66}$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i-1,j}^{n} - 2u_{i,j}^{n} + u_{i+1,j}^{n}}{\Delta x^2} \tag{3.67}$$

$$\frac{\partial^2 u}{\partial y^2} = \frac{u_{i-1,j}^{n} - 2u_{i,j}^{n} + u_{i+1,j}^{n}}{\Delta y^2} \tag{3.68}$$

$$\frac{\partial v}{\partial t} = \frac{v_{i,j}^{n+1} - v_{i,j}^{n}}{\Delta t} \tag{3.69}$$

$$\frac{\partial^2 v}{\partial x^2} = \frac{v_{i-1,j}^{n} - 2v_{i,j}^{n} + v_{i+1,j}^{n}}{\Delta x^2} \tag{3.70}$$

$$\frac{\partial^2 v}{\partial y^2} = \frac{v_{i,j-1}^{n} - 2v_{i,j}^{n} + v_{i,j+1}^{n}}{\Delta y^2} \tag{3.71}$$

The Gray-Scott model is discretized by substituting the above equation 3.65. Equation 3.65 becomes

$$\begin{aligned} \frac{u_{i,j}^{n+1} - u_{i,j}^{n}}{\Delta t} &= D_u \nabla^2 u - u_{i,j}^{n} \left(v_{i,j}^{n}\right)^2 + A\left(1 - u_{i,j}^{n}\right) \\ \frac{v_{i,j}^{n+1} - v_{i,j}^{n}}{\Delta t} &= D_v \nabla^2 v + u_{i,j}^{n} \left(v_{i,j}^{n}\right)^2 - B\left(v_{i,j}^{n}\right) \end{aligned} \tag{3.72}$$

Multiply both sides by Δt and we have:

$$\begin{aligned} u_{i,j}^{n+1} - u_{i,j}^{n} &= \Delta t D_u \nabla^2 u + \Delta t \left[-u_{i,j}^{n} \left(v_{i,j}^{n}\right)^2 + A\left(1 - u_{i,j}^{n}\right)\right] \\ v_{i,j}^{n+1} - v_{i,j}^{n} &= \Delta t D_v \nabla^2 v + \Delta t \left[u_{i,j}^{n} \left(v_{i,j}^{n}\right)^2 - B\left(v_{i,j}^{n}\right)\right] \end{aligned} \tag{3.73}$$

$$u_{i,j}^{n+1} = u_{i,j}^{n} + \Delta t D_u \nabla^2 u + \Delta t \left[-u_{i,j}^{n}\left(v_{i,j}^{n}\right)^2 + A\left(1 - u_{i,j}^{n}\right)\right]$$
$$v_{i,j}^{n+1} = v_{i,j}^{n} + \Delta t D_v \nabla^2 v + \Delta t \left[u_{i,j}^{n}\left(v_{i,j}^{n}\right)^2 - B\left(v_{i,j}^{n}\right)\right] \tag{3.74}$$

where the Laplacian is defined as follows

$$\nabla^2 v = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$
$$\nabla^2 u = \frac{u_{i-1,j}^{n} - 2u_{i,j}^{n} + u_{i+1,j}^{n}}{\Delta x^2} + \frac{u_{i,j-1}^{n} - 2u_{i,j}^{n} + u_{i,j+1}^{n}}{\Delta y^2} \tag{3.75}$$
$$\nabla^2 u = \frac{u_{i-1,j}^{n} - 4u_{i,j}^{n} + u_{i+1,j}^{n} + u_{i,j+1}^{n} + u_{i,j-1}^{n}}{h^2}$$

where $h^2 = \Delta x^2 + \Delta y^2$

Also,

$$\nabla^2 v = \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}$$
$$\nabla^2 v = \frac{v_{i-1,j}^{n} - 2v_{i,j}^{n} + v_{i+1,j}^{n}}{(\Delta x)^2} + \frac{v_{i,j-1}^{n} - 2v_{i,j}^{n} + v_{i,j+1}^{n}}{(\Delta y)^2} \tag{3.76}$$
$$\nabla^2 v = \frac{v_{i-1,j}^{n} - 4v_{i,j}^{n} + v_{i+1,j}^{n} + v_{i,j+1}^{n} + v_{i,j-1}^{n}}{h^2}$$

where $h^2 = (\Delta x)^2 + (\Delta y)^2$

The equation above represents the discretized equation of the Gray-Scott model in 2-Dimensions.

Chapter 4

RESULTS AND DISCUSSION

4.1 Discussion Of The Result

In this project work, the numerical solution of the Gray-Scott reaction-diffusion problems in two spatial dimensional governed by a second-order partial differential equation (PDE) was presented. The finite difference scheme was used to discretize the partial differential equation to a set of ordinary differential equation (ODE). A test for stability was carried out and analyzed. Various curves and plots were used to interpret the results to depict the effect of various parameters on the system.

The Gray-Scott equation was studied in two-dimension, and pulse splitting processes were observed (interaction between chemical species u and v). The interaction was governed by a pair of coupled reaction-diffusion equations

$$\begin{aligned}\frac{\partial u}{\partial t} &= D_u \nabla^2 u - uv^2 + A(1-u).\\ \frac{\partial v}{\partial t} &= D_v \nabla^2 v + uv^2 - Bv.\end{aligned} \tag{4.1}$$

Where $A = F$ and $B = F + K$.

With the initial conditions

$$\begin{aligned}u(x,t) &= 1 - \frac{1}{2}\sin^{100}(\pi(\frac{x-L}{2L}))\\ v(x,t) &= \frac{1}{4}\sin^{100}(\pi(\frac{x-L}{2L}))\end{aligned} \tag{4.2}$$

where $\mathbf{D}_u = 1 = \mathbf{D}_v$, is the diffusion parameters of the two chemical species u and v called activator and inhibitor, with assumptions that the diffusivities are equal and nearly equal ($\mathbf{D}_u = 1 = \mathbf{D}_v = d_1$). The variables $u = u(x,t)$ and $v = v(x,t)$ denote the concentrations of the inhibitor V and the activator U, ∇^2 denotes the Laplacian with respect to $x \in \mathbf{R}$, the parameters A and B are small, $\ll 1$

4.2 Numerical Simulations

In order to illustrate the analysis presented in this project work, the numerical simulation of the two-dimensional gray-scott equation has revealed some different patterns that develop from the relationship between two species u and v in a particular domain defined as L. The results are presented with various parameter values as seen below. One of the regions is considered in showing the patterns because the u and v region produces a similar pattern.

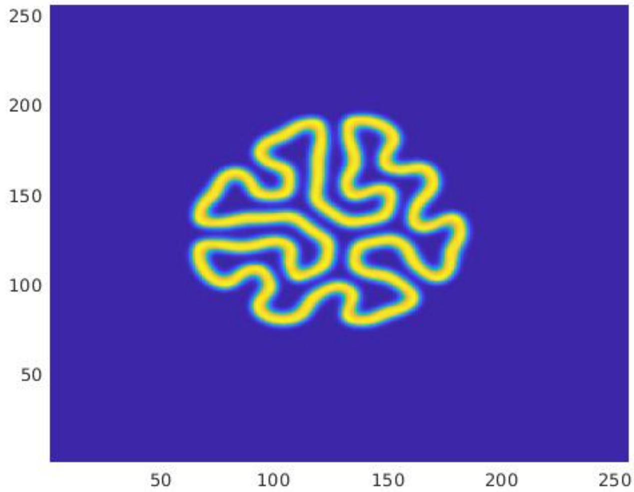

Figure 4.1: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.065$ and $k = 0.0625$

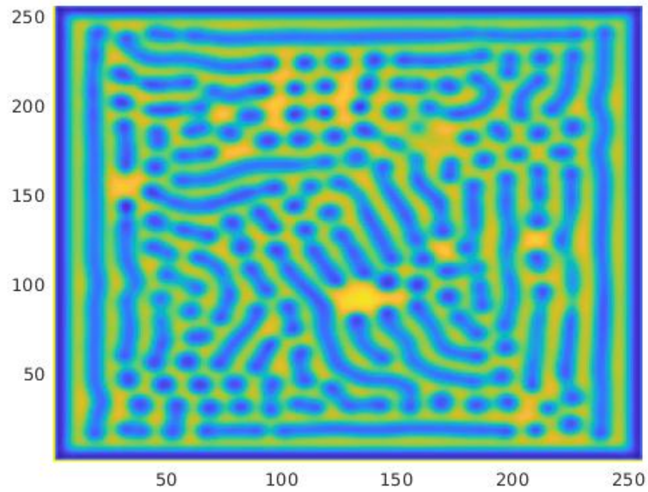

Figure 4.2: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.024$ and $k = 0.056$

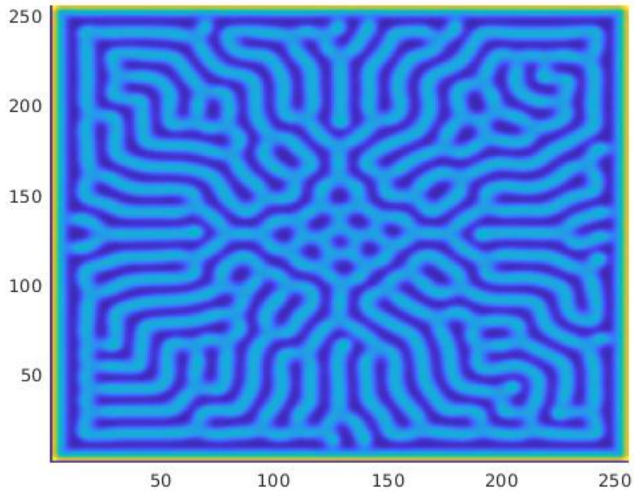

Figure 4.3: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.04$ and $k = 0.006$

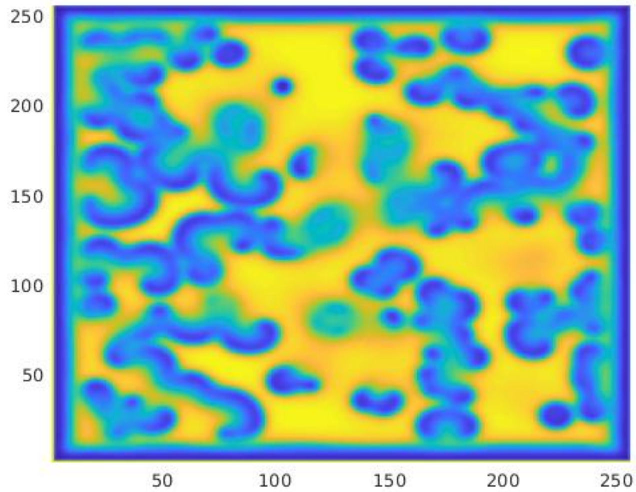

Figure 4.4: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.0172$ and $k = 0.0487$

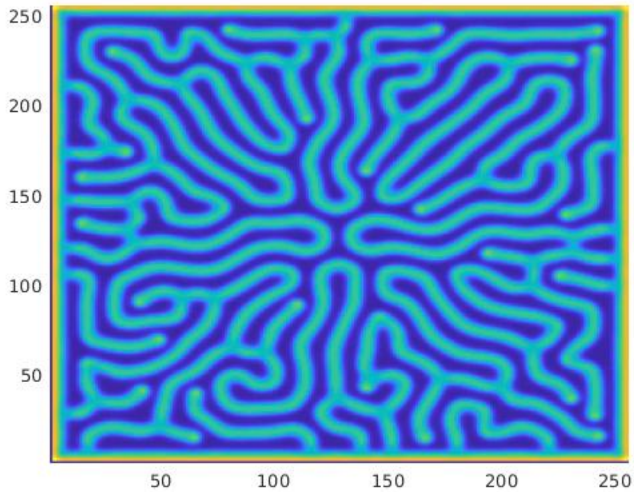

Figure 4.5: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.065$ and $k = 0.0625$

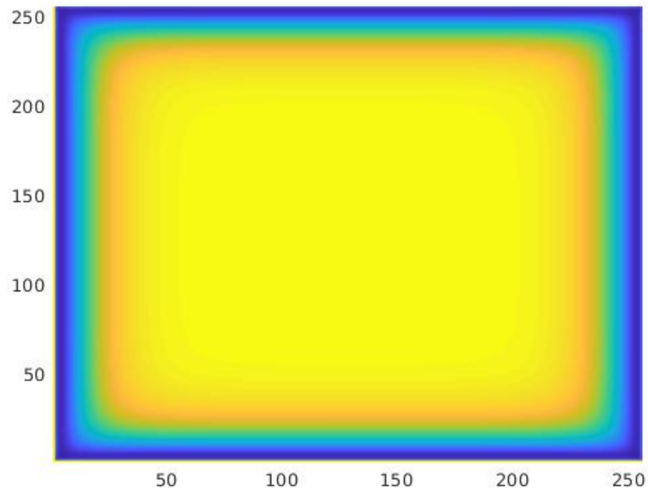

Figure 4.6: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.00143$ and $K = 0.0346$

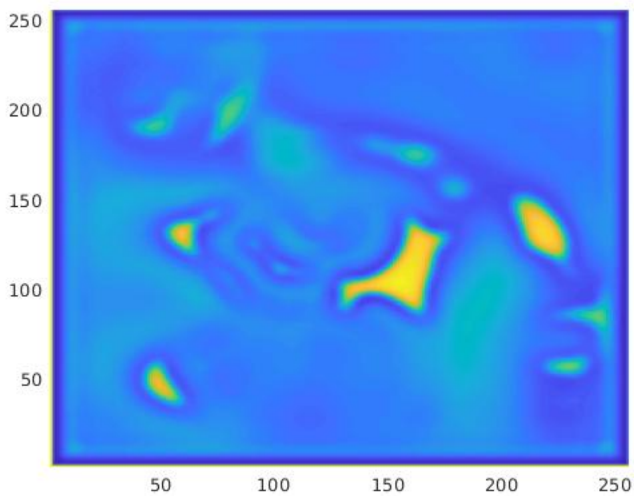

Figure 4.7: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.025$ and $k = 0.05$

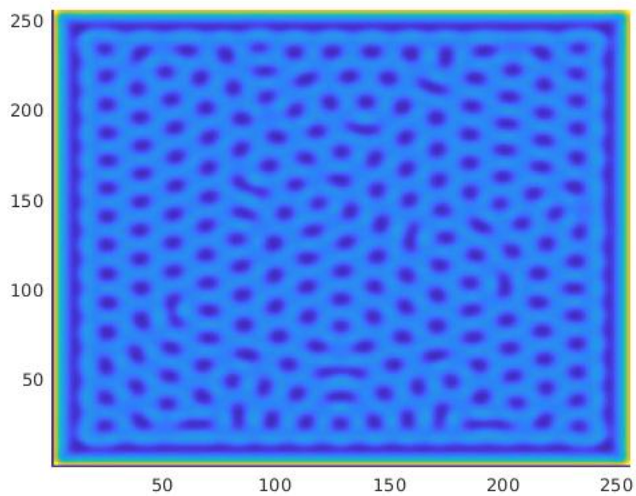

Figure 4.8: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.03$ and $k = 0.055$

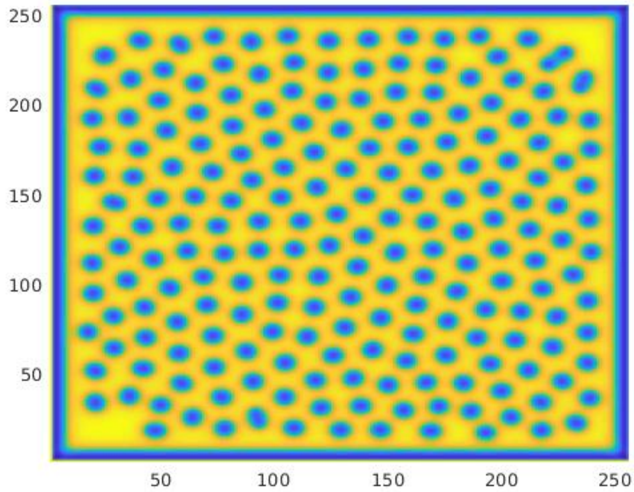

Figure 4.9: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.035$ and $k = 0.065$

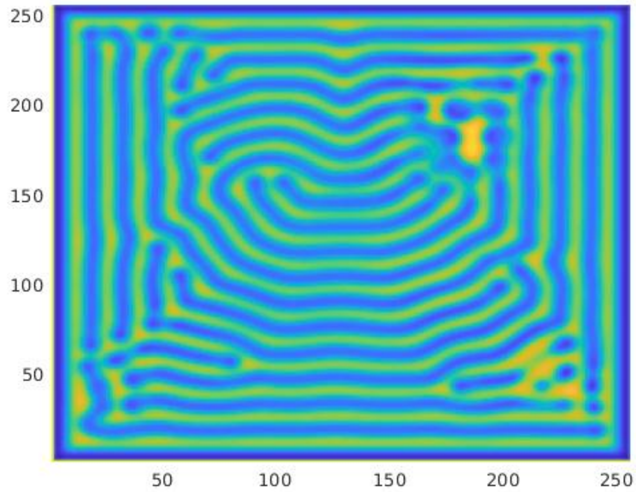

Figure 4.10: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.024$ and $k = 0.055$

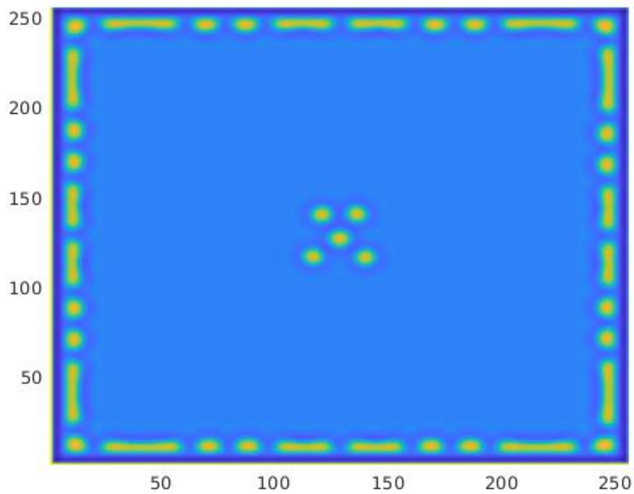

Figure 4.11: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.062$ and $k = 0.06093$

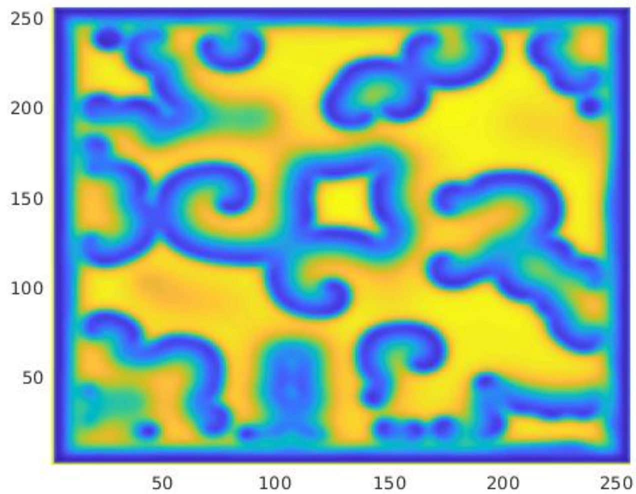

Figure 4.12: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.014$ and $K = 0.045$

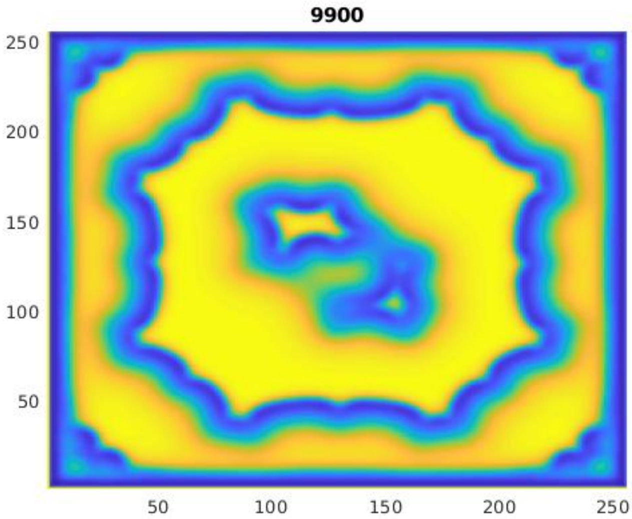

Figure 4.13: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.014$ and $k = 0.045$

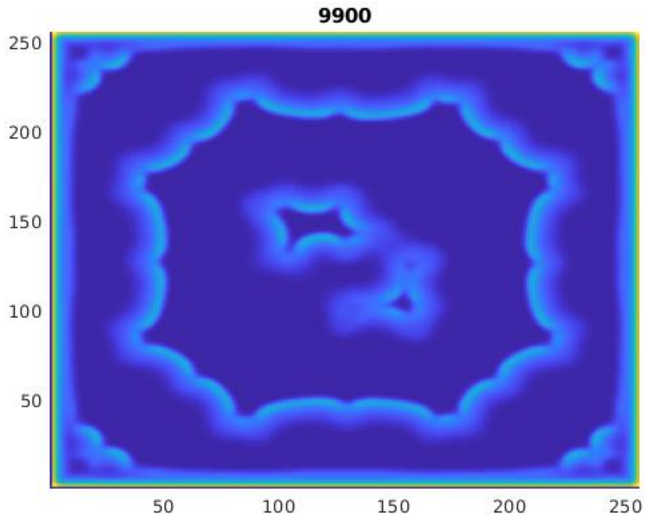

Figure 4.14: plot showing self-replicating patterns and pulse-splitting process for chemical species u and v with domain $L = 2.5$, $h = 0.01$, $dt = 0.8$, $F = 0.014$ and $k = 0.045$

Chapter 5
CONCLUSION AND RECOMMENDATION

The reaction-diffusion problem in the two-dimensional Gray-Scott model has been investigated. The Gray-Scott model is governed by a system of second-order partial differential equation with variable coefficients. This project work aims to obtain a numerical (approximate) solution to the reaction-diffusion problem. The solutions obtained provide vital information on the reaction-diffusion dynamics of the two chemical species u and v in a specified domain. The solutions obtained are analyzed using a numerical approach with the aid of Matlab and surface plots. From the patterns, the following deductions are made

1. The parameters A and B determine the physical process that will dominate the domain or region.

2. The stripe-like patterns double in the number of stripes each time the domain is increased or perturbed.

3. The reaction between the two chemical species is autocatalytic as one of the reaction product is a catalyst for the system.

4. The amplitude of the chemical specie u remains small in regions in which the self-replicating process takes place.

5.1 Recommendation

The following are recommended based on the results obtained from this project work.

A method of approximation which is better when compared to the finite difference scheme may be adopted.

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Appendix

MATLAB Simulation Code

```
%This the  called Gray-Scott model
%Input:  U,V initial concentrations
%        dt  time step
%        h   spacial step
%        Du,Dv diffusion constant
%        k,F   reaction constant, feed rate
%        N     total number of iterations
%Output: U,V   final concentrations
%The explicit finite difference method is used
%The boundary conditions are periodic
%
%Initial conditions
L = 2.5;
h = 0.01;
dt = 0.8;
F = 0.014;K=0.045;
%K=0.095; F=0.056;
%F=0.04; K=0.06;
%F=0.06; K=0.07;%main
%F = 0.0281; K = 0.0596;
%F = 0.0260; K=0.063125;
%F=0.024; K=0.056;
%Du=0.125; Dv=0.05;
%Du=0.018; Dv=10;
%F=0.18; K= 0.057;
%Du=0.01*3; Dv=0.001*4;%main
Du = 2 * 0.00001; Dv = 0.00001;
N = 256;
U = ones(N);
V = zeros(N);
I = (round(N/2) - 10 : round(N/2) + 10);
U(I,I) = 0.5 * ones(length(I)) + 0.01 * rand(length(I)) - 0.01 * rand
   (length(I));
```

```
V(I,I) = 0.25 * ones(length(I)) + 0.01 * rand(length(I)) - 0.01 *
   rand(length(I));
%Boundary conditions
DDU(1,:) = 0; DDU(N,:) = 0; DDU(:,1) = 0; DDU(:,N) = 0;
DDV(1,:)= 0;DDV(N,:)= 0; DDV(:,1) = 0;DDV(: ,N) = 0;
%Finite difference method computation
for k = 1 : 20000
    for i = 2 : N - 1
        for j = 2 : N - 1
            DDU(i,j) = (U(i+1,j) + U(i-1,j) + U(i,j+1) + U(i,j-1) - 4
                * U(i,j)) / h^2;
            DDV(i,j) = (V(i+1,j) + V(i-1,j) + V(i,j+1) + V(i,j-1) - 4
                * V(i,j)) / h^2;
        end
        if mod(i, 200) == 0
            fname=sprintf('uv%d00.mat',i/200);
            %save(fname,'U','V','i')
        end
    end
    RU = Du * DDU - U.* V.^2 + F * (ones(N) - U);
    RV=Dv * DDV + U.* V.^2 -(F+K) * V;
    U=U + dt * RU;
    V=V + dt * RV;
    if mod(k,100) == 0
        fname=sprintf('uv%d00.mat',i/200); %
        %save(fname,'U','V','i')%
        %lighting phong,
        %figure(3);colormap(V);
 shading interp; %
 figure(1);pcolor(U);shading flat;title(num2str(k));
 figure(2);pcolor(V);shading flat;title(num2str(k));
 %pause(0.000001);
    end
    %%%%%%%%%%%%%%%%%%%%%%%%
end
figure(1) %
pcolor(U); %
shading flat;%
figure(2) %
pcolor(V); %
```

```
shading flat; %
 figure(3);pcolor(U); axis image; title('U');
 figure(4);pcolor(V); axis image; title('V');
```