APPLICATION OF NON-LINEAR DIFFERENTIAL EQUATIONS IN AUTO-CATALYTIC CHEMICAL KINETICS

BY

BALCHA AREDA

A THESIS SUBMITTED TO

DEPARTEMANT OF APPLIED MATHEMATICS SCHOOL OF APPLIED NATURAL SCIENCE

OFFICE OF GRADUATE STUDIES

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July 23,2020

ADAMA, ETHIOPIA

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Approval Page

This is to certify that the thesis prepared by Balcha Areda entitled "APPLICATION OF NON LINEAR DIFFERENTIAL EQUATIONS IN AUTO-CATALYTIC CHEMICAL KINETICS" submitted in partial fulfillment of the requirement for the degree of Master of Science in Applied Mathematics with the regulation of the University and meets the accepted standards with respect to originality.

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Abstract

In this study,we have considered the stability nature of a two dimensional non-linear differential equation, popularly known as the Brusselator model and analysis dynamical behavior of the model.The stability of Brusselator model with parameters a *and* b *depend on the concentration chemical corresponding initial conditions is stable if* $b > a^2 + 1$*. So that stability analysis of the equilibrium point of the modified model had be done using Jacobian matrix or Routh-Hurwitz Criteria. We justify the existence of Hopf bifurcation in a two dimensional nonlinear differential equation with the help of Hopf bifurcation theorem and technique of Normal forms to show that supercritical Hopf bifurcation occurs in the system we have considered.The stability of new system formed by hypothesis* b *kept constantly injected into system with rate* v *is stable* $v < 1.21922$ *,besides to all concentration tend toward critical point other wise its unstable and concentration remains bounded or unbounded to large lines while concentration of* x *goes to zero.The numerical solutions of the system of non linear DEs was supplemented by using the built ode45 Mathlab software.*

Key Words:-Non-linear system of differential equations, Brusselator model, MATHLAB, Stability analysis , Hopf-Bifurcation

Chapter 1

Introduction

1.1 Background of the study

Differential equations are extremely important in mathematics and science, since the laws of nature are generally expressed in terms of differential equations.The mathematical description of various processes in chemistry and physics is possible by describing them with the help of differential equations which are based on simple model assumptions and defining the conditions [1]. In chemistry the laws governing chemical kinetics can be written as systems of ordinary differential equations based on the law of mass action. The law of mass action is the proposition that the rate of the chemical reaction is directly proportional to the product of the activities or concentrations of the reactants[1]. It explains and predicts behaviors of solutions in dynamic equilibrium. Specifically, it implies that for a chemical reaction mixture that is in equilibrium, the ratio between the concentration of reactants and products is constant[2].It is assumed that different chemical molecules come into contact by collision before reacting, and that the collision rate is reactively proportional to the number of molecules of each reacting species.

Suppose that two chemicals A and B react to form a product chemical C, written as

$$A + B \xrightarrow{k} C$$

with a constant rate of the reaction k.

For simplicity, we will use the same symbol C, say to refer to both the chemical C and its concentration. From the chemical equation we can easily write the rate equation. It is important to note that most chemical systems are assumed to follow mass action kinetics, meaning that the reaction rate is proportional to the concentration of the reactants. So that dC/dt is the

rate concentration of product C that proportional to the product of the concentrations A and B, with proportionality constant k. That is,

$$\frac{dC}{dt} = kAB.$$

Similarly, the law of mass action enables us to write equations for the time derivatives of the reactant concentrations A and B:

$$\frac{dA}{dt} = -kAB, \quad \frac{dB}{dt} = -kAB.$$

With only one reaction it is easy to see the differential equations governing the concentration of each species.

$$\frac{dC}{dt} = -\frac{dA}{dt} = -\frac{dB}{dt} = kAB.$$

Notice that when using the law of mass action to find the rate-of-change of a concentration, the chemical that the arrow points towards is increasing in concentration (positive sign), the chemical that the arrow points away from is decreasing in concentration (negative sign). The product of concentrations on the right-hand-side is always that of the reactants from which the arrow points away, multiplied by the rate constant that is on top of the arrow[3].
By adding a second chemical equation we will demonstate a slightly more complex system.

$$2A \longrightarrow 3E$$

In this equation species A and E have stoichiometric coefficients greater than one. The differential equations for each species are now:

$$\frac{dA}{dt} = -kAB - 2kA^2, \quad \frac{dE}{dt} = 3kA^2.$$

Note that the rate gives the number of times that a reaction occurs in a volume at a given concentration, while the stoichiometric coefficient tells how many molecules of a species are consumed or produced in each reaction.
A wide variety of chemical reactions can be modeled with coupled (often nonlinear) differential equations. These equations describe the time evolution of the concentrations of the various chemical species: reactants, intermediaries, catalysts, and products. The problem of dealing with chemical reactions of systems involving two variable intermediates, together with a number of initial and final products whose concentrations are assumed to be controlled throughout the reaction process is an important one under quite realistic conditions

and is discussed by Nicolis and Prigogine in[4].

The reaction mechanism to be studied, commonly called the Brusselator model. The Brusselator is a famous theoretical model for a type of autocatalytic reaction and oscillating chemical reaction. The Brusselator model was proposed by Ilya Prigogine and his collaborators (Lefever) at the University of Libre de Bruxelles in 1968[4, 5, 6]. This chemical an autocatalytic reaction in which one of the reactant will generate itself as the reaction proceeds [6].An autocatalytic reaction is one in which a species acts to increase the rate of its producing reaction. Brusselator model is important in real life problem such as :Chemical kinetics, Enzymatic reaction,formation of turing patterns on animal skin, formation of ozone by atomic oxygen through a triple collision.

In 1961, ten years after Belousov's initial experiments, new work was initiated by Zhabotinskii [2]. He quickly reproduced Belousov's results, and soon began working on a similar systems using malic or malonic acids as reductants. Belousov and Zhabotinsky discovered chemical systems exhibiting oscillations. More precisely, they observed that cerium(III) and cerium(IV) were the cycling species: in a mix of potassium bromate, cerium(IV) sulfate, and citric acid in dilute sulfuric acid, the ratio of concentration of the Ce(IV) and Ce(III) ions oscillated. Then Zhabotinskii demonstrated that Ce (III) and Ce (IV) were the cycling species, and he proposed a mechanism for how these cycles occurred. The following two equations show the simplified mechanism.

$$Ce(III) \longrightarrow Ce(IV) \tag{1.1}$$

$$Ce(IV) + CHBr(COOH)_2 \longrightarrow Ce(III) + Br^- + otherproducts \tag{1.2}$$

Equation (1.1) is auto-catalyzed by BrO_3^-, and strongly inhibited by Br^-ions. Therefore, as Ce(IV) is produced in equation(1.1) the rate of equation (1.2) increases. This results in a high concentration of Br^- which inhibits and slows equation , and the cycle begins again(1.1). After the discovery of oscillating chemical reactions, in 1968 Prigogine proposed a virtual oscillating chemical reaction system the Brusselator model[8].

Brusselator model is the reaction mechanism has form of

$$\begin{cases} A \xrightarrow{\upsilon_1} X, \\ B + X \xrightarrow{\upsilon_2} Y + D, \\ 2X + Y \xrightarrow{\upsilon_3} 3X, \\ X \xrightarrow{\upsilon_4} E \end{cases} \tag{1.3}$$

where υ_i are the constant chemical reaction rates.

The rate equations for auto-catalytic reactions are fundamentally nonlinear differential equation.The solution of differerential equation is specific function that satisfies equation. Unfortunately many of them cannot be solved analytically. To investigate the predictions of model of such phenomena it is necessary to approximate their solution numerically. In this thesis we study the Brusselator Model.We will investigate the predictions of model of phenomena numerical and qualitative solution by MATHLAB software.

1.2 Statement of the problem

The dynamics of the oscillating reaction discovered by Belousov and Zhabotinsky [12]can be modeled through the so-called Brusselator model [10]which involves six reactants and products A, B, D, E, X and Y where A and B are reactants (substrates), D and E are products and X and Y are the auto-catalytic reactants of the set of reactions is given as follows

$$\begin{cases} A \xrightarrow{\upsilon_1} X, \\ B + X \xrightarrow{\upsilon_2} Y + D, \\ 2X + Y \xrightarrow{\upsilon_3} 3X, \\ X \xrightarrow{\upsilon_4} E \end{cases} \tag{1.4}$$

where υ_i are the constant chemical reaction rates.

The governing equations of the Brusselator model are obtained from the autocatalytic reaction using law of mass action (i.e. the rate of a chemical reaction is directly proportional to the product of the concentration of reactant) and the set of equations for the change in concentrations of X and Y are found to be

$$\begin{cases} \dot{X} = A + X^2Y - (B+1)X \\ \dot{Y} = BX - X^2Y \end{cases} \tag{1.5}$$

The study was focused on the Brusselator model as the system (1.5) by assuming that A and B are kept constant and with the hypothesis that component B is constantly injected in the mixture with some rate.

This study was intended to answer the following basic questions;

1. What are the basic assumptions to formule mathematical model that describe the dynamics of the auto-catalytic chemical kinetics ?
2. What is qualitative behaviour of mathematical model that describe the auto-catalytic chemical kinetics ?
3. What is numerical result?

1.3 Objectives of the study

1.3.1 General Objective of the Study

The general objective of this study is to investigate the dynamics of auto-catalytic chemical kinetics using non-linear differential equations.

1.3.2 Specific objectives

The specific objectives of this study is to:-

- analyze the stability of model that describe autocatalytic chemical kinetics.
- modify the Brusselator model that describe the auto-catalytic chemical kinetics.
- compute numerical solution of the modified non-linear DEs.

1.4 Significance of the study

The result of this study will help to:

1. Understand how to apply non linear DEs in the auto-catalytic chemical kinetics.
2. Scientific community to further investigation the problem.

Chapter 2

Literature Review

Initially, the Brusselator model was proposed by Prigogine and R. Lefever in 1968[4, 5, 6]. The Brusselator model comes from the mathematical modeling of autocatalytic chemical reaction governed by

$$\alpha \mapsto U \tag{2.1}$$

$$\beta + U \mapsto V + D \tag{2.2}$$

$$2U + V \mapsto 3U \tag{2.3}$$

$$U \mapsto E \tag{2.4}$$

$$\tag{2.5}$$

where α and β are the input chemical, D and E are the output chemical, U and V are the intermediate species. In the 1970s, nonlinear oscillations and bifurcations were discovered first by modelling and then by experiments for the autocatalytic Brusselators and the Belousov-Zhabotinsky chemical reaction [9, 10].

A simple chemical model that exhibits complex dynamics is the Brusselator model, which is an example of an autocatalytic oscillating chemical reaction [13]. This model could present the limit cycle, Hopf bifurcation and also the chaotic behaviour when a certain sinusoidal force acts on the system. This force could be created by the heat convection, microwaves etc, that its behaviour is sinusoidal with a small intensity.

The mechanism for the classical Brusselator chemical model [13] is given as follows:.

$$\begin{cases} A \xrightarrow{\upsilon_1} X, \\ B + X \xrightarrow{\upsilon_2} Y + D, \\ 2X + Y \xrightarrow{\upsilon_3} 3X, \\ X \xrightarrow{\upsilon_4} E \end{cases} \tag{2.6}$$

where υ_i are the constant chemical reaction rates.

The Brusselator chemical reaction model describes a chemical system that converts a reactant A to a final product E through four steps and four intermediate species, X ,B ,Y and D. The steps (2) and (3) are bimolecular and autocatalytic trimolecular reactions respectively. Step (3) is autocatalystic, since two X molecules make three X molecules and it also has an inhibiting factor because, while Y is necessary to make the reaction, in this process Y is also used. Indeed, it is the autocatalystic reaction that causes the chemical oscillations in the Brusselator model. Based on the mechanism of Brusselator reaction, product E is resulted from species X in step (4). In addition, species X is the result of steps (1) and (3). These relationships could show the sensitivity to initial conditions.

The chemical reaction mechanism system (2.6), known as the Brusselator system. It is important in that it admits limit-cycle oscillations and yet contains only two dependent variables (X and Y) thus enabling the use of two-dimensional mathematical systems[6]

In recent decades the Brusselator model has been studied both numerically and analytically. Numerical solution of Brusselator model with or without diffusion is important because analytic solution of Brusselator model is not known yet. Some authors analyze the numerical solution of Brusselator model using various numerical techniques suchas: Decomposition method , second order finite differnce method , collocation method , Runge kutta[19], Twizell et al. [14] developed a second-order method for the numerical solution of the initial-value problems of the Brusselator model. Peng and Wang [15] and Ghergu [16, 17] obtained some conditions for the non-existence and existence of positive non-constant steady states. Kolokolnikov et al.[18] proved the existence of K-periodic, spatially bi-stable structures, mesas and studied their stability. Kang [19] discussed the dynamics of the local map of a discrete version of the Brusselator model, focusing on asymptotic behaviors of bounded trajectories inside the Julia set. Biazar and Ayati [20] considered an Approximation to the solution of the Brusselator system by applying Adomian decomposition method. You [21]

showed the existence of a global attractor for the solution semiflow of the Brusselator equations. Zuo and Wei [22] investigated hopf bifurcations and global steady state bifurcation for a coupled two-cell Brusselator model.

In this study we were treated the concentration of one reactant as description for the structure of the modify model of the steady state solutions of the Brusselator model (2.6). The in-built ODE solver MATHLAB function $ode45$ will used as numerical solution. It gives the good simulation results.

Chapter 3

Mathematical Preliminary

In this chapter, we state some theorems and give the definitions of terminologies which are most crucial for the Thesis as an input.

3.1 Non-linear system of differential equations

Consider a non-linear system of Ordinary Differential Equation (ODE)

$$\frac{du}{dt} = f(u(t)) \tag{3.1}$$

where

$$u = (u_1, u_2, \ldots, u_n)^T, f = (f_1, f_2, \ldots, f_n)^T$$

$f : E \longrightarrow \mathbb{R}^n$ and E is an open subset of $\mathbb{R}^n$.

3.2 Existence and Uniqueness Theorem

The fundamental existence-uniqueness theorem for a non-linear autonomous system of ordinary differential equations

$$\dot{u} = f(u(t)), u(t_0) = u_0 \tag{3.2}$$

under the hypothesis that $f \in C^1(E)$ where E is an open subset of $\mathbb{R}^n$.

Definition 3.2.1 *(The Fundamental Existence-Uniqueness Theorem) [7] Suppose that* $f \in C(E)$ *where E is an open subset of* $\mathbb{R}^n$. *Then u(t) is a solution of the differential equation*

(3.2) on an interval I if u(t) is differentiable on I and if for all $t \in I, u(t) \in E$ and

$$u' = f(u(t)).$$

And given $u_o \in E$, u(t) is a solution of the initial value problem

$$u' = f(u(t)), u(t_0) = u_0$$

on an interval I if $t_o \in I, u(t_o) = u_o$ and u(t) is a solution of the differential equation (3.2) on the interval I .

Definition 3.2.2 ([7]) *A solution $u(t)$ of (3.2) is stable if every solution that starts sufficiently close to $u(t)$ at $t = t_0$ remains close to $u(t)$ for all $t > t_0$. The solution $u(t)$ is unstable if there exists at least one solution starting close to $u(t)$ at $t = t_0$,which does not remain close to $u(t)$ for all $t > t_0$.*

3.2.1 Some stability concepts for ODEs

The goal of stability analysis is to investigate if small perturbations in a system will cause large changes in the behavior of the systems, in which case the system is unstable.Otherwise if small changes in the behavior of the systems, in which case the system said to be asymptotically stable.

For the non-linear autonomous system (3.1), the stability of a solution can be examined if the system is approximated by Linear with Constant Coefficient (LCC) system,which means linearized.

Linearization of nonlinear system

For the non-linear autonomous system (3.1), the stability of a solution can be examined if the system is approximated by Linear with Constant Coefficient (LCC) system. Assume that $u(t)$ is a solution of (3.1). At time $t = t_0$, where $u = u(t_0)$, a small perturbation δu_0 brings us to a new solution trajectory, $u(t) + \delta u(t)$, which is followed for $t > t_0$. The perturbed solution satisfies the ODE system

$$\frac{d(u(t) + \delta u(t))}{dt} = f(u + \delta u),$$

Taylor expansion of the right hand side up to the first-order term gives

$$\frac{du}{dt} + \frac{d\delta u}{dt} = f(u) + \frac{\partial f}{\partial u}\delta u + O(||\delta u||^2). \tag{3.3}$$

In (3.3),the Jacobian is introduced

$$J(u) = \begin{pmatrix} \frac{\partial f_1}{du_1} & \frac{\partial f_1}{du_2} & \cdots \frac{\partial f_1}{du_n} \\ \frac{\partial f_2}{du_1} & \frac{\partial f_2}{du_2} & \cdots \frac{\partial f_2}{du_n} \\ & . & \\ & . & \\ \frac{\partial f_n}{du_1} & \frac{\partial f_n}{du_2} & \cdots \frac{\partial f_n}{du_n} \end{pmatrix}.$$

We obtain, after neglecting the higher order term, the linearized equation

$$\frac{d\delta u}{dt} = J(u)\delta u, \qquad \delta u(t_0) = \delta u_0.$$

If the Jacobian is frozen at $t = t_0$ to a constant matrix J_0, i.e.,

$$J_0 = \frac{\partial f}{\partial u}(u(t_0)).$$

To investigate the stability of critical points, i.e. points satisfying the algebraic equation $f(u) = 0$. Assume critical point u^* is perturbed to a solution $u^* + \delta u(t)$ in the neighborhood of u^*. If all perturbed solutions converge to the critical point u^*, this point is said to be asymptotically stable. If at least one perturbed solution diverges away from the critical point, it is unstable. If the perturbation δu is small,we can approximate $f(u)$ close to the point u^* using Taylor expansion up to the first-order term:

$$f(u^* + \delta u) = f(u^*) + J(u^*)\delta u + O(||\delta u||^2). \tag{3.4}$$

The perturbed solution satisfies the differential equation,i.e.,

$$\frac{du^*}{dt} + \frac{d\delta u}{dt} = f(u^*) + J(u^*)\delta u$$

where we have neglected the higher order terms in (3.3).

As u^* is a constant and $f(u^*) = 0$, we get an ODE system for the perturbation term δu :

$$\frac{d\delta u}{dt} = J(u^*)\delta u$$

This is LCC system of type $\frac{du}{dt} = Au$. where $A \in M^{n\times n}$

Hence, to investigate the stability of a critical point, proceed as follows:

1. Compute a critical point u^* by solving f(u)=0.

2. Form the Jacobian J(u) and compute $J^* = J(u^*)$.

3. Compute the eigenvalues λ_i of J^* and check if $Re(\lambda_i) < 0$.

3.3 Routh-Hurwitz Criteria

Definition 3.3.1 *A matrix $A \in \mathbb{R}^{n\times n}$ is called Hurwitz or asymptotically stable, if and only if $Re(\lambda_i) < 0; \forall i = 1, 2...n$. where $\lambda_i's$ are the eigenvalues of the matrix A [10, 22].*

Given the polynomial;

$$P(\lambda) = \lambda^n + a_1\lambda^{n-1} + \cdots + a_{n-1}\lambda + a_n;$$

where the coefficients a_i are real constants, $\{i = 1, \cdots, n\}$.
Define the n Hurwitz matrices using the coefficients a_i of the characteristic polynomial such that:

$$H_n = \begin{pmatrix} a_1 & 1 & 0 & 0 & \cdots & 0 \\ a_3 & a_2 & a_1 & 1 & \cdots & 0 \\ a_5 & a_4 & a_3 & a_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & a_n \end{pmatrix}$$

where $a_j = 0$ if $j > n$.

$$H_1 = a_1, H_2 = \begin{pmatrix} a_1 & 1 \\ 0 & a_2 \end{pmatrix}, H_3 = \begin{pmatrix} a_1 & 1 & 0 \\ a_3 & a_2 & a_1 \\ 0 & 0 & a_3 \end{pmatrix}$$

All the roots of the polynomial $p(\lambda)$ are negative or have negative real part if the determinants of all Hurwitz matrices are positive, $det(H_j) > 0, j = 1, 2, .., n$.
When $n = 2$ the Routh-Hurwitz Criteria simplify to det $H_1 = a_1 > 0$ and

$$\det(H_2) = \begin{vmatrix} a_1 & 1 \\ 0 & a_2 \end{vmatrix} = a_1 a_2 - 0 > 0$$

$$\det(H_3) = \begin{vmatrix} a_1 & 1 & 0 \\ a_3 & a_2 & a_1 \\ 0 & 0 & a_3 \end{vmatrix} = a_1 a_2 a_3 - a_3^2 > 0$$

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$$\det(H_n) = \begin{vmatrix} a_1 & a_3 & a_5 & . & . & . \\ 1 & a_2 & a_4 & . & . & . \\ 0 & a_1 & a_3 & . & . & . \\ . & & & & & \\ . & & & & & \\ . & & & & & \\ 0 & 0 & 0 & . & . & . & a_k \end{vmatrix} > 0, \text{for k =1, 2, 3, ... ,n.}$$

For a polynomial of degree $n = 2, 3$ and 4, the Routh-Hurwitz Criteria are summarized as follows:

(i) Quadratic equation:$\lambda^2 + a_1\lambda + a_2 = 0$
Stability Criteria: $a_1 > 0, a_2 > 0$

(ii) Cubic equation: $\lambda^3 + a_1\lambda^2 + a_2\lambda + a_3 = 0$
Stability criteria: $a_1 > 0, a_2 > 0, a_3 > 0, a_1 a_2 > a_3 > 0$

(iii) Fourth order equation:$\lambda^4 + a_1\lambda^3 + a_2\lambda^2 + a_3\lambda + a_4 = 0$
Stability criteria: $a_i > 0 (i = 1, 2, 3, 4), a_1 a_2 - a_3 > 0, a_1 a_2 a_3 - a_3^2 - a_1^2 a_4 > 0$

Chapter 4

Analysis of application of non linear DEs in Auto-catalytic chemical kinetics

4.1 Physical Problem and Mathematical Modeling

Let us consider the models involving trimolecular reaction steps which exhibit interesting properties and pose challenging mathematical problems regarding the asymptotic behavior of the solutions. We first study the so-called Brusselator model, which involves six reactants and products $A, B, D, E, X,$ and Y ,such that A and B are reactants, D and E are products or output chemicals while X and Y are the auto-catalytic reactants :

$$\begin{cases} A \xrightarrow{\upsilon_1} X, \\ B + X \xrightarrow{\upsilon_2} Y + D, \text{ bimolecular reaction,} \\ 2X + Y \xrightarrow{\upsilon_3} 3X, \text{trimolecular autocatalytic reaction} \\ X \xrightarrow{\upsilon_4} E \end{cases} \tag{4.1}$$

where υ_i are the constant chemical reaction rates.

The concentrations of the species as functions of time t are denoted by $A(t), B(t), D(t), E(t), X(t),$ and $Y(t)$.

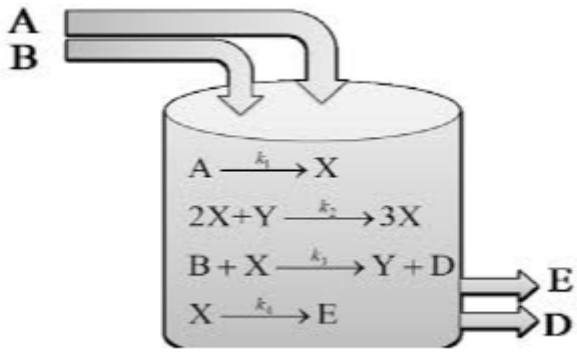

Figure 4.1: Schematic representation of Bruselator model

Mass conservation in the chemical reactions leads to the following differential equations:

$$\begin{cases} \dot{A} = -\upsilon_1 A \\ \dot{B} = -\upsilon_2 BX \\ \dot{D} = \upsilon_2 BX \\ \dot{E} = \upsilon_4 X \\ \dot{X} = \upsilon_1 A - \upsilon_2 BX + \upsilon_3 X^2 Y - \upsilon_4 X \\ \dot{Y} = \upsilon_2 BX - \upsilon_3 X^2 Y \end{cases} \tag{4.2}$$

Under the assumptions that,

- all species are homogeneously distributed in the reactor volume; hence, neither their diffusivities nor any other spatial transport phenomena are considered.
- start by eliminating the two equations governing the production of species D and E, since they are independent of the four others and assumed not to participate in any further reactions so that their concentrations are irrelevant.
- Since the Brusselator is an ideal system, reactions (4.1) can be assumed to be exothermal, and their respective reverse reactions can be assumed to be negligible. Nevertheless, the conditions for oscillation can be met even in the presence of reverse reactions. As noticed by [23] , irreversibility is not a necessary condition for oscillation.This leaves only two varying concentrations, those of the intermediates X and Y, the minimum number required for an oscillatory system.

We are interested in the evolution of the intermediate products, X and Y

$$\begin{cases} \dot{X} = \upsilon_1 A - \upsilon_2 BX + \upsilon_3 X^2 Y - \upsilon_4 X \\ \dot{Y} = \upsilon_2 BX - \upsilon_3 X^2 Y \end{cases} \tag{4.3}$$

It is convenient to express the Brusselator (4.3) in non dimensional form, with some scaling factors that simplify the equations.

The scaling of concentrations and time would be

$$X^* = \frac{X}{X_0}, \quad Y^* = \frac{Y}{Y_0}, \quad t^* = \frac{t}{t_0}$$

where X_0, Y_0 and t_0 are the scaling factors for X, Y and t respectively.

With these scalings, (4.3) can be expressed as

$$\begin{cases} \dot{X^*} = \frac{\upsilon_1 t_0}{X_0} A - t_0 \upsilon_2 BX + \upsilon_3 t_0 X_0 Y_0 X^2 Y - \upsilon_4 t_0 X \\ \dot{Y^*} = \frac{\upsilon_2 t_0 X_0}{Y_0} BX - \upsilon_3 t_0 {X_0}^2 X^2 Y \end{cases} \tag{4.4}$$

where the (*) symbol denotes the scaled variables. Now, there are several possibilities for non dimensionalization depending on which terms we are interested in linearizing. Let us choose the fourth term on the right-hand side (RHS) of (4.4) to scale time as $t_0 = {\upsilon_4}^{-1}$. Then,

$$\begin{cases} \dot{X^*} = \frac{\upsilon_1 t_0}{\upsilon_4 X_0} A - \frac{\upsilon_2}{\upsilon_4} BX^* + \frac{\upsilon_3}{\upsilon_4} X_0 Y_0 X^{*2} Y * -X^* \\ \dot{Y^*} = \frac{\upsilon_2 t_0 X_0}{\upsilon_4 Y_0} BX^* - \frac{\upsilon_3 {X_0}^2}{\upsilon_4} X^{*2} Y^* \end{cases} \tag{4.5}$$

Making the term involving $X^{*2}Y^*$ in (4.5) of order 1, we get

$$\frac{\upsilon_3 {X_0}^2}{\upsilon_4} = 1 \Rightarrow X_0 = (\frac{\upsilon_3}{\upsilon_4})^{\frac{1}{2}}$$

$$\frac{\upsilon_3}{\upsilon_4} X_0 Y_0 = 1 \Rightarrow Y_0 = (\frac{\upsilon_4}{\upsilon_3})^{\frac{1}{2}}$$

Now, scaling terms that

$$a = (\frac{\upsilon_1^2 \upsilon_3}{\upsilon_4^3})^{\frac{1}{2}} A; b = \frac{\upsilon_2}{\upsilon_4} B; x = (\frac{\upsilon_3}{\upsilon_4})^{\frac{1}{2}} X; y = (\frac{\upsilon_3}{\upsilon_4})^{\frac{1}{2}} Y; \tau = \upsilon_4 t$$

with $a > 0, b > 0$.

Table 4.1: Scaling Factors for the variables in the model.

Variable	Scaling
X	$X^* = \frac{X}{X_0}, \quad X_0 = (\frac{\upsilon_3}{\upsilon_4})^{\frac{1}{2}}$
Y	$Y^* = \frac{Y}{Y_0}, \quad Y_0 = (\frac{\upsilon_4}{\upsilon_3})^{\frac{1}{2}}$
t	$t^* = \frac{t}{t_0}, \quad t_0 = {\upsilon_4}^{-1}$
a	$(\frac{\upsilon_1^2 \upsilon_3}{\upsilon_4^3})^{\frac{1}{2}} A$
b	$\frac{\upsilon_2}{\upsilon_4} B$

Then, with these scalings the non dimensional Brusselator becomes

$$\begin{cases} \dot{X^*} = a - bX^* + X^{*2}Y^* - X^* \\ \dot{Y^*} = bX^* - X^{*2}Y^* \end{cases}$$

rearranging terms and dropping the (*) symbol we get with two the intermediate products, x and y in dimensionless form are

$$\begin{cases} x' = a + x^2 y - (b+1)x \\ y' = bx - x^2 y \end{cases} \tag{4.6}$$

Eqn (4.6) have a much simpler form than the original, dimensional forms,(4.3).

For simplicity we will use the shorthand $U(t) = (x(t), y(t))$ for the two-dimensional vector of concentrations. The resulting system of two equations with two unknowns can be written as the initial value problem

$$\begin{cases} U'(t) = F(U(t)) \\ U(0) = U_0 = (x_0, y_0)^T \end{cases} \tag{4.7}$$

where, $U(t) = (x(t), y(t))^T$ is the vector modeling the variations of concentration of substances x and y and obtain

$$F(U) = \begin{pmatrix} a - (b+1)x + x^2 y \\ bx - x^2 y \end{pmatrix}.$$

.

4.1.1 Stationary-state Solutions and their Local Stability

The stability of the system is its propensity to evolve toward a constant or steady solution.The system described by eqn (4.4) does not go to chemical equilibrium because the reactant

concentrations are held constant. Instead we can identify 'stationary states' at which $\frac{dx}{dt}$ and $\frac{dy}{dt}$ equal zero simultaneously. This steady solution $U(t) = Uc$, if it exists,satisfies $U(t) = 0$. Therefore stability of the system be calculated by solving $F(Uc) = 0$. The steady-state is given by computing the resulting system

$$x' = 0, y' = 0.$$

This implies,

$$\begin{aligned} a + x^2y - (b+1)x &= 0 \\ bx - x^2y &= 0 \end{aligned}$$

These is given by the unique solution

$$x = a, y = \frac{b}{a}.$$

Therefore,the steady-state is $U_c = (a, b/a)^T$.

The stability of the system can also be regarded as its ability to relax in finite time to the steady state when a perturbation $\Delta U = U(t) - U_c$ is applied to the solution. In order to study the influence of variations ΔU, we derive a differential equation for ΔU.

Differentiation yields

$$\Delta U' = U'(t) - U_c' = U'(t)$$

since U_c is constant.

Now using Taylor's expansion the system is linearized around the steady state U_c. we obtain $\Delta U' = U'(t) = F(U) = F(Uc) + \nabla F(U)_{Uc}(U - Uc) + O(||U - Uc||^2)$,

where

$$\nabla F(U) = \begin{pmatrix} \frac{\partial F1}{\partial x} & \frac{\partial F1}{\partial y} \\ \frac{\partial F2}{\partial x} & \frac{\partial F2}{\partial y} \end{pmatrix} = \begin{pmatrix} 2xy - (b+1) & x^2 \\ b - 2xy & -x^2 \end{pmatrix}, F(Uc) = 0$$

Assuming small variations ΔU, the term $O(||U - Uc||^2)$ can be neglected, leading to the linear differential system

$$\begin{cases} \Delta U' = J\Delta U, \\ \Delta(0) = \Delta_0, \end{cases} \tag{4.8}$$

where the Jacobian matrix $J = \nabla F_{U_{Uc}}$ is in this case

$$J = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix} \tag{4.9}$$

In the case that J is diagonalizable, it can be decomposed as $J = MDM^{-1}$,where $D_{ij} = \lambda_i \delta_{ij}$ and its integer powers are $J^n = MD^nM^{-1}$ for n > 0.

The exponential of a matrix J is,

$$\exp(J) = 1 + J + \frac{J^2}{2!} + \frac{J^3}{3!} + \cdots = \sum_0^\infty \frac{1}{n!} J^n.$$

Hence,

$$e^J = \sum_{n=0}^{\infty} \frac{1}{n!} J^n = \sum_{n=0}^{\infty} \frac{1}{n!} MD^nM^{-1} = M(\sum_{n=0}^{\infty} \frac{1}{n!} D^n)M^{-1} = Me^DM^{-1}$$

where e^D is the diagonal matrix $(e^D)_{ij} = \delta_{ij} e^{\lambda i}$, formed out of the exponential of the eigenvalues of the matrix J.

So,the differential system (4.8) can be directly integrated:

$$\Delta U' = J\Delta U, \Delta(0) = \Delta_0$$

$$\int \frac{\Delta U'}{\Delta U} = \int J dt$$

$$\ln \Delta U = Jt + \ln \Delta(0)$$

$$\Delta U = e^{Jt}\Delta(0), \quad \Delta(0) = \Delta_0$$

$$\Delta U = e^{tJ}\Delta_0 \tag{4.10}$$

The long-time behavior is obtained by making $t \longrightarrow +\infty$ in the exact solution (4.10) of the linearized system (4.8). If all eigenvalues λ of J have negative real part, then $e^{\lambda t} \longrightarrow 0$ as $t \longrightarrow +\infty$. Therefore the matrix $e^{Jt} = Me^{Dt}M^{-1} \longrightarrow 0$ as $t \longrightarrow +\infty$ and the solution ΔU goes to 0.The Taylor expansion around the critical point is valid in this case, and the solution of the non-linear system (4.7) tends toward the steady-state.

In order to evaluate the stability of the stationary state $(a, \frac{b}{a})$, the eigenvalue equation of the Jacobian matrix J is expressed as the roots of the characteristic polynomial

$$|J - \lambda I| = 0$$

where the λ's are the eigenvalues and I is the identity matrix.

Arranging these values into matrix form gives:

$$det \begin{pmatrix} (b-1)-\lambda & a^2 \\ -b & -a^2-\lambda \end{pmatrix} = 0 \tag{4.11}$$

which has the characteristic equation

$$\lambda^2 + \lambda(a^2 - b + 1). + a^2 \tag{4.12}$$

Equation (4.12) has the form

$$\lambda^2 - \tau\lambda + \delta = 0 \tag{4.13}$$

where, $\tau = b - 1 - a^2$ and $\delta = a^2$ are the trace and determinant of the Jacobian matrix at equilibrium respectively.

After solving for equation (4.13), one obtains

$$\lambda_{\pm} = \frac{\tau \pm \sqrt{\triangle}}{2} \tag{4.14}$$

where $\triangle = \tau^2 - 4\delta = (a^2 - b + 1)^2 - 4a^2$ is the discriminant of the Jacobian at equilibrium. For $\tau > 0$ the fixed point is unstable, while for $\tau < 0$ it is stable. Changing the stabilit y at τ = 0 , we find the steady-state parameter values by the equation $b = 1 + a^2$. The determinant δ is always positive. The linearized equation in the neighborhood of this point is unstable if and only if $b > a^2 + 1$.

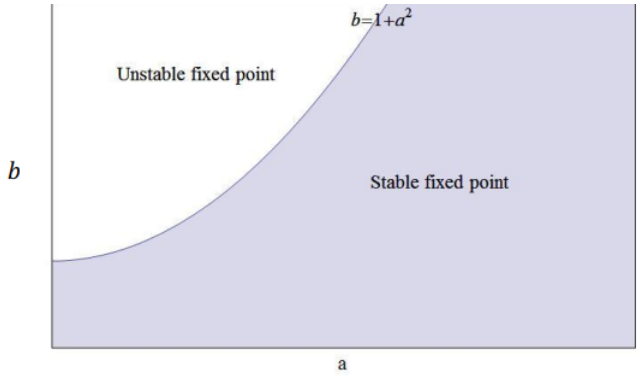

Figure 4.2: Stability regions of the Brusselator system as a function of parameters a and b.

Table 4.2: Nature of the steady state and existence of the limit cycle.

Region	τ	$\triangle$	Eigenvalues	types of critical value	limit cycle exist
1	>0	≥ 0	positive real	unstable node	yes
2	>0	<0	positive real parts	unstable focus	yes
	$=0$		purely imaginary	critical point	no
3	<0	<0	negative real pats	stable focus	no
4	<0	≥ 0	negative real	stable node	No

In particular, if b takes the critical value $b > a^2 + 1$, then the trace is zero, i.e., the equilibrium is on the borderline between a stable and an unstable focus (see fig 4.2). For values of b below the critical value, the equilibrium is stable. Increasing b beyond the critical value destabilizes the equilibrium such that it becomes an unstable focus, and the concentrations of x and y start to oscillate.Since as parameter b increases, the steady state turns from stable node to a stable focus, then it loses its stability (the system evolves towards a limit cycle) and the steady state turns from an unstable focus to an unstable node.

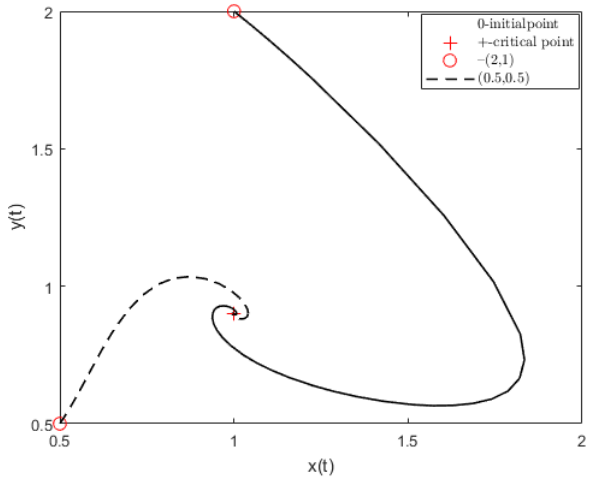

Figure 4.3: Simplified Brusselator model, stable case,a=1,b=0.9, Parametric curves $(x, y)^T$ for two different initial conditions, $(2, 1)^T$and$(0.5, 0.5)^T$.

The figure (4.3)shows the behavior of component y versus the component x for two different initial conditions. The two trajectories converge toward the same critical point of coordinates $(a, \frac{b}{a})$ = (1, 0.9).

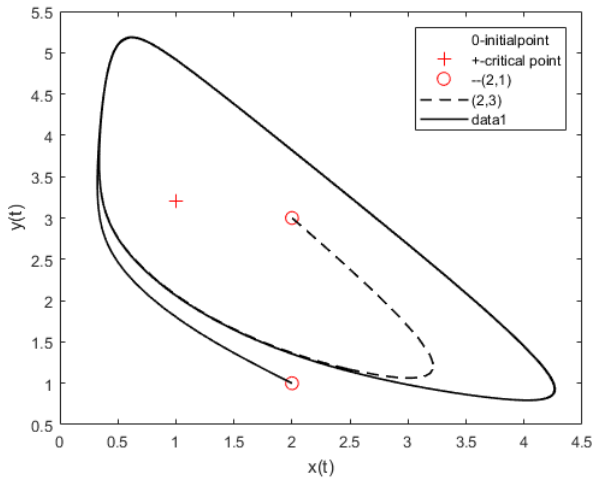

Figure 4.4: Simplified Brusselator model, unstable case a= 1, b = 3.2. Parametric curves $(x, y)^T$ for two different initial conditions, $(2, 1)^T$ and $(2, 3)^T$

Figure (4.4) numerically illustrates that this cycle does not depend on initial conditions but only on the parameters a and b. As they get closer to the instability limit ($b = a^2 + 1$), the limit cycle becomes smaller and eventually collapses into the critical point.
Further,for $b > a^2 + 1$ there must be a limit cycle occurs, when b approaches $a^2 + 1$. Then the limit cycle becomes smaller and smaller ,and finally disappears in the critical point.

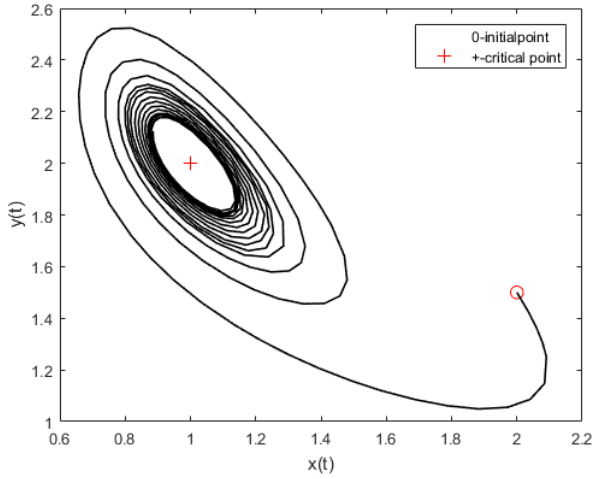

Figure 4.5: Solutions of the Brusselator,a=1,b=3.

For these values of the parameters a and b, the solution is converging toward the equilibrium point. For larger values of b the solution to the equations is a limit cycle in which the values of x and y cycle around the unstable equilibrium point.

4.1.2 Andronov-Hopf bifurcation Analysis

Theorem 4.1.1 (Hopf Bifurcation Criteria,[7, 22]) *Suppose an equilibrium $(a, b/a)$ of the system*

$$x' = f(x, y, a, b)$$
$$y' = g(x, y, a, b)$$

loses stability as the parameter b passes through a critical value b_{AH}(increasing or decreasing) and does so because a pair of complex conjugate eigenvalues

$$\lambda(a, b) = \alpha(a, b) + i\beta(a, b)$$

of the Jacobian evaluated at the equilibrium crosses transversely from the left to the right half complex plane (or vice versa).
By this is meant

$$\alpha(a, b_{AH}) = 0, \beta(a, b_{AH}) \neq 0, \frac{d\alpha}{db} \mid_{b=b_{AH}} \neq 0$$

Then limit cycles bifurcate from the equilibrium at $b = b_{AH}$. These limit cycles exist for b(near and) either greater than or less than b_{AH}. The cycles encircle the equilibrium, have amplitudes that shrinks to zero and periods that approach $\frac{2\pi}{\beta(b_{AH})}$ as $b \longrightarrow b_{AH}$.

To study the stability nature of Hopf bifurcation, we change the coordinate twice: first to bring the point$(a, b/a)$to the origin and then to put the vector field into standard form.
The equilibrium point $(a, b/a)$ undergoes a change in stability as varies when is kept fixed. Let first approximate $f(x, y)$ and $g(x, y)$ linear Taylor series polynomials centered at an equilibrium $(a, \frac{b}{a})$.These polynomials are

$$f(a, \frac{b}{a}) + m(x - a) + n(y - \frac{b}{a})$$
$$g(a, \frac{b}{a}) + c(x - a) + d(y - \frac{b}{a})$$

where coefficients are calculated from the derivatives of f and g by the formulas

$$m = \frac{df}{dx} \mid_{(a,\frac{b}{a})}, n = \frac{df}{dy} \mid_{(a,\frac{b}{a})}, c = \frac{dg}{dx} \mid_{(a,\frac{b}{a})}, d = \frac{dg}{dy} \mid_{(a,\frac{b}{a})} . \tag{4.15}$$

Since $f(a, \frac{b}{a}) = 0$ and $g(a, \frac{b}{a}) = 0$, the Taylor polynomial approximations become

$$f(x, y) \approx m(x - a) + n(y - \frac{b}{a})$$
$$g(x, y) \approx c(x - a) + d(y - \frac{b}{a}).$$

Using the notation

$$(x, y) \to (\bar{x}, \bar{y})$$
$$\bar{x} = x - a, \bar{y} = y - \frac{a}{b},$$

then $x = \bar{x} + a$, $Y = \bar{y} + \frac{a}{b}$

we obtain the autonomous, linear homogeneous system

$$\begin{cases} \bar{X}' = mx + ny \\ \bar{Y}' = cx + dy \end{cases} \tag{4.16}$$

as an approximation to the system $f'(x, y)$ and $g'(x, y)$. This autonomous, linear homogeneous system with coefficients given by the formulas (4.15), is called the linearization of $f'(x, y)$ and $g'(x, y)$ at the equilibrium $(a, \frac{b}{a})$.

If we then rename $\bar{y}' = y'$ and $x' = \bar{x}'$, the system becomes

$$\begin{cases} \bar{x}' = a + (\bar{x} + a)^2(\bar{y} + \frac{b}{a}) - (b + 1)(\bar{x} + a) \\ \bar{y}' = b(\bar{x} + a) - (\bar{x} + a)^2(\bar{y} + \frac{b}{a}). \end{cases} \tag{4.17}$$

This implies

$$\bar{x}' = \bar{x}b - \bar{x} + a^2\bar{y} + \frac{b}{a}\bar{x}^2 + 2\bar{x}\bar{y}a + \bar{x}^2\bar{y}$$
$$\bar{y}' = b\bar{x} + a^2\bar{y} - \frac{b}{a}\bar{x}^2\bar{y} - \bar{x}^2 - 2\bar{x}\bar{y}a.$$

or ,in the normal form

$$\begin{pmatrix} \bar{x}' \\ \bar{y}' \end{pmatrix} = \begin{pmatrix} (b-1) & a^2 \\ -b & -a^2 \end{pmatrix} \begin{pmatrix} \bar{x} \\ \bar{y} \end{pmatrix} + \begin{pmatrix} \frac{b}{a}X'^2\bar{y} + \bar{x}^2 + 2a\bar{y}\bar{x} \\ -\frac{b}{a}X'^2 - \bar{y}\bar{x}^2 - 2A\bar{y}\bar{x} \end{pmatrix}. \tag{4.18}$$

The coefficient matrix of the linear part for (4.17)is

$$J = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix}$$

The eigenvalues of the Jacobian matrix are

$$\lambda_{\pm(a,b)} = \frac{b - a^2 - 1 \pm \sqrt{\triangle}}{2}, with \ \triangle = (a^2 - b + 1)^2 - 4a^2. \tag{4.19}$$

$$\alpha(a, b) = Re(\lambda_{\pm(a,b)}) = \frac{b - 1 + a^2}{2}$$
$$\beta(a, b) = Im(\lambda_{\pm(a,b)}) = \frac{\pm\sqrt{a^2 - b + 1)^2 - 4a^2}}{2}$$

In this case, we expect to see the bifurcation when $b = b_{AH} = 1 + a^2$. For $b < b_{AH}$, the equilibrium point is a stable focus, while it is an unstable focus for $b > b_{AH}$.

An Andronov-Hopf bifurcation will occur when $\alpha(a, b)$ the real part of the eigenvalue of (4.19)changes sign,i.e. when it passes through zero.

Next, we verify the conditions for Hopf bifurcations at $b = b_{AH} = 1 + a^2$

(i) $\alpha(b_{AH}) = 0, \beta(b_{AH}) = \pm ai \neq 0$ (non-hyperbolicity condition: conjugate pair of imaginary eigenvalues)

Therefore, the eigenvectors corresponding to the above eigenvalues are $\begin{pmatrix} 1 \\ \pm ai \end{pmatrix}$.

(ii) $\frac{\partial}{\partial b} Re(\lambda) = d = \frac{1}{2} \neq 0$ (transversality condition: the eigenvalues cross the imaginary axis with non-zero speed).

(iii) Then, using the linear transformation

$$\begin{pmatrix} \bar{x} \\ \bar{y} \end{pmatrix} = T \begin{pmatrix} u \\ v \end{pmatrix}$$

where $T = \begin{pmatrix} 0 & a^2 \\ a & -b+1 \end{pmatrix}$ is the matrix of real and imaginary parts of the eigenvectors of the eigenvalues (4.18) , we obtain the system in standard form as:

$$\begin{pmatrix} u' \\ v' \end{pmatrix} = \begin{pmatrix} 0 & -a \\ a & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} (-3 + 3b + a^2 b - 3a)v^2 \\ ((2-b)av^2 + a^3 uv^2 + (1-b)a^2 v^3 + 2a^2 uv) \end{pmatrix} \tag{4.20}$$

Where the nonlinear parts of the (4.20) are

$$f(u, v) = (-3 + 3b + a^2 b - 3a)v^2$$
$$g(u, v) = ((2-b)av^2 + a^3 uv^2 + (1-b)a^2 v^3 + 2a^2 uv)$$

and we have the following

$f_u = 0, f_{uu} = 0, f_{uuu} = 0, f_v = 0, f_{vv} = 0, f_{uv} = 1, f_{vvv} = 0, g_u = 0, g_{uu} = 0, g_{uuv} = 0, g_v = 0, g_{vv} = 0, g_{vvv} = 6(1-b)a^2, g_{uv} = 2a^2$

Substituting these in the relation

$$l = \frac{1}{16}(f_{uuu} + f_{uvv} + g_{uuv} + g_{vvv}) + \frac{1}{16\omega}(f_{uv}(f_{uu} + f_{vv}) - g_{uv}(g_{uu} + g_{vv}) - f_{uu}g_{uu} + f_{vv}g_{vv})$$

with $f_{uv} = (\frac{\partial^2 f_{B_{AH}}}{\partial u \partial v}) \mid b = b_{AH}(a, \frac{b}{a})$, etc. (genericity condition)

$l = -\frac{a^2(a^2+2)}{8} < 0$

which shows that the Hopf bifurcation is supercritical.

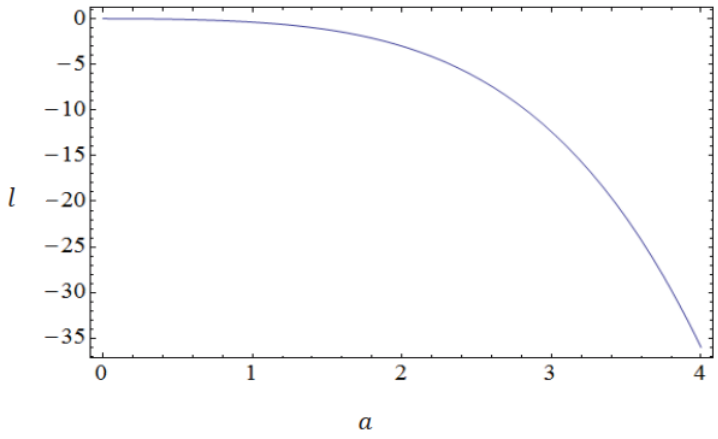

Figure 4.6: Coefficient 'l' vs. parameter 'a' plot.

The bifurcation is therefore supercritical and we have a family of stable periodic orbits. Thus, we can conclude that the system undergoes supercritical Hopf bifurcation for parameter values given by $b = b_{AH} = a^2 + 1$.

Then a unique curve of periodic solutions bifurcates from the origin into the region $b > b_{AH}$ if $ld = -\frac{a^2(a^2+2)}{16} < 0$. The origin is a stable fixed point for $b < b_{AH}$and an unstable fixed point for $b > b_{AH}$ if $d = \frac{1}{2} > 0$ whilst the periodic solutions are unstable if the origin is stable on the side of $b = b_{AH}$ where the periodic solutions exist. The amplitude of the periodic orbits grows like $\sqrt{|\ b\ |}$ whilst their periods tend to $\frac{2\pi}{|a|}$ as $|b|$ tends to $|b_{AH}|$.

Figure (4.7) shows the behavior for $b < b_{AH}$. As expected, we get a stable focus.If we pick a value of b just a bit above b_{AH}, we get a small limit cycle which grows as we increase b figure (4.7-4.10).

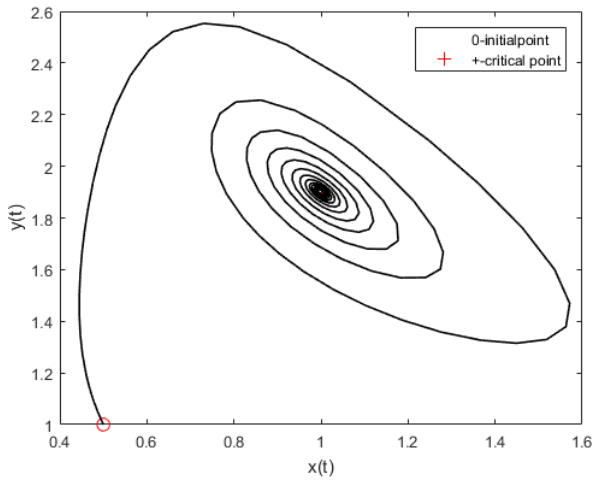

Figure 4.7: A trajectory in the phase plane for the Brusselator with a = 1, b = 1.9.

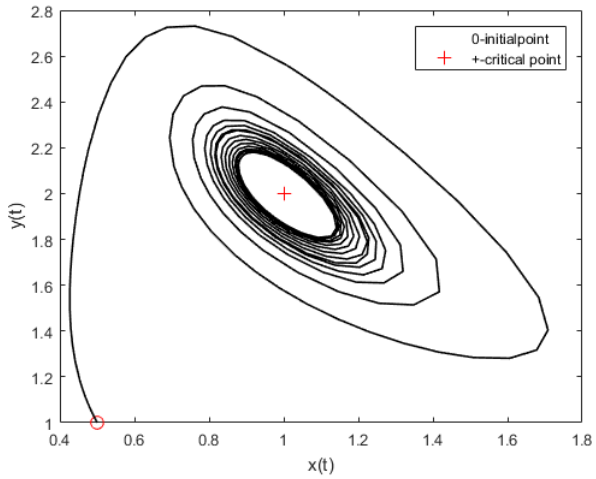

Figure 4.8: A trajectory in the phase plane for the Brusselator with a = 1, b = 2.001.

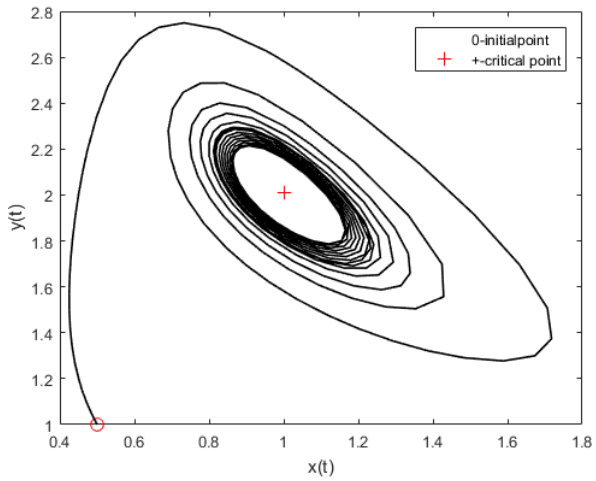

Figure 4.9: A trajectory in the phase plane for the Brusselator with a = 1, b = 2.01.

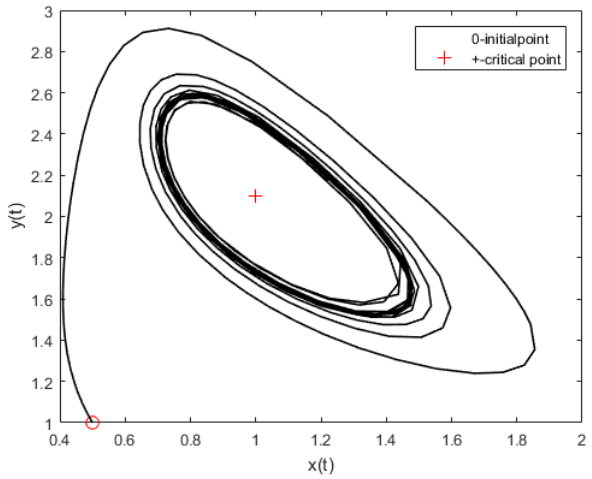

Figure 4.10: A trajectory in the phase plane for the Brusselator with a = 1, b = 2.1.

Figure(4.7-4.10) is an example of this procedure which shows clearly that the limit cycle grows as we move away from the bifurcation. Based on this behavior, we can conclude that the Andronov-Hopf bifurcation is supercritical.

4.2 Model for the Maintained Reaction

Consider now the system (4.1) with the hypothesis that no longer suppose that B is kept constant, but that component B is constantly injected in the mixture with rate v. The concentration of B as a function of time is denoted by z(t). The system of chemical reactions reduces to a new system of three equations:

$$\begin{cases} X' = A - (Z+1)X + X^2Y \\ Y' = XZ - X^2Y \\ Z' = -XZ + \upsilon \end{cases} \tag{4.21}$$

By scaling of the variables,

$$a = (\frac{\upsilon_1^2\upsilon_3}{\upsilon_4^3})^{\frac{1}{2}}A; z = \frac{\upsilon_2}{\upsilon_4}Z; x = (\frac{\upsilon_3}{\upsilon_4})^{\frac{1}{2}}X; y = (\frac{\upsilon_3}{\upsilon_4})^{\frac{1}{2}}Y; \tau = \upsilon_4 t$$

with $a > 0, \upsilon > 0$.

In dimensionless form, the dynamics of the Brusselator reaction can be described by a system of three ODEs are:

$$\begin{cases} x' = a - (z+1)x + x^2y \\ y' = xz - x^2y \\ Z' = -xz + \upsilon \end{cases} \tag{4.22}$$

4.2.1 Stationary-state Solutions and their Local Stability

The problem (4.22) now admits a steady state are given by computing the resulting system

$$x' = 0, y' = 0, z' = 0.$$

This implies,

$$\begin{aligned} a + x^2y - (b+1)x &= 0 \\ xz - x^2y &= 0 \\ -xz + \upsilon &= 0 \end{aligned}$$

We get

$$x = a, y = \frac{\upsilon^2}{a}, z = \frac{\upsilon}{a}.$$

Therefore, the steady state is $U_c = (a, v/a^2, v/a)^T$.

The Jacobian matrix of the right-hand-side function of the system (4.22) is

$$\nabla FU = \begin{pmatrix} \frac{\partial F1}{dx} & \frac{\partial F1}{dy} & \frac{\partial F1}{dz} \\ \frac{\partial F2}{dx} & \frac{\partial F2}{dy} & \frac{\partial F2}{dz} \\ \frac{\partial F3}{dx} & \frac{\partial F3}{dy} & \frac{\partial F3}{dz} \end{pmatrix} = \begin{pmatrix} 2xy - (z+1) & x^2 & -x \\ z - 2xy & -x^2 & x \\ -z & 0 & -x \end{pmatrix}$$

In order to study the stability of the system, this matrix is evaluated at the steady state (with assumption $a = 1, U_c = (1, v, v)^T$).

$$J = \begin{pmatrix} v-1 & 1 & -1 \\ -v & -1 & 1 \\ -v & 0 & -1 \end{pmatrix}$$

This matrix has $\lambda^3 + (3-v)\lambda^2 + (3-2v)\lambda + 1$ as characteristic polynomial by Routh-Hurwitz criteria and satisfies the condition for stability if and only if $v < \frac{(9-\sqrt{17})}{4} = 1.21922$.

Thus when v increases beyond this value, there arises a limit cycle which exists for all values of v up to approximately 1.5. When continues to grow, the limit cycle 'explodes' and $x \longrightarrow 0$ while y and $z \longrightarrow \infty$. So the system (4.4) has a behaviour completely different from the simplified model (4.22)

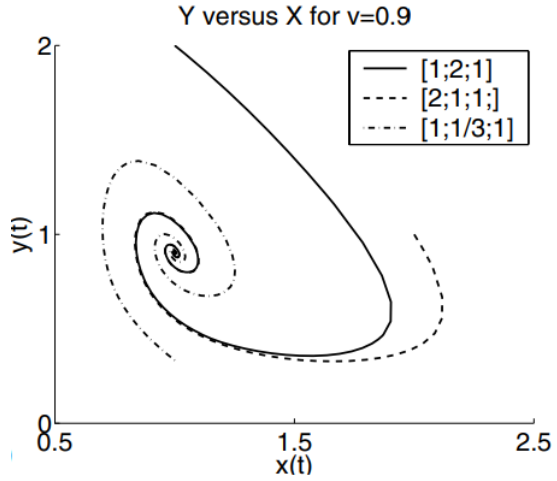

Figure 4.11: Brusselator model, stable case v =0 .9 Parametric curves $(x, y)^T$ for two different initial conditions, $(1, 2, 1)^T$ and $(2, 2, 2)^T$

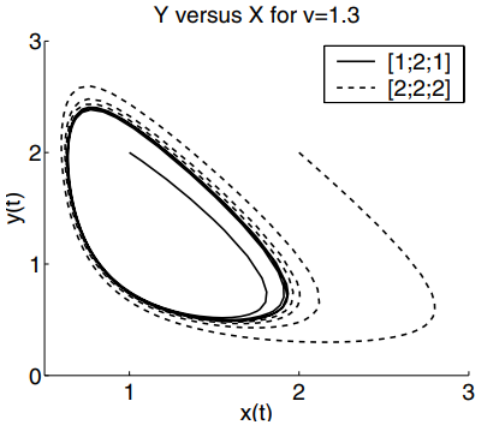

Figure 4.12: Brusselator model, unstable periodic case v =1.3 Parametric curves $(x, y)^T$ for two different initial conditions, $(1, 2, 1)^T$ and $(2, 2, 2)^T$

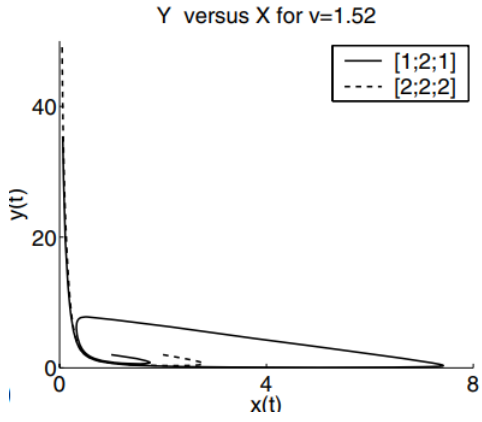

Figure 4.13: Brusselator model, unstable periodic case v =1.52 Parametric curves $(x, y)^T$ for two different initial conditions, $(1, 2, 1)^T$ and $(2, 2, 2)^T$

For instance the numerical solution if v = 0.9, the system is stable; therefore all three concentrations tend toward their equilibrium value $(U_c = (1, 0.9, 0.9)^T)$ and which shows the variations of y as a function of x, also points out the convergence toward the critical point, starting from several different initial conditions. For v = 1.3, the system is unstable, but the concentrations remain bounded. Their variation as a function of time is periodic and tends toward a limit cycle .Eventually, for $v > 1.5$, the system is unstable and divergent and the values of the concentrations y and z are unbounded for large times while the concentration x goes to 0. Thus when v increases beyond this value, there arises a limit cycle which exists for all values of v up to approximately 1.5.

Chapter 5

Conclusion

We have considered the stability nature of two dimensional non-linear differential equation, popularly known as the Brusselator model and analysis dynamical behavior of the model.The stability of Brusselator model with parameters a and b (4.4) depend on the concentration chemical corresponding initial conditions is stable if $b > a^2 + 1$ .The stability of new system (4.19) formed by hypothesis b kept constantly injected into system with rate v is stable $v < 1.21922$,besides to all concentration tend toward critical point other wise its unstable and concentration remains bounded or unbounded to large lines while concentration of x goes to zero. We justify the existence of Hopf bifurcationin a two dimensional nonlinear differential equation (4.4) with the help of Hopf bifurcation theorem and used the technique of Normal forms to show that supercritical Hopf bifurcation occurs in the system we have considered.

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