

# Pattern formation in the Brusselator model of chemical reactions

by

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Submitted in partial fulfillment of the requirements for the degree

Magister Scientiae

in the Department of Mathematics and Applied Mathematics  
in the Faculty of Natural and Agricultural Sciences

University of Pretoria  
Pretoria

March 2016

## DECLARATION

I, the undersigned, declare that the dissertation, which I hereby submit for the degree Magister Scientiae at the University of Pretoria, is my own work and has not previously been submitted by me for a degree at this or any other tertiary institution.

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**Date:**

# Summary

The Brusselator model is widely used to illustrate and study basic features of models of chemical reactions involving trimolecular steps. We provide the necessary mathematical theory related to Reaction-Diffusion systems in general and to the Brusselator model in particular. Specifically, the issues of local and global existence of solutions, their uniqueness and regularity are discussed in detail. The theoretical and numerical investigation presented further in the thesis provides an insight into the asymptotic behavior of the solutions of this model, characterizing the parameter region for each of the three qualitatively different cases: homogeneous steady state, Turing pattern and bulk oscillations. Particular attention is given to the supercritical Hopf bifurcation parameter domain where no substantial theory is available. This study was largely motivated by the observations of Young, Zhabotinsky and Epstein that Turing patterns eventually (for sufficiently small ratio of the diffusion coefficients) dominate the Hopf bifurcation induced bulk oscillations. In this work we confirm this observation and further establish more precisely the shape of the boundary separating the Turing pattern domain and the bulk oscillations domain in the parameter space. The obtained results are used in revealing an essential mechanism generating oscillating patterns in the coupled Brusselator model. It can be considered as a model of the reaction sequences in two thin layers of gel that meet at an interface. Each layer contains the same reactants with the same kinetics but with different diffusion coefficients. The occurrence of oscillating patterns is due to the fact that for the same values of the parameters of the model but with different diffusion coefficients the one system can be in the Turing pattern domain while the other is in the bulk oscillations domain. Hence, roughly speaking, one layer provides a pattern while the other layer drives the oscillations.

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The second law of thermodynamics states that an isolated system in time will eventually reach the state of "thermodynamic equilibrium", this corresponds to maximum disorder. The question that naturally arises is how is it then possible for evolutionary processes to increase in complexity and order as time progress. The keywords here are - isolated system. The Nobel Laureate Ilya Prigogine [8] wrote the following on this issue: "From the simplest bacterial cell to man, maintenance of life requires a continuous exchange of energy and matter with the surrounding world. Living organisms belong, therefore, to the class of open systems". This is why we have countless examples where non-equilibrium are the source of order. Describing this spatial and temporal self-organization observed in physical systems is vital in order to understand physical and biological processes.

The main situation of interest for us here is the case of chemical reactions. Chemical reactions can oscillate spontaneously. In the 1950's when Soviet biochemist Boris Belousov announced this discovery he sounded more like an alchemist in pursuit of the philosopher's stone. He chanced upon this oscillating chemical reaction while looking for an inorganic analogue of the biochemical citric acid cycle. Luckily, Woodstock and the moon landing (officially) have already happened and we can now claim mathematically without the patronage for immortality potion recipes that this is indeed true. When Belousov finally managed to publish his discovery in an obscure Russian medical meeting, it was still thought that all solutions of chemical reagents must go monotonously to a homogeneous stable equilibrium. It was only later when Anatol Zhabotinsky presented his work at a conference in Prague in 1968, that he confirmed Belousov's claim. In fact it became known as the Belousov-Zhabotinsky reaction. Thirty years after the initial discovery Belousov and Zhabotinsky were awarded the Lenin Prize, the most prestigious award in the Soviet Union for accomplishments relating to science, literature, arts, architecture, and

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technology. This, unfortunately was 10 years after Belousov's death.

The Belousov-Zhabotinsky reaction involves more than twenty elementary reaction steps. Prigogine [8] wrote in his monograph that "the relation between the direction of time and dynamics is a subject of a highly technical character." Luckily Tyson (1985) reduced this system and it's analysis. Ilya Prigogine and his collaborators proposed an elegant model, known as the Brusselator. Essentially this is a theoretical auto-catalytic reaction described with only two differential equations. This approximation neglects the consumption of reactants but still exhibits the same properties observed in more complicated models such as the BZ-reaction. Should this consumption be included without replenishment then we will observe eventual "thermodynamic equilibrium". Therefore this simplified model captures a time interval of interesting reactant dynamics, much like a tape recorder playing an infinitely looping video clip. Isolating this interaction gives us the opportunity to mathematically describe the empirical observations.

Another striking phenomenon of instability of the "thermodynamic equilibrium" was first described by Allen Turing. His paper on the chemical basis of morphogenesis [19], published in 1952, was one of the first examples ever that studied instability with respect to diffusion. However, this work remained unknown outside the context of morphogenesis and was criticized on various ground. It is said that the origin of criticism arose from a bad choice of examples in the paper. However, the criticism does not touch on the essential ideas. Prigogine showed keen insight and immense enthusiasm when he wrote that "there is a deep and unexpected relation between the "chemistry" as studied by molecular biology and the "space-time structure" as determined by the mathematical properties of kinetic equations when various conditions are satisfied. It is this relation between chemistry, thermodynamics and mathematics that is so fascinating in the study of self-organization." He then continues to speculate that pre-biotic evolution corresponds essentially to a succession of instabilities leading to a level of increasing complexity, and allows for some philosophical ramblings when he states that in general evolution can be viewed as a problem in structural instability.

The Brusselator is the main focus for this thesis. This study was largely motivated by the article [24] dealing with the interplay between the reaction kinetics and the diffusion properties of the reactants. Change in the kinetic terms induces transition from stable steady state to oscillations, the so called Hopf bifurcation. Increasing the difference of the diffusion coefficients changes the stability of the spatially homogeneous steady state from stable to unstable (Turing bifurcation) and leading to the appearance of stable spatially heterogeneous steady states called Turing patterns. It's observed in [24] that Turing patterns eventually (for sufficiently small ratio of the diffusion coefficients) dominate the Hopf bifurcation induced bulk oscillations. In our work we confirm this observation and further establish more precisely the shape of the boundary separating the Turing pattern domain and the bulk oscillations



domain in the parameter space. The obtained results are used in revealing an essential mechanism generating oscillating patterns in the coupled Brusselator model. It can be considered as a model of the reaction sequences in two thin layers of gel that meet at an interface. Each layer contains the same reactants with the same kinetics but with different diffusion coefficients. The occurrence of oscillating patterns is due to the fact that for the same values of the reaction parameters but with different diffusion coefficients the one system can be in the Turing pattern domain while the other system is in the bulk oscillation domain. Hence, roughly speaking, one layer provides a pattern while the other layer drives the oscillations.

We provide the necessary mathematical theory related to Reaction-Diffusion systems in general and to the Brusselator model in particular. Specifically, the issues of local and global existence of solutions, their uniqueness and regularity are discussed in detail. The thesis is organised as follows Chapter 2 gives necessary background theory from Functional Analysis, Sobolev spaces, and Semigroup Theory. Chapter 3 deals with the existence, uniqueness and regularity of solutions of the abstract Cauchy problem. Chapter 4 looks at the qualitative analysis of reaction-diffusion systems. In Chapter 5 we apply and verify the theory using the Brusselator model. Lastly, Chapter 6 contains a numerical investigation of the interplay between the Hopf bifurcation and Turing instability in the Brusselator model and the coupled Brusselator model. This chapter was published as an article in the Elsevier journal *Mathematics and Computers in Simulation* [1].



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# Mathematical Preliminaries

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In this chapter we provide some of the essential mathematical background needed for proving the results in the subsequent chapters. The preliminaries on Functional Analysis are based on the book [5]. The short introduction to Sobolev spaces follows mostly [9]. The reference for most of the Semigroup theory is the book [10].

## 2.1 Functional Analysis

**Definition 2.1.1.** Let  $X$  be a vector space. A real valued function  $\langle \cdot, \cdot \rangle : X \times X \rightarrow \mathbb{R}$  is called an **inner product** if it has the following properties. Suppose  $x, y, z \in X$ , with  $\alpha, \beta \in \mathbb{R}$

- (a)  $\langle x, x \rangle \geq 0$
- (b)  $\langle x, y \rangle = \langle y, x \rangle$
- (c)  $\langle \alpha x + \beta y, z \rangle = \alpha \langle x, z \rangle + \beta \langle y, z \rangle$
- (d)  $\langle x, x \rangle = 0$  if and only if  $x = 0$

A vector space  $X$  with an inner product defined on it is shortly called an inner product space.

**Definition 2.1.2.** Let  $X$  be a vector space. A real valued function  $\|\cdot\| : X \rightarrow \mathbb{R}$  is called a **norm** if it has the following properties. Suppose  $x, y \in X$ , with  $\alpha \in \mathbb{R}$

- (a)  $\|x\| \geq 0$
- (b)  $\|\alpha x\| = |\alpha| \|x\|$

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$$(c) \|x + y\| \leq \|x\| + \|y\|$$

$$(d) \|x\| = 0 \text{ if and only if } x = 0$$

A vector space with a norm defined on it is shortly called a normed space

**Remark 1.** It is easy to show that an inner product on  $X$  defines a norm on  $X$  given by  $\|x\| = \langle x, x \rangle^{1/2}$

The convergence is defined in terms of norm as follows

**Definition 2.1.3.** Let  $X$  be a normed space. A sequence  $(x_n)$  in  $X$  is called **convergent** if there exists an  $x \in X$  such that for every  $\epsilon > 0$  there exist  $N(\epsilon) \in \mathbb{N}$  such that  $\|x_n - x\| < \epsilon$  for all  $n > N(\epsilon)$ . The element  $x$  is called the limit of  $(x_n)$  and we write  $\lim_{n \rightarrow \infty} x_n = x$

Linked to the concept of convergence is the concept of Cauchy sequence.

**Definition 2.1.4.** Let  $X$  be a normed space. A sequence  $(x_n)$  in  $X$  is called **Cauchy** if for every  $\epsilon > 0$  there exists  $N(\epsilon) \in \mathbb{N}$  such that  $\|x_n - x_m\| < \epsilon$  for all  $n, m > N(\epsilon)$

It is easy to see that every convergent sequence is a Cauchy sequence [5, pg.29, Theorem 1-4.5]. However the inverse is only true for the so called complete spaces.

**Definition 2.1.5** (Completeness). A normed space is called **complete** if every Cauchy sequence is convergent.

**Definition 2.1.6** (Hilbert space, Banach Space). An inner product space which is complete is called a Hilbert space. A normed space which is complete is called a Banach space.

Clearly, every Hilbert space is a Banach space. The completeness of normed spaces plays an important role in the existence of solution theory of PDEs discussed in Chapter 3. However, there we only deal with the issue of completeness of subspaces of given Hilbert spaces. In this case the completeness can be described by the next theorem.

**Theorem 2.1.1.** A subspace  $Y$  of a Banach space  $X$  is complete if and only if  $Y$  is closed in  $X$ .

*Proof.* [5, pg.67] □

**Theorem 2.1.2** (Cauchy-Schwartz inequality).

$$\|\langle x, y \rangle\| \leq \langle x, x \rangle^{1/2} \langle y, y \rangle^{1/2}$$

*Proof.* [5, pg.13] □

In finite dimensional vector spaces we have some very convenient properties as illustrated with the following theorems,

**Theorem 2.1.3.** *Suppose  $X$  is a finite dimensional vector space. Any two norms  $N_1, N_2$  are equivalent, that is there exist positive constants  $c_1$  and  $c_2$  such that.*

$$c_1 N_1(x) \leq N_2 \leq c_2 N_1(x)$$

*Proof.* [5, pg.75] □

**Remark 2.** *This equivalence of norms is not the case for an infinite dimensional vector space, which we can easily see if we consider the space  $L^2[0, 1]$  with norms*

$$\|f\| = \left( \int_0^1 f(x)^2 \right)^{\frac{1}{2}}, \quad \|f\|_{\infty} = \sup_{0 \leq x \leq 1} f(x).$$

*Consider,*

$$f(x) = \begin{cases} 1, & x = 0, \\ 0, & x \in (0, 1]. \end{cases}$$

*Clearly equivalence of norms collapses since  $\|\cdot\| = 0$  and  $\|\cdot\|_{\infty} = 1$ .*

## 2.2 Sobolev Spaces

We will concern ourselves mainly with the space  $L^2(\Omega)$ . This space was introduced by D. Hilbert in 1912 in connection with integral equations and is the earliest example of a Hilbert space. We assume that  $\Omega$  is an open subset of  $\mathbb{R}^n$ .

**Definition 2.2.1.** *A nonnegative measurable function  $f$  on  $\Omega$  is called Lebesgue integrable if its Lebesgue integral  $\int_{\Omega} f d\mu$  is finite.*

**Remark 3.** *For more on this the following light reading is recommended [2].*

**Definition 2.2.2.** *The vector space  $L^2(\Omega)$  consists of all the functions  $f$  such that  $f^2$  is Lebesgue integrable.*

**Theorem 2.2.1.** *The space  $L^2(\Omega)$  is complete w.r.t to the inner product,*

$$\langle f, g \rangle = \int_{\Omega} f g d\mu.$$

*Proof.* [2, pg. 118, Theorem 10] □

The above inner product defines a norm,  $\|f\| = \langle f, f \rangle^{1/2}$ , which is referred to as the  $L^2$ -norm. The following function space plays an important role in approximation theory of PDEs.

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**Definition 2.2.3.** A function  $f$  is in  $C_0^\infty(\Omega)$  if it is in  $C^\infty(\Omega)$  and the closure of the set  $\{x \in \Omega \mid f(x) \neq 0\}$  is contained in  $\Omega$ .

**Theorem 2.2.2.**  $C_0^\infty(\Omega)$  is dense in  $L^2(\Omega)$  with respect to the  $L^2$ -norm

*Proof.* [9, pg.49 Theorem 2.7] □

The next step to defining a Sobolov space is the idea of weak derivative, which is a generalization of the classical definition of a derivative.

**Definition 2.2.4.** Suppose  $u \in L^2(\Omega)$  and suppose there exists a  $v \in L^2(\Omega)$  such that

$$(u, \partial^\alpha \phi) = (-1)^{|\alpha|} (v, \phi) \quad \forall \phi \in C_0^\infty(\Omega).$$

Then  $v$  is called the weak derivative of order  $\alpha$  of  $u$  and is denoted by  $D^\alpha u$ . The set of functions in  $L^2(\Omega)$  with weak derivatives up to order  $m$  is denoted by  $W^m(\Omega)$ .

**Remark 4.** In Definition 2.2.4 we use the notation  $\partial^\alpha = \partial_1^{\alpha_1} \dots \partial_n^{\alpha_n}$  where  $\alpha = (\alpha_1, \dots, \alpha_n)$  is a vector of non-negative integers. Then  $|\alpha| = \alpha_1 + \dots + \alpha_n$  is the order of the derivative.

For clarity we consider the following example

**Example 2.2.1.** Suppose  $\Omega \subset \mathbb{R}^2$  and  $\alpha = (3, 2)$ , then we have  $\partial^\alpha u = \partial_1^3 \partial_2^2 u$  with the order of derivative  $|\alpha| = 5$

**Theorem 2.2.3.** Suppose  $u, v \in W^m(\Omega)$  then  $W^m(\Omega)$  is an inner product space with inner product defined as,

$$(u, v)_m = \sum_{|\alpha| \leq m} (D^\alpha u, D^\alpha v)$$

We finally reach the point of defining a Sobolov space, their importance comes from the fact that solutions of PDEs are found in Sobolov spaces and not necessarily continuous spaces with classical derivatives.

**Definition 2.2.5.** The vector space  $W^m(\Omega)$  with inner product  $\langle \cdot, \cdot \rangle_m$  is called a **Sobolov space**.

**Theorem 2.2.4.** The Sobolev space  $W^m(\Omega)$  is complete

**Definition 2.2.6.** Let  $H^m(\Omega)$  be the closure of  $C^m(\Omega)$  with respect to the  $W^m(\Omega)$  norm defined as  $\|\cdot\|_m = \sqrt{\langle u, u \rangle_m}$

**Definition 2.2.7.** Suppose  $\Omega \subset \mathbb{R}^n$ , then  $\Omega$  is called **star shaped** if there exists a  $p \in \Omega$  such that for any  $x \in \Omega$  the set  $\{tp + (1-t)x \mid t \in [0, 1]\} \subset \Omega$ .

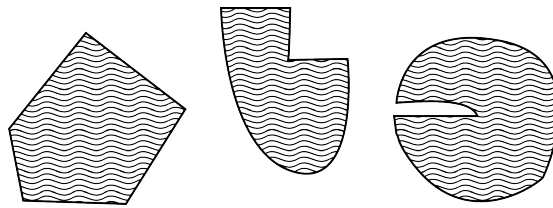
**Theorem 2.2.5.** If  $\Omega$  is star shaped, then  $H^m(\Omega) = W^m(\Omega)$

Next we describe the cone condition which is a sufficient condition for the domain in order to apply the Sobolev Embedding theorem,

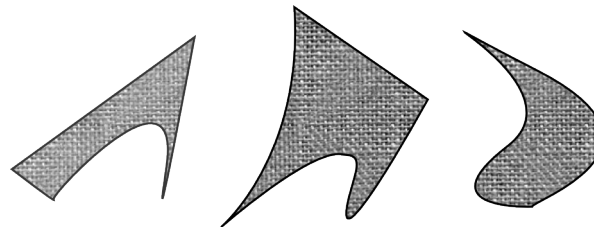
**Definition 2.2.8.** [9, pg. 60] An open bounded domain  $\Omega$  is said to satisfy the **cone condition** if there exists a cone  $C_r(x)$  of fixed dimensions, with radius  $r$  and vertex  $x$ , such that, when any point  $x \in \Omega$  is used as the vertex of the cone, the cone can be oriented so that all its points lie in  $\Omega$ .

**Remark 5.** In order to test if the cone condition holds for a domain  $\Omega \subset \mathbb{R}^2$ , one can think of an isosceles triangle with fixed dimensions. If, for each point  $x \in \Omega$  we can orientate the triangle in a such a way that it is completely contained in  $\Omega$ , then the cone condition is satisfied.

**Example 2.2.2.** We illustrate the cone condition for domains  $\Omega \subset \mathbb{R}^2$  with the figures below.



**Figure 2.1:** Domains that satisfy the cone condition



**Figure 2.2:** Domains that do not satisfy the cone condition

**Theorem 2.2.6.** Suppose  $\Omega$  is star shaped, then  $\Omega$  satisfy the cone condition.

We now state the Sobolev Embedding Theorem. This tells us what sort of regularity to expect from functions contained in specific Sobolev spaces.

**Theorem 2.2.7** (Sobolev Embedding Theorem(a)). Let  $u \in W^m(\Omega)$ ,  $\Omega$  bounded in  $\mathbb{R}^n$  and satisfying the cone condition, with  $2m \leq n$ . Let  $\Gamma_s$  be a smooth  $s$ -dimensional manifold of  $\Omega$  such that  $n - 2m < s \leq n$ . Then,

- (a)  $u \in L^k(\Gamma_s)$  for any  $k$  such that  $k < 2s/(n - 2m)$
- (b) The embedding of  $W^m(\Omega)$  into  $L^k(\Gamma_s)$  is compact

*Proof.* [9, pg.80, Theorem 3.9]

□

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**Theorem 2.2.8** (Sobolev Embedding Theorem(b)). *Let  $u$  be an arbitrary function in  $W^m(\Omega)$ ,  $\Omega$  bounded in  $\mathbb{R}^n$  and satisfying the cone condition. Then,*

(a) *If  $2m > n$  and  $0 < \|\beta\| < m - n/2$ , then  $D^\beta u(x)$  is continuous and a constant  $C_0$  can be found such that,*

$$\sup_{x \in \Omega} |D^\beta u(x)| \leq C_0 \|u\|_{W^m(\Omega)}$$

(b) *The embedding of  $W^m(\Omega)$  into  $\bar{C}^\beta(\Omega)$  is compact*

(c)  *$W^m(\Omega) \subset \bar{C}^{m-n/2-1}(\Omega)$*

*Proof.* [9, pg.80, Theorem 3.10]

□



## 2.3 Semigroup theory

The first paper on semigroups according to G.B Preston [13] was that of A.K Suschkewitch published in 1928 titled "On finite semigroups which are not necessarily cancellative", note this is translated from German using modern terminology. Since E. Hille and K. Yoshida established the characterization of generators of  $C_0$ -semigroups in the 1940s, semigroups of linear operators have developed into a beautiful abstract theory. Although sometimes difficult to apply, the fact that this abstract theory has many applications in partial differential equations provides motivation for its necessity as an integral discipline of both functional analysis and differential equations.

### 2.3.1 Semigroups of Linear Operators

**Definition 2.3.1.** *Let  $X$  be a Banach space. A family of bounded linear operators  $T(t)$  from  $X$  to  $X$  defined for  $t \geq 0$  is a **semigroup of bounded linear operators** on  $X$  if the following properties hold.*

(a)  $T(0) = I$ , ( $I$  is the identity operator on  $X$ )

(b)  $T(t + s) = T(t)T(s)$  for every  $t, s \geq 0$

**Definition 2.3.2.** *A semigroup of bounded linear operators,  $T(t)$ , is called **uniformly continuous** if,*

$$\lim_{t \rightarrow 0} \|T(t) - I\| = 0.$$

**Definition 2.3.3.** *Let  $X$  be a Banach space. A semigroup of bounded linear operators,  $T(t)$ , is called a **strongly continuous** semigroup of bounded linear operators if,*

$$\lim_{t \rightarrow 0^+} T(t)x = x \text{ for every } x \in X.$$

A strongly continuous semigroup of bounded linear operators,  $T(t)$ , is also called a  $C_0$ -semigroup.

**Remark 6.** *If  $T(t)$  is a  $C_0$ -semigroup then  $T(t)$  is not necessarily uniformly continuous.*

We consider following theorems for a  $C_0$ -semigroup to be continuous w.r.t time  $t$  for a fixed  $x \in X$ .

**Theorem 2.3.1.** *Let  $T(t)$  be a  $C_0$ -semigroup. There exist constants  $\alpha \geq 0$  and  $M \geq 1$  such that*

$$\|T(t)\| \leq Me^{\alpha t} \text{ for } 0 \leq t < \infty$$

## 2. MATHEMATICAL PRELIMINARIES

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*Proof.* [10, pg.4, Theorem 2.2] □

**Theorem 2.3.2.** *If  $T(\cdot)$  is a  $C_0$ -semigroup and  $x$  an arbitrary element in  $X$ , then  $T(\cdot)x \in C([0, \infty], X)$ .*

*Proof.* Let  $t \geq h > 0$  for an arbitrary  $x \in X$ , then we have,

$$\|T(t+h)x - T(t)x\| = \|T(t)T(h)x - T(t)x\| \leq \|T(t)\| \|T(h)x - x\|$$

Since  $T(\cdot)$  is a  $C_0$ -semigroup it follows from Theorem 2.3.1 that,

$$\|T(t+h)x - T(t)x\| \leq Me^{\alpha t} \|T(h)x - x\| \quad (2.1)$$

Similarly,

$$\begin{aligned} \|T(t)x - T(t-h)x\| &= \|T(t-h)T(h)x - T(t-h)x\| \\ &\leq \|T(t-h)\| \|T(h)x - x\| \\ &\leq Me^{\alpha(t-h)} \|T(h)x - x\| \end{aligned} \quad (2.2)$$

Then from (2.1) and (2.2) we have  $T(t)x$  is continuous for any  $t > 0$ . □

The application of this abstract theory to PDEs is closely related to the idea of an infinitesimal generator. This idea is essential in providing us with existence and uniqueness of solutions of abstract Cauchy problems.

**Definition 2.3.4.** *Consider a semigroup  $T(\cdot)$ . For  $h > 0$  we define a linear operator  $A_h$  as  $A_h x = h^{-1}(T(h) - I)x$ . Let*

$$D(A) = \{x \in X \mid \lim_{h \rightarrow 0} A_h x \text{ exists}\}$$

and define the operator  $A$  with domain  $D(A)$  as,

$$Ax = \lim_{h \rightarrow 0} A_h x \text{ for } x \in D(A).$$

The operator  $A$  is called the **infinitesimal generator** of  $T(\cdot)$ .

**Remark 7.** *We see that  $Ax$  is in a sense the right derivative of  $T(\cdot)x$  at 0*

The following two theorems provide us with useful properties of the infinitesimal generator of a  $C_0$ -semigroup.

**Theorem 2.3.3.** *Let  $T(\cdot)$  be a  $C_0$ -semigroup. If  $A$  is the infinitesimal generator of  $T(\cdot)$  then  $D(A)$  is a subspace of  $X$  and  $A$  is a closed linear operator.*

*Proof.* [10, pg.5] □

**Theorem 2.3.4.** *Suppose  $T(t)$  is a  $C_0$ -semigroup and let  $A$  be its infinitesimal generator. Then*

(a) For  $x \in X$ ,

$$\lim_{h \rightarrow 0^+} \frac{1}{h} \int_t^{t+h} T(s)x ds = T(t)x$$

(b) For  $x \in X$ ,  $\int_0^t T(s)x ds \in D(A)$  and

$$A \left( \int_0^t T(s)x ds \right) = T(t)x - x$$

(c) For  $x \in D(A)$ ,  $T(t)x \in D(A)$  and

$$\frac{d}{dt} T(t)x = AT(t)x = T(t)Ax$$

(d) For  $x \in X$ ,

$$T(t)x - T(s)x = \int_s^t T(\tau)Ax d\tau = \int_s^t AT(\tau)x d\tau$$

*Proof.* [10, pg. 5] □

We have from Theorem 2.3.1 that if  $T(t)$  is a  $C_0$ -semigroup there exist  $\alpha \geq 0$  and  $M \geq 1$  such that  $\|T(t)\| \leq Me^{\alpha t}$  for  $t \geq 0$ . Now if  $\alpha = 0$  then  $T(t)$  is called **uniformly bounded**, in fact if  $M = 1$  then we have the following definition.

**Definition 2.3.5.** A semigroup  $T(t)$  is called a  $C_0$  **semigroup of contractions** if,  $\|T(t)\| \leq 1$ , for  $t \in [0, \infty]$

**Definition 2.3.6.** Suppose  $A$  is a linear operator on  $X$ , the set of all complex numbers  $\lambda$  for which  $(\lambda I - A)$  is invertible on  $X$  is called the **resolvent set**  $\rho(A)$  of  $A$ . Also, the family  $A_\lambda = (\lambda I - A)^{-1}$ ,  $\lambda \in \rho(A)$  of bounded linear operators is called the **resolvent** of  $A$ .

Next we present the very important Hille-Yosida theorem which provides the necessary conditions for a linear operator to be an infinitesimal generator of a  $C_0$ -semigroup of contractions. The theorem is named after the mathematicians Einar Hille and Kosaku Yosida who both independently discovered the result around 1948.

**Theorem 2.3.5** (Hille-Yosida). A linear (unbounded) operator  $A$  is the infinitesimal generator of a  $C_0$ -semigroup of contractions if and only if the following conditions are satisfied.

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(a)  $A$  is closed and  $D(A)$  is dense in  $X$

(b) The resolvent set  $\rho(A)$  of  $A$  contains  $\mathbb{R}^+$  and for every  $\lambda > 0$

$$\|(\lambda I - A)^{-1}\| \leq \lambda^{-1}$$

*Proof.* [10, pg.8, Theorem 3.1] □

We present here some ideas contained in the proof of the Hille-Yosida theorem which lead to consequence. However the complete proof is quite elaborate and the reader can use the above reference should there be any further enquiry. The ideas presented are used to show that the conditions of the Hille-Yosida theorem are sufficient for  $A$  to be an infinitesimal generator.

**Definition 2.3.7.** For every  $\lambda > 0$  of the resolvent set  $\rho(A)$ ,  $A_\lambda$  of  $A$  is defined by

$$A_\lambda = \lambda(\lambda I - A)^{-1}A$$

$A_\lambda$  is called the **Yosida approximation** of an infinitesimal generator because of the following lemma.

**Lemma 2.3.6.** Let  $A$  satisfy the conditions of Theorem 2.3.5. If  $A_\lambda$  is the Yosida approximation of  $A$ , then

$$\lim_{\lambda \rightarrow \infty} A_\lambda x = Ax, \text{ for } x \in D(A).$$

*Proof.* [10, pg.10, Lemma 3.3] □

A consequence of Theorem 2.3.5 and its proof is that we can define a  $C_0$ -semigroup in terms of its infinitesimal generator using its Yosida approximation,

**Corollary 2.3.7.** Let  $A$  be the infinitesimal generator of  $T(t)$ , a  $C_0$ -semigroup of contractions. If  $A_\lambda$  is the Yosida approximation of  $A$ , then

$$T(t)x = \lim_{\lambda \rightarrow \infty} e^{tA_\lambda}x \text{ for } x \in X$$

*Proof.* [10, pg.11, Corollary 3.5] □

**Remark 8.** Applying the Hille-Yosida theorem is often challenging, the Lumer-Phillips theorem is much more suitable for this task. We will return to the Lumer-Phillips theorem at a later stage.

## 2.3.2 The abstract Cauchy problem

### 2.3.2.1 The homogeneous initial value problem

**Definition 2.3.8.** Let  $X$  be a Banach space and let  $A$  be a linear operator from  $D(A) \subset X$  into  $X$ . Given  $x \in X$ , finding a solution  $u(t)$  to the initial value problem

$$\begin{cases} \frac{du(t)}{dt} = Au(t) & t > 0, \\ u(0) = x. \end{cases}$$

is called the **abstract Cauchy problem** for  $A$ .

**Theorem 2.3.8.** Let  $A$  be the infinitesimal generator of a  $C_0$ -semigroup  $T(t)$ . Then  $u(t) = T(t)x$  is the unique solution to the abstract Cauchy problem for  $A$  with initial value  $u(0) = x$ .

*Proof.* It is clear from Theorem 2.3.4 that if  $A$  is an infinitesimal generator of a  $C_0$  semigroup the solution of the abstract Cauchy problem is  $u(t) = T(t)x$ . We verify this with a few simple steps:

$$u(t) = T(t)x \Rightarrow \frac{d}{dt}u(t) = \frac{d}{dt}T(t)x = Au(t).$$

For the initial condition we have  $u(0) = T(0)x = x$ . We proceed to prove uniqueness. Suppose  $u(t) = T(t)x$ ,  $v(t) = S(t)x$  are both solutions to the abstract Cauchy problem for  $A$ . Let  $z(t) = u(t) - v(t)$ , then we have

$$\left\| \frac{d}{dt}z(t) \right\| = \|Az(t)\| \leq \|A\| \|z(t)\|.$$

It follows from Gronwall's Inequality, that

$$\|z(t)\| \leq Ce^{\int_0^t \|A\| T(t) dt}$$

Now since  $z(0) = 0$  we have that  $C = 0$ . Therefore  $v(t) = u(t)$  □

### The inhomogeneous initial value problem

We consider the following initial value problem

$$\begin{cases} \frac{du(t)}{dt} = Au(t) + f(t), & t > 0 \\ u(0) = x \end{cases} \quad (2.3)$$

where  $f : [0, \bar{T}] \rightarrow X$ . We assume that  $A$  is the infinitesimal generator of a  $C_0$  semigroup  $T(t)$  so that the corresponding homogeneous equation, i.e  $f = 0$ , has a unique solution for every initial value  $x \in D(A)$ . Let us now consider the various notions of solution.

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**Definition 2.3.9.** [10, pg. 105] A function  $u$  is a **classical solution** of (2.3) on  $[0, \bar{T}]$  if  $u \in (C^1[0, \bar{T}], X)$ , i.e  $u$  is continuous on  $[0, \bar{T}]$ , continuously differentiable on  $[0, \bar{T}]$ ,  $u(t) \in D(A)$  for  $0 < t < \bar{T}$  and (2.3) is satisfied.

We consider (2.4) as a generalized solution if (2.3) is not differentiable on  $[0, T)$ . In order to prove this we first state the following useful proposition.

**Proposition 2.3.9.** Suppose  $T(\cdot)$  is a  $C_0$  semigroup with infinitesimal generator  $A$  and the function  $f$  is differentiable. Consider the function  $g$  given by  $g(t) = T(t + s)f(t)$ . If  $t + s > 0$ , then  $g$  is differentiable at  $t$  and

$$g'(t) = AT(t + s)f(t) + T(t + s)f'(t)$$

*Proof.*

$$\begin{aligned} h^{-1}(g(t + h) - g(t)) &= h^{-1}(T(t + s + h)f(t + h) \\ &\quad - T(t + s)f(t)) \\ &= h^{-1}T(t + s)(T(h)f(t + h) - f(t)) \\ &= h^{-1}T(t + s)(T(h)f(t + h) \\ &\quad - T(h)f(t)) + T(t + s)h^{-1}(T(h) - I)f(t) \end{aligned}$$

Now taking the limit,  $h \rightarrow 0+$  on both sides we get,

$$g'(\theta) = AT(\theta + \beta)f(\theta) + T(\theta + \beta)f'(\theta)$$

□

**Theorem 2.3.10.** Let  $A$  be the infinitesimal generator of a  $C_0$ -semigroup  $T(t)$ . Let  $x \in X$  and suppose  $f$  is integrable on  $X$ . The function  $u \in C([0, \bar{T}], X)$  given by

$$u(t) = T(t)x + \int_0^t T(t - s)f(s)ds, \quad 0 \leq t \leq \bar{T} \quad (2.4)$$

is a **mild solution** of the initial value problem (2.3) on  $[0, \bar{T}]$ .

*Proof.* Similiar to the proof in [10, pg.106]. Let  $g(s) = T(t - s)u(s)$  with  $t - s > 0$ . It follows from Proposition 2.3.9 that  $g(s)$  is differentiable. Therefore we have,

$$\begin{aligned} \frac{dg}{ds} &= -AT(t - s)u(s) + T(t - s)u'(s) \\ &= -AT(t - s)u(s) + T(t - s)Au(s) + T(t - s)f(s) \\ &= T(t - s)f(s) \end{aligned}$$

If  $f$  is integrable then,  $T(t-s)f(u(s))$  is integrable since  $f(u(s)) \in X \Rightarrow T(t-s)f(s) \in X$ . Now from Theorem 2.3.4(d), the equivalent of the fundamental theorem of calculus it follows that  $u(t) = T(t)x + \int_0^t T(t-s)f(s)ds$   $\square$

**Definition 2.3.10.** [10, pg. 109] A function  $u$  which is differentiable almost everywhere on  $[0, \bar{T}]$  with  $u'$  integrable on  $X$  is called a **strong solution** of the initial value problem (2.3) if  $u(0) = x$  and  $u'(t) = Au(t) + f(t)$  a.e on  $[0, \bar{T}]$ .

**Theorem 2.3.11.** Let  $A$  be the infinitesimal generator of a  $C_0$  semigroup  $T(t)$  on  $X$ . If  $f : [0, \bar{T}] \rightarrow X$  is continuously differentiable then the solution (2.4) of (2.3) with  $u_0 \in D(A)$  is a classical solution.

*Proof.* [10, pg.107]  $\square$

Suppose  $f$  is just locally Lipschitz then we have the following regularity theorem,

**Theorem 2.3.12.** Let  $A$  be the infinitesimal generator of a  $C_0$  semigroup  $T(t)$ . If  $f : [0, \bar{T}] \rightarrow X$  is differentiable a.e on  $[0, \bar{T}]$  and  $f'$  is integrable then for every  $x \in D(A)$  the initial value problem (2.3) has a unique strong solution.

*Proof.* [10, pg.109]  $\square$



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# Existence and uniqueness of the solution of the semilinear abstract Cauchy problem 3

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The question of existence and uniqueness is practically an important one and deeply mathematical. A formal proof for the existence of our solution assures us that our numerical approximation might have some validity. Suppose we don't know if we have a solution defined in finite time, then we won't be sure if the physical system will behave in the manner that our model predicts. Another important concept is that of global existence, having certainty of existence of solution for all  $t > 0$  means that it won't blow-up in space. This can be of dire consequence for some physical models like combustion or pressure models should we design a physical system based on a model without global existence. Another issue is non-uniqueness since this implies that we don't know how the model with initial setting will behave. This in turn ruins the predictive capabilities and possible usefulness of such model. We deal with these issues in the sections that follow.

We consider the abstract Cauchy problem for semilinear equations, of the form,

$$\begin{cases} \frac{du(t)}{dt} = Au + f(u), \\ u(0) = x, \end{cases} \quad (3.1)$$

where  $f : X \rightarrow X$  is locally Lipschitz. We also assume that  $A$  is the infinitesimal generator of a  $C_0$  semigroup. Using the same arguments as in Theorem 2.3.10 we see that,  $u \in C([0, \bar{T}], X)$  is a solution of (3.1) provided that for every  $t \in [0, \bar{T}]$  we have

$$u(t) = T(t)x + \int_0^t T(t-s)f(u(s))ds. \quad (3.2)$$

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### 3.1 Local existence of solutions

The first step to prove existence and uniqueness is to write the desired model in the form (3.1) using the ideas of Semigroup Theory. In order to achieve this abstraction we state and prove a list of useful propositions. The aim of the application of the propositions is to show that the model satisfy the conditions of the Lumer-Phillips theorem which we state and prove after the propositions. Applying the Lumer-Phillips theorem grants our abstracted model with the very important infinitesimal generator of a  $C_0$ -semigroup of contractions. This allows us to use a standard contraction mapping argument to show existence and uniqueness for a small interval in time. In this section we assume that the operator  $A$  is linear as well as dissipative, i.e.  $\langle Ax, x \rangle \leq 0$  for any  $x \in X$ . Further,  $Q, Y, Z$  denote linear operators. The domain, the range and the nullspace of a linear operator  $Q$  are denoted by  $\mathcal{D}(Q)$ ,  $\mathcal{R}(Q)$  and  $\mathcal{N}(Q)$ , respectively. The adjoint operator of  $Q$  is denoted by  $Q^*$ .

**Proposition 3.1.1.** *Let  $\lambda > 0$  and let  $\bar{A} = \lambda I - A$ . Then we have  $\lambda \|x\|^2 \leq \langle \bar{A}x, x \rangle$ .*

*Proof.* It follows from the dissipativity assumption that,  $\lambda \|x\|^2 \leq \lambda \|x\|^2 - \langle Ax, x \rangle = \langle \lambda x, x \rangle - \langle Ax, x \rangle = \langle \lambda x - Ax, x \rangle = \langle (\lambda I - A)x, x \rangle$   $\square$

**Proposition 3.1.2.** *Let  $Z$  be a linear operator. If  $\mathcal{D}(Z)$  is dense in a Hilbert space  $X$ , then  $\mathcal{R}(Z)^\perp = \mathcal{N}(Z^*)$ .*

*Proof.* Suppose that  $y \in \mathcal{R}(Z)^\perp$  then by definition we have  $\langle Zx, y \rangle = 0$ . Also, by definition of an adjoint operator we have,  $\langle Zx, y \rangle = \langle x, Z^*y \rangle \forall x \in \mathcal{D}(Z)$ . Since  $\mathcal{D}(Z)$  is dense in  $X$  we have  $Z^*y = 0 \Rightarrow y \in \mathcal{N}(Z^*) \Rightarrow \mathcal{R}(Z)^\perp \subseteq \mathcal{N}(Z^*)$ . Now, suppose  $y \in \mathcal{N}(Z^*)$  then by definition  $Z^*y = 0$ . Then,  $\forall x \in X$  we have  $0 = \langle x, 0 \rangle = \langle Z^*y, x \rangle = \langle Zx, y \rangle \Rightarrow y \in \mathcal{R}(Z)^\perp \Rightarrow \mathcal{N}(Z^*) \subseteq \mathcal{R}(Z)^\perp$ . Therefore  $\mathcal{R}(Z)^\perp = \mathcal{N}(Z^*)$   $\square$

**Proposition 3.1.3.**

*For every  $\lambda > 0$ , the nullspace of the adjoint operator of  $\bar{A} = \lambda I - A$  is trivial that is,  $\mathcal{N}(\bar{A}^*) = \{0\}$ .*

*Proof.* By Proposition 3.1.1 we have,  $\langle \bar{A}x, x \rangle \geq \lambda \|x\|^2$ . Now by definition of an adjoint operator,  $\langle x, \bar{A}^*x \rangle \geq \lambda \|x\|^2$ . Suppose that  $x \in \mathcal{N}(\bar{A}^*)$  then  $\langle x, \bar{A}^*x \rangle = \langle x, 0 \rangle = 0 \geq \lambda \|x\|^2 \Rightarrow \|x\| = 0 \Rightarrow x = 0$  by properties of a norm. Therefore  $\mathcal{N}(\bar{A}^*)$  is trivial.  $\square$

**Proposition 3.1.4.** *Let  $W$  be any closed subspace of a Hilbert space  $X$ . Then,*

$$W \oplus W^\perp = X$$

*Proof.* [5, pg.146] □

**Proposition 3.1.5.** *Let  $W$  be a closed subspace of  $X$ . Then  $(W^\perp)^\perp = W$ .*

*Proof.* Let  $x \in (W^\perp)^\perp, y \in W^\perp$  and  $z \in W$  then,  $\langle x, y \rangle = 0$  and  $\langle y, z \rangle = 0$  by definition, therefore  $z \in W \Rightarrow z \in (W^\perp)^\perp$ . Now since a orthogonal space is always closed it follows that  $(W^\perp)^\perp = W \Rightarrow W \subseteq (W^\perp)^\perp$ . Now  $(W^\perp)^\perp \subseteq X$ , so for any  $x \in (W^\perp)^\perp \exists y \in W^\perp, z \in W$  such that  $x = y + z$ , by proposition 3.1.4. Now, we have  $y = x - z$ , since  $z \in W \subseteq (W^\perp)^\perp$  and  $(W^\perp)^\perp$  is a vector space we have that  $y \in (W^\perp)^\perp$ . By assumption  $y \in W^\perp$  therefore,  $\langle y, y \rangle = 0 \Rightarrow y = 0 \Rightarrow x = z$ . Since  $x$  is arbitrary we have  $(W^\perp)^\perp \subseteq W$ . Therefore  $(W^\perp)^\perp = W$ . □

**Proposition 3.1.6.**

(i) *Let  $\lambda > 0$  and  $\bar{A} = \lambda I - A$ . If  $\langle \bar{A}x, x \rangle \geq \lambda \|x\|^2$  then  $\bar{A} = \lambda I - A$  is invertible.*

(ii) *Let  $\lambda > 0$  and  $\bar{A} = \lambda I - A$ . Suppose  $\mathcal{D}(\bar{A})$  is complete and  $\langle \bar{A}x, x \rangle \geq \lambda \|x\|^2$ . Then  $\mathcal{R}(\bar{A})$  is closed.*

(iii) *Supopose  $\mathcal{R}(\bar{A})$  is closed then  $\mathcal{R}(\bar{A}) = X$*

*Proof.*

(i) Follows directly from Proposition 3.1.3.

(ii) Suppose  $(x_n)$  is a Cauchy sequence in  $\mathcal{R}(\bar{A})$  then, by Proposition 2.1.6,  $\|x_n - x_m\| = \|\bar{A}\bar{A}^{-1}x_n - \bar{A}\bar{A}^{-1}x_m\| \geq \|\bar{A}^{-1}x_n - \bar{A}^{-1}x_m\|$ . Therefore  $(\bar{A}^{-1}x_n)$  is a Cauchy sequence  $\Rightarrow \lim_{n \rightarrow \infty} \bar{A}^{-1}x_n = z \in \mathcal{D}(\bar{A})$ , since  $\mathcal{D}(\bar{A}) = X$ , a complete space.  $\bar{A}z = \bar{A} \lim_{n \rightarrow \infty} \bar{A}^{-1}x_n = \lim_{n \rightarrow \infty} \bar{A}\bar{A}^{-1}x_n = \lim_{n \rightarrow \infty} x_n$ . This implies that  $\bar{A}z = x \in \mathcal{R}(\bar{A})$  and since  $(x_n)$  was arbitrary we have that  $\mathcal{R}(\bar{A})$  is closed.

(iii) By Proposition 3.1.5, we have  $\mathcal{R}(\bar{A}) = (\mathcal{R}(\bar{A})^\perp)^\perp$  therefore  $\mathcal{R}(\bar{A}) = (\mathcal{N}(\bar{A}^*))^\perp = \{0\}^\perp = X$ . □

**Proposition 3.1.7.** *Suppose  $Q, Y$  are closed linear operators then,*

(i)  *$Z = Q + Y$  is a closed linear operator.*

(ii)  *$kQ$  is a closed linear operator, for some  $k \in \mathbb{N}$*

*Proof.* (i) Suppose  $(x_n) \in \mathcal{D}(Q) \cap \mathcal{D}(Y)$  where  $x_n \rightarrow x$  as  $n \rightarrow \infty$ . We have  $Zx_n = (Q + Y)x_n = Qx_n + Yx_n$ . Let  $n \rightarrow \infty$  then we have  $Qx_n \rightarrow Qx$  and  $Yx_n \rightarrow Yx$ , since both are closed linear operators. Therefore  $Zx_n \rightarrow Qx + Yx = (Q + Y)x = Zx \Rightarrow Z$  is a closed linear operator. Similiar argument holds for (ii). □

Next we state and prove a special case of the Lumer-Phillips theorem.

### 3. EXISTENCE AND UNIQUENESS OF THE SOLUTION OF THE SEMILINEAR ABSTRACT CAUCHY PROBLEM

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**Theorem 3.1.8** (Lumer-Phillips). *A dissipative linear (unbounded) operator  $A$  is the infinitesimal generator of a  $C_0$  semi-group of contractions if the following conditions are satisfied*

- (i)  $\mathcal{D}(A)$  is dense in  $X$
- (ii) For each  $\lambda > 0$ ,  $\mathcal{R}(\lambda I - A) = X$

*Proof.* The aim here is to show that the properties of the Hille-Yosida theorem hold. We have that,  $(\lambda I - A)^{-1}$  is a bounded linear operator of  $X$  for each  $\lambda > 0$  bounded by  $\|(\lambda I - A)^{-1}\| \leq \lambda^{-1}$ . Next we proceed to show that  $A$  is a closed operator. Since the  $\mathcal{N}(\lambda I - A)$  is trivial we have that the operator  $\lambda I - A$  is injective. Now, together with  $\mathcal{R}(\lambda I - A) = X$  implies that  $\lambda I - A$  is a closed operator. This implies that  $A$  is a closed operator {From Proposition 3.1.9, in this case we let  $kQ = -(\lambda I - A)$  and  $Y = \lambda I$  such that  $Z = kQ + Y = A$ } Therefore both the conditions of the Hille-Yosida theorem is satisfied and we have that the dissipative operator  $A$  is the infinitesimal generator of a  $C_0$  semi-group of contractions.  $\square$

**Remark 9.** *We see therefore from the previous propositions that if we have a dissipative linear (unbounded) operator  $A$  and the domain of  $A$  is not just dense but also complete, that is  $\mathcal{D}(A) = X$ , then the second condition is also satisfied. This is especially useful for the application of the Lumer-Phillips theorem.*

**Definition 3.1.1.** [5, pg. 299] *An element  $x \in X$  is called a fixed point of a mapping  $\Psi : X \rightarrow X$  if  $x \in X$  is mapped onto itself, that is,*

$$\Psi x = x$$

**Definition 3.1.2.** [5, pg. 300 Definition 5.1-1] *Let  $M$  be a normed space. A positive mapping  $\Psi : X \rightarrow X$  is called a contraction on  $M$  if there is a positive real number  $\alpha < 1$  such that for all  $x, y \in M$*

$$\|\Psi x - \Psi y\| \leq \alpha \|x - y\|$$

**Theorem 3.1.9** (Banach Fixed Point Theorem). *Consider a Hilbert space  $X$ . Let  $\Psi : X \rightarrow X$  be a contraction on  $X$ . Then  $\Psi$  has precisely one fixed point.*

*Proof.* [5, pg. 300 Theorem 5.1-2]  $\square$

**Theorem 3.1.10.** *Let  $u_0 \in X$ . Then there exists a  $\delta > 0$ , such that (3.1) has a unique solution  $u \in C([0, \delta]; X)$ .*

*Proof.* based on [15] pg.115 . Let  $\delta > 0$  be arbitrary. We define a mapping  $\Psi$  from  $C([0, \delta], X)$  into itself,

$$(\Psi u)(t) = T(t)x + \int_0^t e^{(t-s)A} f(u(s)) ds, \quad 0 \leq t \leq \delta$$

We define  $S = \{u \in C([0, \delta], X), u(0) = x, \|u(t) - T(t)x\| \leq 1\}$ . Let

$$M = \sup_{\|u(t) - T(t)x\| \leq 1} \|f(u)\|$$

$$\begin{aligned} \|(\Psi u)(t) - T(t)x\| &= \left\| \int_0^t T(t-s) f(u(s)) ds \right\| \\ &\leq t \|T\| M \end{aligned}$$

We used here that, since  $T$  is a  $C_0$ -semigroup of contractions, we have  $\|T\| \leq 1$ . We see that  $\Psi$  maps  $S$  into  $S$  if we choose  $\delta \leq 1/2M$ . Furthermore,

$$\begin{aligned} \|\Psi u(t) - \Psi v(t)\| &= \left\| \int_0^t T(t-s) (f(u(s)) - f(v(s))) ds \right\| \\ &\leq \int_0^t \|T\| \|f(u(s)) - f(v(s))\| ds \\ &\leq \|T\| L \int_0^t \|u(s) - v(s)\| ds \\ &\leq tL \sup_{0 \leq t \leq \delta} \|u - v\|. \end{aligned}$$

We see that  $\Psi$  is a contraction on  $S$ . Let  $\delta \leq \min\{1/2M, 1/2L\}$ ,

$$\sup_{0 \leq t \leq \delta} \|\Psi u(t) - \Psi v(t)\| \leq 1/2 \sup_{0 \leq t \leq \delta} \|u(t) - v(t)\|.$$

It follows from Theorem 3.1.9 that  $\Psi$  has a fixed point. □

## 3.2 Global existence of solutions

### 3.2.1 Invariant Regions

Invariant regions are key to proving the existence of solutions for all  $t > 0$ . In this section we define invariant regions and state general theorems that will be used later on to prove global existence of specific systems.

**Definition 3.2.1.** A solution  $u(t)$  of (3.1) defined on  $[0, \bar{T})$  is called *maximal* if it cannot be produced beyond  $\bar{T}$ , that is, for any solution  $v(t)$ ,  $t \in [0, T_1]$  with  $u(0) = v(0)$  we have  $T_1 \leq \bar{T}$ .

### 3. EXISTENCE AND UNIQUENESS OF THE SOLUTION OF THE SEMILINEAR ABSTRACT CAUCHY PROBLEM

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**Definition 3.2.2.** A closed subset  $\Sigma \subset X$  is called an **invariant set** of (3.1) if for every  $x \in \Sigma$  the maximal solution on:  $[0, \bar{T}) \rightarrow X$ ,  $u$  of (3.1) with  $u(0) = x$  we have  $u(t) \in \Sigma$ ,  $t \in [0, \bar{T})$ .

**Corollary 3.2.1.** A closed subset  $\Sigma \subset X$  is invariant, provided that the directional vector of  $f$  of (3.1) points strictly into  $\Sigma$  on  $d\Sigma$ .

*Proof.* [15, pg. 202 Corollary 14.8] □

**Theorem 3.2.2.** Let  $f : X \rightarrow X$  be locally Lipschitz continuous in  $u$ . If  $A$  is the infinitesimal generator  $C_0$ -semigroup  $T(t)$  on  $X$  then for every  $u_0 \in X$  there is a  $\bar{T} \leq \infty$  such that the initial value problem (3.1) has a unique mild solution  $u$  on  $[0, \bar{T})$ . Moreover, if  $\bar{T} < \infty$  then

$$\lim_{t \rightarrow \bar{T}} \|u(t)\| = \infty$$

.

*Proof.* [10, Theorem 1.4, pg. 185] □

**Corollary 3.2.3** (Global existence). Suppose that the conditions in Theorem 3.2.2 hold. If  $\Sigma$  is a bounded invariant region, then for every  $x \in \Sigma$  the solution of (3.1) with  $u_0 \in \Sigma$  exist for all  $t \geq 0$  and  $u(t) \in \Sigma, t \geq 0$ .

**Theorem 3.2.4** (Regularity). Let  $A$  be the infinitesimal generator of a  $C_0$ -semigroup  $T(t)$  on  $X$ . If  $f : X \rightarrow X$  is continuously differentiable from  $X$  into  $X$  then the mild solution of (3.1) with  $u_0 \in \mathcal{D}(A)$  is a classical solution of the initial value problem.

*Proof.* [10, Theorem 1.5, pg. 187] □

# Peculiarities of reaction diffusion equations 4

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## 4.1 General Setting

In [7] Nicolis and De Wit describe reaction-diffusion systems based on the assumption of decoupling between two kinds of processes occurring on significantly variant scales. We can think of the evolution of the macroscopic variables, such as the concentrations or temperature described separately from the dynamics of interaction at the molecular level. This approach, referred to as the mean field description, takes the form,

$$\frac{\partial w}{\partial t} = f + D\nabla^2 w \quad (4.1)$$

$f : R^n \rightarrow R^n$  and  $D$  a  $n \times n$  diagonal matrix, where the two terms in the right hand side stand, successively, for the effect of reaction and of diffusion. For simplicity it is assumed that there is no effects due to external forces, that there are no cross effects in transport, that is why  $D$  is a diagonal matrix, and that Fick's or Fourier's laws adequately describe mass and heat diffusion. .

In the absence of spatial degrees of freedom diffusion is not possible. This implies that  $D$  is a zero matrix. Therefore the equations can be reduced to a set of coupled non-linear ordinary differential equations. Due to the possible intrinsic non-linearity of the reaction function  $f$ , complex behaviour persists, because of this, this reduced form of (4.1) has provided some of the earliest and most widely used models of bifurcation and chaos theories.

In the presence spatial degrees of freedom, that is  $D$  is a non-zero diagonal matrix, the equations (4.1) define a set of coupled non-linear partial differential equations of the parabolic type. Assuming physically viable boundary conditions they generate a wealth of spatial and temporal patterns. In order to demonstrate this Nicolis and De Wit [7] provide the following partial list of possible solutions that these type of equations possess.

#### 4. PECULIARITIES OF REACTION DIFFUSION EQUATIONS

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- (i) Wave fronts. The spatial coupling of elements possessing two stable steady states or a stable and an unstable one, gives rise to a wave front propagating from the stable or the most stable state toward the unstable or the least stable one. In the presence of locally oscillating or excitable kinetics the front may take some unexpected forms, from cylindrically symmetric patterns to spiral ones.
- (ii) Space-dependent stationary solutions. These arise through a symmetry-breaking instability of the homogeneous state, first proposed by Turing as a universal mechanism of biological morphogenesis.
- (iii) Synchronization, clustering and spatio-temporal chaos. These dynamical behaviours result from the spatial coupling of local elements each in a regime of periodic or chaotic oscillations, depending on the relative strength of diffusion and reactive terms.
- (iv) Composite patterns, such as localized structures and defects. They arise from the interference between two or more mechanisms of instability, as it happens for instance when a Turing instability interacts with one leading to time oscillations or to multiple steady states

This gives us reason to justify the statement that reaction-diffusion systems are at the forefront for understanding the origin of endogenous rhythmic and patterning phenomena observed in nature and in technological applications.

## 4.2 Turing Patterns in a two species model

In this section we'll focus our attention on the second item of the above list, these spatially inhomogeneous solutions was proposed as a model for the chemical basis of morphogenesis by Allen Turing [19] in one of the most important papers in theoretical biology of the previous century. His idea as described in [6] was that if in the absence of diffusion in (4.1) we have a stable uniform steady state then, with spatial degrees of freedom, inhomogeneous patterns can evolve due to a notable difference in the diffusion of the reactants. Murray [6] points out that diffusion is usually considered a stabilising process which is why this was such a novel concept. We consider the equation (4.1) with  $n = 2$  in the form,

$$u_t = \nabla^2 u + f(u, v) \quad v_t = d\nabla^2 v + g(u, v)$$

with Neumann boundary conditions,  $\nabla u = 0, \nabla v = 0$ . We are interested in this diffusion driven instability but to understand this mechanism we first discuss the stability conditions and linearisation of a reaction-diffusion system without diffusion. Therefore we have,

$$u_t = f(u, v) \quad v_t = g(u, v)$$



with the homogeneous steady state solution  $(u_0, v_0)$ , this implies that,

$$f(u_0, v_0) = 0 \quad g(u_0, v_0) = 0$$

We proceed to do a phase-plane analysis on a small perturbation of the homogeneous steady state in order to tell us more about the stability of the system. Let,

$$w = \begin{pmatrix} u - u_0 \\ v - v_0 \end{pmatrix}$$

for  $|w|$  small enough we have,

$$w_t = Jw, \quad J = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}_{u_0, v_0}$$

$J$  is called the stability matrix. This clearly indicates that we now look for solutions of the form

$$w = e^{\lambda t}$$

where  $\lambda$  is an eigenvalue of  $J$ . We see that if  $Re\lambda < 0$  then we have stability since  $w \rightarrow 0$  as  $t \rightarrow \infty$ . This leads us to the following linear stability theorem,

**Theorem 4.2.1.** *Suppose  $f, g : \mathbb{R}^2 \rightarrow \mathbb{R}$  and  $f, g$  are differentiable then the spatially homogeneous system defined as,*

$$u_t = f(u, v) \quad v_t = g(u, v)$$

*with steady state  $(u_0, v_0)$  and stability matrix  $J = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}_{u_0, v_0}$  will be linearly stable if the following conditions are satisfied,*

- (a)  $f_u + g_v < 0$
- (b)  $f_u g_v - f_v g_u > 0$

*Proof.* [6, pg. 82] □

The above Theorem is applicable to the behaviour of non-linear systems due to the Hartman-Grobman Theorem [16]. In a nutshell this theorem states that the dynamics of a non-linear system are equivalent to its linearisation when close enough to a hyperbolic fixed point. It shows that there exist a bijection from the solutions of the non-linear system to the solutions of the linearised one. Therefore, it can be said that the systems are locally topologically conjugate or in short, equivalent.

We state the Hartman-Grobman Theorem without proof including the required definitions for the sake of completeness.

#### 4. PECULIARITIES OF REACTION DIFFUSION EQUATIONS

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**Definition 4.2.1.** A fixed point is said to be **hyperbolic** if all eigenvalues of the stability matrix have non-zero real parts.

**Definition 4.2.2.** A bijective mapping between two manifolds is called a **homeomorphism** if it and its inverse are continuous.

**Definition 4.2.3.** A homeomorphism is called a **diffeomorphism** if both it and its inverse is differentiable.

**Theorem 4.2.2** (Hartman-Grobman Theorem). If  $G$  is a diffeomorphism with hyperbolic fixed point  $\bar{U}$  then there exists  $\delta > 0$ , a neighbourhood  $\mathcal{N}$  of the origin and a homeomorphism  $\mathcal{F} : B(\bar{U}, \delta) \rightarrow \mathcal{N}$  such that  $\mathcal{F}(G(U)) = \partial G(\bar{U})\mathcal{F}(U)$  for all  $U \in B$

### Inhomogeneous steady states

Now we can proceed to linearise a reaction system with diffusion,

$$w_t = Aw + D\nabla^2 w, \quad D = \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix} \quad (4.2)$$

with steady state  $w = 0$ . Also assume that  $d > 0$  in order for diffusion to physically make sense. If  $d < 0$  then either activator or inhibitor would contract on it's own and the activation-inhibition mechanism would no longer be applicable. In order to solve this system we define  $W$ , a time-independent solution of the spatial eigenvalue problem given by,

$$\nabla^2 W + k^2 W = 0, \quad (n \cdot \nabla)W = 0 \text{ on } \partial\Omega \quad (4.3)$$

where  $k$  is the eigenvalue. Suppose  $\Omega = [0, a]$ , then  $W = \cos(m\pi x/a)$ , where  $n$  is an integer.  $W$  clearly satisfies the zero flux boundary conditions and  $k = m\pi/a$ . The eigenvalue  $k$  is called the wavenumber since we can calculate the wavelength  $\omega = 2\pi/k = a/m$ .

**Remark 10.** The reason for choosing zero flux boundary conditions is to make sure that the inhomogeneous steady state that arise is due to the diffusion and not the boundary conditions.

Let  $W_k$  be the eigenfunction corresponding to the wavenumber  $k$ . We look for solutions of the form

$$w = \sum_k c_k e^{\lambda_k t} W_k \quad (4.4)$$

where the constants  $c_k$  are determined by a Fourier expansion of the initial conditions in terms of  $W_k$ . Note that  $\lambda_k$  is the eigenvalue which determines temporal growth. Now substituting (4.4) into (4.2) and using (4.3) we get,

$$\begin{aligned} \lambda W_k &= AW_k + D\nabla^2 W_k \\ &= AW_k - Dk^2 W_k \end{aligned}$$

In order to obtain the nontrivial solutions of  $W_k$  we determine  $\lambda$  as a root of a polynomial equation,

$$|\lambda I - A + Dk^2| = 0 \quad (4.5)$$

Writing out the left hand side,

$$\begin{aligned} & \left| \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix} - \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} + k^2 \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix} \right| \\ &= (\lambda^2 - f_u + k^2)(\lambda - g_v + k^2d) - f_v k^2 \\ & \quad + k^2\lambda - k^2g_v + k^4d - f_v g_u \\ &= \lambda^2 + \lambda[k^2(1 + d) - (f_u + g_v)] + h(k^2) \end{aligned} \quad (4.6)$$

where

$$h(k^2) = dk^4 - k^2(df_u + g_v) + |A| \quad (4.7)$$

then the roots of (4.5) are obtained in terms  $k$  in the form,

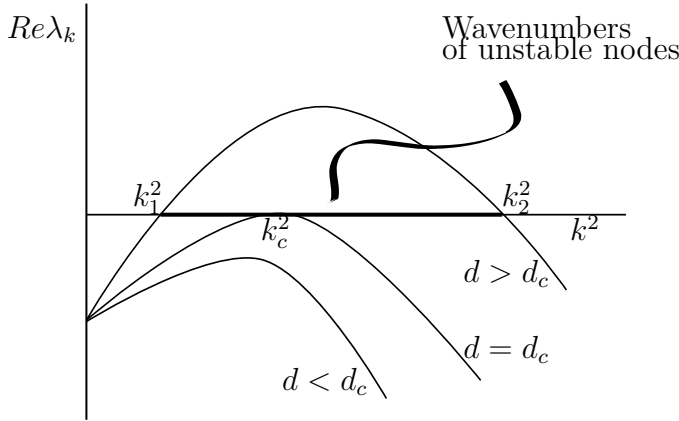
$$2\lambda = -[k^2(1 + d) - (f_u + g_v)] \pm \{[k^2(1 + d) - (f_u + g_v)]^2 - 4h(k^2)\}^{1/2} \quad (4.8)$$

**Remark 11.** *It is important to note the following. Since  $Re\lambda$  is now a function of  $k$ , and we have a solution of the form (4.4) it follows that for certain wavenumbers  $k$ ,  $W_k$  will grow exponentially while the rest will tend towards zero. The key assumption here is that  $W_k$  is bounded by the reaction kinetics therefore it will reach a stable solution. We note that even though diffusion is the cause of an instability it will eventually reach a stable inhomogeneous solution due to this boundedness.*

Let the conditions (a) and (b) in Theorem 4.2.1 hold. Then it follows from the theorem that the steady state  $(u_0, v_0)$  is stable. We will now proceed to show that diffusion can cause the steady state to become unstable. This can happen if the coefficient of  $\lambda$  in (4.6) is negative or if  $h(k^2) < 0$ . First we look at the coefficient of  $\lambda$ , that is  $k^2(1 + d) - (f_u + g_v)$ . Now for the first term we have that  $d > 0$ , this guarantees that  $k^2(1 + d) > 0$ . Looking at the second term we have that  $(f_u + g_v) < 0$ , this implies the positivity of  $\lambda$ 's coefficient. Therefore the only possibility left is  $h(k^2) < 0$ . We have from condition (b) that  $|A| > 0$  therefore we are left with the coefficient of  $k^2$ , namely  $(df_u + g_v) > 0$ . This is only possible if  $d \neq 1$  since condition (a) requires  $f_u + g_v < 0$ . Note that  $(df_u + g_v) > 0$  is a necessary but not sufficient condition for instability. In order for  $h(k^2) < 0$  we need  $h(k_m^2) < 0$  where  $h(k_m^2) < h(k^2)$  for all  $k$ . Therefore we proceed to differentiate  $h$  in terms of  $k^2$  to obtain,

$$h'(k^2) = 2dk^2 - (df_u + g_v)$$

#### 4. PECULIARITIES OF REACTION DIFFUSION EQUATIONS



**Figure 4.1:** Relationship between the real part of the eigenvalue,  $Re\lambda_k$ , and corresponding wavenumber,  $k^2$  with diffusion,  $d$ , acting as the driving force behind the activation of a band of wavenumbers.

Setting this equal to zero and solving  $k^2$  to obtain  $k_m^2$  and substituting back into  $h(k^2)$  leads to the following,

$$k_m^2 = \frac{df_u + g_v}{2d}, \quad h_m = |A| - \frac{df_u + g_v}{4d} \quad (4.9)$$

Therefore we see that the condition  $h(k^2) < 0$  implies that

$$|A| < \frac{(df_u + g_v)^2}{4d} \quad (4.10)$$

So in order to calculate the critical diffusion coefficient ratio  $d_c$  we let  $|A| = \frac{(df_u + g_v)^2}{4d}$  and obtain,

$$\begin{aligned} 4d(f_u g_v - f_v g_u) &= d^2 f_u^2 + 2df_u g_v + g_v^2 \\ 2df_u g_v - 4df_v g_u &= d^2 f_u^2 + g_v^2 \\ 0 &= d^2 f_u^2 - 2d(f_u g_v - 2f_v g_u) + g_v^2 \\ 0 &= d^2 f_u + 2d(2f_v g_u - f_u g_v) + g_v^2 \end{aligned}$$

Thus we have to solve the following polynomial, with  $d_c$  being the appropriate root,

$$f_u^2 d_c^2 + 2(2f_v g_u - f_u g_v) d_c + g_v^2 = 0$$

Now assuming that  $d > d_c$  we can use the roots of  $h(k^2)$  in order to calculate the interval of the activated wavenumbers (i.e  $\lambda(k) > 0$ ), given by

$$\begin{aligned} k_1^2 &= \frac{1}{2d} [(df_u + g_v) - \{(df_u + g_v)^2 - 4d|A|\}^{1/2}] < k^2 \\ &< \frac{1}{2d} [(df_u + g_v) + \{(df_u + g_v)^2 - 4d|A|\}^{1/2}] = k_2^2 \end{aligned}$$

Therefore we can now place bounds on the wavenumbers of our general solution (i.e  $k_1 < k < k_2$ ),

$$w = \sum_{k_1}^{k_2} c_k e^{\lambda_k t} W_k \quad (4.11)$$

Lastly, we state all the conditions necessary for diffusion driven instability of a two species reaction diffusion system,

- (i)  $f_u g_v - f_v g_u > 0$
- (ii)  $f_u + g_v < 0$
- (iii)  $df_u + g_v > 0$
- (iv)  $\frac{(df_u + g_v)}{4d} > |A|$

### 4.3 Limit Cycles of the reaction system

**Definition 4.3.1.** A closed trajectory is called a **limit cycle** if at least one other trajectory spirals towards the limit cycle as time approaches either infinity or negative infinity. We can divide limit cycles into stable, unstable and semi-stable, see the following for illustration

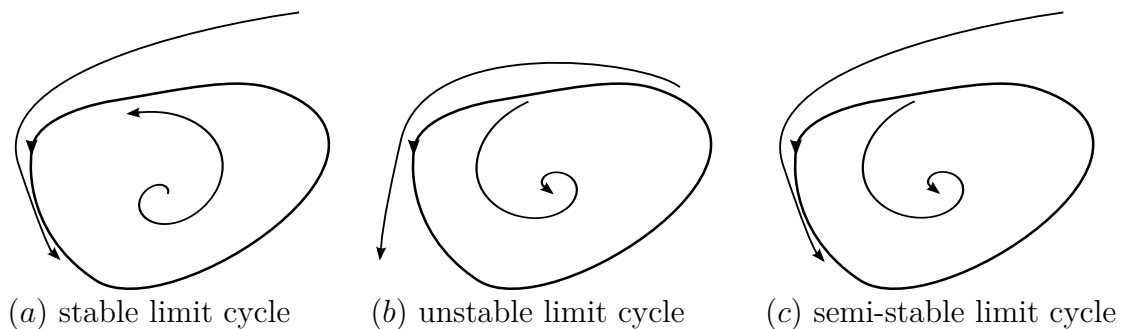


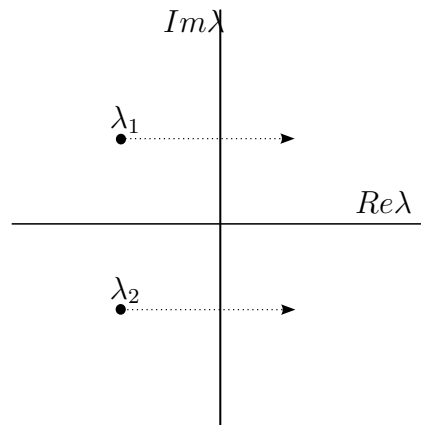
Figure 4.2

Limit cycles is self-sustaining without any periodic forcing (i.e external input). The Poincare-Bendixson theorem is used to show that limit cycles exist.

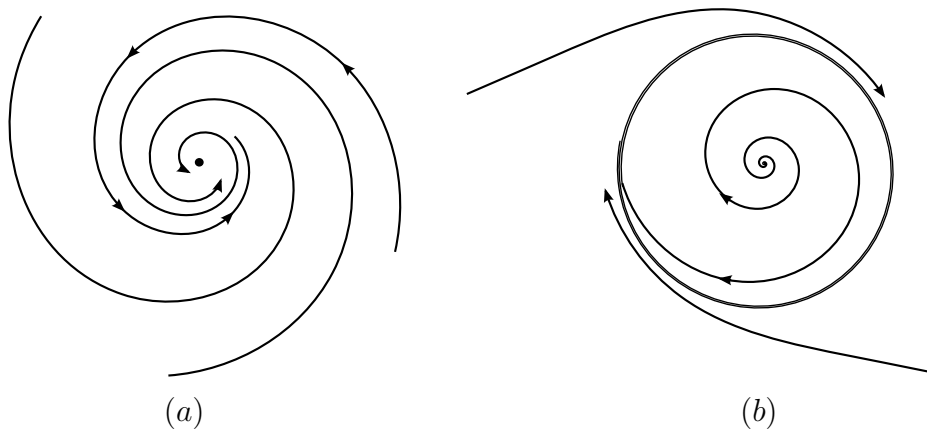
**Theorem 4.3.1** (Poincare-Bendixson). Suppose that  $\Omega$  is a closed bounded subset of the plane,  $x = f(x)$  is a continuously differentiable vector field on an open set containing  $\Omega$ ,  $\Omega$  does not contain any fixed points and there exists a trajectory  $C$  that is contained in  $\Omega$ , (i.e  $C$  starts in  $\Omega$  and stays in  $\Omega$  for all  $t > 0$ ). Then there exists a stable limit cycle contained in  $\Omega$ .

#### 4. PECULIARITIES OF REACTION DIFFUSION EQUATIONS

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**Figure 4.3:** Illustration of requirement for Hopf bifurcation



**Figure 4.4:** See definition 4.3.2

*Proof.* [11]

□

**Remark 12.** *In order to apply the Poincare-Bendixson theorem one constructs a trapping region, that is a closed connected set such that the vector field points "inward".*

#### 4.3.1 Hopf Bifurcation

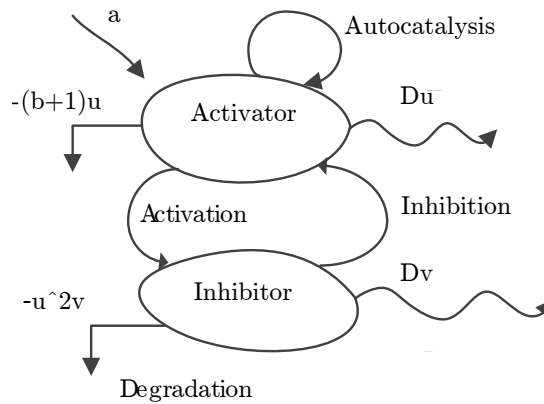
Suppose a two-dimensional system has a stable fixed point. A **Hopf Bifurcation** occur when the eigenvalues are complex conjugates and simultaneously cross the imaginary axis into the right half plane.

**Remark 13.** *Hopf bifurcations can occur in phase spaces of any dimension  $n \geq 2$ , but we will focus on the two dimensional case.*

**Definition 4.3.2.** *Suppose a two-dimensional system has a stable fixed point. When a stable spiral [Figure 4.4(a)] changes into an unstable spiral surrounded by a limit cycle [Figure 4.4(b)] it is called a **Hopf Bifurcation**.*

## 5.1 Introduction to the Brusselator model

This introduction provides broader context for the Brusselator model by briefly discussing activator-inhibitor type of reaction-diffusion equations. The chemical detail and history of the Brusselator model are elaborated on in Chapter 6.



**Figure 5.1:** Schematic representation of the Brusselator model:  $u$  acts as the activator whilst  $v$  is the inhibitor.  $u$  is kept at a constant concentration of  $a$  through continuous replenishment.  $u$  is diminished through the term  $-(b+1)u$  and auto-catalysis is described by the term  $u^2v$ .  $v$  is diminished through the term  $-u^2v$  and replenished due to  $bu$ . Note that the diffusion of the inhibitor is always greater than the activator,  $D_v > D_u$ .

Gierer and Meinhardt,[3], states that many aspects of morphogenesis can be explained in terms of activating and inhibiting substances. They provide the example of the induction of organs by small transplants. The induction can be seen as the short range activation. Whereas the long range inhibition is the existence of organs around the transplant. Another example of this

## 5. THE BRUSSELATOR MODEL

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would be the formation of sand dunes. a Small elevated area of sand will cause more sand to gather there as the wind blows over the area. This we can think of as the positive feedback. The sand also act as the inhibitor, since the removal of the sand will cause existence of less elevated areas. These areas are sheltered from the wind hence inhibiting the growth of the sand dune. The Brusselator model falls under this type of reaction kinetics known as Activator-inhibitor models. The model describes the concentration of a short-range auto catalytic substance, the activator, that regulates the production of its long-range antagonist, the inhibitor.

We state the Brusselator equations here without derivation for easy reference.

$$\begin{aligned}\frac{\partial u}{\partial t} &= a - (b + 1)u + u^2v + D_u \nabla^2 u \\ \frac{\partial v}{\partial t} &= bu - u^2v + D_v \nabla^2 v\end{aligned}\tag{5.1}$$

In the following sections of this chapter we will refer to the Brusselators' reaction kinetics as follow,

$$\begin{aligned}f(u, v) &= a - (b + 1)u \\ g(u, v) &= bu - u^2v\end{aligned}\tag{5.2}$$

### 5.2 Existence and uniqueness of the solution of the Brusselator model

In order to write the Brusselator model as an abstract Cauchy problem we define the following operators. Let  $w = (u, v)$ ,

$$A = D\nabla^2, \quad D = \begin{pmatrix} D_u \\ D_v \end{pmatrix}, \quad F(w) = \begin{pmatrix} f(w) \\ g(w) \end{pmatrix}$$

Therefore we write (5.1) as,

$$\frac{\partial w}{\partial t} = Aw + F(w)$$

It is clear that  $A$  is a linear operator and we define it more generally in terms of weak derivatives. Therefore we have an unbounded linear operator  $A : W^2(\Omega) \rightarrow L^2(\Omega)$ .

**Example 5.2.1.** *It's easy to see that  $A$  is unbounded if we consider the following example. Let  $f(x) = \sin(nx)$ ,  $n \in \mathbb{N}$  with  $x \in [0, 1]$ , now consider  $f''(x) = -n^2 \sin(nx)$  which implies unboundedness of the operator  $A$  where  $Af(x) = f''(x)$ ,*



## 5.2. Existence and uniqueness of the solution of the Brusselator model

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Our aim is to show that  $A$  is an infinitesimal generator of a  $C_0$ -semigroup, we achieve this by applying the Lumer-Phillips theorem. Therefore we proceed to show that the two conditions of the Lumer-Phillips theorem ( Theorem 3.1.8 ) are satisfied. We first deal with the density of  $\mathcal{D}(A)$  assuming that  $\Omega$  is an open set of  $\mathbb{R}^2$ . It clearly follows that  $C_0^\infty(\Omega) \subset W^2(\Omega)$  by definition and  $C_0^\infty(\Omega)$  is dense in  $L^2(\Omega)$  by Theorem 2.2.2. The second condition is a bit more elaborate, we first show that  $A$  is dissipative and then if  $\mathcal{D}(A)$  is complete we have  $\mathcal{D}(\lambda I - A) = X$ , as shown in Section 2.3. We proceed to show the dissipativity of  $A$  for  $\Omega$  as a square in  $\mathbb{R}^2$ . The dissipativity for  $A$  with Von Neumann or Dirichlet boundary conditions follows from integration by parts,

$$\langle Aw, w \rangle = D \langle \nabla^2 w, w \rangle = -D \langle \nabla w, \nabla w \rangle + D \int_{\Omega} \nabla w \cdot w$$

clearly the last term is cancelled since either  $\nabla w = 0$  on  $\partial\Omega$  or  $w = 0$  on  $\partial\Omega$ , therefore we have

$$\langle Aw, w \rangle = -D \langle \nabla w, \nabla w \rangle = -D \|\nabla w\|^2 \leq 0$$

This proves that  $A$  is a dissipative operator for  $\Omega$ , and we can apply the Lumer-Phillips theorem, Theorem 3.1.8. In chemical reactions we are more often concerned with the behaviour of the kinetics. Therefore, in order to exclude any boundary effects, we assume periodic boundary conditions (PBC) on a rectangular domain  $\Omega = [0, a] \times [0, a]$ . That is,

$$u|_{x=0} = u|_{x=a}, \quad u|_{y=0} = u|_{y=a}, \tag{5.3}$$

$$v|_{x=0} = v|_{x=a}, \quad v|_{y=0} = v|_{y=a}. \tag{5.4}$$

We can think of two-dimensional PBC as equal to that of a world map of some video games (think Pacman or Snake) when an object passes through one side then it re-appears on the opposite side with the same velocity vector. Another way to describe it topologically is if we can fold the two dimensional domain into a three dimensional doughnut with consequence that no boundary conditions exist.

We use the following trick in order to prove the dissipativity of  $A$  on a rectangular domain with PBC. One of the variables are kept fixed, let this be  $x^*$ . Then we integrate w.r.t to  $y$  as follow,

$$\begin{aligned} \int_0^a \frac{\partial^2}{\partial y^2} w(x^*, y) \cdot w(x^*, y) dy = \\ - \int_0^a \frac{\partial}{\partial y} w(x^*, y) \cdot \frac{\partial}{\partial y} w(x^*, y) dy + \frac{\partial}{\partial y} y w(x^*, y) w(x^*, y) \Big|_0^a \end{aligned}$$

## 5. THE BRUSSELATOR MODEL

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Now notice that due to the periodic boundary conditions we have  $\frac{\partial}{\partial y}w(x^*, 0)w(x^*, 0) = \frac{\partial}{\partial y}w(x^*, a)w(x^*, a)$ . We then integrate over  $u$  to obtain

$$\int_0^a \int_0^a \frac{\partial^2}{\partial y^2} w(x, y) \cdot w(x, y) dy dx = - \int_0^a \int_0^a \frac{\partial}{\partial y} w(x, y) \cdot \frac{\partial}{\partial y} w(x, y) dy dx$$

Similarly, the same is done for partial derivative of  $x$ ,

$$\int_0^a \int_0^a \frac{\partial^2}{\partial x^2} w(x, y) \cdot w(x, y) dy dx = - \int_0^a \int_0^a \frac{\partial}{\partial x} w(x, y) \frac{\partial}{\partial x} w(x, y) dy dx$$

Now adding them together we get,

$$\begin{aligned} \int_0^a \int_0^a \left( \frac{\partial^2}{\partial y^2} w(x, y) + \frac{\partial^2}{\partial x^2} w(x, y) \right) \cdot w(x, y) dy dx = \\ - \int_0^a \int_0^a \frac{\partial}{\partial y} w(x, y) \frac{\partial}{\partial y} w(x, y) + \frac{\partial}{\partial x} w(x, y) \frac{\partial}{\partial x} w(x, y) dy dx \end{aligned}$$

Adding the diffusion matrix and simplifying the notation we get,

$$\int_{\Omega} D \nabla^2 w \cdot w = -D \int_{\Omega} \nabla w \cdot \nabla w$$

Now it easy to see that,

$$\langle D \nabla^2 w, w \rangle = D \langle \nabla w, \nabla w \rangle \leq 0$$

Therefore we have that  $A$  is a dissipative operator on a rectangular domain. Now it follows from the Lumer-Phillips theorem, Theorem 3.1.8 that  $A$  is a  $C_0$ -semigroup of contractions. It is clear that  $F$  is locally lipschitz continuous therefore local existence and uniqueness follows from Theorem 3.1.10. We will show global existence when we construct an invariant region in section 5.4. The regularity of the solution w.r.t time follows from Theorem 3.2.4, that is  $w \in (C^1[0, \bar{T}], W^2)$ . The regularity w.r.t to space follows from Theorem 2.2.8(b). Clearly  $\Omega$  satisfies the cone condition and with  $m = 2$ ,  $n = 2$  we have  $W^2(\Omega) \subset \bar{C}(\Omega)$ .

Now to conclude this section. We have shown that there exists a unique solution that is continuous in space and differentiable in time on a rectangular domain with periodic boundary conditions. In terms of the physical aspects of the Brusselator model it implies plausibility since any discontinuity in space or time would be hard to explain with our current understanding of diffusion and chemical reaction-kinetics.

## 5.3 Turing Patterns in the Brusselator model

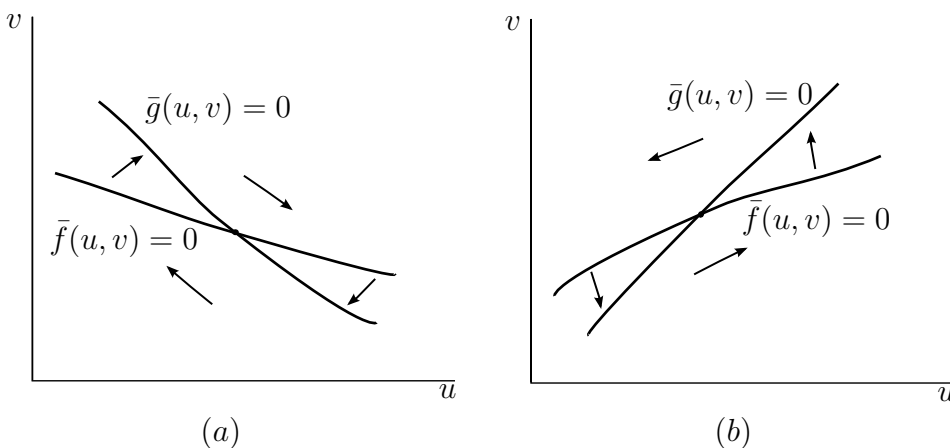
The question whether a system is capable of producing Turing patterns heavily leans not just on the diffusion but also on the dimensionless reaction kinetics. That is, the system has to be equivalent to some activation-inhibition interpretation coupled with unequal diffusion. We will refer to the Turing conditions as stated at the end of Section 4.2 in order to deduce the two broad types of reaction kinetics that produce Turing Patterns. It is clear from conditions, (ii) and (iii) that  $f_u$  and  $g_v$  must be of opposite sign, since the diffusion will cause the instability it follows that  $f_u > 0$  and  $g_v < 0$ . The first condition,  $f_u g_v - f_v g_u > 0$  leads us to the two different types, since the only condition is that  $f_v$  and  $g_u$  needs to be of opposite sign.

We show the two different phase planes near each systems fixed point in Figure 5.2. The signs of the stability matrices for the two systems will look as follow, for Figure 5.2 (a) we have,

$$\begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}_{u^*,v^*} = \begin{pmatrix} + & + \\ - & - \end{pmatrix}$$

for Figure 5.2 (b) we have,

$$\begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}_{u^*,v^*} = \begin{pmatrix} + & - \\ + & - \end{pmatrix}$$



**Figure 5.2:** Schematic illustration of the phase-planes around the fixed point for each type of diffusion driven instability

**Remark 14.** *The signs of the phase plane will also affect the rolls  $u$  and  $v$  play as activator and inhibitor. This in turn will affect whether the pattern*

## 5. THE BRUSSELATOR MODEL

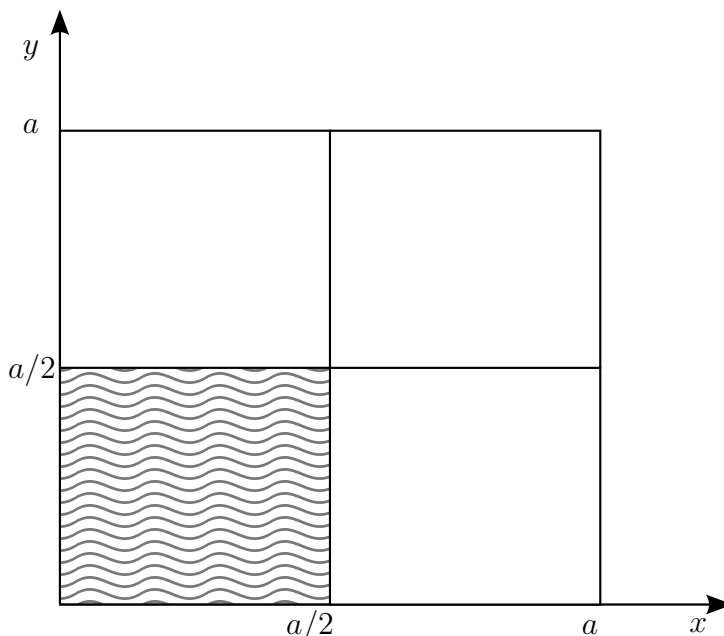
formation of  $u$  and  $v$  are in or out of phase. The implication of this phase transition is fundamental to biological applications. An in-depth discussion of this can be pursued in the book of Murray [6, pg. 87].

In Figure 5.5 we verify the nullclines of the Brusselator around its fixed point, we see that indeed it adheres to one of the two broad types of Activator-inhibitor models shown in Figure 5.2. Now that we've verified the qualitative behaviour of the reaction-kinetics we proceed to establish the Turing conditions for the specific case of the Brusselator model. First we want the uniform state to be stable in the absence of diffusion, that is,  $f_u + g_v < 0 \Rightarrow b < 1 + a^2$ , and  $f_u g_v - f_v g_u > 0 \Rightarrow a^2 > 0$ . Now bringing the diffusion into consideration we have the conditions,  $df_u + g_v > 0 \Rightarrow 1 + \frac{1}{d}a^2 < b$ , but we see from the condition  $|A| - \frac{(df_u + g_v)^2}{4d} < 0$  that,  $(1 + \frac{a}{\sqrt{d}})^2 < b$ . It is easy to see that if  $(1 + \frac{a}{\sqrt{d}})^2 < b$  then  $\frac{a^2}{d} + 1 < b$  will also hold.

In chapter 6 we kept the following parameter fixed,

$$a = 3, \quad D_v = 10,$$

and varied  $b$  and  $D_u$  to investigate the pattern formation. In Chapter 6 we assume PBC whereas in the theory we've derived the Turing conditions for Neumann boundary conditions. We show here how one can extend a rectangular domain with Neumann boundary condition such that the Turing Pattern theory is still applicable for a rectangular domain with PBC.



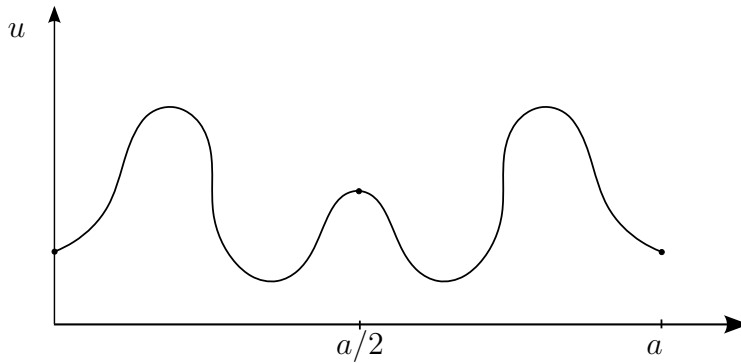
**Figure 5.3:** We illustrate how to extend  $\Omega = [0, a/2] \times [0, a/2]$  in order to have an appropriate domain on which we can define our function  $\bar{w}_k$ .

### 5.3. Turing Patterns in the Brusselator model

Let  $w_k$  be defined on  $\Omega = [0, a/2] \times [0, a/2]$ . Now,

$$\bar{w}_k = \begin{cases} w_k(x, y), & 0 \leq x \leq \frac{a}{2}, 0 \leq y \leq \frac{a}{2} \\ w_k(a - x, y), & \frac{a}{2} \leq x \leq a, 0 \leq y \leq \frac{a}{2} \\ w_k(x, a - y), & 0 \leq x \leq \frac{a}{2}, \frac{a}{2} \leq y \leq a \\ w_k(a - x, a - y), & \frac{a}{2} \leq x \leq a, \frac{a}{2} \leq y \leq a \end{cases} \quad (5.5)$$

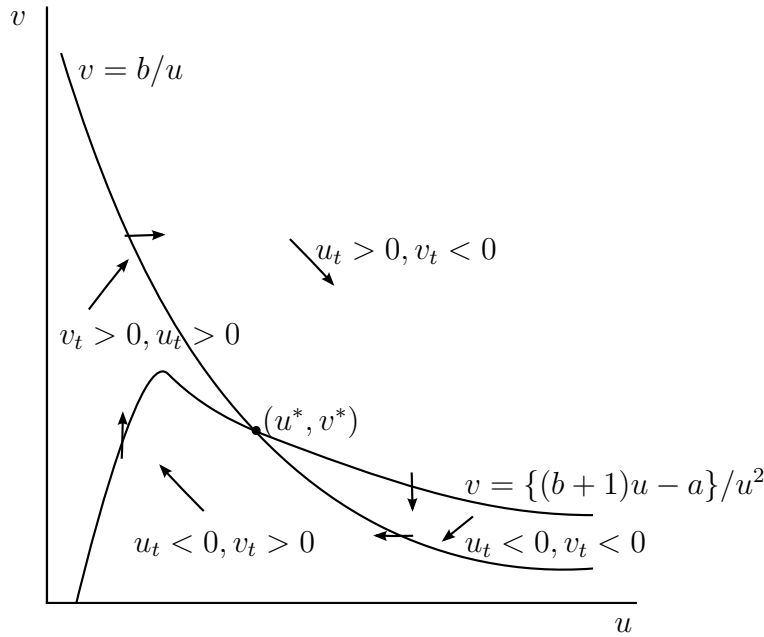
We see from the way  $\bar{w}_k$  is defined on  $[0, a] \times [0, a]$  that we have PBC. We illustrate this with a one-dimensional domain  $[0, a]$  in Figure 5.4.



**Figure 5.4:** Let  $\Omega = [0, a]$ , and let  $w_k$  be defined on  $[0, a/2]$ . Now let  $\bar{w}_k = \{w_k(x), 0 \leq x \leq \frac{a}{2}; w_k(a - x), \frac{a}{2} \leq x \leq a\}$ . We see from the way  $\bar{w}_k$  is defined that it's reflexive around  $a/2$ . Thus,  $\bar{w}_k(0) = \bar{w}_k(a)$  implying PBC.

See Figure 6.1 and Figure 6.4a for a comprehensive numerical investigation on the typical Turing patterns observed in the Brusselator model (5.1) as parameters  $(b, D_v)$  are varied.

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**Figure 5.5:** In order to plot the nullclines we set  $f(u, v) = 0, g(u, v) = 0$  and write it as explicit functions of  $v$ . Therefore we get  $u_t = 0$  on  $v = \{(b+1)u - a\}/u^2$  and  $v_t = 0$  on  $v = b/u$ .

### 5.4 Hopf bifurcation in the Brusselator model

We first calculate the fixed point  $(u^*, v^*)$ . Setting  $f(u, v) = 0$  we get that  $a - (b+1)u + u^2v = 0 \implies bu = a + u^2v - u$ . Substituting this into  $g(u, v)$  we get  $u = a$ , and solving for  $v$  we get  $v = b/a$ . Therefore  $(u^*, v^*) = (a, b/a)$ . In order to linearise the problem we calculate the partial derivatives,

$$\begin{aligned} f_u &= 2uv - (b+1), & f_v &= u^2 \\ g_u &= b - 2uv, & g_v &= -u^2 \end{aligned}$$

Therefore we get the stability matrix of the system as,

$$A_{u^*, v^*} = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}_{u^*, v^*} = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix}$$

We proceed to calculate the characteristic polynomial,

$$|A - \lambda I| = \lambda^2 + (a^2 - (b-1))\lambda + a^2$$

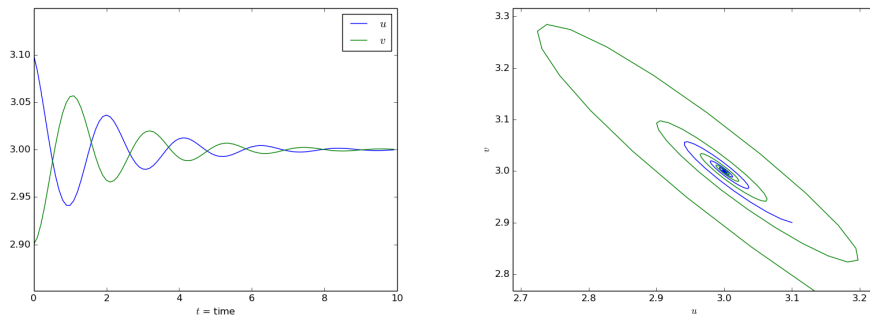
Solving the roots of the characteristic polynomial we get,

$$\lambda_1, \lambda_2 = -(1 + a^2 - b) \pm \{(1 + a^2 - b)^2 - 4a^2\}^{1/2} \quad (5.6)$$

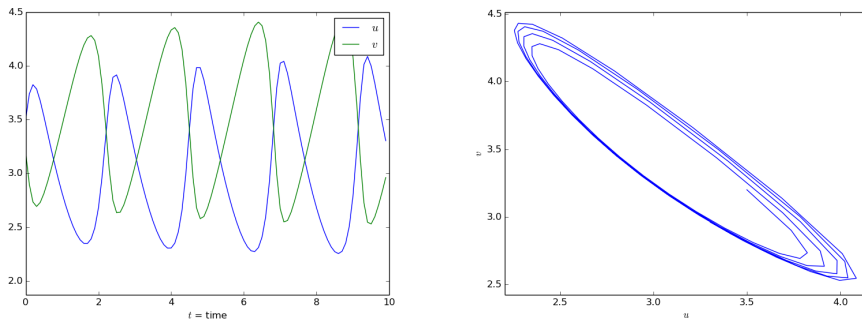
## 5.4. Hopf bifurcation in the Brusselator model

It is clear from (5.6) that  $Re(\lambda) < 0$  if  $b < a^2 + 1$ , and if  $b_h = a^2 + 1$  we have that  $Re(\lambda) = 0$ , this we call the hopf bifurcation point (crossing over from the left imaginary plane to the right imaginary plane, see Figure 4.3 ). This implies that for  $b > a^2 + 1$  the equilibrium  $(u^*, v^*)$  is unstable since  $Re\lambda > 0$  and all non equilibrium solutions will approach a stable limit cycle. We numerically investigated the system of ODEs (5.2) in order to verify the Hopf bifurcation.

**Remark 15.** *More depth and detail on the analysis of bifurcations can be found in the book by Strogatz [17, pg. 251]*



**Figure 5.6:** Parameters:  $(a, b) = (3, 9)$ , stable fixed point  $(u^*, v^*) = (3, 3)$ ,  $(u_0, v_0) = (3.1, 2.9)$

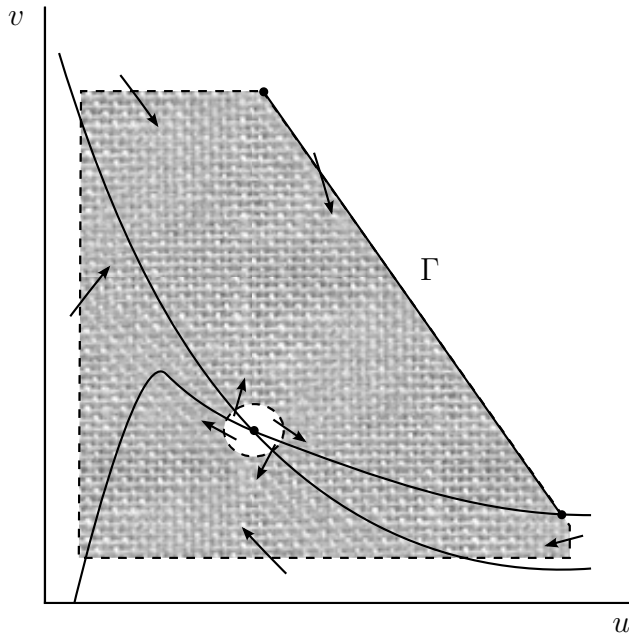


**Figure 5.7:** Parameters:  $(a, b) = (3, 12)$ , unstable fixed point  $(u^*, v^*) = (3, 12/3)$ ,  $(u_0, v_0) = (3.5, 3.3)$

We see from Figure 5.6 and Figure 5.7 that a Hopf bifurcation does indeed occur as described in the previous chapter. Next we prove that a limit cycle exist for (5.2) with parameters  $(a, b) = (3, 12)$  and unstable fixed point  $(u^*, v^*) = (3, 4)$ , through constructing a region. This approach can be used for any unstable fixed point but the details needs to be changed. In other words this is not a general method of proving the existence for all unstable fixed points.

We proceed to construct an invariant region, see Figure 5.8. The problem is the right-hand side of the region since a vertical line of a rectangular domain

## 5. THE BRUSSELATOR MODEL



**Figure 5.8:** Constructed invariant region for the Brusselator model with parameters:  $(a, b) = (3, 12)$ , unstable fixed point  $(u^*, v^*) = (3, 12/3)$ . See above paragraph for details on the line segment  $\Gamma$ .

won't satisfy the invariant condition (i.e vectors pointing inwards). This is clear from Figure 5.5. Therefore we show that there exists a line segment  $\{\Gamma : v = -u + c, u \in [\alpha, \beta], c \in \mathfrak{R}\}$  such that  $|v_t| > |u_t|$ . This would imply that on the line segment  $\Gamma$  the ratio of the rate of change  $v_t/u_t > 1$ , therefore the vectors on  $\Gamma$  points into the region. Let  $\{\Gamma : v = -u + 15.5\}$ , this ensures that the line segment is above  $v = 12/u$  on  $[\alpha, \beta]$ . Since  $u_t > 0, v_t < 0$  we have  $|v_t| - |u_t| = -v_t - u_t > 0$ . Substituting  $\Gamma$ , we obtain  $-v_t - u_t = -12u + u^3 - 15.5u^2 - 3 + 13u - u^3 + 15u^2 = -3 + u \implies u > 3$ . Therefore we choose  $\alpha = 3.5$  and  $\beta_f < \beta < \beta_g$ , where  $\beta_f$  is the intersection of  $\Gamma$  with  $v = \{13u - 3\}/u^2$  on the  $u$ -axis and  $\beta_g$  is the intersection of  $\Gamma$  with  $v = 12/u$  on the  $u$ -axis. It is clear from Figure 5.8 that vectors on the rest of the boundary of the region, point inwards. Therefore we have an invariant region. Now if we exclude the fixed point then it follows from the Poincare-Bendixson theorem, Theorem 4.3.1, that there exists a limit cycle in the invariant region.

**Remark 16.** *The Poincare-Bendixson theorem only holds if the fixed point is repellent, since a stable spiral is a possible solution trajectory if the fixed point is stable and attractive.*

**Remark 17** (Global Existence). *It follows from Corollary 3.2.3 that there exist a solution for all  $t > 0$ .*



# Stationary and oscillatory patterns in a coupled Brusselator model 6

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*The content of this chapter is published in the article [1].*

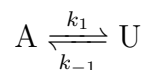
## Abstract

This paper presents a numerical investigation into the pattern formation mechanism in the Brusselator model focusing on the interplay between the Hopf and Turing bifurcations. The dynamics of a coupled Brusselator model is studied in terms of wavelength and diffusion, thus providing insight into the generation of stationary and oscillatory patterns. The expected asymptotic behaviour is confirmed by numerical simulations. The observed patterns include inverse labyrinth oscillations, inverse hexagonal oscillations, dot hexagons and parallel lines.

## 6.1 Introduction

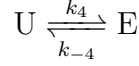
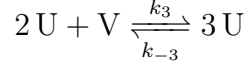
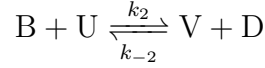
Models involving termolecular reaction steps exhibits interesting properties and pose challenging mathematical problems regarding the asymptotic behaviour of the solutions. It is well-known that models of reaction sequences with two intermediates and only uni- and bimolecular steps do not admit limit cycles [8, Section 7.1]. Therefore, for instability to occur in the thermodynamic branch (the solution in equilibrium) one needs to use cubic reaction rates [4], [21], [8].

The following reaction sequence was studied by Prigogine and Lefever in 1968 [14]:



## 6. STATIONARY AND OSCILLATORY PATTERNS IN A COUPLED BRUSSELATOR MODEL

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We note that the third step in the sequence involves a cubic nonlinear reaction term. Under the assumptions that

- (i) D and E are removed from the reaction domain the instant they are produced (or equivalently,  $k_{-2} = k_{-4} = 0$ ),
- (ii) the nonlinear reaction is irreversible ( $k_{-3} = 0$ ),
- (iii) A is in sufficient abundance,

the dynamics of the reaction sequence is represented in [14] by two rate equations:

$$\begin{aligned} \frac{\partial U}{\partial \hat{t}} &= k_1 A - (k_2 B + k_4)U + k_3 U^2 V + \hat{D}_u \nabla^2 U \\ \frac{\partial V}{\partial \hat{t}} &= k_2 B U - k_3 U^2 V + \hat{D}_v \nabla^2 V \end{aligned} \quad (6.1)$$

By scaling of the variables,

$$\begin{aligned} t &= k_4 \hat{t} & u &= \left(\frac{k_3}{k_4}\right)^{\frac{1}{2}} U & v &= \left(\frac{k_3}{k_4}\right)^{\frac{1}{2}} V \\ a &= \left(\frac{k_1^2 k_3}{k_4^3}\right)^{\frac{1}{2}} A & b &= \frac{k_2}{k_4} B & D_i &= \frac{\hat{D}_i}{k_4} \end{aligned} \quad (6.2)$$

the model (6.1) is simplified to the following model involving only two parameters.

$$\begin{aligned} \frac{\partial u}{\partial t} &= a - (b + 1)u + u^2 v + D_u \nabla^2 u \\ \frac{\partial v}{\partial t} &= bu - u^2 v + D_v \nabla^2 v \end{aligned} \quad (6.3)$$

The system (6.3) of reaction diffusion partial differential equations is known as the trimolecular model or the Brusselator model, the latter term coined by Tyson in 1973 [20]. This model has been widely used to illustrate and study basic features of chemical reaction models involving trimolecular steps. In some sense it plays in the settings of these models a pivotal role similar to the role the harmonic oscillator and the Heisenberg model play in ferromagnetism [8].

This paper presents a numerical investigation into the pattern formation mechanism in the Brusselator model. The next section (Section 2) is devoted to studying the interplay between the two bifurcations in the model, namely the Hopf bifurcation and the Turing bifurcation. This investigation is largely motivated by the observations in [24] that Turing patterns eventually (for sufficiently small ratio of the diffusion coefficients) dominate the Hopf bifurcation induced oscillations. The numerical simulations yield a hyperbola-like shaped boundary between the two regions. Oscillatory patterns are observed only in a small area near the horizontal part of curve. Based on these results, Section 3 deals with pattern formation in a coupled Brusselator model, that is, two systems of the form (6.3) linked via linear interaction terms. The study of the dynamics of this model in terms of wavelength and diffusion provides insight into generation of stationary and oscillatory patterns. The expected asymptotic behaviour is confirmed by numerical simulations. The observed patterns include inverse labyrinth oscillations, inverse hexagonal oscillations, dot hexagons and parallel lines. In Section 4 we provide some concluding remarks and directions for future work. For completeness of the exposition, details on the numerical method used for the simulations are presented in the Appendix.

## 6.2 Turing and Hopf bifurcations in the Brusselator model

The system (6.3) has one spatially homogeneous steady state,  $u^* = a$ ,  $v^* = \frac{b}{a}$ . Its stability is influenced by two factors: the appearance of spatially homogeneous limit cycle (Hopf bifurcation) and the ratio of the diffusion coefficients (Turing instability). We recall them briefly.

The spatially homogeneous solutions of (6.3) satisfy the system of ODEs

$$\begin{aligned}\frac{du}{dt} &= a - (b + 1)u + u^2v, \\ \frac{dv}{dt} &= bu - u^2v.\end{aligned}\tag{6.4}$$

Linear stability analysis yields that  $(u^*, v^*)$  is an asymptotically stable equilibrium of (6.4) if  $b < a^2 + 1$  with Hopf bifurcation at  $b = a^2 + 1$ . This means that for  $b > a^2 + 1$  the equilibrium is unstable and all nonequilibrium solutions approach a stable limit cycle.

Turing instability refers to the fact that the steady state  $(u^*, v^*)$  is unstable when the ratio of the diffusion coefficients is sufficiently small/large. Following the standard approach, e.g. as presented in [6], we obtain the Turing instability

## 6. STATIONARY AND OSCILLATORY PATTERNS IN A COUPLED BRUSSELATOR MODEL

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conditions in the form,

$$b < b_H := a^2 + 1 \quad (6.5)$$

$$b > b_T := \left(1 + a\sqrt{\frac{D_u}{D_v}}\right)^2 \quad (6.6)$$

We note that (6.5) and (6.6) hold simultaneously only if  $\frac{D_u}{D_v} < 1$ , which implies that the activator,  $u$ , diffuses slower than the inhibitor,  $v$ . Further, for any fix values of  $a$  and  $b > 1$ , stable patterns are formed when  $\frac{D_u}{D_v}$  is sufficiently small so that  $b > b_T$ . Therefore, in the subcritical Hopf parameter domain given by (6.5) we have two qualitatively different options for the dynamics of the model (6.3): (i) stable spatially homogenous steady state  $(u^*, v^*)$  and (ii) formation of stable spatial patterns, with the respective parameter subdomains separated by the bifurcation line  $b = b_T$ .

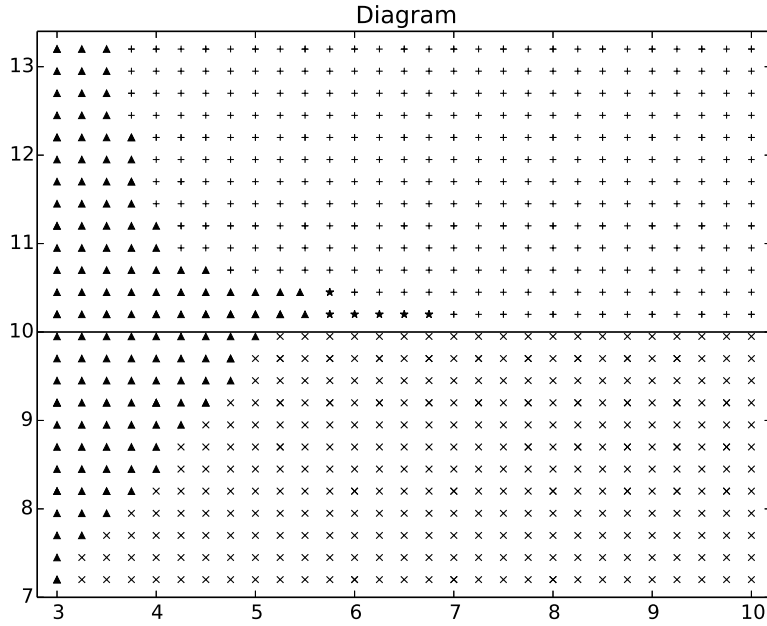
Our main interest is in the asymptotic properties of the model (6.3) in the supercritical Hopf domain  $b > b_H$ . In this parameter domain the model (6.3) has a spatially homogeneous limit cycle, so called bulk oscillations, corresponding to the limit cycle of (6.4). We investigate numerically the asymptotic behavior of the solutions of (6.3) with a focus on the disappearing of oscillations and formation of stable patterns when  $\frac{D_u}{D_v}$  is sufficiently small. The numerical method used for the simulations is presented in the Appendix. The system (6.3) is considered for  $x \in [0, 200] \times [0, 200]$  with periodic boundary conditions

$$u|_{x_1=0} = u|_{x_1=200}, \quad u|_{x_2=0} = u|_{x_2=200}, \quad (6.7)$$

$$v|_{x_1=0} = v|_{x_1=200}, \quad v|_{x_2=0} = v|_{x_2=200}. \quad (6.8)$$

Following the approach in [24], we fix the values of  $D_v$  and  $a$  and vary  $b$  and  $D_u$ . More precisely, we consider  $b \in [7.2, 13.2]$ ,  $D_u \in [3, 10]$  with independent increments of 0.25 each, while keeping  $D_v = 10$  and  $a = 3$ . The system (6.3) is solved with initial conditions which are random perturbations of the spatially homogeneous steady state. The points of the parameter grid are given in Figure 6.1. At any parameter point, irrespective of the initial condition, the computed solution eventually settles in one of the following stable states: spatially homogeneous steady state, bulk oscillations, oscillating patterns or stationary Turing patterns. Different markers in the Figure 6.1 indicate which one of these asymptotic behaviors is observed (see Legend). Interactive form of this figure is available on [18]. Clicking a marker on the diagram plays a video of a typical evolution of the solution for the respective values of the parameters  $b$  and  $D_u$ .

Below the Hopf bifurcation line  $b = b_H$ , and as expected, the line  $b = b_T$  separates a stable steady state region and a Turing patterns region. Interestingly, above the line  $b = b_H$ , there is a very well pronounced separation line  $b = b_{T^*}$  between the bulk oscillations region and the pattern formation region. Mostly, the patterns are stationary. The exception is a narrow area between



**Figure 6.1:** Classification of the numerical simulations of the Brusselator model into the following classes: SS - Stable stationary state, O - Bulk Oscillations, OP - Oscillating patterns, TP - Turing patterns. Interactive form of the figure is available in [18]

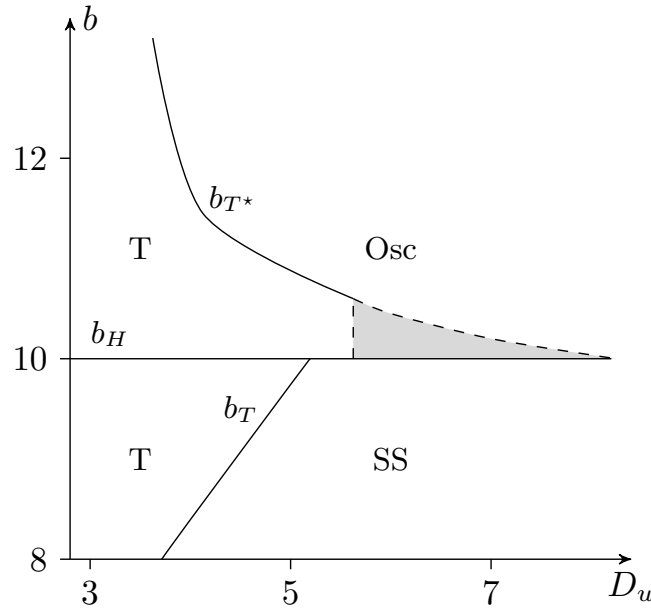
the lines  $b = b_H$  and  $b = b_{T^*}$ , where oscillating patterns occur. Schematically the different regions and dividing lines are presented in Figure 6.2. The line  $b = b_{T^*}$  which separates the bulk oscillations region and the pattern formation region has a hyperbola-like shape. This implies that for any fixed  $b > b_H$ , a stable stationary pattern is formed provided the fraction  $\frac{D_u}{D_v}$  is sufficiently small. Further, the simulations indicate a possible vertical asymptote at a value of,  $D_u$  in (3.4, 3.6), that is for  $D_u$  smaller than this value a stable pattern is formed irrespective of the value of  $b$ .

### 6.3 The coupled Brusselator model

The coupled Brusselator model comprises two systems of the form (6.3) coupled via linear reaction terms. Its general form is

$$\begin{aligned}
 \frac{\partial u_i}{\partial t} &= D_{u_i} \nabla^2 u_i + \alpha(u_j - u_i) + f(u_i, v_i) \\
 \frac{\partial v_i}{\partial t} &= D_{v_i} \nabla^2 v_i + \beta(v_j - v_i) + g(u_i, v_i)
 \end{aligned}
 \tag{6.9}$$

## 6. STATIONARY AND OSCILLATORY PATTERNS IN A COUPLED BRUSSELMATOR MODEL



**Figure 6.2:** Schematic representation of the regions in Figure 6.1: T - stable Turing patterns, Osc - bulk oscillations, SS: stable steady state

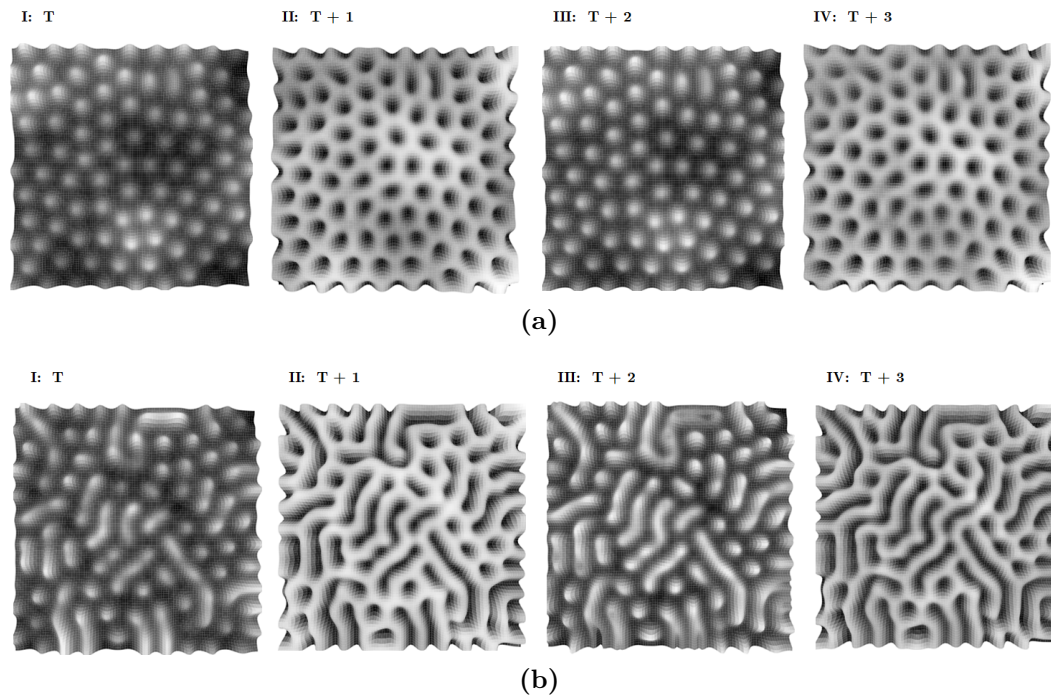
with  $i, j = 1, 2, i \neq j$ . The reactions  $f$  and  $g$  are as in (6.3), namely  $f(u, v) = a - (1 + b)u + u^2v$  and  $g(u, v) = bu - u^2v$ . The system (6.9) can be considered as a model of the reaction sequences in two thin layers of gel that meet at an interface. Each layer contains the same set of reactants with the same kinetics but with different diffusion parameters. The difference in diffusion can be owed to either physical (viscosity or density of the gel) or chemical (complex formation) factors. We note that the model represents two diffusion processes, referred to as horizontal and vertical diffusion. Horizontal diffusion is the diffusion in the two dimensional spatial domain of one layer and is described by the Laplacian term in each equation of (6.9). The vertical diffusion is the interaction between the two layers represented by the linear terms  $\alpha(u_j - u_i)$  and  $\beta(v_j - v_i)$ ,  $i, j = 1, 2, i \neq j$ . Yang et al. [23, ] studied the stable spatial resonance and superposition patterns in this coupled system. The spatial resonance of two wavelengths in the interacting layers produce stationary patterns, known as "black/white-eyes". Whereas the superposition patterns combines stripes and/or spots of varying size layered on top of each other. They also report a three-phase oscillatory interlacing hexagonal lattice pattern, known as "twinkling-eye" pattern, which occurs due to resonance between a Turing mode and its subharmonic.

Here we show a mechanism of generating oscillating patterns in the coupled model which is based on the asymptotic properties of a single layer model as presented in Figure 6.2. More precisely, oscillating patterns are obtained

Figure	$a$	$b$	$\alpha$	$D_{u1}$	$D_{v1}$	$D_{u2}$	$D_{v2}$	$k_1$	$k_2$
3a	3	10.2	0.1	4	10	10	10	0.83	0.1
3b	3	10.2	0.1	5	10	10	10	0.68	0.1
3c	3	13.2	0.1	3	10	10	10	1.25	0.4
4bI	3	10.2	1	6	10	30	100	0.56	0.33
4bII	3	10.2	1	6	10	37	100	0.56	0.28
4bIII	3	10.2	1	6	10	41	100	0.56	0.26
4bIV	3	10.2	1	6	10	44	100	0.56	0.24

**Table 6.1:** Parameters used in simulations of coupled Brusselator model ( $\alpha = \beta$ )

by coupling a layer with bulk oscillations and a layer with a Turing pattern. Roughly speaking, the one layer provides patterns while the other one drives the oscillations. It is important to observe that due to the shape of the curve  $b = b_{T^*}$  in Figure 6.2 one can indeed obtain two layers of such different properties by just varying  $D_u$ . This property is essential since the two coupled layers in (6.9) differ only in their diffusion coefficients.

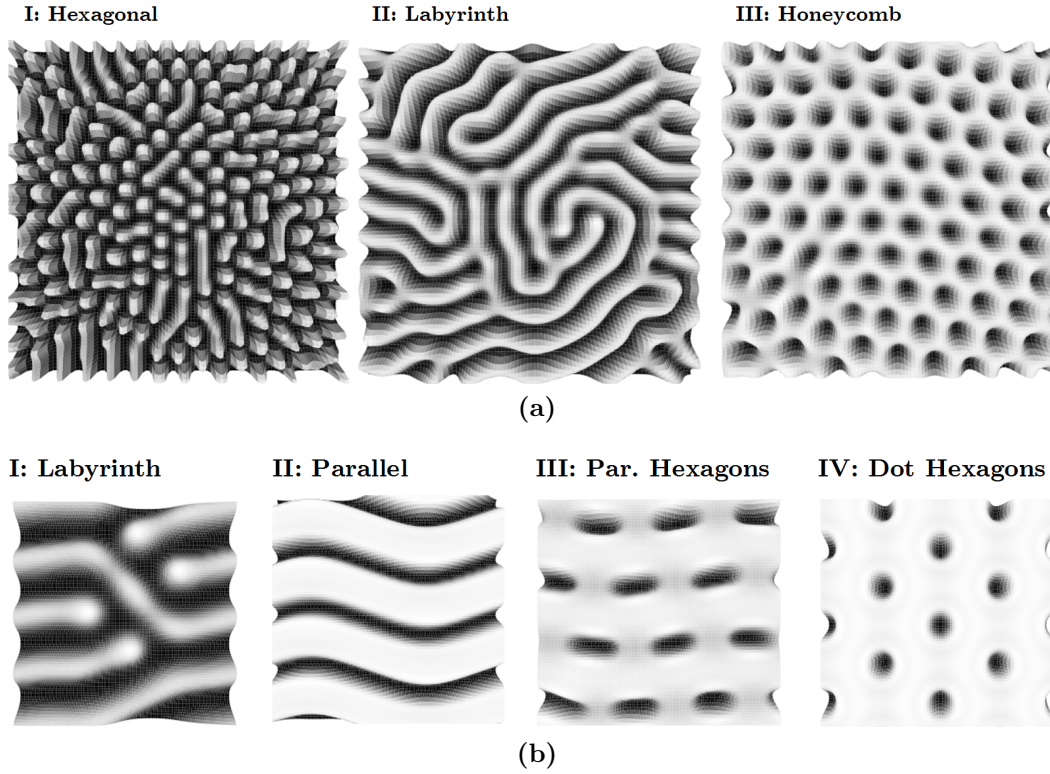


**Figure 6.3:** Oscillating pattern in a coupled Brusselator model (a) Honeycomb-inverse pattern oscillations (b) Labrynth-inverse pattern oscillations

The parameters used in our simulations are given in Table 1. In the first set of simulations we varied the diffusion  $D_{u1}$  in the first layer while keeping the rest of the parameters fixed. We observe an oscillating pattern when we



## 6. STATIONARY AND OSCILLATORY PATTERNS IN A COUPLED BRUSSELTOR MODEL



**Figure 6.4:** Stationary patterns in the coupled Brusselator model: (a) typical patterns observed in a single layer Brusselator model; (b) patterns that occur due to interaction of two Turing modes with various wavelengths

couple a strong bulk oscillating layer with a Turing pattern layer, see Figure 6.3a and Figure 6.3b. Typical Turing patterns observed in a single layer Brusselator model (Figure 6.4a) oscillate through inverting the concentration of each previous time step. Increasing  $b$  leads to a temporal separation of the Turing patterns and the bulk oscillations with the system spending longer periods in a set pattern.

The second set of simulations shows deviation from the typical Turing patterns of a single layer, Figure 6.4b, due to the interacting Turing modes on different scales. The wavenumber was derived from the linearized system in the form

$$k_i = \sqrt{\frac{1}{2} \left( \frac{f_u}{D_u} + \frac{g_v}{D_v} \right)} = \sqrt{\frac{1}{2} \left( \frac{b-1}{D_u} - \frac{a^2}{D_v} \right)}.$$

We kept the short wavelengths fixed (wavenumber  $k_1 = 0.56$ ) while varying the long wavelengths. The long wavelength was achieved by increasing both diffusion coefficients  $D_{u_2}$  and  $D_{v_2}$ , thus providing for the layer to remain in the Turing domain. The stationary patterns progress from Labyrinth patterns through to Dot Hexagonal patterns with Parallel lines occurring when the



wavelength ratio  $\frac{k_1}{k_2} = 2$ . Hexagons first appear when the wavelength ratio  $\frac{k_1}{k_2} > 2$ . When  $\frac{k_1}{k_2} > 2.3$ , we observe a clear dot hexagonal pattern, as seen in Figure 6.4bIII.

## 6.4 Conclusion

The numerical investigation in this paper provides insight into the asymptotic behavior of the solutions of a single layer Brusselator model, characterizing the parameter region for each of the three qualitatively different cases. Particular attention is given to the supercritical Hopf bifurcation parameter domain where no substantial theory is available. The obtained results are used further in revealing an essential mechanism generating oscillating patterns in the coupled Brusselator model. Future work is envisaged on the analysis of the single and coupled model using a theoretical approach similar to Rashkov's [25], with the aim of producing a more complete classification of the stationary and oscillating patterns as well as their generating mechanisms.

## 6.5 Appendix

The Alternating-Direction Implicit method (ADI) uses the concept of operator splitting or time splitting. The idea is to divide each timestep into two steps of size  $\Delta t/2$ , where in each substep, a different dimension is treated implicitly. This leads to a set of equations for each substep similar to the set of equations for the implicit one dimensional case. The Peaceman-Rachford variant [12] of the ADI method consists of solving (6.9), with the prediction substep ( $\Delta t/2$ ) using the backward Euler method for the  $x$  derivative terms and the forward Euler method for the  $y$  derivative terms. The correction substep ( $\Delta t$ ) then proceeds to swap the Euler methods around using the forward Euler method for  $x$  derivative terms and the backward Euler method for the  $y$  derivative terms. We illustrate the substeps below,

$$\frac{u_{l,m}^{n+\frac{1}{2}} - u_{l,m}^n}{\Delta t/2} = D_u \left( \frac{u_{l+1,m}^{n+\frac{1}{2}} - 2u_{l,m}^{n+\frac{1}{2}} + u_{l-1,m}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{u_{l,m+1}^n - 2u_{l,m}^n + u_{l,m-1}^n}{\Delta y^2} \right) + F(u_{l,m}^n, v_{l,m}^n)$$

$$\frac{u_{l,m}^{n+1} - u_{l,m}^{n+\frac{1}{2}}}{\Delta t/2} = D_u \left( \frac{u_{l+1,m}^{n+\frac{1}{2}} - 2u_{l,m}^{n+\frac{1}{2}} + u_{l-1,m}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{u_{l,m+1}^{n+1} - 2u_{l,m}^{n+1} + u_{l,m-1}^{n+1}}{\Delta y^2} \right) + F(u_{l,m}^{n+\frac{1}{2}}, v_{l,m}^{n+\frac{1}{2}})$$

(6.10)

where  $F(u, v) = \alpha(u_j - u_i) + f(u_i, v_i)$ , we note that the same holds for  $v$ .

## 6. STATIONARY AND OSCILLATORY PATTERNS IN A COUPLED BRUSSELATOR MODEL

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Using periodic boundary conditions for the system (6.9) the first step in (6.10) is reduced to solving for  $m = 1, 2, \dots, M$ , a linear tridiagonal cyclic system of the form,

$$\begin{pmatrix} 1+2r & -r & 0 & \dots & & -r \\ -r & 1+2r & -r & \dots & & \\ & & & \dots & & \\ & & & \dots & -r & 1+2r & -r \\ -r & & & \dots & 0 & -r & 1+2r \end{pmatrix} \cdot \begin{pmatrix} u_{1,m}^{n+\frac{1}{2}} \\ u_{2,m}^{n+\frac{1}{2}} \\ \dots \\ u_{L-1,m}^{n+\frac{1}{2}} \\ u_{L,m}^{n+\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \dots \\ f_{L-1} \\ f_L \end{pmatrix} \quad (6.11)$$

where  $r = \frac{D_u \Delta t}{2\Delta x^2}$ ,  $s = \frac{D_v \Delta t}{2\Delta y^2}$ ,  $f_i = -su_{i-1,m} + (1+2s)u_{i,m} - su_{i+1,m} + \frac{\Delta t}{2} F(u_{i,m}^n, v_{i,m}^n)$ ,  $i = 1, 2, \dots, L$ . The second step in (6.10) is implemented similarly by interchanging  $x$  and  $y$ . In order to solve the systems efficiently we use the Sherman-Morrison formula [22, Section 2.7.1], handling the coefficient matrix as a tridiagonal matrix plus a correction. This requires us to define the following two vectors. Let  $P$  be the tridiagonal matrix in (6.11),

$$\varphi_1 = \begin{pmatrix} \gamma \\ 0 \\ \vdots \\ 0 \\ p_{L,M} \end{pmatrix} \quad \varphi_2 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ p_{1,1}/\gamma \end{pmatrix} \quad (6.12)$$

where  $\gamma = -p_{1,2}$ . We can now solve the tridiagonal matrix with the following steps:

- (i) Solve  $P' \cdot u = f$
- (ii) Set up the vector  $\varphi_1$ .
- (iii) Solve  $P' \cdot z = \varphi_1$ .
- (iv) Obtain the form,  $\Psi = \varphi_2 \cdot u_m / (1 + \varphi_2 \cdot z)$
- (v) Use the form  $\Psi$  to obtain the new values of  $u_m$ , i.e  $u_m = u_m - \Psi \cdot z$

where  $P' = P$  but with the following two terms modified.

$$p'_{1,2} = p_{1,2} - \gamma \quad p'_{L,M} = p_{L,M} - p_{L,M} \frac{p_{1,1}}{\gamma} \quad (6.13)$$

## 6.6 Acknowledgement

This work has been supported by the SARChI Chair in Mathematical Models and Methods in Bioengineering and Biosciences and the National Research Foundation of South Africa. The authors would like to thank the anonymous reviewers for their contributions to improving the quality of the paper.



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In the dissertation we presented an application of Semigroup theory. Although the theory is often regarded as ornamental we demonstrated its application to nonlinear chemical dynamics. A sound theoretical framework was set-up through relevant concepts in Functional Analysis, and Sobolev spaces. This framework allowed us to show existence, uniqueness and regularity of the solution of activator-inhibitor type reaction diffusion equations, in particular the Brusselator model. The existence theory can be extended to a general class of locally Lipschitz reaction functions. We then investigated possible behaviour of the solution and the mechanisms that drive it. The typical behaviour of the solution that we discussed include Turing patterns, limit cycles and bifurcations.

Furthermore, a numerical investigation was conducted to determine pattern formation mechanism of the coupled Brusselator model. Here we extended the understanding of the pattern formation through the classification of a single layered Brusselator model. The numerical investigation provides an insight into the asymptotic behavior of the solutions of this model, characterizing the parameter region for each of the three qualitatively different cases: homogeneous steady state, Turing pattern and bulk oscillations. Particular attention was given to the supercritical Hopf bifurcation parameter domain where no substantial theory is available. We confirmed the observations that Turing patterns eventually (for sufficiently small ratio of the diffusion coefficients) dominate the Hopf bifurcation induced bulk oscillations. Our work provides a more accurate description of the shape of the boundary separating the Turing pattern domain and the bulk oscillations domain in the parameter space. We showed that the oscillating patterns is due to the fact that for the same values of the parameters  $a$  and  $b$  but with different diffusion coefficients the one system can be in the Turing pattern domain while the other in the bulk oscillations domain. Hence, roughly speaking, one layer provides a pattern while the other

## 7. CONCLUSION

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layer drives the oscillations.

Further possible research involves the empirical study of the pattern formation in the general reaction diffusion model with other practically relevant reaction functions considered. The aim is to compile a catalogue of pattern formations which can be a useful reference in biological and chemical modelling. This can also be extended further to include other spatial operators such as advection and integral operators. The threshold conditions on the model parameters for the appearance of the various patterns will also need to be determined. The empirical investigation on the possible patterns and conditions under which they occur will help to formulate conjectures. A fruitful theoretical study of the formulated conjectures will produce mathematical proofs.

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