A Thesis for the Degree of Ph.D. in Engineering

Mathematical analysis for the reaction–diffusion equations of Belousov–Zhabotinsky reaction

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Contents

Chapter 1

Introduction

1.1 Abstract

The research subject of this thesis is a reaction–diffusion equation that describes a chemical reaction called Belousov–Zhabotinsky (BZ) reaction. The BZ system is a kind of reaction–diffusion system which was discovered by B.P. Belousov in 1951, and it was studied in detail by A.M. Zhabotinsky later. The BZ system has remained a prototype for nonlinear chemical systems. The interesting aspect of BZ reaction to be observed is the changing of color in the reaction by temporal and spatial processing. It demonstrates the oscillations, consecutive pulses from the source center, and also self-organizing patterns. Oregonator model was proposed by R.J. Field et al (1972) to capture the features of BZ reaction without dealing with the intermediate details in three processes by five reactions. A three variables simplified model of the Oregonator model was proposed by R. J. Field and R. M. Noyes in 1972. After that, a two variables simplified model of the Oregonator model was proposed by J. J. Tyson and P.C. Fife in 1980. In this thesis, we study mathematically the reaction–diffusion equations of Keener–Tyson type for BZ reaction. Regarding the reaction–diffusion equations of BZ reaction we obtain the following two results.

(i) The time-global existence of unique smooth positive solutions to the reaction-diffusion equations of the Keener-Tyson model for the Belousov–Zhabotinsky reaction in the whole space is established with bounded nonnegative initial data. Deriving estimates of semigroups and time

evolution operators, and applying the maximum principle, the unique existence and the positivity of solutions are ensured by construction of time-local solutions from certain successive approximation. Invariant regions and large time behavior of solutions are also discussed. Here, our main issue is to ensure the positivity of trigger function. The Keener–Tyson model is a two-variable partial differential equation with a reaction term and a diffusion term, where the reaction term is in the form of a fraction, hence there is a difficulty at the stage of showing positiveness for the solution determined by the successive approximation sequence. In this thesis we devised a rigorous proof of it.

(ii) Besides, the existence of positive solutions to the system of ordinary differential equations related to the Belousov–Zhabotinsky reaction is established. The Keener–Tyson model is a two-variable partial differential equation with a reaction term and a diffusion term, where the reaction term is in the form of a fraction, hence when performing numerical calculations, if the denominator of the fraction takes a value close to 0 or a negative value, an error may occur in the numerical calculation. The key idea is to use a new successive approximation of solutions, then ensuring its positivity. To obtain the positivity and invariant region for numerical solutions, the system is discretized as difference equations of explicit form, employing operator splitting methods with linear stability conditions. Algorithm to solve the alternate solution is given.

1.2 Outline of this thesis

In this section, the outline of this thesis is presented.

The main topic of this thesis is reaction–diffusion equation. We discuss Belousov–Zhabotinsky reaction-diffusion equation, which is separated into 2 chapters. The first one corresponds to Chapter 3, and second one is drawn in Chapter 4.

Chapter 2 presents global information about the case in this thesis. This chapter includes 3 sections, where the diffusion-reaction is explained by the process and gives the extension for its derivation. The general information for Belousov–Zhabotinsky reaction is presented in Section 2.2, and the detail of it written in Section 2.3 Appendix.

The information in chapter 3 is spelled out by 5 sections. This chapter tells us about a well-posedness for the reaction-diffusion equations of Belousov–Zhabotinsky reaction. Some theorems are given in this chapter, and also the proof of each theorem is elucidated.

Chapter 4 includes 6 sections. This section discusses numerical solutions for Belousov–Zhabotinsky reaction. Listed in introduction, objectives, results, ordinary differential equations, difference equations, and at the end, the algorithm for numerical solutions is given.

Chapter 2

Reaction–diffusion phenomena

One of the phenomena in this world showing nonlinear dynamics is Belousov–Zhabotinsky reaction, which has diffusion processing in chemistry. The goal of this chapter is to explain about reaction-diffusion for Belousov–Zhabotinsky reaction.

2.1 Reaction–diffusion equation

Diffusion is the process by which matter is transported from one part of a system to another part as a result of random molecular movement. The classical experiment presents in a tall cylindrical vessel filled with iodine, and water is poured on top, carefully, and slowly. So that no convection currents are set up. First, the colored part is separated sharply, with a well-defined boundary. Later it is found that the upper part becomes colored, and getting fainter towards the top. It shows us that there is a transfer processing of iodine molecules from the lower to the upper part of the vessel taking place in the absence of convection current [3].

Mathematical theory of diffusion is isotropic substances in based on the hypothesis that the rate of transfer of diffusing substance through unit area of a section is proportional to the concentration gradient, i.e.

$$F = -D\nabla u, \tag{2.1.1}$$

where F is the rate of transfer per unit area of section, u is the concentration of diffusing substance, and D is a positive constant called as the diffusion coefficient.

From the equation of continuity

$$\frac{\partial u}{\partial t} = \nabla \cdot F,$$

and (2.1.1), the following diffusion equation is obtained [3]:

$$\frac{\partial u}{\partial t} = D\Delta u,$$

where Δ is the Laplacian operator. We have used the notation $\Delta := \sum_{i=1}^{n} \partial_i^2$, where $\partial_i := \partial/\partial x_i$ for $i = 1, \ldots, n$.

By introducing the reaction term $f(u)$ which is a function of u, the reaction–diffusion equation take the form [22]:

$$\frac{\partial u}{\partial t} = D\Delta u + f(u). \tag{2.1.2}$$

2.2 Belousov–Zhabotinsky reaction

The Belousov–Zhabotinsky (BZ) is a kind of reaction-diffusion system which was discovered by B.P. Belousov in 1951, and it was studied in detail by A.M. Zhabotinsky later. The BZ system has remained a prototype for nonlinear chemical systems. The changing of color in the reaction by temporal and spatial processing, this reaction demonstrates the oscilations, consecutive pulses from a source center, and also self-organizing patterns. The fascinating aspects of investigation on this system not only lie in the understanding of chemical reaction, but also in complexities of nonlinear dynamic systems from mathematical perspective [2].

The BZ reaction is created by a trigger wavefront (converting the medium from a reduced to an oxidized state) and a phase wave back (converting the medium from an oxidized to a reduced state) [27]. The BZ reaction is named after Russian workers who first studied in this reaction involves isothermal oxidation of malonic acid in aqueous solution in the presence of bromate ions, sulfuric acid, and a cation couple such as Ce^{3+} and Ce^{4+}. The mechanism for

BZ reaction which comprises eleven reactions (listed in [8]), presented that the reaction divided into autocatalytic as indicated by the reproduction of $HBrO_2$. One of them is written as the following reaction:

$$\mathrm{BrO_2 + Ce^{3+} + H^+ \;\leftrightarrow\; HBrO_2 + Ce^{4+}}. \tag{2.2.1}$$

We saw that $HBrO_2$ is produced autocatalytically in reaction (2.2.1), and Ce^{3+} is rapidly oxidized to Ce^{4+} [8]. Here Ce^{3+} and Ce^{4+} make the color of the solution white (or colorless) and yellow, respectively. Moreover, ferroin and ferriin make the color of red and blue in the reaction, respectively. When ferriin could stay either high or low concentrations in an open system with a ferroin reservoir, or when ferroin changed slowly, the bistability referred to attracting as red and blue in the bromate - CHD - ferroin medium [2]. Figure 1 represents one kind of pattern of the diffusivities in BZ reaction.

Source: https://www.youtube.com/watch?v=LL3kVtc-4vY

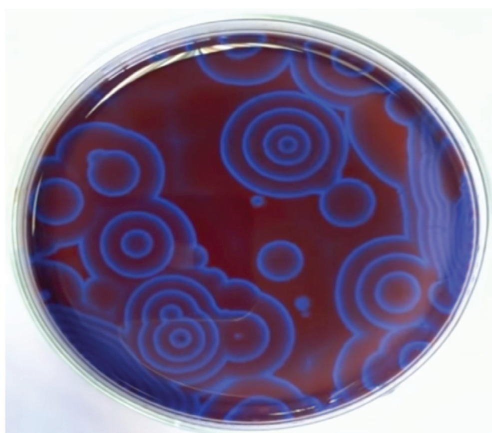

Figure 1. Pattern in the BZ reaction medium in a petri dish.

Oregonator model was proposed by R.J. Field *et al* (1972) to capture the features of BZ reaction without dealing with the intermediate details in three processes by five reactions [6]. A three variables simplified model of the Oregonator model was proposed by R. J. Field and R. M. Noyes in 1972 [4]. After that, a two variables simplified model of the Oregonator model was proposed by J. J. Tyson and P.C. Fife in 1980 [26].

In the next chapter, we consider the following initial value problem of the reaction-diffusion equations of Keener-Tyson type for BZ reaction [27]:

$$\text{(BZ)} \quad \begin{cases} \dfrac{\partial u}{\partial t} = \Delta u + \dfrac{1}{\varepsilon} u\,(1-u) - hv\dfrac{u-q}{u+q}, & \text{in } \mathbb{R}^{\mathrm{n}} \times (0,\infty) \\ \dfrac{\partial v}{\partial t} = d\Delta v + u - v, & \text{in } \mathbb{R}^{\mathrm{n}} \times (0,\infty) \\ u\,|_{t=0} = u_0, \quad v\,|_{t=0} = v_0 & \text{in } \mathbb{R}^{\mathrm{n}}. \end{cases}$$

Here, $u = u(x,t)$ and $v = v(x,t)$ denote for the concentration of $HBrO_2$ and Fe^{3+} (ferriin) in the vessel, respectively. $u_0 = u_0(x)$ and $v_0 = v_0(x)$ are given nonnegative bounded functions. We denote ε, h, q, and d for some positive constants. The derivation of BZ is shown in Section 2.3 Appendix.

2.3 Appendix

2.3.1 Derivation

In this section, we show the derivation of BZ according to [2]. All reactions of Oregonator model were considered to be irreversible and forward rate constants were assigned to four of the reactions. The rate constant and stoichiometry of the fifth reaction were treated as expendable parameters [5]. In Chen investigation (see [2]), it found that there are three stages occur in the whole lifespan of system called as transitional period, induction period, and main period. Each stage has unique characteristics and corresponding bifurcation points. The reactions in BZ system (see [2]) of the bromate-CHD-ferroin are separated in the following three processes A, B, and C:

$$\text{A} \begin{cases} \mathrm{BrO_3^-} + \mathrm{Br^-} + 2\mathrm{H^+} & \rightarrow & \mathrm{HBrO_2} + \mathrm{HOBr} & \text{(R1)} \\ \mathrm{HBrO_2} + \mathrm{Br^-} + \mathrm{H^+} & \rightarrow & 2\mathrm{HOBr} & \text{(R2)} \end{cases}$$

$$\text{B} \begin{cases} \mathrm{BrO_3^-} + \mathrm{HBrO_2} + \mathrm{H^+} & \leftrightarrow & 2\mathrm{BrO_2^*} + \mathrm{H_2O} & \text{(R3)} \\ \mathrm{BrO_2^*} + \mathrm{ferroin} + \mathrm{H^+} & \leftrightarrow & \mathrm{HBrO_2} + \mathrm{ferriin} & \text{(R4)} \\ 2\mathrm{HBrO_2} & \rightarrow & \mathrm{BrO_3^-} + \mathrm{HOBr} + \mathrm{H^+} & \text{(R5)} \end{cases}$$

$$
\mathrm{C}\left\{\begin{array}{llll}
\text{ferriin} + \text{CHD} + \text{BrCHD} & \leftrightarrow & \text{ferroin} + \text{H}^+ + \text{BrCHD}^* & \\
 & & + \ \text{CHD}^* & \text{(R6)} \\
\text{BrCHD}^* + \text{CHD}^* + \text{H}_2\text{O} & \rightarrow & h\text{Br}^- + \text{CHD} + \text{others} & \text{(R7)} \\
\text{BrCHD} + \text{H}^+ + \text{H}_2 & \rightarrow & \text{Br}^- + \text{H}_2\text{Q (hydroquinone)} & \\
 & & + \ \text{others} & \text{(R8)}
\end{array}\right.
$$

Here the symbol * represents that the molecule becomes an excited state by absorbing light. We can understand the processes A, B, and C as follows [11]. In the process A, the action of Br^- produces $HBrO_2$. In the process B, $HBrO_2$ produces BrO_2^*, and ferriin is generated due to the oxidation of BrO_2^* to ferroin. In the process C, ferroin is generated due to the reduction of BrCHD to ferriin. Br^- is also generated. Therefore Br^- reactivates the process A and repeats the cycle. Notice that we can show that (2.2.1) is the reaction which running at process B, written as (R4).

To understand the process of modeling in the intermediate chemical species of BZ reaction, we considered in the following rate equations:

$$
\left\{\begin{array}{lcl}
\dfrac{dX}{dt} & = & -k_3HAX + k_{-3}U^2 + k_4HU(C-Z) - k_{-4}XZ \\
 & & -2k_5X^2 - k_2HXY + k_1H^2AY, \\
\dfrac{dY}{dt} & = & -k_2HXY - k_1H^2AY + hk_7R + k_8B_0H, \\
\dfrac{dZ}{dt} & = & k_4HU(C-Z) - k_{-4}XZ - k_6BZ \\
 & & +k_{-6}HR(C-Z), \\
\dfrac{dU}{dt} & = & 2k_3HAX - 2k_{-3}U^2 - k_4HU(C-Z) + k_{-4}XZ, \\
\dfrac{dR}{dt} & = & k_6BZ - k_{-6}HR(C-Z) - k_7R,
\end{array}\right. \tag{2.3.1}
$$

where $A = [\mathrm{BrO_3^-}]$, $B = [\mathrm{CHD}] + [\mathrm{BrCHD}]$, $B_0 = [\mathrm{BrCHD}]$, $C = [\text{ferroin}] + [\text{ferriin}]$, $H = [\mathrm{H^+}]$, $U = [\mathrm{BrO_2^*}]$, $R = [\mathrm{BrCHD^*}] + [\mathrm{CHD^*}]$, $X = [\mathrm{HBrO_2}]$, $Y = [\mathrm{Br^-}]$, $Z = [\text{ferriin}]$, $h =$ unknown stoichiometric parameter, rate constant k_m corresponds to reaction (R_m) where $m = 1, 2, 5, 7, 8$, k_n and k_{-n} correspond to reaction (R_n) where $n = 3, 4, 6$, and [ ] represents the concentration of a chemical species.

R changes so fast, due to $k_6 \ll k_7 \ll k_{-6}$, that it will be approximated with its steady-state. By using scaled dimensionless parameter and variables (see [2]), rate equations are written as:

$$\begin{cases} \varepsilon \dfrac{dx}{dt} &= -x - x^2 - xy + qy + u(c-z) + K_{-3}u^2 - K_{-4}xz, \\ \varepsilon\sigma \dfrac{dy}{dt} &= -qy - xy + \dfrac{hz}{1+\rho(c-z)} + \beta, \\ \dfrac{dz}{dt} &= u(c-z) - K_{-4}xz - \dfrac{z}{1+\rho(c-z)}, \\ \varepsilon\mu \dfrac{du}{dt} &= 2x + K_{-4}xz - u(c-z) - 2K_{-3}u^2. \end{cases} \tag{2.3.2}$$

For $\sigma, \mu \ll 1$, we obtain new system:

$$\begin{cases} \varepsilon \dfrac{dx}{dt} &= x(1-x) - \left[\dfrac{hz}{1+\rho(c-z)} + \beta\right] \dfrac{x-q}{x+q} - K_{-3}{u_0}^2, \\ \dfrac{dz}{dt} &= 2x - 2K_{-3}{u_0}^2 - \dfrac{z}{1+\rho(c-z)}. \end{cases}$$

with steady states y and u:

$$\begin{aligned} y_0 &= \frac{1}{q+x}\left[\frac{hz}{1+\rho(c-z)} + \beta\right], \\ u_0 &= \frac{2x(2+K_{-4}z)}{(c-z) + \sqrt{(c-z)^2 + 8K_{-3}x(2+K_{-4}z)}}. \end{aligned}$$

The corresponding PDE system for medium with diffusion is

$$\begin{cases} \varepsilon \dfrac{dx}{dt} &= x(1-x) - \left[\dfrac{hz}{1+\rho(c-z)} + \beta\right] \dfrac{x-q}{x+q} - K_{-3}{u_0}^2 + \Delta x, \\ \dfrac{dz}{dt} &= 2x - 2K_{-3}{u_0}^2 - \dfrac{z}{1+\rho(c-z)} + \delta\Delta z. \end{cases} \tag{2.3.3}$$

The theory of wave propagation in excitable media is usually based on a pair of reaction–diffusion equation. By changing variable x and z in (2.3.3) being u and v respectively, and assume that $\beta, \rho \to 0$, $K_{-3} = 0$ and a little bit modify, then (2.3.3) be rewritten as:

$$\begin{cases} \varepsilon \dfrac{\partial u}{\partial t} = \varepsilon^2 \Delta u + u(1-u) - fv\dfrac{u-q}{u+q}, \\ \dfrac{\partial v}{\partial t} = \Delta v + u - v. \end{cases} \tag{2.3.4}$$

By divided both of sides in the first equation of (2.3.4) with ε, and define $h := f/\varepsilon$ then we obtain BZ equations seem like in Section 2.2.

2.3.2 Nullclines

By putting any values to (2.3.4), and $f = \varepsilon h$, we can show the nullclilnes of ordinary differential equations (2.3.4) in Figure 2.

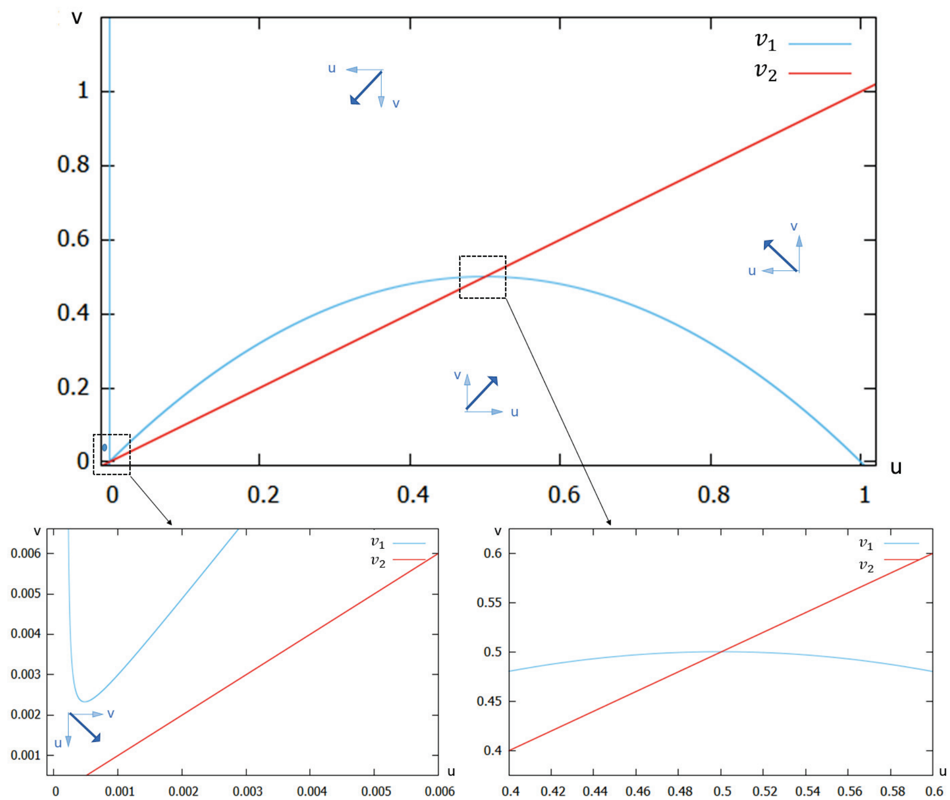

Figure 2. Nullclines of ordinary differential equations (2.3.4) with $q = 0.0002$, $h = 16.145$, and $\varepsilon = 0.032$, $v_1 = (u(1-u)(u+q))/(f(u-q))$, and $v_2 = u$.

Chapter 3

A well-posedness for the reaction–diffusion equations of Belousov–Zhabotinsky reaction

In this chapter, the time-global existence of unique smooth positive solutions to the reaction-diffusion equation of Keener-Tyson model for the Belousov-Zhabotinsky reaction in the whole space is established with bounded nonnegative initial data. By deriving estimates of semigroups and time evolution operators, and by applying the maximum principle, the unique existence and the positivity of solutions are ensured by the construction of time-local solutions from certain successive approximation. Invariant regions and large time behavior of solutions are also discussed.

3.1 Introduction

We consider the initial value problem of reaction-diffusion equations BZ in chapter 2, Section 2.2. For example of constant values, by [2] we have $\varepsilon = 0.032$, $q = 2.0 \times 10^{-4}$, and $d = 0.6 \times \varepsilon$. Note that in BZ, h (or f) stands for the excitability which governs dynamics of a pattern formulation. In fact, a spiral pattern appears for large value of h. Besides a ripple (concentric circle) pattern is developed for small value of h.

It has already been known the solvability of BZ in the abstract setting of L^2-framework by Yagi and his collaborators [25, 28]. In our framework, we may treat more various data, including the trivial solution of BZ. Furthermore, the invariant region and large time behavior of solutions are concerned. For applying the estimates of maximum principle type, we argue certain successive approximation of solutions. And at the end, to obtain uniform bounds, and to ensure positivity, some estimates for semigroups and time evolution operators are derived by arguments of relatively compact perturbation from Laplacian, via smoothing properties of the heat semigroup.

3.2 Objectives

In BZ reaction, the complexities of nonlinear dynamic systems from a mathematical perspective, such as the bifurcation and the oscillations, made this topic interesting to be studied. Here, our aim is to establish the well-posedness theory and some basic properties of solutions to BZ, in terms of functional analysis. Here, our main issue is to ensure the positivity of u.

3.3 Semigroups and time evolution operators

Let $n \in \mathbb{N}$, $1 \leq p < \infty$, and $L^p := L^p(\mathbb{R}^n)$ be the space of all p-th integrable functions in $\mathbb{R}^n$ with the norm $\|f\|_p := \left(\int_{\mathbb{R}^n} |f(x)|^p dx \right)^{1/p}$. Let L^∞ be the space of all bounded functions with the norm $\|f\|_\infty := \operatorname{ess.sup}_{x \in \mathbb{R}^n} |f(x)|$. Define BUC as the space of all bounded uniformly continuous functions. Since L^∞ is a Banach space, so is its closed subset BUC, as well as $C(I; BUC)$ for closed interval $I \subset \mathbb{R}$. For $k \in \mathbb{N}$, let $W^{k,\infty}$ be a set of all bounded functions whose k-th derivatives are also bounded.

In the whole space $\mathbb{R}^n$, for $w_0 \in L^\infty(\mathbb{R}^n)$ the heat equation

$$\text{(H)} \quad \begin{cases} \partial_t w = \Delta w & \text{in} \quad \mathbb{R}^n \times (0, \infty), \\ w|_{t=0} = w_0 & \text{in} \quad \mathbb{R}^n \end{cases}$$

admits a time-global unique smooth solution

$$\begin{aligned} w &:= w(t) := w(x,t) := (e^{t\Delta}w_0)(x) := (H_t * w_0)(x) \\ &:= \int_{\mathbb{R}^n} (4\pi t)^{-n/2} \exp(-|x-y|^2/4t) w_0(y) dy \end{aligned}$$

in $C_w((0,\infty); L^\infty)$, where $H_t := H_t(x) := (4\pi t)^{-n/2} \exp(-|x|^2/4t)$ is the heat kernel. Since $\|H_t\|_1 = 1$ for $t > 0$, by Young's inequality we have $\|w(t)\|_\infty \leq \|H_t\|_1 \|w_0\|_\infty \leq \|w_0\|_\infty$ for $t > 0$. In particular, if $w_0(x) \geq c$ for all $x \in \mathbb{R}^n$ with some $c \in \mathbb{R}$, then $w(x,t) \geq c$ holds true for $x \in \mathbb{R}^n$ and $t > 0$; so-called the maximum principle. Furthermore, if additionally $w_0 \in BUC$ and $w_0 \not\equiv c$, then $w(x,t) > c$ for $x \in \mathbb{R}^n$ and $t > 0$; so-called the strong maximum principle.

We easily see that for $k \in \mathbb{N}$, there exists a positive constant C such that $\|\partial_i^k e^{t\Delta} w_0\|_\infty \leq C t^{-k/2} \|w_0\|_\infty$ for $t > 0$ and $1 \leq i \leq n$. So, $w(t) \in C^k$ for $k \in \mathbb{N}$ and $t > 0$, which implies that $w(t) \in C^\infty(\mathbb{R}^n)$ for $t > 0$, and then $w \in C^\infty(\mathbb{R}^n \times (0,\infty))$.

In general, for $w_0 \in L^\infty$, there is a lack of the continuity of solutions to (H) in time at $t = 0$. Note that $e^{t\Delta} w_0 \to w_0$ in L^∞ as $t \to 0$, if and only if $w_0 \in BUC$.

3.4 Results

The time-global existence of unique smooth positive solutions to the reaction-diffusion equations of the Keener-Tyson model for the Belousov-Zhabotinsky reaction in the whole space is established with bounded nonnegative initial data (u_0, v_0). Due to semigroup theory, reaction-diffusion equations BZ are formally equivalent to the integral equations:

$$u(t) = e^{t\Delta} u_0 + \int_0^t e^{(t-s)\Delta} \left[\frac{u(s)\{1-u(s)\}}{\varepsilon} - hv(s) \frac{u(s)-q}{u(s)+q} \right] ds, \tag{3.4.1}$$

$$v(t) = e^{dt\Delta} v_0 + \int_0^t e^{d(t-s)\Delta} \left[-v(s) + u(s) \right] ds, \tag{3.4.2}$$

since Δ generates a (C_0) semigroup $\{e^{t\Delta}\}_{t\geq 0}$ in $BUC(\mathbb{R}^n)$, so-called the heat semigroup. To show the uniqueness, this expression is useful. Once we establish the existence of solutions to the integral equations (3.4.1) and (3.4.2), it is easy to confirm that solutions to the integral equations satisfy BZ in the classical sense by the standard argument from smoothing property of the heat semigroup.

Theorem 3.4.1 *Let $n \in \mathbb{N}$, $\varepsilon, h, d > 0$, and let $q \in (0,1)$. Put $\bar{u} \in (q,1)$ is a root of $g(u) := u(1-u)(u+q) - \varepsilon hq(u-q) = 0$, and $S := (q, \bar{u})^2$. Let $u_0, v_0 \in BUC(\mathbb{R}^n)$.*

1. *If $u_0(x) \geq 0$ and $v_0(x) \geq 0$ for $x \in \mathbb{R}^n$, then there exists a pair (u,v) of time-global unique nonnegative classical solutions to BZ in $C([0,\infty); BUC(\mathbb{R}^n))$.*
2. *If $(u_0(x), v_0(x)) \in S$ for $x \in \mathbb{R}^n$, then $(u(x,t), v(x,t)) \in S$ for $x \in \mathbb{R}^n$ and $t > 0$.*
3. *If $u(x,t_*) \geq c_*$ and $v(x,t_*) \geq c_*$ for $x \in \mathbb{R}^n$ with some $t_* \geq 0$ and $c_* > 0$, then there exists a $T_\sharp \geq t_*$ such that $(u(x,t), v(x,t)) \in S$ for $x \in \mathbb{R}^n$ and $t \geq T_\sharp$.*

3.5 Proof of Theorem 3.4.1

Here we will give a rigorous proof of the existence of time-global unique nonnegative classical solutions in L^∞-setting.
Let us introduce the notion of an invariant region. A set $\Omega \subset \mathbb{R}^2$ is called an invariant region, if a pair (u,v) of solutions to BZ always remains in Ω. Theorem 3.4.1 (1) implies that $[0,\infty)^2$ is an invariant region. Furthermore, the assertion (2) tells us that the square domain $S := (q, \bar{u})^2$ is an invariant region. It will be seen that $[0,m]^2$ for $m \geq 1$ are also invariant regions in Proposition 3.5.2.

We easily notice that there are two nonnegative steady states (solutions independent of x and t): the trivial solution $(0,0)$ and a non-trivial one $(\widetilde{u}, \widetilde{u})$, where $\widetilde{u}$ is a positive root of $\widetilde{g}(u) := (1-u)(u+q) - \varepsilon h(u-q) = 0$.

Note that $(\widetilde{u}, \widetilde{u}) \in S$. The linear stability or instability theories may be found around $(\widetilde{u}, \widetilde{u})$ in [28]. In addition, the assertion (3) leads us to give large time behaviors of solutions. In fact, some global attractors are in S. Moreover, the trivial solution is clearly unstable, which follows from the strong maximum principle.

For proving the existence theory, one can release the condition of uniform continuity for initial data. Indeed, for $u_0, v_0 \in L^\infty(\mathbb{R}^n)$, there exists a pair of time-global unique smooth nonnegative solutions to BZ. However, in this case, there is a lack of the continuity of solutions in time at $t = 0$. So, the solutions belong to $C_w((0,\infty); L^\infty(\mathbb{R}^n))$, i.e., $C([\delta,\infty); L^\infty(\mathbb{R}^n))$ for $\delta > 0$.

For proving Theorem 3.4.1 (1), we first show the existence of time-local unique nonnegative classical solutions. To construct time-local solutions, the key idea is to use the certain successive approximation. One may easily see that the solution is smooth in t and x. Once we obtain time-local well-posedness, it is rather easy to extend the solution time-globally, since a priori bounds are derived uniformly in time and space by the maximum principle. Global bounds of solutions follow from the behaviors of those to the corresponding ordinary differential equations of the logistic type.

Let us consider the following initial value problem associated with the second equation of BZ:

$$(\mathrm{P_V}) \begin{cases} \partial_t \psi = d\Delta\psi - \psi + \varphi & \text{in} \quad \mathbb{R}^n \times (0,\infty), \\ \psi|_{t=0} = \psi_0 & \text{in} \quad \mathbb{R}^n. \end{cases}$$

Here, $\varphi := \varphi(x,t)$ is a given bounded function. We are now in a position to state the time-global solvability of this problem, and derive upper and lower bounds for the solutions ψ.

Lemma 3.5.1 *Let $n \in \mathbb{N}$, $d > 0$, $c \geq 0$, and let $\varphi \in L^\infty(\mathbb{R}^n \times (0,\infty))$ with $\varphi(x,t) \geq c$ for $x \in \mathbb{R}^n$ and $t > 0$. If $\psi_0 \in BUC$ with $\psi_0(x) \geq c$ for $x \in \mathbb{R}^n$, then there exists a time-global unique solution to* $(\mathrm{P_V})$ *in $C([0,\infty); BUC)$ with $\psi(x,t) \geq c$ for $x \in \mathbb{R}^n$ and $t > 0$, enjoying*

$$\|\psi(t)\|_\infty \leq \|\psi_0\|_\infty + t \max_{0 \leq \tau \leq t} \|\varphi(\tau)\|_\infty \quad \text{for} \ \ t > 0. \tag{3.5.1}$$

Proof. Let $L := d\Delta - 1$. One may see that L generates a (C_0) semigroup

$\{e^{tL}\}_{t\geq 0}$ in BUC with

$$\|e^{tL}\|_{\mathcal{L}(L^\infty)} := \|e^{tL}\|_{L^\infty\to L^\infty} := \sup_{\psi_0\in L^\infty,\not\equiv 0} \frac{\|e^{tL}\psi_0\|_\infty}{\|\psi_0\|_\infty} \leq e^{-t} \quad \text{for } t>0,$$

since $e^{tL} = e^{-t}e^{dt\Delta}$. So, for $\psi_0 \in BUC$, $(\mathrm{P_V})$ is written as

$$\psi(t) = e^{tL}\psi_0 + \int_0^t e^{(t-s)L}\varphi(s)ds. \tag{3.5.2}$$

The existence of a time-global unique solution follows from this formula. Taking L^∞-norm into (3.5.2) above, the upper bound estimate (3.5.1) is easily obtained.

We next show the lower bound. If $\varphi \equiv \psi_0 \equiv c$, then $\psi \equiv c$ is a unique solution to $(\mathrm{P_V})$. So, by (3.5.2), $\chi := \psi - c$ satisfies

$$\chi(t) = e^{tL}(\psi_0 - c) + \int_0^t e^{(t-s)L}\left\{\varphi(s) - c\right\} ds \geq 0$$

for $x \in \mathbb{R}^n$ and $t > t_\flat$. Thus, $\psi \geq c$. $\square$

Remark 3.5.1 (i) If φ has some regularity, e.g. $\varphi \in L^\infty([0,\infty); W^{1,\infty})$, then ψ becomes a classical solution; C^1 in t and C^2 in x; see the proof of Lemma 3.5.3 in below. Moreover, if φ is smooth in t and x, then the solution ψ is also smooth in t and x.
(ii) If either $\varphi(x,t) > c$ in some open set around $x_\flat \in \mathbb{R}^n$ and $t_\flat \in [0,\infty)$ or $\psi_0 \not\equiv c$, then $\psi(x,t) > 0$ for $x \in \mathbb{R}^n$ and $t > t_\flat$ by the strong maximum principle.

In what follows, we recall some theories and estimates for time evolution operators. Let us consider the following autonomous problem:

$$(\mathrm{P_A}) \begin{cases} \partial_t\xi = \Delta\xi - \eta(x,t)\xi & \text{in } \mathbb{R}^n\times(0,\infty), \\ \xi|_{t=0} = \xi_0 & \text{in } \mathbb{R}^n. \end{cases}$$

Here, $\eta := \eta(x,t)$ is a given bounded function. We now establish the time-local solvability of $(\mathrm{P_A})$ with upper bounds of $\xi(t)$.

Lemma 3.5.2 *Let $n \in \mathbb{N}$, $a > 0$. Assume that $\eta \in L^\infty(\mathbb{R}^n \times [0,\infty))$ with $|\eta(x,t)| \le a$ for $x \in \mathbb{R}^n$ and $t > 0$. If $\xi_0 \in BUC$, then there exist a $T_* > 0$ and a time-local unique solution to* $(\mathrm{P_A})$ *in $C([0,T_*];BUC)$, having $\|\xi(t)\|_\infty \le \dfrac{4}{3}\|\xi_0\|_\infty$ holds for $t \in [0,T_*]$.*

Proof. The proof is based on the standard iteration. Set $\xi_1(t) := e^{t\Delta}\xi_0$,

$$\xi_{\ell+1}(t) := e^{t\Delta}\xi_0 - \int_0^t e^{(t-s)\Delta}\eta(s)\ \xi_\ell(s)ds$$

for $\ell \in \mathbb{N}$, successively. Obviously, $\|\xi_1(t)\|_\infty \le \|\xi_0\|_\infty$ for $t > 0$. Taking $\|\cdot\|_\infty$ into above, $\|\xi_{\ell+1}(t)\|_\infty \le \dfrac{4}{3}\|\xi_0\|_\infty$ holds for $\ell \in \mathbb{N}$, at least when $t \in \left[0, \dfrac{1}{4a}\right]$. So, we also see that $\left\{\xi_\ell\right\}_{\ell=1}^\infty$ is a Cauchy sequence in $C([0,T_*];BUC)$ with some $T_* \ge \dfrac{1}{4a}$. One can easily check that $\xi = \lim_{\ell\to\infty}\xi_\ell$ is a solution to $(\mathrm{P_A})$. The uniqueness follows from the Gronwall inequality, as usual. □

Let $A := A(x,t) := \Delta - \eta(x,t)$. By using time evolution operators $\left\{U(t,s)\right\}_{0\le s\le t}$ associated with A, then the solution to $(\mathrm{P_A})$ can be rewritten as $\xi(t) = U(t,0)\xi_0$; see e.g. the book of Tanabe [23]. The upper bound above implies $\|U(t,0)\|_{L^\infty\to L^\infty} \le 4/3$ for $0 \le t \le \dfrac{1}{4a}$, as well as $\|U(t,s)\|_{L^\infty\to L^\infty} \le 4/3$ for $0 \le s \le t \le \dfrac{1}{4a}$.

Now, we begin to discuss a classical solution to $(\mathrm{P_A})$. Let $\nabla := (\partial_1,\ldots,\partial_n)$.

Lemma 3.5.3 *Adding the assumption in Lemma* 3.5.2*, suppose $t^{1/2}\nabla\eta(t) \in L^\infty(\mathbb{R}^n \times [0,\infty))$. Then ξ is a classical solution to* $(\mathrm{P_A})$.

Proof. Although the argument is rather standard, we give a proof. It is easy to see that $\|\nabla\xi(t)\|_\infty \le Ct^{-1/2}$ for $t \in (0,T_*]$ with $T_* \le 1$ by

$$\xi(t) = e^{t\Delta}\xi_0 - \int_0^t e^{(t-s)\Delta}\eta(s)\xi(s)ds,$$

taking ∇ and $\|\cdot\|_\infty$ into above. So, the key is to derive estimates for the second spatial derivatives. One easily has

$$\begin{aligned}\|\nabla^2\xi(t)\|_\infty &\le \|\nabla^2 e^{t\Delta}\xi_0\|_\infty + \int_0^t \|\nabla^2 e^{(t-s)\Delta}\eta(s)\xi(s)\|_\infty ds \\ &\le Ct^{-1}\|\xi_0\|_\infty + \int_0^t (t-s)^{-1/2}\|\nabla\left\{\eta(s)\xi(s)\right\}\|_\infty ds \\ &\le Ct^{-1}\|\xi_0\|_\infty + \int_0^t (t-s)^{-1/2} C s^{-1/2} ds \le Ct^{-1}\end{aligned}$$

for $t \in (0, T'_*]$ with $T'_* \le T_* \le 1$ and constant C depending only on n, $\|\xi_0\|_\infty$, $\sup_{0\le\tau\le T'_*}\|\eta(\tau)\|_\infty$ and $\sup_{0\le\tau\le T'_*}\tau^{1/2}\|\nabla\xi(\tau)\|_\infty$. The estimate for $\partial_t\xi$ can also be derived, similarly. By uniqueness, ξ becomes a classical solution as long as it exists, at least up to T_*. $\square$

In here, a kind of linearized problem of the first equation of BZ with a non-autonomous term is considered.

$$(\mathrm{P_N})\quad \begin{cases} \partial_t\xi = \Delta\xi - \eta(x,t)\{\xi - c\} + \zeta(x,t) & \text{in}\quad \mathbb{R}^n\times(0,\infty), \\ \xi|_{t=0} = \xi_0 & \text{in}\quad \mathbb{R}^n. \end{cases}$$

Here, $\zeta := \zeta(x,t)$ is a given bounded function; $c \ge 0$ is a constant. By deriving estimates of semigroups and time evolution operators, and by applying the maximum principle, the unique existence and the positivity of solutions are ensured by the construction of time-local solutions.

Lemma 3.5.4 *Let $n \in \mathbb{N}$, a, $b > 0$ and $c \ge 0$. Assume that η, $\zeta \in L^\infty(\mathbb{R}^n \times [0,\infty))$ satisfying $t^{1/2}\nabla\eta$ and $t^{1/2}\nabla\zeta$ are bounded, $|\eta| \le a$ and $0 < \zeta \le b$ for $x \in \mathbb{R}^n$ and $t > 0$. If $\xi_0 \in BUC$ with $\xi_0(x) \ge c$ for $x \in \mathbb{R}^n$, then there exist a $T_\dagger > 0$ and a time-local unique classical solution to $(\mathrm{P_N})$ in $C([0,T_\dagger]; BUC)$ with $\xi(x,t) > c$, and $\|\xi(t)\|_\infty \le 2\|\xi_0\|_\infty$ for $x \in \mathbb{R}^n$ and $t \in [0, T_\dagger]$.*

Proof. Let $\theta := \xi - c$ and $\theta_0 := \xi_0 - c \ge 0$. So, θ satisfies

$$\partial_t\theta = \Delta\theta - \eta(x,t)\theta + \zeta(x,t), \qquad \theta|_{t=0} = \theta_0,$$

which is also rewritten as

$$\theta(t) = U(t,0)\theta_0 + \int_0^t U(t,s)\zeta(s)ds. \tag{3.5.3}$$

When $\theta_0 \equiv 0$, it is easy to show $\theta > 0$. So, let us assume $\|\theta_0\|_\infty > 0$. By Lemma 3.5.2 and Lemma 3.5.3, we can show the existence of a time-local unique classical solution to (3.5.3), having the upper bound estimate:

$$\begin{aligned}\|\theta(t)\|_\infty &\leq \|U(t,0)\theta_0\|_\infty + \int_0^t \|U(t,s)\zeta(s)\|_\infty ds \\ &\leq \frac{4}{3}\|\theta_0\|_\infty + \frac{4}{3}t \max_{0\leq\tau\leq t} \|\zeta(\tau)\|_\infty \leq 2\|\theta_0\|_\infty\end{aligned}$$

for $t \in (0, T_\dagger]$ with some $T_\dagger \leq \min\{T_*, \|\theta_0\|_\infty/2b\}$. Once we have $\xi(t) \geq c$, it is clear that $\|\xi(t)\|_\infty \leq 2\|\xi_0\|_\infty$ in $[0, T_\dagger]$.

The lower bound of solutions follows from the maximum principle for a classical solution. We suppose that there exists $(\hat{x}, \hat{t}) \in \mathbb{R} \times (0, T_*]$ such that $\xi(\hat{x}, \hat{t}) = c$. Without loss of generality, $\hat{t}$ is taken as the first time when ξ touches to c. At $(\hat{x}, \hat{t})$, we see that $\partial_t \xi \leq 0$ in the left hand side of $(\mathrm{P_N})$, however, $\Delta\xi \geq 0$, $\zeta > 0$ and $\eta\{\xi - c\} = 0$ in the right hand side. This contradicts to that ξ is a classical solution to $(\mathrm{P_N})$. We can apply Oleinik's technique to avoid the situation for the case $\xi(\hat{x}, \hat{t}) \to c$ as $|\hat{x}| \to \infty$; see [9] or [10]. Note that even if $\theta_0 = \xi_0 - c \equiv 0$, then $\theta = \xi - c > 0$ by the positivity of ζ. Therefore, $\xi(x,t) > c$ for $x \in \mathbb{R}^n$ and $t \in [0, T_\dagger]$. $\square$

3.5.1 Time-local solvability

By deriving estimates of semigroups and time evolution operators, and by applying the maximum principle, the unique existence and the positivity of solutions are ensured by the construction of time-local solutions from certain successive approximation. We will give the complete proof of the time-local solvability in this section.

Proposition 3.5.1 *Let $n \in \mathbb{N}$, ε, h, $d > 0$, and let $q \in (0,1)$. If u_0, $v_0 \in BUC(\mathbb{R}^n)$ with $q \leq u_0(x) \leq 1$ and $q \leq v_0(x) \leq 1$ for $x \in \mathbb{R}^n$, then there exist $T_0 > 0$ and time-local unique classical solutions (u, v) to BZ in $C([0, T_0]; BUC(\mathbb{R}^n))$ with $q \leq u(x,t) \leq 2m$ and $q \leq v(x,t) \leq 2m$ for $x \in \mathbb{R}^n$ and $t \in [0, T_0]$, where $m := \max\{\|u_0\|_\infty, \|v_0\|_\infty\} \leq 1$. Furthermore, $T_0 \geq C/m$ with some constant $C > 0$ independent of m.*

Proof. We employ an iteration argument. For making the approximation sequences, we begin with

$$u_1(t) := e^{t\Delta}u_0 \quad \text{and} \quad v_1(t) := e^{dt\Delta}v_0.$$

For $\ell \in \mathbb{N}$, we successively define

$$\begin{aligned} u_{\ell+1}(t) &:= U_\ell(t,0)u_0 + \int_0^t U_\ell(t,s)\left[\frac{u_\ell(s)}{\varepsilon} + \frac{hqv_\ell(s)}{u_\ell(s)+q}\right]ds, \\ v_{\ell+1}(t) &:= e^{tL}v_0 + \int_0^t e^{(t-s)L}u_\ell(s)ds. \end{aligned}$$

Here, we put $A_\ell := \Delta - \eta_\ell$ with $\eta_\ell(x,t) := \dfrac{u_\ell(x,t)}{\varepsilon} + \dfrac{hv_\ell(x,t)}{u_\ell(x,t)+q}$, and $\{U_\ell(t,s)\}_{t\geq s\geq 0}$ is the time evolution operator associated with A_ℓ. Note that $u_{\ell+1}$ and $v_{\ell+1}$ formally satisfy

$$\partial_t u_{\ell+1} = A_\ell u_{\ell+1} + \zeta_\ell = \Delta u_{\ell+1} + \frac{u_\ell(1-u_{\ell+1})}{\varepsilon} - hv_\ell \frac{u_{\ell+1}-q}{u_\ell+q}, \tag{3.5.4}$$

with $u_{\ell+1}|_{t=0} = u_0$ and $\zeta_\ell(x,t) := \dfrac{u_\ell(x,t)}{\varepsilon} + \dfrac{hqv_\ell(x,t)}{u_\ell(x,t)+q} \geq 0$;

$$\partial_t v_{\ell+1} = Lv_{\ell+1} + u_\ell = d\Delta v_{\ell+1} - v_{\ell+1} + u_\ell, \tag{3.5.5}$$

with $v_{\ell+1}|_{t=0} = v_0$ for positive functions u_ℓ and v_ℓ.
In what follows, we derive estimates for u_ℓ, v_ℓ, $\partial_i u_\ell$ and $\partial_i v_\ell$. We put

$$\begin{aligned} K_{1,\ell} &:= K_{1,\ell}(T) := \sup\nolimits_{0\leq t\leq T} \|u_\ell(t)\|_\infty, \\ K_{2,\ell} &:= K_{2,\ell}(T) := \sup\nolimits_{0\leq t\leq T} \|v_\ell(t)\|_\infty, \\ K_{3,\ell} &:= K_{3,\ell}(T) := \sup\nolimits_{0\leq t\leq T} t^{1/2}\|\partial_i u_\ell(t)\|_\infty, \\ K_{4,\ell} &:= K_{4,\ell}(T) := \sup\nolimits_{0\leq t\leq T} t^{1/2}\|\partial_i v_\ell(t)\|_\infty, \end{aligned}$$

for $T > 0$, $1 \leq i \leq n$ and $\ell \in \mathbb{N}$. For deriving the uniform estimates, we will use the induction argument for ℓ.

For $\ell = 1$, by $q \leq u_0 \leq m$ and $q \leq v_0 \leq m$, we easily see that $q \leq u_1(t) \leq \|u_0\|_\infty$, $q \leq v_1(t) \leq \|v_0\|_\infty$, $t^{1/2}\|\partial_i u_1(t)\|_\infty \leq \|u_0\|_\infty$ and $t^{1/2}\|\partial_i v_1(t)\|_\infty \leq \|v_0\|_\infty$ for $t > 0$ and $1 \leq i \leq n$ by the maximum principle and estimates for the heat kernel. Thus,

$$K_{j,1} \leq m \quad \text{for} \quad T > 0 \text{ and } 1 \leq j \leq 4. \tag{3.5.6}$$

For $\ell = 2$, before estimating u_2 and v_2, we give bounds for η_1 and ζ_1. By $u_1 \geq q$, $v_1 \geq q$ and conditions of (3.5.6), it holds that

$$\|\eta_1\|_\infty \leq \big(\frac{1}{\varepsilon} + \frac{h}{q}\big)m =: a_1 \quad \text{and} \quad 0 \leq \zeta_1 \leq \big(\frac{1}{\varepsilon} + h\big)m := b_1.$$

So, by Lemma 3.5.2 and Lemma 3.5.4, it holds that

$$\begin{aligned}
\|u_2(t)\|_\infty &\leq \|U_1(t,0)u_0\|_\infty + \int_0^t \|U_1(t,s)\zeta_1(s)\|_\infty \, ds \\
&\leq \frac{4}{3}\, \|u_0\|_\infty + \int_0^t \frac{4}{3}\, b_1 \, ds \\
&\leq 2m
\end{aligned}$$

provided that $t \leq T_{\dagger,2}$ with some $T_{\dagger,2} > 0$. Furthermore, since u_2 is a classical solution to (3.5.4) with $\ell = 1$ by Lemma 3.5.3, with $c = q$, we can apply the maximum principle to obtain $u_2(x,t) \geq q$ for $x \in \mathbb{R}^n$ and $t \in [0, T_{\dagger,2}]$. To get the estimate for $K_{3,2} = \sup_t t^{1/2}\|\partial_i u_2(t)\|_\infty$, we use the expression by the heat semigroup:

$$u_2(t) = e^{t\Delta}u_0 + \int_0^t e^{(t-s)\Delta}\left[-\eta_1(s)u_2(s) + \zeta_1(s)\right] ds.$$

Hence, it holds that

$$t^{1/2}\|\partial_i u_2(t)\|_\infty \leq \|u_0\|_\infty + t^{1/2}\int_0^t (t-s)^{-1/2}[a_1\|u_2(s)\|_\infty + b_1] ds \leq 2m$$

for $t \in (0, T'_{\dagger,2}]$ with some $T'_{\dagger,2} \leq T_{\dagger,2}$. On the other hand, by Lemma 3.5.1, with $c = 0$, it holds that

$$q \leq v_2(x,t) \leq \|v_0\|_\infty + t \sup_{0 \leq \tau \leq t} \|u_1(\tau)\|_\infty \leq 2m$$

for $x \in \mathbb{R}^n$ and $t \in [0,1]$. For deriving the estimate for $\partial_i v_2$, we appeal to the heat semigroup, again, to obtain

$$t^{1/2}\|\partial_i v_2(t)\|_\infty \leq \|v_0\|_\infty + t^{1/2}\int_0^t \|\partial_i e^{(t-s)\Delta}\left[-v_2(s) + u_1(s)\right]\|_\infty \, ds \leq 2m$$

for $t \in (0, T_{\flat,2}]$ with $T_{\flat,2} \leq 1$. So, letting $T_2 := \min\{T'_{\dagger,2}, T_{\flat,2}\}$, we have

$$u_2 \geq q, \quad v_2 \geq q, \quad K_{j,2} \leq 2m \quad \text{for} \quad T \leq T_2, \quad 1 \leq j \leq 4. \tag{3.5.7}$$

As the similar discussion, then there exists a $T_0 \le T_2$ such that

$$u_3 \ge q, \quad v_3 \ge q, \quad K_{j,3} \le 2m \quad \text{for} \quad T \le T_0, \quad 1 \le j \le 4. \tag{3.5.8}$$

Note $T_0 \ge C/m$ with some $C > 0$. The proof is essentially the same as that for $\ell \ge 4$ in below. So, the detail is omitted in here.

Let $\ell \ge 4$. We now assume that

$$u_\ell \ge q, \quad v_\ell \ge q, \quad K_{j,\ell} \le 2m \quad \text{for} \quad T \le T_0, \quad 1 \le j \le 4 \tag{3.5.9}$$

hold. We will compute estimates for $u_{\ell+1}$ and $v_{\ell+1}$. By assumption,

$$\|\eta_\ell\|_\infty \le \big(\frac{1}{\varepsilon} + \frac{h}{q}\big)2m =: a \quad \text{and} \quad 0 \le \zeta_\ell \le \big(\frac{1}{\varepsilon} + h\big)2m := b$$

hold for $t \in [0, T_0]$. Hence, by Lemma 3.5.2 and Lemma 3.5.4, one can see that

$$\begin{aligned}
\|u_{\ell+1}(t)\|_\infty &\le \|U_\ell(t,0)u_0\|_\infty + \int_0^t \|U_\ell(t,s)\zeta_\ell(s)\|_\infty \, ds \\
&\le \frac{4}{3}m + \int_0^t \frac{4}{3} b \, ds \\
&\le 2m
\end{aligned}$$

for $t \in [0, T_0]$. Note that we took $T_0 \le m/2b$ in here. Since u_ℓ is a classical solution to (3.5.4), we can apply the maximum principle to obtain $u_{\ell+1}(x,t) \ge 0$ for $x \in \mathbb{R}^n$ and $t \in [0, T_0]$. For using the expression

$$u_{\ell+1}(t) = e^{t\Delta}u_0 + \int_0^t e^{(t-s)\Delta}\left[-\eta_\ell(s)u_{\ell+1}(s) + \zeta_\ell(s)\right] ds,$$

we take ∂_i and $\|\cdot\|_\infty$ into above to obtain that

$$t^{1/2}\|\partial_i u_{\ell+1}(t)\|_\infty \le \|u_0\|_\infty + t^{1/2}\int_0^t (t-s)^{-1/2}[a\|u_{\ell+1}(s)\|_\infty + b] \, ds \le 2m$$

for $t \in [0, T_0]$ by (3.5.1). Besides, by Lemma 3.5.1,

$$q \le v_{\ell+1}(x,t) \le \|v_0\|_\infty + t \sup_{0 \le \tau \le t} \|v_\ell(\tau)\|_\infty \le 2m$$

holds for $x \in \mathbb{R}^n$ and $t \in [0, T_0]$. By the heat semigroup, we obtain

$$t^{1/2} \|\partial_i v_{\ell+1}(t)\|_\infty \leq \|v_0\|_\infty + t^{1/2} \int_0^t \|\partial_i e^{(t-s)\Delta} \left[-v_{\ell+1}(s) + u_\ell(s) \right] \|_\infty \, ds \leq 2m$$

for $t \in [0, T_0]$. Therefore,

$$u_{\ell+1} \geq q, \quad v_{\ell+1} \geq q, \quad K_{j,\ell+1} \leq 2m \quad \text{for} \quad T \leq T_0, \quad 1 \leq j \leq 4.$$

Thus, (3.5.9) holds true for all $\ell \in \mathbb{N}$.

One may see that u_ℓ and v_ℓ are continuous in $t \in [0, T_0]$ for $\ell \in \mathbb{N}$. It is also easy to see that $\left\{ u_\ell, v_\ell, t^{1/2} \partial_i u_\ell, t^{1/2} \partial_i v_\ell \right\}_{\ell=1}^\infty$ are Cauchy sequences in $C([0, T_0]; BUC)$, taking T_0 small again, necessarily. We denote $(u, v, \hat{u}, \hat{v})$ by the limit functions of $(u_\ell, v_\ell, t^{1/2} \nabla u_\ell, t^{1/2} \nabla v_\ell)$ as $\ell \to \infty$. The coincidences $\hat{u} = t^{1/2} \nabla u$ and $\hat{v} = t^{1/2} \nabla v$ hold, obviously. The uniqueness follows from the Gronwall inequality, directly. Furthermore, by construction, $q \leq u(x,t) \leq 2m$ and $q \leq v(x,t) \leq 2m$ for $x \in \mathbb{R}^n$ and $t \in [0, T_0]$, as well as (u, v) is a pair of the time-local unique classical solutions to BZ. This completes the proof of Proposition 3.5.1. $\square$

Remark 3.5.2 (i) For $k \in \mathbb{N}$, it is possible to construct $u(t), v(t) \in C^k(\mathbb{R}^n)$ for $t \in (0, T_k]$, if T_k is chosen small enough. Nevertheless, the solution is unique as long as it exists, one can extend the existence time of the solution up to T_0 having bounds for k-th derivatives. We hence confirm that $u(t) \in C^k(\mathbb{R}^n)$ for all $k \in \mathbb{N}$ and $t \in (0, T_0]$, which means that $u(t), v(t) \in C^\infty(\mathbb{R}^n)$ in $t \in (0, T_0]$, as well as $u, v \in C^\infty(\mathbb{R}^n \times (0, T_0])$.

(ii) This iteration procedure also works for proving $u \geq 0$ and $v \geq 0$, provided if $u_0 \geq 0$ and $v_0 \geq 0$. Since $u_\ell \geq 0$ and $v_\ell \geq 0$ hold for $\ell \in \mathbb{N}$ by Lemma 3.5.1 and Lemma 3.5.4 with $c = 0$, as the same way as above, we ensure that the limits also satisfy $0 \leq u(x,t) \leq 2m$ and $0 \leq v(x,t) \leq 2m$ for $x \in \mathbb{R}^n$ and $t \in [0, T_0]$.

3.5.2 Invariant region

This section mainly concerns the invariant region and large time behaviour of BZ solutions. In this subsection, invariant regions are discussed. We first show that the solutions obtained by Proposition 3.5.1 can be extended time-globally. Also besides, invariant regions and large time behavior of solutions can be shown in the proposition 3.5.2.

Proposition 3.5.2 *Let $n \in \mathbb{N}$, ε, h, $d > 0$ and $q \in (0,1)$. If u_0, $v_0 \in BUC(\mathbb{R}^n)$ with $0 \leq u_0(x) \leq m$ and $0 \leq v_0(x) \leq m$ for $x \in \mathbb{R}^n$ with some $m \geq 1$, then there exists a time-global unique classical solutions (u,v) to BZ in $C([0,\infty); BUC(\mathbb{R}^n))$ with $0 \leq u(x,t) \leq m$ and $0 \leq v(x,t) \leq m$ for $x \in \mathbb{R}^n$ and $t > 0$.*

Proof. By Proposition 3.5.1, we have already obtained a pair of time-local unique classical solutions $(u(x,t), v(x,t)) \in [0,2m]^2$ for $x \in \mathbb{R}^n$ and $t \in [0,T_0]$. In what follows, we will derive the a priori estimates $u \leq m$ and $v \leq m$ for $t \in [0,T_0]$. It is enough to consider the local behavior of solutions. Using the same argument in the proof of Lemma 3.5.4, there does not exist $(\tilde{x},\tilde{t})$ such that $u(\tilde{x},\tilde{t}) > m$ by $m \geq 1$. So, we have $u \leq m$. Furthermore, since $u \leq m$ and $v_0 \leq m$, one can also see that $v > m$ never happened. So, $v \leq m$.

Gathering the time-local solvability, uniqueness and upper bounds, we can extend the solution up to $t \in [0,2T_0]$. Repeating this argument infinitely many times, we obtain a time-global unique classical solution $(u,v) \in [0,m]^2$.
□

Note that Theorem 3.4.1 (1) immediately follows from Proposition 3.5.2. And also, this implies that $[0,m]^2$ is an invariant region for $m \geq 1$. We are now in a position to show that $S := (q,\bar{u})^2$ is an invariant region.

Proof of Theorem 3.4.1 (2)

Let $(u_0,v_0) \in S$. By Proposition 3.5.1, Remark 3.5.2 (ii) and Proposition 3.5.2, we have obtained a time-global unique smooth solutions having the lower and upper bounds $(u,v) \in [q,1]^2$. So, it is required to show that

u and v never touched to $\bar{u} \in (q,1)$. We assume that there exists $(\bar{x},\bar{t})$ such that $u(\bar{x},\bar{t}) = \bar{u}$. Without loss of generality, we take $\bar{t} \in (0,\infty)$ is the first time, and $\bar{x} \in \mathbb{R}^n$. Since $u, v \geq q$ and $\bar{u}$ is a positive root of $g(u) = 0$, at $(\bar{x},\bar{t})$ we see that $\partial_t u > 0$, $\Delta u \leq 0$ and $\dfrac{1}{\varepsilon}u(1-u) - hv\dfrac{u-q}{u+q} \leq 0$. This contradicts to that u is a solution. One can avoid the case $u(x,t) \to \bar{u}$ at $|x| \to \infty$ by Oleinik's technique.

Similarly, if there exists $(\bar{x},\bar{t})$ such that $v(\bar{x},\bar{t}) = \bar{u}$, then at $(\bar{x},\bar{t})$ we see that $\partial_t v > 0$, $d\Delta v \leq 0$ and $-v + u \leq -v + \bar{u} = 0$. This is a contradiction. It is also easy to see that u and v never touched to q, as the same arguments above. Therefore, $(u,v) \in S$. $\square$

In BZ equations, it is possible to occur that the solution running for a large value of time. Finally, we will give the remaining parts of the proof of Theorem 3.4.1. We will discuss the large time behaviors of BZ solutions.

Proof of Theorem 3.4.1 (3)

We now put $m := \max\{\|u_0\|_\infty, \|v_0\|_\infty\} > 1$ and $c_* \in (0,q)$, without loss of generality. Applying Lemma 3.5.1, Lemma 3.5.4, with $c = c_*$, and Proposition 3.5.2. It is easy to see that $c_* \leq u(x,t) \leq m$ and $c_* \leq v(x,t) \leq m$ for $x \in \mathbb{R}^n$ and $t > t_*$. Let $\rho := \rho(t)$ be the solution to the following ordinary differential equation of logistic type:

$$\rho' = \frac{1}{\varepsilon}\rho(1-\rho) \quad \text{for} \quad t > t_*, \quad \rho(t_*) = c_*.$$

Note that $0 < c_* < q < 1$, and then ρ is monotone increasing. So, there exists a $T_{\sharp 1} > t_*$ such that $\rho(T_{\sharp 1}) = q$. By the argument of the maximum principle, $u(x,t) \geq \rho(t)$ for $x \in \mathbb{R}^n$ and $t \in [t_*, T_{\sharp 1}]$, that is to say, ρ is a subsolution of u up to $T_{\sharp 1}$.

We secondly consider that $\sigma := \sigma(t)$ is the solution to

$$\sigma' = G_m(\sigma) := \frac{1}{\varepsilon}\sigma(1-\sigma) - hm\frac{\sigma - q}{\sigma + q} \quad \text{for} \quad t > T_{\sharp 1}, \quad \sigma(T_{\sharp 1}) = q.$$

Note that there exists $q_1 \in (q,1)$ such that $G_m(q_1) = 0$, and $\sigma(t)$ converges to q_1 as t tend to infinite. Since σ is monotone increasing, for $q_2 \in (q, q_1)$, then there exists a $T_{\sharp 2} \geq T_{\sharp 1}$ such that $\sigma(T_{\sharp 2}) = q_2$. Again, σ is a subsolution of u, we thus see that $u(x,t) \geq q_2 > q$ for $x \in \mathbb{R}^n$ and $t \geq T_{\sharp 2}$.

Thirdly, we derive a lower bound of v. Let $\nu := \nu(t)$ be a solution to differential equation

$$\nu' = -\nu + q_2 \quad \text{for} \quad t > T_{\sharp 2}, \quad \nu(T_{\sharp 2}) = c_*.$$

Obviously, ν is monotone increasing, and $\nu(t)$ converges to q_2 as t running to infinity. Hence, for $q_3 \in (q, q_2)$, there exists a $T_{\sharp 3} \geq T_{\sharp 2}$ such that $\nu(T_{\sharp 3}) = q_3$. Since ν is a subsolution of v, we have $v(x,t) \geq q_3 > q$ for $x \in \mathbb{R}^n$ and $t \geq T_{\sharp 3}$.

In what follows, we shall derive upper bounds of u and v. Let us define $\kappa := \kappa(t)$ as the solution to

$$\kappa' = G_*(\kappa) := \frac{1}{\varepsilon}\kappa(1-\kappa) - hq_3\frac{\kappa - q}{\kappa + q} \quad \text{for} \quad t > T_{\sharp 3}, \quad \kappa(T_{\sharp 3}) = m.$$

Note that κ is monotone decreasing, and $\kappa(t)$ converges to κ_* as t tend to infinite, where $\kappa_* \in (q, \bar{u})$ satisfies $G_*(\kappa) = 0$. For $u_* \in (\kappa_*, \bar{u})$, there exists a $T_{\sharp 4} \geq T_{\sharp 3}$ such that $\kappa(T_{\sharp 4}) = u_*$. Since $v \geq q_3$ for $t \geq T_{\sharp 3}$, it holds that $u(x,t) \leq \kappa(t)$ for $x \in \mathbb{R}^n$ and $t \geq T_{\sharp 3}$. That is to say, κ is a supersolution of u. Moreover, $u(x, T_{\sharp 4}) \leq u_*$ for $x \in \mathbb{R}^n$. We thus see that $u(x,t) \leq u_* < \bar{u}$ for $x \in \mathbb{R}^n$ and $t \geq T_{\sharp 4}$.

Since $u \leq u_* < \bar{u}$ for $t \geq T_{\sharp 4}$, there exists a $T_\sharp \geq T_{\sharp 4}$ such that $v(x, T_\sharp) \leq \bar{u}$ for $x \in \mathbb{R}^n$, by observing a supersolution of v:

$$\mu' = -\mu + u_* \quad \text{for} \quad t > T_{\sharp 4}, \quad \mu(T_{\sharp 4}) = m.$$

Hence, $v(x,t) < \bar{u}$ for $x \in \mathbb{R}^n$ and $t > T_\sharp$.

Note that S is an invariant region by Theorem 3.4.1 (2). Therefore, summing up the arguments above, $(u(x,t), v(x,t)) \in S$ for $x \in \mathbb{R}^n$ and $t > T_\sharp$. This completes the proof of Theorem 3.4.1 (3). $\square$

Remark 3.5.3 (i) Looking at the proof above, we find the following fact. Let $\bar{\kappa} \in (q, \bar{u})$ be a root of $\kappa(1-\kappa)(\kappa + q) - \varepsilon h q_1(\kappa - q) = 0$. For $q_\natural \in [q, q_1)$ and $u_\natural \in (\bar{\kappa}, \bar{u}]$, then there exists a $T_\natural \geq t_*$ such that $(u(x,t), v(x,t)) \in S_\natural := (q_\natural, u_\natural)^2 \subset S$ for $x \in \mathbb{R}^n$ and $t \geq T_\natural$. Note that $S_\natural$ is an invariant region depending on m.

(ii) The assumption $u(t_*), v(t_*) \geq c_*$ are crucial. Indeed, it seems to be difficult to show $(u,v) \in S$ for large t, when $u_0 \geq 0$, $v_0 \geq 0$ and either $u_0 \not\equiv 0$ or $v_0 \not\equiv 0$ only.

Chapter 4

Positivity-preserving numerical methods for Belousov–Zhabotinsky reaction

In this chapter, the existence of positive solutions to the system of ordinary differential equations related to the Belousov-Zhabotinsky reaction is established. Our idea is to use a new successive approximation of solutions, ensuring its positivity. To obtain the positivity and invariant region for numerical solutions, the system is discretized as difference equations of explicit form, employing operator splitting methods with linear stability conditions. An algorithm to solve the alternate solution is given.

4.1 Introduction

We consider the reaction-diffusion equations of Keener-Tyson model for Be lousov–Zhabotinsky reaction BZ in chapter 2, Section 2.2. There are many literatures on structure-preserving numerical methods for partial differential equations; see e.g. [7] and references therein. Moreover, the researchers on reaction-diffusion equations often discuss the positivity of numerical solutions, when the time-step size Δt is small enough; the reader can find it in e.g. [29]. From this viewpoint, it has been known that Mimura and his collaborators obtained the positive numerical solutions to the system of some reaction-diffusion equations; see [16, 17]. However, it seems to be new that a numerical scheme leads us to invariant regions. Also besides, there are many numerical results on BZ reaction; see e.g. [24] and references therein. On the other hand, here our scheme is an explicit method which has the features as aiming at application to validated numerics, in the future.

4.2 Objective

Continuing from Chapter 3, the interesting one on BZ reaction, the positivity of u is a critical issue. The goal of this study is to give a new discretization scheme for some reaction-diffusion equations, which priori ensures the positivity-preserving. Our aim is to establish similar results for numerical solutions to the difference equations discretized BZ of special type.

4.3 Results

The virtue of using the following new successive approximation of BZ solutions is to be ensured the positivity of the solutions, automatically. Here, we emphasize that this technique can be applied to construct the positivity (or, non-negative) of solutions to ordinary differential equations and positive numerical solutions to finite difference equations.

$$\begin{aligned}
\partial_t u_{\ell+1} &= \Delta u_{\ell+1} + \frac{1}{\varepsilon} u_\ell (1 - u_{\ell+1}) - h v_\ell \left(\frac{u_{\ell+1} - q}{u_\ell + q} \right), \\
\partial_t v_{\ell+1} &= d\Delta v_{\ell+1} - v_{\ell+1} + u_\ell,
\end{aligned}$$

for $\ell \in \mathbb{N}$ with $u_{\ell+1}|_{t=0} = u_0$ and $v_{\ell+1}|_{t=0} = v_0$, starting at $u_1 := e^{t\Delta} u_0$ and $v_1 := e^{dt\Delta} v_0$ with nonnegative initial data u_0, $v_0 \in BUC(\mathbb{R}^n)$.

The construction of time-local positive solutions to the system of first-order ordinary differential equation (ODE), deal with the following system:

$$\text{(P)} \qquad u_i' = -f_i(\mathbf{u}) u_i + g_i(\mathbf{u}), \quad t > 0, \quad u_i(0) = a_i, \quad i = 1, \dots, m,$$

for natural number of m.

Let X, Y be metric spaces, then $F : X \to Y$ is called *Lipschitz* (continuous) if there exist a number $\Lambda > 0$ such that $\|F(x_1) - F(x_2)\| \le \Lambda \|x_1 - x_2\|$ for all $x_1, x_2 \in X$. Furthermore, F is called *locally Lipschitz* (continuous) if for every $x \in X$ there exists some $\epsilon > 0$ such that F is Lipschitz continuous on the ϵ-neighborhood of x.

Theorem 4.3.1 *If $f_i, g_i \geq 0$ are locally Lipschitz continuous and $a_i \geq 0$, then there exists a time-local unique solution $u_i \geq 0$ to* (P)*.*

To obtain the positivity and invariant region for numerical solutions, the system is discretized as difference equations of explicit form. We argue the numerical algorithm for positive solutions. We first discuss a discretization of (P). To obtain positive solutions, we choose the following difference equations (DE), mixing the forward and backward Euler methods:

$$\text{(DE)} \qquad \frac{\mathbf{u}^{k+1} - \mathbf{u}^k}{\Delta t} = -F(\mathbf{u}^k)\mathbf{u}^{k+1} + \mathbf{g}(\mathbf{u}^k), \quad k \in \mathbb{N}_0 := \mathbb{N} \cup \{0\},$$

where $\mathbf{u}^k = \left(u_1^k, \ldots, u_m^k\right)$, $t_k := k\Delta t$ for $\Delta t > 0$ and $u_i^0 = a_i \geq 0$ for $i = 1, \ldots, m$.

Theorem 4.3.2 *If $f_i, g_i \geq 0$ are Lipschitz continuous, $\Delta t > 0$ and $u_i^0 \geq 0$, then the numerical solution $u_i^k \geq 0$ to* (DE) *exists for $k \in \mathbb{N}$.*

In the end, employing operator splitting methods with linear stability conditions for solving the discretized reaction–diffusion equation. First, we will state the results on numerical solutions of BZ to discretized equations. Let us consider the discretization,

$$\text{(D}_\text{o}\text{)} \qquad \begin{cases} \dfrac{u_j^{k+1} - u_j^k}{\Delta t} = \dfrac{u_j^k(1 - u_j^{k+1})}{\varepsilon} - h\, v_j^k\, \dfrac{u_j^{k+1} - q}{u_j^k + q}, \\ \dfrac{v_j^{k+1} - v_j^k}{\Delta t} = -v_j^{k+1} + u_j^k \end{cases}$$

for $j = 1, \ldots, J-1$ and $k \in \mathbb{N}_0$. On the other hand, for the discretization of the heat equations, we use the standard FTCS (forward difference for time and second-order central difference for space),

$$\text{(D}_\text{h}\text{)} \qquad \begin{cases} \dfrac{\tilde{u}_j^{k+1} - \tilde{u}_j^k}{\Delta t} = \dfrac{\tilde{u}_{j+1}^k - 2\tilde{u}_j^k + \tilde{u}_{j-1}^k}{\Delta x^2}, \\ \dfrac{\tilde{v}_j^{k+1} - \tilde{v}_j^k}{\Delta t} = d\dfrac{\tilde{v}_{j+1}^k - 2\tilde{v}_j^k + \tilde{v}_{j-1}^k}{\Delta x^2} \end{cases}$$

for $j = 1, \ldots, J-1$ and $k \in \mathbb{N}_0$.

Theorem 4.3.3 *Let $\varepsilon, h, \Delta t, \Delta x > 0$, $d \geq 0$ and $q \in (0,1)$. Define u_j^k, v_j^k as numerical solutions to alternate* $(\mathrm{D_o})$ *and* $(\mathrm{D_h})$*. If $u_j^0, v_j^0 \in (q,1)$ for j, then $u_j^k, v_j^k \in (q,1)$ for j and k, provided if $\Delta t/\Delta x^2 \leq 1/\max\{2, 2d\}$.*

4.4 Ordinary differential equations

The construction of time-local positive solutions to the system of first order ordinary differential equations (ODE) is discussed in this section. We deal with system ODE nonlinear (P) in Section 4.3.

Throughout this processing, for simplicity of notation, $t = 0$ is the initial time, $' := d/dt$, $\mathbf{u} := \big(u_1, \ldots, u_m\big)$. Here, $u_i = u_i(t)$ are unknown functions for $t > 0$ and $i = 1, \ldots, m$. Besides, $a_i \geq 0$ are given initial data, $f_i \geq 0$ and $g_i \geq 0$ are also given function. We often rewrite (P) into the following vector valued ODE:

$$(\mathrm{P}') \quad \begin{cases} \mathbf{u}' & = -F(\mathbf{u})\mathbf{u} + \mathbf{g}(\mathbf{u}), \quad t > 0, \\ \mathbf{u}(0) & = \mathbf{a}. \end{cases}$$

Here, we have denoted $\mathbf{a} := \big(a_1, \ldots, a_m\big)$, $\mathbf{g} := \big(g_1, \ldots, g_m\big)$, and F is the diagonal $m \times m$ matrix whose (i,i)-component is f_i.
When $m = 2$, $u := u_1$, $v := u_2$, $a_1 := u_0$, $a_2 := v_0$ and

$$F := \begin{pmatrix} u/\varepsilon + hv/(u+q) & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathbf{g} := \begin{pmatrix} u/\varepsilon + hqv/(u+q) \\ u \end{pmatrix}$$

are taken, then (P) is equivalent to the uniform-in-space BZ. The model problem (P) is often used to describe dynamics of nonlinear chemical or biological systems, for example, the Lotka-Volterra type equations of prey-predator models with density-dependent inhibition (Holling's type II or type IV), epidemic SIV (or, SHIV) models and the Gierer-Meinhardt model. We especially treat fractional nonlinear terms, and the denominator takes on the value of zero for negative solutions. Hence, the positivity of solutions to (P) is strongly required, and so is even in its approximation.

4.4.1 Proof of Theorem 4.3.1

We consider the nonlinear system (P) in Section 4.3. Let $a_i \geq 0$ for $i = 1, \dots, m$. For the sake of simplicity, let us assume that $\mathbf{a} \neq \mathbf{0}$ and $g_i(\mathbf{v}) > 0$ for $\mathbf{v} \neq \mathbf{0}$. Making the approximation sequences $\{u_i^\ell\}_{\ell=1}^\infty$ for $i = 1, \dots, m$, we begin with $\mathbf{u}^1(t) := \mathbf{a}$ for $t \geq 0$. For each $\ell \in \mathbb{N}$, we successively define $\mathbf{u}^{\ell+1}$ as the solution to the system of linear non-autonomous ODE:

$$\text{(SA)} \qquad \left(\mathbf{u}^{\ell+1}\right)' = -F(\mathbf{u}^\ell)\mathbf{u}^{\ell+1} + \mathbf{g}(\mathbf{u}^\ell), \quad t > 0, \quad \mathbf{u}^{\ell+1}(0) = \mathbf{a}$$

with vectors of nonnegative $\mathbf{u}^\ell$ and $\mathbf{a}$. So, (SA) is equivalent to the integral equation

$$\text{(INT)} \qquad \mathbf{u}^{\ell+1}(t) = \mathbf{a} - \int_0^t F(\mathbf{u}^\ell(s))\mathbf{u}^{\ell+1}(s)ds + \int_0^t \mathbf{g}(\mathbf{u}^\ell(s))ds.$$

Heuristically, if F is a constant matrix, then $\mathbf{v}' = -F\mathbf{v}$, $t > 0$, $\mathbf{v}(0) = \mathbf{a}$ admits a solution $\mathbf{v}(t) = e^{-Ft}\mathbf{a}$. In this situation, we thus have

$$\mathbf{u}^{\ell+1}(t) = e^{-Ft}\mathbf{a} + \int_0^t e^{-F(t-s)}\mathbf{g}(\mathbf{u}^\ell(s))ds.$$

For general matrix-valued functions F, one may construct $\mathbf{u}^{\ell+1}$ for each $\ell \in \mathbb{N}$ by perturbation theory, at least time-locally.

Obviously, $u_i^1 \geq 0$ for $i = 1, \dots, m$ and $\|\mathbf{u}^1(t)\| = \|\mathbf{a}\|$ for $t \geq 0$. Here, we have used the max norm for vectors $\|\mathbf{v}\| := \max_{i=1,\dots,m} |v_i|$ for $\mathbf{v} := \big(v_1, \dots, v_m\big)$, as well as to matrices $\|F\| := \max_{i,j=1,\dots,m} |f_{ij}|$ for $F := \big(f_{ij}\big)$. In what follows, we will show the positivity and boundedness of $u_i^{\ell+1}$ by induction in ℓ. For $\mathbf{u}^2$, it holds true that

$$\begin{aligned} \|\mathbf{u}^2(t)\| &\leq \|\mathbf{a}\| + \int_0^t \|F(\mathbf{u}^1(s))\| \cdot \|\mathbf{u}^2(s)\|ds + \int_0^t \|\mathbf{g}(\mathbf{u}^1(s))\|ds \\ &\leq \|\mathbf{a}\| + \|F(\mathbf{a})\| \cdot t \cdot \max_{0\leq s\leq t} \|\mathbf{u}^2(s)\| + t \cdot \|\mathbf{g}(\mathbf{a})\|. \end{aligned}$$

Taking $\max_{0\leq t\leq \tau}$ in both hand side, we have

$$\|\mathbf{u}^2(t)\| \leq 2\|\mathbf{a}\| \quad \text{for} \quad t \in [0, T_2],$$

with $T_2 := \min\big\{1/(3\|F(\mathbf{a})\|), \|\mathbf{a}\|/(3\|\mathbf{g}(\mathbf{a})\|)\big\}$. In addition, we can also obtain that $u_i^2 \geq 0$. Indeed, let us assume that there exists a $t_* \in (0, T_2]$ such that $u_i^2(t_*) = 0$ for some $i = 1, \ldots, m$. Without loss of generality, t_* is the first time when u_i^2 touches 0. So, at t_*, we see that $(u_i^2)' \leq 0$, $f_i(\mathbf{u}^1)u_i^2 = 0$, and $g_i(\mathbf{u}^1) > 0$. This contradicts to the fact that $\mathbf{u}^2$ is a solution to (SA) with $\ell = 1$.

Let $\ell \geq 2$. Assume that $\|\mathbf{u}^\ell(t)\| \leq 2\|\mathbf{a}\|$ and $u_i^\ell(t) \geq 0$ hold for $t \in [0, T_0]$ and $i = 1, \ldots, m$, where $T_0 > 0$ will be determined later. We now argue on $\mathbf{u}^{\ell+1}$. By assumption, it is easy to see that

$$
\begin{aligned}
\|\mathbf{u}^{\ell+1}(t)\| &\leq \|\mathbf{a}\| + \int_0^t \|F(\mathbf{u}^\ell(s))\| \cdot \|\mathbf{u}^{\ell+1}(s)\| ds + \int_0^t \|\mathbf{g}(\mathbf{u}^\ell(s))\| ds \\
&\leq \|\mathbf{a}\| + M_f \cdot t \cdot \max_{0 \leq s \leq t} \|\mathbf{u}^{\ell+1}(s)\| + t \cdot M_g \\
&\leq 2\|\mathbf{a}\| \quad \text{for} \quad t \in [0, T_0],
\end{aligned}
$$

with $T_0 := \min\big\{1/(3M_f), \|\mathbf{a}\|/(3M_g)\big\}$, where

$$
M_f := \sup_{\|\mathbf{v}\| \leq 2\|\mathbf{a}\|,\, \mathbf{v} \geq \mathbf{0}} \|F(\mathbf{v})\|, \quad M_g := \sup_{\|\mathbf{v}\| \leq 2\|\mathbf{a}\|,\, \mathbf{v} \geq \mathbf{0}} \|\mathbf{g}(\mathbf{v})\|.
$$

In addition, we can also see that $u_i^{\ell+1} \geq 0$ for i by the same contradiction argument above. This means that $\|\mathbf{u}^\ell(t)\| \leq 2\|\mathbf{a}\|$ and $u_i^\ell \geq 0$ hold for all $\ell \in \mathbb{N}$ and $i = 1, \ldots, m$ for $t \in [0, T_0]$.

It is straightforward to get the continuity of solutions. One may also see that $\big\{\mathbf{u}_\ell\big\}_{\ell=1}^\infty$ is a Cauchy sequence in $C([0, T_0]; \mathbb{R}^m)$. So, the limit $\big(u_1(t), \ldots, u_m(t)\big) = \mathbf{u}(t) = \lim_{\ell \to \infty} \mathbf{u}^\ell(t)$ exists for $t \in [0, T_0]$, and satisfies (P); $u_i(t) \geq 0$ for $i = 1, \ldots, m$ by construction. The uniqueness follows from Gronwall's inequality, directly. $\square$

Note that the proof is easy, if $a_i > 0$ for all i. In Theorem 4.3.1, it is not needed to use either the existence of stable solutions to (P), comparison principle, nor a priori estimates by Lyapunov functions.

4.5 Difference equations

Before we argue the numerical algorithm for positive solutions, we saw that the discretization of (P), mixing the forward and backward Euler methods, is written as (DE), see Section 4.3. Obviously, (DE) is a mimic of (SA). Also besides, we see that the numerical solution $\mathbf{u}^k$ to (DE) tends to the solution $\mathbf{u}(t)$ to (P) at $t = t_k$ for each k as $\Delta t \to 0$.

4.5.1 Proof of Theorem 4.3.2

Let us consider (DE) in Section 4.3. Here, we rewrite (DE) into the explicit form as

$$u_i^{k+1} = \frac{u_i^k + g_i(\mathbf{u}^k)\mathit{\Delta} t}{1 + f_i(\mathbf{u}^k)\mathit{\Delta} t}, \quad k \in \mathbb{N}_0, \quad i = 1, \ldots, m.$$

So, $u_i^{k+1} \geq 0$, if $u_i^k \geq 0$. Thus, one can prove it by induction. □
The advantage of Theorem 4.3.2 is that we may take arbitrary large $\mathit{\Delta} t$.

The spirit of (DE) is still valid on the numerical methods for construction of nonnegative solutions to the partial differential equations. For simplicity, let $n = 1$, and consider the discretization $\mathbf{u}_j^k$ of $\mathbf{u}(x_j, t_k)$ for $x_j := j\mathit{\Delta} x$ and $t_k := k\mathit{\Delta} t$ satisfying

$$\frac{\mathbf{u}_j^{k+1} - \mathbf{u}_j^k}{\mathit{\Delta} t} = d\frac{\mathbf{u}_{j+1}^k - 2\mathbf{u}_j^k + \mathbf{u}_{j-1}^k}{\mathit{\Delta} x^2} - F(\mathbf{u}_j^k)\mathbf{u}_j^{k+1} + \mathbf{g}(\mathbf{u}_j^k) \tag{4.5.1}$$

with nonnegative initial data. So, it is easy to see that all element of $\mathbf{u}_j^k$ is nonnegative for all j and k, provided if the linear stability condition $\mathit{\Delta} t/\mathit{\Delta} x^2 \leq 1/(2d)$ for $d > 0$ in the Lax-Richtmyer sense is assumed. Note that the similar scheme has also been introduced by Mimura in [16], and [17], for ensuring the postivity of numerical solutions, basically. In fact, Mimura argued the reaction-diffusion equation of following type:

$$\frac{\mathbf{u}_j^{k+1} - \mathbf{u}_j^k}{\mathit{\Delta} t} = \mathcal{D}\frac{\mathbf{u}_{j+1}^k - 2\mathbf{u}_j^k + \mathbf{u}_{j-1}^k}{\mathit{\Delta} x^2} + \widetilde{F}(\mathbf{u}_j^k)\mathbf{u}_j^{k+1} \tag{4.5.2}$$

with nonnegative diagonal matrix $\mathcal{D}$. From this procedure, we can also get positive solutions, under the linear stability conditions. However, it is not clear whether the invariant region for numerical solutions to (4.5.1) and (4.5.2) is derived, in general.

4.6 Numerical solutions to BZ

We will derive invariant regions for numerical solutions to BZ. For the sake of simplicity, let $n = 1$, and let us consider BZ in bounded interval $x \in [0, L]$ for $L > 0$ with the homogeneous Neumann boundary conditions $\partial_x u(0, t) = \partial_x u(L, t) = 0$ or, the periodic boundary conditions $u(x, t) = u(x + L, t)$ for

$t > 0$. For discretization of BZ, we put $u_j^k \approx u(x_j, t_k)$ and $v_j^k \approx v(x_j, t_k)$ for $j = 0, \ldots, J$ and $k \in \mathbb{N}_0$, taking e.g. the average of integration. Here, $J \in \mathbb{N}$, $x_j := j\Delta x$, $t_k := k\Delta t$ for $\Delta x > 0$ and $\Delta t > 0$; $L = J\Delta x$.

We sometimes employ the algorithm of operator splitting methods (OSM) for solving the discretized reaction-diffusion equation and related problems. By using $(\mathrm{D_o})$ and $(\mathrm{D_h})$ in Section 4.3, at $j = 0$ and $j = J$, we give certain definition by boundary conditions. Our algorithm is to solve alternate $(\mathrm{D_o})$ and $(\mathrm{D_h})$. That is to say, a pair of the series $\left\{u_j^k, v_j^k\right\}$ is given as

1. Put $u_j^0 \approx u_0(x_j)$ and $v_j^0 \approx v_0(x_j)$, the average of integration.
2. Construct u_j^1, v_j^1 by $(\mathrm{D_o})$ with $k = 0$.
3. Construct $\tilde{u}_j^1, \tilde{v}_j^1$ by $(\mathrm{D_h})$ with $\tilde{u}_j^0 := u_j^1$ and $\tilde{v}_j^0 := v_j^1$.
4. Construct u_j^2, v_j^2 by $(\mathrm{D_o})$ with $u_j^1 := \tilde{u}_j^1$ and $v_j^1 := \tilde{v}_j^1$.
5. Construct $\tilde{u}_j^2, \tilde{v}_j^2$ by $(\mathrm{D_h})$ with $\tilde{u}_j^1 := u_j^2$ and $\tilde{v}_j^1 := v_j^2$.
6. Repeat this process.

If $d = 0$, then we skip the steps of construction $\tilde{v}_j^k$, that is, $\tilde{v}_j^k := v_j^k$.

4.6.1 Proof of Theorem 4.3.3

Considering $(\mathrm{D_o})$ and $(\mathrm{D_h})$ in Section 4.3, here we will give proof of Theorem 4.3.3. By Theorem 4.3.2 and the linear stability conditions, it holds that $u_j^k, v_j^k \geq 0$ for all j and k. The induction in k is used. Let $u_j^k, v_j^k \in (q, 1)$. We first check that $u_j^{k+1}, v_j^{k+1} > q$ by $(\mathrm{D_o})$. It turns out that

$$\begin{aligned} u_j^{k+1} - q &= \frac{u_j^k + u_j^k \Delta t/\varepsilon + hqv_j^k \Delta t/(u_j^k + q)}{1 + u_j^k \Delta t/\varepsilon + hv_j^k \Delta t/(u_j^k + q)} - q \\ &= \frac{(u_j^k - q) + (1 - q)u_j^k \Delta t/\varepsilon}{1 + u_j^k \Delta t/\varepsilon + hv_j^k \Delta t/(u_j^k + q)} > 0 \end{aligned}$$

by $u_j^k > q$ and $q \in (0, 1)$. Similarly, we have

$$v_j^{k+1} - q = \frac{v_j^k + u_j^k \Delta t}{1 + \Delta t} - q = \frac{(v_j^k - q) + (u_j^k - q)\Delta t}{1 + \Delta t} > 0.$$

One can also easily see that

$$
\begin{aligned}
1-u_j^{k+1} &= \frac{(1-u_j^k)+(1-q)hv_j^k\mathit{\Delta}t/(u_j^k+q)}{1+u_j^k\mathit{\Delta}t/\varepsilon+hv_j^k\mathit{\Delta}t/(u_j^k+q)} > 0,\\
1-v_j^{k+1} &= \frac{(1-v_j^k)+(1-u_j^k)\mathit{\Delta}t}{1+\mathit{\Delta}t} > 0.
\end{aligned}
$$

On $(\mathrm{D_h})$, it is well-known that the linear stability condition yields the maximum principle for numerical solution, that is, $\tilde{u}_j^{k+1}, \tilde{v}_j^{k+1} \in (q,1)$, if $\tilde{u}_j^k, \tilde{v}_j^k \in (q,1)$. This completes the proof. $\square$

Remark 4.6.1 (i) This assertion implies that $S_{\mathit{\Delta}} := (q,1)^2$ is an invariant region for numerical solutions to alternate $(\mathrm{D_o})$ and $(\mathrm{D_h})$.

(ii) One can easily see that $\mathbb{R}_+^2$ is also an invariant region by positivity-preserving.

(iii) The numerical solutions converge to solutions to PDE BZ as $\mathit{\Delta}t \to 0$ with order $O(\mathit{\Delta}t)$, as the same as the standard scheme and equation (4.5.2).

(iv) The similar results on the predator-prey models are also obtained. The reader can find the details on PDE in [20] and references therein.

(v) We believe that one may take initial data, more freely. In fact, if $u_j^0, v_j^0 \geq 0$ for j, and if $u_{j'}^0, v_{j''}^0 > 0$ for some j' and j'', then there exists a $k' \in \mathbb{N}_0$ such that $u_j^k, v_j^k \in (q,1)$ for $k \geq k'$ and j. This means that absorbing sets for numerical solutions always exist in $S_{\mathit{\Delta}}$.

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