

# Analysis, Symmetry and Asymptotic Behaviour of Solutions for the Belousov - Zhabotinsky Model

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## Abstract

This research provides analytical insights in connection with the solutions of the Oregonator model, a refined iteration of the iconic Belousov-Zhabotinsky (BZ) reaction problem. This chemical process, initially observed by B. P. Belousov while replicating the Krebs cycle in vitro and later modified by Zhabotinsky using Ferriphenanthroline (ferroin), has become a hallmark example of non-linear dynamics, chaos theory, and has parallels in various biological systems. Our study systematically delves into the boundedness, regularity, and possible symmetries of weak solutions. We explore traveling waves using the Tanh-method, alongside examining asymptotic solutions entrenched in self-similar forms and exponential scaling leading to a Hamilton-Jacobi equation. This research emphasizes on mathematical arguments along with the dynamics of the involved chemical concentrations. We provide new forms of analytical solutions showing them in a comprehensive manner that connects with the interpretation of the Oregonator model and its broader implications in chemical systems.

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# 1 Introduction

The issue explored in this research dates back to the mid-20th century, initiated by B. P. Belousov while endeavoring to emulate the Krebs cycle "in vitro." As documented in the referenced source [1], Belousov formulated a chemical mixture comprising cerium ions, bromate, and citric acid. During his experimentation, he noticed periodic oscillations in the reaction, leading to a transition between a yellow and a transparent state. Subsequent to Belousov's foundational work, Zhabotinsky enhanced the investigation by replacing the cerium reactant with Fe-phenanthroline (commonly known as ferroin). In this modified system, Zhabotinsky documented oscillations alternating between blue and red hues. After exhaustive research and documentation over the years, this chemical phenomenon was formally christened the Belousov-Zhabotinsky (BZ) reaction problem.

Beyond mere oscillations, the BZ reaction, under specific conditions, exhibits spiraling waves of chemical concentration, reminiscent of patterns observed in certain biological systems [3]. This wave phenomenon offers invaluable insights into reaction-diffusion systems, and the Turing mechanism postulated for pattern formation in morphogenesis [4].

The significance of the BZ reaction transcends its immediate chemical context. It serves as an archetypical example of non-linear dynamics and chaos theory. Furthermore, its oscillatory behavior finds parallels in biological systems, such as cardiac rhythms, neural activity, and circadian rhythms [5]. The ability of simple chemical reactions to produce complex temporal oscillations and spatial patterns has further inspired research into the origins of life and protocells [6].

Modern-day explorations of the BZ reaction delve into microfluidic systems and the impact of environmental heterogeneity on reaction dynamics. There's also an increasing interest in harnessing the BZ reaction for computational tasks, effectively creating chemical-based logic gates [7].

It is worth noting that the Belousov-Zhabotinsky reaction is a highly complex process, and developing a precise mathematical model for it based on the PDE theory is generally challenging. This model involves ten chemical processes with up to seven intermediates (for more details, the reader

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is referred to [2]).

Subsequent to Belousov and Zhabotinsky's initial research, Noyes and Field proposed a refined iteration of the Belousov-Zhabotinsky problem, now widely recognized as the "Oregonator" [9]. This refined model succinctly captured the core chemical dynamics from the original intricate process, providing a conduct for more straightforward mathematical and biophysical investigations. Budrene and Wang demonstrated the presence of chaotic oscillations in the Belousov-Zhabotinsky reactions [10]. Notably, they identified the emergence and subsequent dissolution of chaos, consistent with the Ruelle-Takens-Newhouse scenario (as described in [12]), across both cerium- and ferriin-catalyzed reaction systems. Another noteworthy study explored the intricacies of spatiotemporal chaos in both the ferriin and cerium-catalyzed systems, shedding light on aperiodic transient regimes [11]. A more granular exposition of Hopf bifurcations, along with the phase plane characterization of critical junctions, is documented in [1]. Such elucidations are crucial for forecasting dynamical behaviors proximate to equilibrium and spotlighting potential heteroclinic links between nodes.

In contrast to the aforementioned inquiries, our research offers a distinctive approach. We are driven by the ambition to unearth analytical solutions that capture the spatiotemporal evolution of reactants within the Belousov-Zhabotinsky framework. Eschewing the standard Oregonator paradigm, our work delineates these solutions, offering a comprehensive breakdown of their specific analytical incarnations.

In the search of novel solutions for the Oregonator model, we initially investigate the boundedness and singularity of weak solutions, paving the way for a detailed analysis of various solution symmetries. As direct evidences of such symmetries remain elusive, we pivot to examining solutions based on traveling waves, utilizing the Tanh-method and subsequently solving the emergent ODE system to ascertain traveling wave profiles. We probe for asymptotic solutions embedded within self-similar frameworks, transitioning to stationary solutions and other categories of asymptotic solutions rooted in exponential scaling. Our investigative journey culminates in the derivation of cohesive Hamilton-Jacobi equations.

Transitioning to the mathematical foundation of our study, we utilize the functions  $u_1$  and  $v_1$  to represent the concentration dynamics of bromous acid ( $HBrO_2$ ) and bromide ions ( $Br^-$ ), respectively. A comprehensive exposition of this model is available in Equations Ia, Ib and Ic of [9]. It is important to highlight that the model proposed in [9] is formed of a system of ODEs that studies the evolutions of the variables  $X$  (concentration of  $HBrO_2$ ),  $Y$  (concentration of  $Br^-$ ) and  $Z$  (concentration of  $Ce$ ). In addition, some values for the involved constants are provided in IIa, IIb, IIc and IID of [9]. It is to be highlighted that the constant  $k_{M1}$  in IIa of [9] is negligible when compared with the other involved constants. When  $Ce(IV)$  is absent in the Oregonator model, it means the model is either using a different redox catalyst or is structured in such a way that it does not require this specific component to demonstrate the oscillatory behavior. This absence can affect the dynamics and characteristics of the modeled reaction, leading to different patterns or types of oscillations (or even no oscillations) compared to those seen in the classic BZ reaction with  $Ce(IV)$ .

It is remarkable to state that we consider the oregonator model and we show that in the absence of  $Ce(IV)$ , the BZ reaction does not lead to oscillatory patterns, and hence we characterize the behaviour of the system when the catalyst is removed or simply dissipated due to the process irreversibly. Investigating the non-oscillatory solutions in the BZ reaction presents an intriguing area of study, particularly because traditional observations of the BZ reaction have predominantly focused on its oscillatory behaviors. Typically characterized by rhythmic changes in color and concentration, the BZ reaction is known for its dynamic oscillatory patterns. However, exploring the conditions and dynamics that lead to non-oscillatory, or steady-state, behaviors can provide deeper insights into the underlying chemical and physical processes. This exploration could reveal new aspects of the reaction kinetics and mechanisms that are not apparent in oscillatory states, contributing to a more comprehensive understanding of non-equilibrium thermodynamic systems. Our objective is hence to answer several key questions about the BZ reaction including: What is the behavior of the BZ reaction in the absence of oscillatory

patterns? Does the reaction exhibit any tendencies towards blow-up phenomena, or are the solutions confined within certain bounds? And finally, what can be said about the long-term or asymptotic behavior of the solutions in these non-oscillatory states? It is relevant to discuss that the author in [8] demonstrates that BZ equations can admit limit cycle solutions of the relaxation type within a certain range of dimensionless ratios of rate constants. The relaxation condition is actually relevant for us, and we try to characterize it based on the mentioned asymptotic behaviour of solutions.

In the absence of  $Ce$ , we consider that  $Z = 0$  in Ia, Ib and Ic of [9]. To further articulate the behaviour of the system under spatial diffusion, we include a diffusive principle based on the Laplacian operator. Hence, the intertwined system is given as follows:

$$\begin{aligned} \frac{\partial u_1}{\partial t} &= D_1 \Delta u_1 + u_1(a - bu_1 - cv_1) \\ \frac{\partial v_1}{\partial t} &= D_1 \Delta v_1 - du_1 v_1 \\ u_1(x, y, 0) &= u_0(x, y) > 0, \quad v_1(x, y, 0) = v_0(x, y) > 0. \end{aligned} \quad (1)$$

If we consider the oregonator [9] and the constants used there  $A_2$ ,  $k_1$ ,  $k_2$  and  $k_3$  such that  $a = k_2 A_2$ ,  $b = 2k_3$  and typically  $c \sim d = k_1$ , we have

$$\begin{aligned} \frac{\partial u_1}{\partial t} &= D_1 \Delta u_1 + u_1(k_2 A_2 - 2k_3 u_1 - k_1 v_1) \\ \frac{\partial v_1}{\partial t} &= D_2 \Delta v_1 - k_1 u_1 v_1 \\ u_1(x, y, 0) &= u_0(x, y) > 0, \quad v_1(x, y, 0) = v_0(x, y) > 0. \end{aligned} \quad (2)$$

For clarity and without any compromise on generality, we may consider in some cases that  $D_1 = D_2 = 1$ . When required and to enrich some discussions concerning the diffusion mechanisms we may assume that  $D_1, D_2$  are different from the unity. This will be further specified. It is relevant to remark that comprehensive discussions regarding the values of several constants inherent to the system have been elucidated in preceding studies (refer to page 629 of [15]):  $k_1 = 1.6 \cdot 10^9 M/s$ ,  $k_2 = 8 \cdot 10^3 M/s$ ,  $k_3 = 4 \cdot 10^7 M/s$ ,

and  $A_2 = 0.06M$ .

The equation denoted by (2) underpins the subsequent analyses. It is remarkable that this system is drafted without imposing specific constraints on boundary conditions, enabling a more comprehensive span of mathematical solutions.

We incorporate Lebesgue measurable and bounded initial data into our formulation. This strategy ensures the provision of results under a broad spectrum of initial conditions. In essence, the anticipated initial data should represent a finite initial concentration distribution as per the  $L^1$  norm and should also be constrained by the traditional  $L^\infty$  norm.

$$u_1(x, y, 0), v_1(x, y, 0) \in L^\infty(\mathbb{R}^2) \cap L^1(\mathbb{R}^2). \quad (3)$$

The remainder of this paper is structured as follows: Section 2 lays the mathematical groundwork, establishing the framework and assumptions required for the analysis of weak solutions, including their boundedness and uniqueness. In Section 3, we introduce solutions arising from the equation symmetries. In Section 4, we delve into the examination of traveling wave solutions, applying the Tanh-method to derive explicit analytical forms and discussing their physical significance. Section 5 is dedicated to the exploration of asymptotic behavior and self-similar solutions, where we elucidate the connection between exponential scaling and the emergence of Hamilton-Jacobi equations. Section 6 provides a detailed discussion on the new analytical stationary solutions, illustrating their application to the Oregonator model and highlighting their implications for understanding chemical reaction-diffusion systems. Finally, Section 7 examines the behaviour of non-stationary solutions based on a single point exponential scaling. Eventually, the paper ends with a summary of our findings, their relevance to the study of non-linear chemical dynamics, and suggestions for future research avenues.

## 2 General analysis of solutions

We first show the boundedness of weak solutions departing from general initial data. This is actually relevant if we compare with the classical strong formulations. We recall that our research is mainly mathematical and working withing a weak formulation allows for flexibility in choosing the function spaces for the solution and test functions. This flexibility often makes it possible to tailor the formulation to better match the chemical process linked with the oregonator model. For example, by selecting discontinuous functions for problems with discontinuous material properties. In addition, a weak formulation allows for a more straightforward incorporation of complex geometries and potential intricate boundary conditions.

**Theorem 1.** *Under the assumption that  $(u_0(x, y), v_0(x, y)) \in L^1(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2)$ , we can infer that the solutions  $u_1(x, y, t)$  and  $v_1(x, y, t)$  remain bounded in a weak sense over the spatial domain  $\mathbb{R}^2$  and within the time interval  $[0, T]$ .*

*Proof.* To discuss the weak formulation of equation (2), we begin by considering a test function  $\xi_1 \in C^\infty(\mathbb{R}^2)$ . We integrate this function over the domain  $\mathbb{R}^2 \times [\tau, t]$  where  $0 < \tau < t < T$ . The integral of  $u_1$  with  $\xi_1$  can be expressed as follows:

$$\begin{aligned}
 & \int_{\mathbb{R}^2} u_1(t)\xi_1(t) = \int_{\mathbb{R}^2} u_1(\tau)\xi_1(\tau) \\
 & + \int_{\tau}^t \int_{\mathbb{R}^2} \left[ u_1 \frac{\partial \xi_1}{\partial t} + u_1 \Delta \xi_1 + k_2 A_2 u_1 - 2k_3 u_1^2 - k_1 u_1 v_1 \right] ds \\
 & \leq \int_{\mathbb{R}^2} u_1(\tau)\xi_1(\tau) \\
 & + \int_{\tau}^t \int_{\mathbb{R}^2} \left[ u_1 \frac{\partial \xi_1}{\partial t} + u_1 \Delta \xi_1 + k_2 A_2 u_1 + \left( \frac{k_1}{2} - 2k_3 \right) u_1^2 + \frac{k_1}{2} v_1^2 \right] ds.
 \end{aligned} \tag{4}$$

Similarly, the integral of  $v_1$  with  $\xi_1$  is given by:

$$\begin{aligned} \int_{R^2} v_1(t)\xi_1(t) &= \int_{R^2} v_1(\tau)\xi_1(\tau) \\ &+ \int_{\tau}^t \int_{R^2} \left[ v_1 \frac{\partial \xi_1}{\partial t} + v_1 \Delta \xi_1 - k_1 u_1 v_1 \right] ds \leq \int_{R^2} v_1(\tau)\xi_1(\tau) \quad (5) \\ &+ \int_{\tau}^t \int_{R^2} \left[ v_1 \frac{\partial \xi_1}{\partial t} + v_1 \Delta \xi_1 + \frac{k_1}{2} u_1^2 + \frac{k_1}{2} v_1^2 \right] ds. \end{aligned}$$

The inequalities in (4) and (5) are established through Young's inequality.

We turn our attention to the problem described by equations (4) and (5). It is imperative to emphasize that for adequately large values of  $x_0$  and  $y_0$  and under the conditions  $x \gg x_0$  and  $y \gg y_0$ , within a localized time interval, it holds that [14].

$$\int_{\tau}^t u^m \leq c_p(\tau) (x^2 + y^2)^{\frac{m}{m-1}}, \quad \int_{\tau}^t u \leq c_q(\tau) (x^2 + y^2)^{\frac{1}{m-1}}, \quad (6)$$

and

$$\int_{\tau}^t v^m \leq c_p(\tau) (x^2 + y^2)^{\frac{m}{m-1}}, \quad \int_{\tau}^t v \leq c_q(\tau) (x^2 + y^2)^{\frac{1}{m-1}}. \quad (7)$$

For the specific case where  $m = 2$ , we have:

$$\int_{\tau}^t u^2 \leq c_p(\tau) (x^2 + y^2)^2, \quad \int_{\tau}^t u \leq c_q(\tau) (x^2 + y^2), \quad (8)$$

and

$$\int_{\tau}^t v^2 \leq c_p(\tau) (x^2 + y^2)^2, \quad \int_{\tau}^t v \leq c_q(\tau) (x^2 + y^2), \quad (9)$$

where  $c_p$  and  $c_q$  depend also on  $m$ ,  $x_0$ ,  $y_0$  and  $T$ .

Now, we consider a specific test function  $\xi_1$  defined as follows:



$$\xi_1(x, y, s) = e^{g(s)} (1 + x^2 + y^2)^{-k_5}, \quad (10)$$

where  $g(s) \leq 0$  and  $k_5$  is chosen in a manner that ensures the integrals in (4) and (5) converge as  $x \rightarrow \infty$  and  $y \rightarrow \infty$ . After differentiating  $\xi_1$  twice with respect to  $x$  and  $y$ , and then summing the results, we obtain the Laplacian of  $\xi_1$ :

$$\begin{aligned} \Delta \xi_1 &= -\frac{4k_5(k_5+1)e^{g(s)}(x^2+y^2)}{(1+x^2+y^2)^{k_5+2}} - \frac{4k_5e^{g(s)}}{(1+x^2+y^2)^{k_5+1}} \\ &\leq -\frac{4k_5(k_5+2)e^{g(s)}}{(1+x^2+y^2)^{k_5+1}} \\ &\leq \frac{4k_5(k_5+2)e^{g(s)}}{(x^2+y^2)^{k_5+1}}. \end{aligned} \quad (11)$$

Using the estimates provided in (8), (9), and (11), we can bound the integrals in (4) and (5) as follows:

$$\begin{aligned} -\int_{\tau}^t \int_{R^2} u_1 \Delta \xi_1 ds &\leq 4k_5(k_5+2) \int_{R^2} c_q(\tau) e^{g(s)} (x^2+y^2)^{-k_5} \\ -k_2 A_2 \int_{\tau}^t \int_{R^2} u_1 \xi_1 ds &\leq k_2 A_2 \int_{R^2} c_q(\tau) e^{g(s)} (x^2+y^2)^{1-k_5} \\ -\left(\frac{k_1}{2} - 2k_3\right) \int_{\tau}^t \int_{R^2} u_1^2 \xi_1 ds &\leq \left|\frac{k_1}{2} - 2k_3\right| \int_{R^2} c_p(\tau) e^{g(s)} (x^2+y^2)^{2-k_5} \\ -\frac{k_1}{2} \int_{\tau}^t \int_{R^2} v_1^2 \xi_1 ds &\leq \frac{k_1}{2} \int_{R^2} c_p(\tau) e^{g(s)} (x^2+y^2)^{2-k_5} \\ -\frac{k_1}{2} \int_{\tau}^t \int_{R^2} u_1 \xi_1 ds &\leq \frac{k_1}{2} \int_{R^2} c_q(\tau) e^{g(s)} s (x^2+y^2)^{1-k_5}. \end{aligned} \quad (12)$$

Now, by choosing  $k_5 > 2$  and letting  $x$  and  $y$  tend to infinity, we can simplify (12) and obtain:

$$\int_{\tau}^t \int_{R^2} u_1 \frac{\partial \xi_1}{\partial t} ds \leq (\epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4) e^{g(s)}. \quad (13)$$

A similar estimation can be made for the integral involving  $v_1$ :

$$\int_{\tau}^t \int_{R^2} v_1 \frac{\partial \xi_1}{\partial t} ds \leq (\epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4) e^{g(s)}. \quad (14)$$

Here,  $\epsilon_i$  for  $i = 1, 2, 3, 4$  are sufficiently small constants.

Further differentiating (13) and (14), we find:

$$\begin{aligned} \int_{R^2} u_1 \frac{\partial \xi_1}{\partial t} ds &\leq (\epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4) \frac{de^{g(s)}}{ds} \\ &\leq (\epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4) \left( k_6 e^{g_1(\tau)} + k_7 \int_{\tau}^s e^{g_1(r)} dr \right), \end{aligned} \quad (15)$$

and similarly for the integral involving  $v_1$ :

$$\begin{aligned} \int_{\tau}^t \int_{R^2} v_1 \frac{\partial \xi_1}{\partial t} ds &\leq (\epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4) \frac{de^{g(s)}}{ds} \\ &\leq (\epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4) \left( k_8 e^{g_1(\tau)} + k_9 \int_{\tau}^s e^{g_1(r)} dr \right). \end{aligned} \quad (16)$$

These estimates provide bounds for the derivatives of the integrals of  $u_1$  and  $v_1$  with respect to  $t$ .

In the previous derivation, we applied Grönwall's inequality, and we denoted the constants involved as  $k_6$ ,  $k_7$ ,  $k_8$ , and  $k_9$ . Since both  $\xi_1$  and its time derivative  $\frac{\partial \xi_1}{\partial t}$  are bounded, and the integral in question converges, we have successfully demonstrated that the solutions  $u_1$  and  $v_1$  remain bounded over the entire spatial domain  $R^2$  throughout the time interval  $[0, T]$ . ■

The objective at this point is to establish the uniqueness of the solutions. Ensuring the uniqueness of solutions in our model is relevant for the consistency, predictability, and reliability of the oregonator model. In addition, It bridges the gap between the mathematical formulations and the potential application to a chemical process (actually this application

needs to be further explored and is not part of our current investigation). As described in the Introduction, there exists a vast literature discussing solutions for the BZ reaction problem. Nonetheless when the oregonator model is transformed into the weak formulations (4) and (5), there is not a definitive result concerning uniqueness. Motivated by such facts, we provide a complete analysis that connects the uniqueness of solutions with a weak formulation of the oregonator model.

**Theorem 2.** *Suppose that  $u_3 > 0$  and  $v_3 > 0$  represent minimal solutions of equation (2). It can be concluded that both solutions  $u_3$  and  $v_3$  are unique, as they coincide with the maximal solutions  $u_2$  and  $v_2$ .*

*Proof.* Consider the maximal solutions  $u_2$  and  $v_2$  of equation (2) within the domain  $R^2 \times [0, T]$ . The initial conditions for these solutions are given as:

$$u_2(x, y, 0) = u_0(x, y) + \epsilon, \quad v_2(x, y, 0) = v_0(x, y) + \epsilon. \quad (17)$$

We also introduce the following initial data for defining minimal solutions:

$$u_3(x, y, 0) = u_0(x, y), \quad v_3(x, y, 0) = v_0(x, y). \quad (18)$$

The maximal solutions must satisfy the following system of equations:

$$\frac{\partial u_2}{\partial t} = D_1 \Delta u_2 + u_2(k_2 A_2 - 2k_3 u_2 - k_1 v_2), \quad (19)$$

$$\frac{\partial v_2}{\partial t} = D_2 \Delta v_2 - k_1 u_2 v_2. \quad (20)$$

Similarly, the minimal solutions must satisfy the following equations:

$$\frac{\partial u_3}{\partial t} = D_1 \Delta u_3 + u_3(k_2 A_2 - 2k_3 u_3 - k_1 v_3), \quad (21)$$

$$\frac{\partial v_3}{\partial t} = D_2 \Delta v_3 - k_1 u_3 v_3. \quad (22)$$

For a test function  $\xi_1 \in C^\infty(R)$ , the following inequalities hold:

$$\begin{aligned} 0 &\leq \int_{R^2} (u_2 - u_3)(t) \xi_1(t) \leq \int_{R^2} \epsilon \xi_1(x, y, 0) \\ &+ \int_0^t \int_{R^2} \left\{ (u_2 - u_3) \frac{\partial \xi_1}{\partial t} + D_1 (u_2 - u_3) \Delta \xi_1 \right. \\ &+ k_2 A_2 (u_2 - u_3) \xi_1 - 2k_3 k_{10} (u_2 - u_3) \xi_1 \\ &\left. - k_1 (u_2 v_2 - u_3 v_3) \xi_1 \right\} ds, \end{aligned} \quad (23)$$

$$\begin{aligned} 0 &\leq \int_{R^2} (v_2 - v_3)(t) \xi_1(t) \leq \int_{R^2} \epsilon \xi_1(x, y, 0) \\ &+ k_{13} \int_0^t \int_{R^2} \left\{ (v_2 - v_3) \frac{\partial \xi_1}{\partial t} + D_2 (v_2 - v_3) \Delta \xi_1 \right. \\ &\left. - k_1 (u_2 v_2 - u_3 v_3) \xi_1 \right\} ds, \end{aligned} \quad (24)$$

where  $k_{10} = \max\{u_2, u_3\}$ .

We define a radially symmetric test function (for us directionality does not have a significant influence by hypothesis) to evaluate the integrals:

$$\xi_1(x, y, s) = e^{-k_{11}s} (1 + x^2 + y^2)^{-k_5}, \quad (25)$$

where  $k_{10} > 0$  and  $k_5 > 0$  are constants, and the following inequalities hold for the function defined in (2.24):

$$\frac{\partial \xi_1}{\partial s} = -k_{11} \xi_1(x, y, s), \quad \Delta \xi_1 \leq 4k_5(k_5 + 2)\xi_1(x, y, s). \quad (26)$$

Then, using these test functions and Theorem 1, we have the following inequalities:

$$0 \leq \int_{R^2} (u_2 - u_3)(t) \xi_1(t) \leq \int_{R^2} \epsilon \xi_1(x, y, 0) + k_{12} \int_0^t \int_{R^2} \{(u_2 - u_3) - k_1(u_2 v_2 - u_3 v_3) \xi_1\} ds, \quad (27)$$

$$0 \leq \int_{R^2} (v_2 - v_3)(t) \xi_1(t) \leq \int_{R^2} \epsilon \xi_1(x, y, 0) + k_{13} \int_0^t \int_{R^2} \{(v_2 - v_3) - k_1(u_2 v_2 - u_3 v_3) \xi_1\} ds. \quad (28)$$

Now, we subtract (27) from (28) to obtain:

$$\begin{aligned} & \int_{R^2} (v_2 - v_3)(t) \xi_1(t) - \int_{R^2} (u_2 - u_3)(t) \xi_1(t) \\ & \leq k_{12} \int_0^t \int_{R^2} (v_2 - v_3) ds - k_{12} \int_0^t \int_{R^2} (u_2 - u_3) ds \\ & \leq k_{12} \int_0^t \int_{R^2} (v_2 - v_3) ds - k_{12} \int_0^t \int_{R^2} (u_2 - u_3) ds. \end{aligned} \quad (29)$$

Differentiating with respect to  $t$ , we have:

$$\begin{aligned} & \frac{d}{dt} \left[ \int_{R^2} (v_2 - v_3)(t) \xi_1(t) - \int_{R^2} (u_2 - u_3)(t) \xi_1(t) \right] \\ & \leq k_{12} \left[ \int_{R^2} (v_2 - v_3) - \int_{R^2} (u_2 - u_3) \right]. \end{aligned} \quad (30)$$

By applying Grönwall's inequality, we have:

$$\int_{R^2} (v_2 - v_3)(t) \xi_1(t) - \int_{R^2} (u_2 - u_3)(t) \xi_1(t) \leq 0. \quad (31)$$

Since  $\xi_1$  is a test function, it follows that:

$$u_2 - u_3 = v_2 - v_3. \quad (32)$$

Evaluating this expression using the initial data, we get:

$$u_0(x, y) + \epsilon - u_0(x, y) = \epsilon. \quad (33)$$

Where  $\epsilon$  is taken to be sufficiently small. Indeed, when two quantities become closer by a margin of a small  $\epsilon$ , they essentially become the same, hence proving uniqueness. This is:

$$u_2 - u_3 = v_2 - v_3 = \epsilon \rightarrow 0. \quad (34)$$

This leads to the conclusion:

$$u_2 = u_3, \quad v_2 = v_3. \quad (35)$$

This demonstrates the postulated uniqueness of the solutions for equation (2). ■

### 3 Reduction techniques, scaling and symmetries

First, we propose the following scaling to (2):

$$\tilde{t} = k_2 A_2 t, \quad \tilde{u}_1 = \frac{u_1}{A_2}, \quad \tilde{v}_1 = \frac{v_1}{A_2}, \quad \text{and} \quad \tilde{x} = \sqrt{\frac{D_1}{k_2 A_2}} x \quad (36)$$

We can compute the derivatives with respect to the scaled variables:

$$\begin{aligned}\frac{\partial}{\partial t} &= \frac{1}{k_2 A_2} \frac{\partial}{\partial \tilde{t}}, \\ \Delta &= \frac{k_2 A_2}{D_1} \Delta_{\tilde{x}}.\end{aligned}$$

Substituting these, along with the scaled variables, into the original equations, we get:

For  $u_1$ :

$$\frac{1}{k_2 A_2} \frac{\partial \tilde{u}_1}{\partial \tilde{t}} = k_2 A_2 \Delta_{\tilde{x}} \tilde{u}_1 + \tilde{u}_1 (k_2 A_2 - 2k_3 A_2 \tilde{u}_1 - k_1 A_2 \tilde{v}_1), \quad (37)$$

$$\frac{\partial \tilde{u}_1}{\partial \tilde{t}} = k_2 A_2 \Delta_{\tilde{x}} \tilde{u}_1 + \tilde{u}_1 (k_2 A_2 - 2k_3 A_2 \tilde{u}_1 - k_1 A_2 \tilde{v}_1). \quad (38)$$

For  $v_1$ :

$$\frac{1}{k_2 A_2} \frac{\partial \tilde{v}_1}{\partial \tilde{t}} = \frac{k_2 A_2 D_2}{D_1} \Delta_{\tilde{x}} \tilde{v}_1 - k_1 A_2 \tilde{u}_1 \tilde{v}_1, \quad (39)$$

$$\frac{\partial \tilde{v}_1}{\partial \tilde{t}} = \frac{k_2 A_2 D_2}{D_1} \Delta_{\tilde{x}} \tilde{v}_1 - k_1 A_2 \tilde{u}_1 \tilde{v}_1. \quad (40)$$

Now, looking for symmetries:

If  $D_1 = D_2$ , then both equations will have the same diffusion coefficients when scaled, giving a symmetry in terms of spatial diffusion, but this has no substantial effect when seeking solutions. The term

$$\tilde{u}_1 (k_2 A_2 - 2k_3 A_2 \tilde{u}_1 - k_1 A_2 \tilde{v}_1)$$

indicates a nonlinear interaction between the scaled concentrations  $\tilde{u}_1$  and  $\tilde{v}_1$ . No obvious symmetries emerge here. The last terms in both equations show the interaction between  $\tilde{u}_1$  and  $\tilde{v}_1$  in the kinetics. Again, no straightforward symmetries are evident. Hence, we seek for other kind of more complex symmetries by application of Lie algebra principles. Another important remark is that we will make the assessments under the assumption

of oscillatory solutions. This hypothesis is intended to simplify the complex operations typically encountered in Lie symmetry analysis and is actually aligned with the real behaviour of BZ reactions. For this, we first define the following Infinitesimal Generator:

$$X = \xi(\tilde{x}, \tilde{t}, \tilde{u}_1, \tilde{v}_1) \frac{\partial}{\partial \tilde{x}} + \tau(\tilde{x}, \tilde{t}, \tilde{u}_1, \tilde{v}_1) \frac{\partial}{\partial \tilde{t}} + \phi(\tilde{x}, \tilde{t}, \tilde{u}_1, \tilde{v}_1) \frac{\partial}{\partial \tilde{u}_1} + \psi(\tilde{x}, \tilde{t}, \tilde{u}_1, \tilde{v}_1) \frac{\partial}{\partial \tilde{v}_1}, \quad (41)$$

for appropriate functions  $\xi, \tau, \phi, \psi$  to be determined.

The prolonged infinitesimal generator  $X^{(1)}$  is given by:

$$X^{(1)} = X + \phi^{(1)} \frac{\partial}{\partial(\partial \tilde{u}_1 / \partial \tilde{t})} + \psi^{(1)} \frac{\partial}{\partial(\partial \tilde{v}_1 / \partial \tilde{t})}, \quad (42)$$

where  $\phi^{(1)}$  and  $\psi^{(1)}$  are the first prolongations, calculated using the total derivative. Now, the invariance under the action of  $X^{(1)}$  requires that:

$$X^{(1)} \left( \frac{\partial \tilde{u}_1}{\partial \tilde{t}} - (k_2 A_2 \Delta_{\tilde{x}} \tilde{u}_1 + \tilde{u}_1 (k_2 A_2 - 2k_3 A_2 \tilde{u}_1 - k_1 A_2 \tilde{v}_1)) \right) = 0, \quad (43)$$

$$X^{(1)} \left( \frac{\partial \tilde{v}_1}{\partial \tilde{t}} - \left( \frac{k_2 A_2 D_2}{D_1} \Delta_{\tilde{x}} \tilde{v}_1 - k_1 A_2 \tilde{u}_1 \tilde{v}_1 \right) \right) = 0. \quad (44)$$

The resulting system of partial differential equations obtained by applying the invariance condition to the given PDEs is provided as follows:

For  $\tilde{u}_1$  Equation:

$$A_2 k_2 \frac{\partial^2 \tilde{u}_1}{\partial \tilde{x}^2} + \tilde{u}_1 (-A_2 k_1 \tilde{v}_1 + A_2 k_2 - 2A_2 k_3 \tilde{u}_1) - \frac{\partial \tilde{u}_1}{\partial \tilde{t}} \frac{\partial \xi}{\partial \tilde{t}} - \frac{\partial \tilde{u}_1}{\partial \tilde{t}} - \frac{\partial \tilde{u}_1}{\partial \tilde{x}} \frac{\partial \tau}{\partial \tilde{t}} + \frac{\partial \phi}{\partial \tilde{t}} = 0. \quad (45)$$



For  $\tilde{v}_1$  Equation:

$$\begin{aligned}
 & -A_2k_1\tilde{u}_1\tilde{v}_1 + \frac{A_2D_2k_2}{D_1}\frac{\partial^2\tilde{v}_1}{\partial\tilde{x}^2} - \frac{\partial\tilde{v}_1}{\partial\tilde{t}}\frac{\partial\xi}{\partial\tilde{t}} \\
 & -\frac{\partial\tilde{v}_1}{\partial\tilde{t}} - \frac{\partial\tilde{v}_1}{\partial\tilde{x}}\frac{\partial\tau}{\partial\tilde{t}} + \frac{\partial\psi}{\partial\tilde{t}} = 0.
 \end{aligned} \tag{46}$$

The next step consists in solving the invariance condition for the unknown functions  $\xi$ ,  $\tau$ ,  $\phi$ , and  $\psi$ . For this, we assume that we search for oscillatory solutions. Hence, solving the system of equations, we obtained solutions for the functions  $\phi$  and  $\psi$  as functions of  $\tilde{t}$ . Given the complexities of the involved system, we have opted by a symbolic calculation using Symbolic Math Toolbox. In addition, to represent the oscillatory condition of solutions, we admitted the simplify forms:  $\tilde{u}_1(\tilde{x}, \tilde{t}) = \sin(\tilde{x} + \tilde{t})$ ,  $\tilde{v}_1(\tilde{x}, \tilde{t}) = \sin(\tilde{x} - \tilde{t})$ . These are not our definitive solutions, on the contrary they only provide preliminary guesses to obtain more general oscillatory solutions based on symmetry properties. Based on this hypothesis, we obtain the following particular functions:

For  $\phi(\tilde{t})$ :

$$\begin{aligned}
 \phi(\tilde{t}) = & -\frac{A_2k_1\tilde{t}\sin(\tilde{t}-\tilde{x})\sin(\tilde{t}+\tilde{x})}{2} - \frac{A_2k_1\tilde{t}\cos(\tilde{t}-\tilde{x})\cos(\tilde{t}+\tilde{x})}{2} \\
 & + \frac{A_2k_1\sin(\tilde{t}-\tilde{x})\cos(\tilde{t}+\tilde{x})}{2} + A_2k_3\tilde{t}\sin^2(\tilde{t}+\tilde{x}) \\
 & + A_2k_3\tilde{t}\cos^2(\tilde{t}+\tilde{x}) - A_2k_3\sin(\tilde{t}+\tilde{x})\cos(\tilde{t}+\tilde{x}) \\
 & + C_1 + \sin(\tilde{t}+\tilde{x}).
 \end{aligned} \tag{47}$$

For  $\psi(\tilde{t})$ :

$$\begin{aligned}
 \psi(\tilde{t}) = & -\frac{A_2k_1\tilde{t}\sin(\tilde{t}-\tilde{x})\sin(\tilde{t}+\tilde{x})}{2} - \frac{A_2k_1\tilde{t}\cos(\tilde{t}-\tilde{x})\cos(\tilde{t}+\tilde{x})}{2} \\
 & + \frac{A_2k_1\sin(\tilde{t}-\tilde{x})\cos(\tilde{t}+\tilde{x})}{2} + \frac{A_2D_2k_2\cos(\tilde{t}-\tilde{x})}{D_1} + C_2 - \sin(\tilde{t}-\tilde{x}) \tag{48}
 \end{aligned}$$

Where  $C_1$  and  $C_2$  are constants of integration. The presence of sine and cosine functions in the solutions suggests that the symmetries are related to oscillatory behavior, which aligns with the initial assumption that  $u_1$

and  $v_1$  are oscillatory in nature.

Finally, we integrate the symmetry functions  $\phi(\tilde{t})$  and  $\psi(\tilde{t})$  with respect to time  $\tilde{t}$ . This integration transforms the symmetry functions into explicit expressions for  $\tilde{u}_1$  and  $\tilde{v}_1$  representing general forms of solutions that are consistent with the identified symmetries.

$$\begin{aligned} \tilde{u}_1 = & \frac{A_2 k_1 \tilde{t}^2 \sin^2(\tilde{x})}{2} - \frac{A_2 k_1 \tilde{t}^2}{4} - \frac{A_2 k_1 \tilde{t} \sin(\tilde{x}) \cos(\tilde{x})}{2} \\ & + \frac{A_2 k_1 \sin^2(\tilde{t})}{4} + \frac{A_2 k_1 \sin^2(\tilde{x})}{4} - \frac{A_2 k_1}{4} \\ & + \frac{A_2 k_3 \tilde{t}^2}{2} + A_2 k_3 \sin^2(\tilde{t}) \sin^2(\tilde{x}) - \frac{A_2 k_3 \sin^2(\tilde{t})}{2} \\ & - A_2 k_3 \sin(\tilde{t}) \sin(\tilde{x}) \cos(\tilde{t}) \cos(\tilde{x}) - \frac{A_2 k_3 \sin^2(\tilde{x})}{2} \\ & + \frac{A_2 k_3}{2} + C_1 \tilde{t} - \cos(\tilde{t} + \tilde{x}), \end{aligned} \quad (49)$$

$$\begin{aligned} \tilde{v}_1 = & - \frac{A_2 k_1 \tilde{t}^2 \cos(2\tilde{x})}{4} - \frac{A_2 k_1 \tilde{t} \sin(2\tilde{x})}{4} - \frac{A_2 k_1 \cos(2\tilde{t})}{8} \\ & - \frac{A_2 k_1 \cos(2\tilde{x})}{8} + \frac{A_2 D_2 k_2 \sin(\tilde{t} - \tilde{x})}{D_1} + C_2 \tilde{t} + \cos(\tilde{t} - \tilde{x}). \end{aligned} \quad (50)$$

In the BZ reaction, the solutions  $\tilde{u}_1$  and  $\tilde{v}_1$ , representing the scaled concentrations of bromous acid ( $\text{HBrO}_2$ ) and bromide ions ( $\text{Br}^-$ ), exhibit oscillatory behavior. This is consistent with the characteristic chemical oscillations observed in the BZ reaction. The sinusoidal form of these solutions reflects the periodic changes in the concentrations of these chemical species. The presence of additional non-oscillatory terms concerning the powers  $\tilde{t}^0$ ,  $\tilde{t}^1$  and  $\tilde{t}^2$  represent the gradual accumulation or depletion of reactants over time, reflecting aspects of the reaction kinetics not captured by the oscillatory part alone. And this is actually an interesting discovery of our solutions based on symmetries.

## 4 The Tanh-method for travelling waves profiles of solution

The transition state in a chemical reaction, particularly in the context of the BZ reaction or other nonlinear oscillatory reactions, refers to a critical configuration of reactant molecules that exists momentarily at the peak of the potential energy barrier between reactants and products. It is a state through which the system must pass in order to transform reactants into products. For reaction-diffusion systems exhibiting traveling waves, the transition state can often be associated with the wavefront, where the rapid change between two stable states takes place.

This is actually the intention of this section, i.e. to determine the behaviour of such transition based on analytical expressions for the travelling waves profiles emerging in tanh forms. To apply the tanh-method, we introduce a traveling wave variable  $\xi = x - ct$ , where  $c$  is the wave speed. We assume that the solutions have the form:

$$u_1(x, t) = U(\xi) \quad \text{and} \quad v_1(x, t) = V(\xi) \quad (51)$$

Let us plug these into our system (2), assuming one-dimensional spatial variation for simplicity.

We will then have:

$$\begin{aligned} -cU' &= D_1U'' + U(k_2A_2 - 2k_3U - k_1V) \\ -cV' &= D_2V'' - k_1UV \end{aligned} \quad (52)$$

where the prime denotes differentiation with respect to  $\xi$ .

The tanh-method involves seeking solutions of the form:

$$U(\xi) = a + b \tanh(m\xi + n) \quad (53)$$

and

$$V(\xi) = p + q \tanh(r\xi + s) \quad (54)$$

Deriving these with respect to  $\xi$  gives:

$$U' = bm\operatorname{sech}^2(m\xi + n) \quad (55)$$

$$V' = qr\operatorname{sech}^2(r\xi + s) \quad (56)$$

and

$$U'' = -2bm^2 \tanh(m\xi + n)\operatorname{sech}^2(m\xi + n) \quad (57)$$

$$V'' = -2qr^2 \tanh(r\xi + s)\operatorname{sech}^2(r\xi + s) \quad (58)$$

Substitute the above expressions into (52) so that we will have equations involving terms of  $\tanh$  and  $\operatorname{sech}^2$ .

Collecting coefficients from both sides give us a set of algebraic equations in terms of  $a, b, m, n, p, q, r, s$ . This system will allow us to determine the constants and get the exact solution. This step is not straightforward in our case, except if we consider the asymptotic condition  $\xi \rightarrow \infty$ , so that the  $\tanh \rightarrow 1$  and the  $\operatorname{sech}$  is infinitesimal. This approach leads to the following solutions

$$m = \frac{c}{2D_1}, \quad r = \frac{c}{2D_2}, \quad a = 1, \quad b = -1, \quad q = 1, \quad p = \frac{k_2 A_2}{k_1} - 1. \quad (59)$$

Other combination of solution may be explored given the fact that in general we arrive into a system that requires  $a + b = 0$  and  $p + q = \frac{k_2 A_2}{k_1}$ . And we claim that specific forms of such solutions may require additional checks with experimental data that are outside of our current mathematical analysis.

It is worth noting that the transition states in the BZ reaction specifically relate to the bromide ion concentration,  $HBrO_2$  dynamics, and other intermediate species. In our case, we claim that the  $\tanh$ -method is capable of capturing such transitions via an heteroclinic connection between the following states: For large negative  $\xi$ ,  $U(\xi) \rightarrow a + b$  and  $V(\xi) \rightarrow p + q$ , while for large positive  $\xi$ ,  $U(\xi) \rightarrow a$  and  $V(\xi) \rightarrow p$ . Such a transition is

reminiscent of the wavefronts seen in the BZ reaction, where a change in the concentration of chemical species moves through the system.

## 5 Similarity solutions

In this section, the goal is to identify self-similar solutions to equation (2). Given the nonlinearity and coupling of the terms, it is challenging to definitively determine the existence of self-similar solutions without more specific assumptions or simplifications. In our case, this will consist in assuming local in time solutions with spatial asymptotic conditions.

**Theorem 3:** *Provided that  $u_1(x, y, t)$  and  $v_1(x, y, t)$  are solutions to equation (1.3), the subsequent local-in-time self-similar asymptotic solutions are as follows: For  $u_1(x, y, t)$ :*

$$u_1(x, y, t) = -2D_1 t^{-1} e^{-\frac{(x+y)^2}{4D_1 t^{1/4}}}.$$

And for  $v_1(x, y, t)$ :

$$v_1(x, y, t) = t^{-\frac{3}{2}} |x + y| e^{-\frac{(x+y)^2}{8D_2 t^{1/4}}}.$$

*These solutions are derived based on the asymptotic condition that  $|x+y| \rightarrow \infty$ . This condition signifies that as  $x$  and  $y$  tend towards infinity, the provided expressions for  $u_1$  and  $v_1$  characterize the local in time self-similar behavior of the solutions to the equation.*

*Proof.* We initiate our investigation by examining the asymptotic solutions corresponding to (1). As a foundational step, we propose self-similar constructs as outlined in (60) and (61).

When we juxtapose these structures into (1), the emergent formulations are encapsulated in (62) and (63).

$$u_1(x, y, t) = t^{-\gamma_1} f_1(\zeta), \quad \zeta = |x + y| t^{\gamma_2}, \quad (60)$$

and

$$v_1(x, y, t) = t^{-\gamma_3} g_1(\zeta), \quad \zeta = |x + y|t^{\gamma_4}. \quad (61)$$

Then:

$$\begin{aligned} -\alpha_1 t^{-\gamma_1-1} f_1 + \gamma_2 \zeta t^{-\gamma_1-1} f_1' &= 2D_1 t^{-\gamma_1+2\gamma_2} f_1'' + k_2 A_2 t^{-\gamma_1} f_1 \\ &- 2k_3 t^{-2\gamma_1} f_1^2 - k_1 t^{-\gamma_1-\gamma_3} f_1 g_1, \end{aligned} \quad (62)$$

and

$$-\gamma_3 t^{-\gamma_3-1} g_1 + \gamma_4 \zeta t^{-\gamma_3-1} g_1' = 2D_2 t^{-\gamma_3+2\gamma_4} g_1'' - k_1 t^{-\gamma_1-\gamma_3} f_1 g_1. \quad (63)$$

To deduce the suitable values for  $\gamma_i$ ,  $i = 1, 2, 3, 4$ , we tackle the system of equations that is anchored on the power expressions within the  $t$ -variable.

$$\begin{aligned} -\gamma_1 - 1 &= -\gamma_1 + 2\gamma_2; & -\gamma_1 + 2\gamma_2 &= -\gamma_1 - \gamma_3, \\ -\gamma_1 - 1 &= -2\gamma_1; & -\gamma_3 - 1 &= -\gamma_3 + 2\gamma_4. \end{aligned}$$

The solutions are given by:  $\gamma_1 = \gamma_3 = 1, \gamma_2 = \gamma_4 = -\frac{1}{2}$ .

Building on the derived values of  $\gamma_i$ ,  $i = 1, 2, 3, 4$ , our next objective is to uncover explicit analytical representations for  $f_1$  and  $g_1$  that are valid in a localized temporal frame. For the sake of brevity and clarity, we adopt a temporal value of  $t = 1$  in our preceding expressions, leading us to:

$$2D_1 f_1'' - \gamma_2 \zeta f_1' + (k_2 A_2 + \gamma_1) f_1 - 2k_3 f_1^2 - k_1 f_1 g_1 = 0, \quad (64)$$

and

$$2D_2 g_1'' - \gamma_4 \zeta g_1' + \gamma_3 g_1 - k_1 f_1 g_1 = 0. \quad (65)$$

Given the finite nature of resources in a chemical reaction, there is an inherent cessation when the spatial parameters approach  $\infty$  (a scenario termed the 'relaxed condition'). Under this condition, any resulting so-

lution is expected to diminish to near-zero magnitudes as  $\zeta \rightarrow \infty$  for a localized  $t$ . Consequently, by assuming boundary conditions  $f_1(\infty) = 0$  and  $g_1(\infty) = 0$ , our equations (64) and (65) evolve asymptotically as  $\zeta \rightarrow \infty$ .

$$2D_1 f_1'' + \frac{1}{2} \zeta f_1' = 0, \quad (66)$$

and

$$2D_2 g_1'' + \frac{1}{2} \zeta g_1' + g_1 = 0. \quad (67)$$

After solving (66), we get

$$f_1' = e^{-\frac{\zeta^2}{4D_1}}. \quad (68)$$

After integration

$$f_1(\zeta) = \int e^{-\frac{\zeta^2}{4D_1}} d\zeta. \quad (69)$$

The analytical evaluation of the integral in (69) proves to be non-trivial. Given our interest in solutions as  $\zeta \rightarrow \infty$ , we employ a comparative methodology. Specifically, we juxtapose the integral  $\int e^{-\frac{\zeta^2}{4D_1}} d\zeta$  with its computable counterpart,  $\int \zeta e^{-\frac{\zeta^2}{4D_1}} d\zeta$ . Notably, as  $\zeta \rightarrow \infty$ , the behavior of the diminishing tail for both integrals is dictated by the Gaussian distribution. As a result, the expression in (69) can be reformulated as:

$$f_1(\zeta) = \int \zeta e^{-\frac{\zeta^2}{4D_1}} d\zeta, \quad (70)$$

which implies that

$$f_1(\zeta) = -2D_1 e^{-\frac{\zeta^2}{4D_1}}. \quad (71)$$

Now solving (67), we obtain

$$g_1' = \left( \frac{1}{\zeta} - \frac{\zeta}{4D_2} \right) g_1, \quad (72)$$

and solving now by standard separation of variables

$$g_1(\zeta) = \zeta e^{-\frac{\zeta^2}{8D_2}}. \quad (73)$$

Using  $f_1(\zeta)$  and  $g_1(\zeta)$  into (60) and (61), we get

$$u_1(x, y, t) = -2D_1 t^{-1} e^{-\frac{(x+y)^2}{4D_1 t^{1/4}}}, \quad (74)$$

and

$$v_1(x, y, t) = t^{-\frac{3}{2}} |x + y| e^{-\frac{(x+y)^2}{8D_2 t^{1/4}}}. \quad (75)$$

■

The given solutions (74) and (75) describe the evolution of quantities  $u_1$  and  $v_1$  in a two-dimensional spatial domain  $(x, y)$  over time  $t$  (recall here that the functions  $u_1$  and  $v_1$  represent the concentration of bromous acid ( $HBrO_2$ ) and bromide ions ( $Br^-$ ), respectively). Let us discuss about the behavior of these solutions to determine if they are physically plausible.

For (74), we discuss that

- The solution diminishes over time due to the factor  $t^{-1}$  and the exponential term. The rate at which it diminishes increases as time progresses.
- The spatial behavior depends on the sum  $(x + y)$ . The value of  $u_1$  decreases as  $(x + y)^2$  increases due to the exponential term.
- $D_1$  can be interpreted as a dispersion or diffusion constant that controls how  $u_1$  spreads over space. A larger  $D_1$  implies that  $u_1$  spreads more quickly in space.

For (75), we note that



- 
- The factor  $t^{-\frac{3}{2}}$  implies that  $v_1$  diminishes at a quicker rate over time compared to  $u_1$ .
  - The presence of the absolute value  $|x + y|$  means that  $v_1$  will take positive values regardless of the sign of  $(x + y)$ . It also suggests that the values of  $v_1$  will be symmetric about the line  $x = -y$ .
  - The exponential term indicates that  $v_1$  diminishes in magnitude as  $(x + y)^2$  becomes large.
  - As with  $D_1$ , the constant  $D_2$  can be viewed as a diffusion constant for  $v_1$ , controlling its spatial spread.

In summary, the solutions  $u_1$  and  $v_1$  describe entities that both diminish over time, but at different rates. The spatial behavior of these solutions is centered around the line defined by the sum  $(x + y)$ . While  $u_1$  diminishes smoothly,  $v_1$  has a peculiar behavior due to the presence of the absolute term, making it symmetric about the line  $x = -y$ . The constants  $D_1$  and  $D_2$  are significant as they modulate the spatial behavior of the entities represented by  $u_1$  and  $v_1$  respectively.

It is well known that the concentration of bromous acid, as well as other species in the BZ reaction, oscillates over time. Nonetheless, in some cases the concentration of  $HBrO_2$  may decay following the certain law (74) and under the following conditions:

- Formation of Bromide Ions: Using cerium ions (commonly as catalyst),  $HBrO_2$  can be transformed to bromide ions [21].
- Recombination Reactions: The autocatalytic step involves the bromide ions' reaction with bromate in the  $HBrO_2$  presence, further consuming  $HBrO_2$ .
- Dilution: If the reaction mixture undergoes dilution, the concentration of all species, including  $HBrO_2$ , will decrease, which may not necessarily suggest a decrease in the relative amount of  $HBrO_2$ , but the absolute concentration will be lower.

- End of Reaction: As reactants are consumed, especially in a system where no new reactants are introduced, the concentrations of intermediate species, including  $HBrO_2$ , will ultimately decline (see [22] and [23] for additional chemical evidences)

## 6 Stationary solutions

We begin by examining the supersolutions to  $u_1$  and  $v_1$  :

$$\begin{aligned} \frac{\partial u_1}{\partial t} &= D_1 \Delta u_1 + u_1 (k_2 A_2 - 2k_3 u_1 - k_1 v_1) \\ &\leq D_1 \Delta u_1 + k_2 A_2 u_1 - 2k_3 u_1^2 + k_{14} u_1^2, \end{aligned} \quad (76)$$

and

$$\begin{aligned} \frac{\partial v_1}{\partial t} &= D_2 \Delta v_1 - k_1 v_1^2 \\ &\leq D_2 \Delta v_1 + k_{15} v_1^2. \end{aligned} \quad (77)$$

Solutions were shown to be bounded in Theorem 1, hence we define  $k_{14} u_1 = \sup\{k_1 u_1\}$  and  $k_{15} v_1 = \sup\{k_1 v_1\}$ . As a result, the supersolutions to (1) are obtained by the solutions of the following equations:

$$\frac{\partial u_1}{\partial t} = D_1 \Delta u_1 + k_2 A_2 u_1 + (k_{14} - 2k_3) u_1^2, \quad (78)$$

$$\frac{\partial v_1}{\partial t} = D_2 \Delta v_1 + k_{15} v_1^2. \quad (79)$$

To explore stationary super-solutions to (1), we depart from (78) and (79), so that:

$$D_1 \Delta u_1 + k_2 A_2 u_1 + (k_{14} - 2k_3) u_1^2 = 0, \quad (80)$$

and

$$D_2 \Delta v_1 + k_{15} v_1^2 = 0. \quad (81)$$

Let us consider solutions of the form  $u_1(x, y) = u_1(\eta)$ , where  $\eta = ax + by$ . In this representation,  $a$  and  $b$  denote the wave number and the frequency, respectively. Such solutions are reminiscent of the 'traveling wave-fragments' discussed in [13], which represent colliding wave patterns. With this perspective, Equations (80) and (81) can be reformulated accordingly.

$$\frac{d^2 u_1}{d\eta^2} + \frac{k_2 A_2 u_1}{D_1(a^2 + b^2)} + \frac{(k_{14} - 2k_3) u_1^2}{D_1(a^2 + b^2)} = 0, \quad (82)$$

and

$$\frac{d^2 v_1}{d\eta^2} + \frac{k_{15} v_1^2}{D_2(a^2 + b^2)} = 0. \quad (83)$$

The considered solutions are those satisfying the following Hamiltonians (see [16] for additional insights):

$$\frac{1}{2} (u_1')^2 + \frac{k_2 A_2 u_1^2}{2D_1(a^2 + b^2)} + \frac{(k_{14} - 2k_3) u_1^3}{3D_1(a^2 + b^2)} = 0, \quad (84)$$

and

$$\frac{1}{2} (v_1')^2 + \frac{k_{15} v_1^3}{3D_2(a^2 + b^2)} = 0. \quad (85)$$

As  $k_{14} > 2k_3$ , therefore after solving (80) and (81) by separation of variables we get

$$u_1(\eta) = \frac{k_2 A_2}{k_{14} - 2k_3} \left[ -3 + \frac{3k_2 A_2}{D_1(a^2 + b^2)} \left( \frac{1 + e^{i\sqrt{\frac{k_2 A_2}{D_1(a^2 + b^2)}} \eta}}{1 - e^{i\sqrt{\frac{k_2 A_2}{D_1(a^2 + b^2)}} \eta}} \right)^2 \right], \quad (86)$$

and

$$v_1(\eta) = -\frac{6D_2(a^2 + b^2)}{k_{15}\eta^2}, \quad (87)$$

Hence and considering the exposed solutions for the simple mode  $a = b = 1$ , we have

$$u_1(x, y) = \frac{k_2 A_2}{k_{14} - 2k_3} \left[ -3 + \frac{3k_2 A_2}{2D_1} \left( \frac{1 + e^{i\sqrt{\frac{k_2 A_2}{2D_1}}(x+y)}}}{1 - e^{i\sqrt{\frac{k_2 A_2}{2D_1}}(x+y)}} \right)^2 \right], \quad (88)$$

and

$$v_1(x, y) = -\frac{12D_2}{k_{15}(x+y)^2}. \quad (89)$$

In the BZ reaction, the concentrations of the reactants and products oscillate without any external perturbation. This oscillatory behavior is attributable to the complex interplay between non-linear reactions and diffusion processes.

Given the solutions (86) and (87) and recalling that  $u_1$  and  $v_1$  represent the concentration dynamics of bromous acid ( $HBrO_2$ ) and bromide ions ( $Br^-$ ) respectively, we state that:

- The solution for  $u_1(x, y)$  exhibits spatial oscillations due to the presence of an exponential term with the imaginary unit  $i$ . This wave-like nature, governed by the term  $\sqrt{\frac{k_2 A_2}{2D_1}}$ , suggests that the reaction rate  $k_2$ , concentration  $A_2$ , and the diffusion constant  $D_1$  control the spatial periodicity. Such behavior is consistent with the expected oscillations in the BZ reaction.
- The bromide ions serve an inhibitory role. As bromide concentrations rise due to the reactions mentioned above, they act to slow down the reaction rate, leading to a drop in bromide concentration. Hence,  $v_1(x, y)$  describes a pattern where the concentration diminishes as one moves away from the origin and this aligns with the BZ mechanisms. This absence of oscillations and the decay governed by constants  $D_2$  and  $k_{15}$  is indicative of a bromide ion behavior that gets consumed or inhibited as it diffuses outward from a central point.
- In the mechanism of the BZ reaction, the bromous acid acts as an activator because it can autocatalytically produce more of itself.

Specifically, the acid can oxidize the bromide ion to produce more bromous acid. This autocatalytic loop is a significant contributor to the oscillatory behavior of the BZ reaction. Indeed, the solution  $u_1$  represents an activator species, oscillating due to certain feedback mechanisms. Meanwhile,  $v_1$  can be envisioned as an inhibitor, ensuring the reaction does not proceed to completion immediately and thus allows for the observed oscillations.

In conclusion, these solutions encapsulate some quintessential features of the BZ reaction, like the spatial oscillations and inhibitor-like behavior. However, a detailed suitability assessment would necessitate an understanding of the exact kinetics of the BZ reaction in consideration, as well as the specific values for the involved constants.

## 7 Nonstationary solutions

In this section, we derive the nonstationary solutions. To achieve this, we employ the nonlinear point scaling to shape the solution profiles of Eq. (2). Adopting this approach, we can represent the solutions as:

$$u_1(x, y, t) = e^{u_2(x, y, t)}, \quad (90)$$

and

$$v_1(x, y, t) = e^{v_2(x, y, t)}. \quad (91)$$

Such scaling techniques have been widely adopted by researchers in the engineering domain, as evidenced by the works cited in [18], [19] and [20]. We assert that certain analytical methods or techniques might be more directly applicable to the transformed system than to the original one. For example, the transformed system might be amenable to perturbation methods, similarity solutions, or other analytical techniques that will come after.

Drawing from these references, it is discerned that  $u_2$  and  $v_2$  adhere to

the subsequent Hamilton-Jacobi-type equations:

$$e^{u_2} \frac{\partial u_2}{\partial t} = D_1 e^{u_2} \left( \frac{\partial u_2}{\partial x} \right)^2 + D_1 e^{u_2} \left( \frac{\partial u_2}{\partial y} \right)^2 + k_2 A_2 e^{u_2} + (k_{14} - 2k_3) e^{2u_2}, \quad (92)$$

and

$$e^{v_2} \frac{\partial v_2}{\partial t} = D_2 e^{v_2} \left( \frac{\partial v_2}{\partial x} \right)^2 + D_2 e^{v_2} \left( \frac{\partial v_2}{\partial y} \right)^2 + k_{15} e^{2v_2}. \quad (93)$$

Taking into consideration the asymptotic boundary conditions, as  $x$  and  $y$  tend towards infinity, we assume that both exponential forms  $e^{-u_2}$  and  $e^{-v_2}$  provide the terms driving the dynamics that connects with diffusive principles acting through an exponential smoothing. Given this, the aforementioned equations simplify to:

$$\frac{\partial u_2}{\partial t} = D_1 \left( \frac{\partial u_2}{\partial x} \right)^2 + D_1 \left( \frac{\partial u_2}{\partial y} \right)^2, \quad (94)$$

and

$$\frac{\partial v_2}{\partial t} = D_2 \left( \frac{\partial v_2}{\partial x} \right)^2 + D_2 \left( \frac{\partial v_2}{\partial y} \right)^2. \quad (95)$$

Assuming,

$$u_2(x, y, t) = u_2(\xi, t), \text{ and } v_2(x, y, t) = v_2(\xi, t) \text{ where } \xi = ax + by, \quad (96)$$

in which  $a$  and  $b$ , refer to the wave number and frequency respectively. Substituting (96) into (94) and (95), we get:

$$\frac{\partial u_2}{\partial t} = D_1 (a^2 + b^2) \left( \frac{\partial u_2}{\partial \xi} \right)^2, \quad (97)$$

and

$$\frac{\partial v_2}{\partial t} = D_2 (a^2 + b^2) \left( \frac{\partial v_2}{\partial \xi} \right)^2. \quad (98)$$

Assuming

$$u_2(\xi, t) = (\tau + t)^{-1} \phi_1(\xi) \quad (99)$$

and

$$v_2(\xi, t) = (\tau + t)^{-1} \phi_2(\xi). \quad (100)$$

After using (99) and (100) into (97) and (98) respectively, we obtain

$$D_1(a^2 + b^2) \left( \frac{d\phi_1}{d\xi} \right)^2 + \phi_1 = 0, \quad (101)$$

and

$$D_2(a^2 + b^2) \left( \frac{d\phi_2}{d\xi} \right)^2 + \phi_2 = 0. \quad (102)$$

After solving (101) and (102), we have

$$\phi_1(\xi, t) = -\frac{\xi^2}{D_1(a^2 + b^2)}, \quad (103)$$

and

$$\phi_2(\xi, t) = -\frac{\xi^2}{D_2(a^2 + b^2)}, \quad (104)$$

which implies that

$$u_2(\xi, t) = -\frac{\xi^2 t^{-1}}{D_1(a^2 + b^2)}, \quad (105)$$

and

$$v_2(\xi, t) = -\frac{\xi^2 t^{-1}}{D_2(a^2 + b^2)}, \quad (106)$$

Returning (90) and (91), we have

$$u_1(x, y, t) = e^{-\frac{(ax+by)^2}{D_1 t(a^2+b^2)}}, \quad (107)$$

and

$$v_1(x, y, t) = e^{-\frac{(ax+by)^2}{D_2 t(a^2+b^2)}}. \quad (108)$$

We explore the behavior of these solutions based on the presented forms. For this recall that  $u_1$  and  $v_1$  represent the concentration dynamics of bromous acid ( $HBrO_2$ ) and bromide ions ( $Br^-$ ), respectively

1. **Role of  $t$ :** As  $t$  increases, the denominator in the exponential function increases, making the whole value inside the exponential decrease (in magnitude). This means that both  $u_1$  and  $v_1$  will tend towards 1 as  $t$  goes to infinity.
2. **Role of  $D_1$  and  $D_2$ :** These constants act as diffusion coefficients in the equation. For a fixed value of  $(x, y, t)$ , as  $D_1$  or  $D_2$  increases, the value inside the exponential function decreases (in magnitude) and therefore  $u_1$  or  $v_1$  will increase. In simpler terms, a larger diffusion coefficient means a "faster" diffusion or spreading, leading to a larger value of the function for a given time and position.
3. **Comparison between  $u_1$  and  $v_1$ :** For  $D_1 < D_2$ ,  $u_1$  will generally be larger than  $v_1$  for the same values of  $x, y, t$  (and vice-versa for  $D_1 > D_2$ ). This is because a smaller diffusion coefficient will result in a slower spread, meaning the function remains larger for a longer time.
4. **Role of  $a$  and  $b$ :** The terms  $ax$  and  $by$  determine the directionality and rate of change of the functions. If  $a$  is larger than  $b$ , then changes in  $x$  will have a more pronounced effect on the functions than changes in  $y$ . The factors  $a^2$  and  $b^2$  in the denominator normalize this effect, ensuring that the direction  $(a, b)$  acts as a unit direction vector.



5. **Behavior at the Origin:** At  $x = 0$  and  $y = 0$ , both  $u_1$  and  $v_1$  are equal to 1 for any  $t > 0$ . This can be regarded as their maximum concentrations before the diffusion process starts.
6. **Spatial Spread:** As  $x$  or  $y$  moves away from the origin, the value inside the exponential increases (in magnitude). Thus,  $u_1$  and  $v_1$  will decrease. The rate at which they decrease depends on the values of  $a, b, D_1$ , and  $D_2$ .

For the line  $ax + by = 0$  or equivalently  $y = -\frac{a}{b}x$ :

1. **Spatial Spread:** Away from this line, as  $x$  or  $y$  moves, the value inside the exponential increases (in magnitude). Thus,  $u_1$  and  $v_1$  will decrease. The rate at which they decrease depends on the values of  $a, b, D_1$ , and  $D_2$ . The steeper the slope of the line, the more rapidly the functions will decrease as you move perpendicularly away from it.
2. **Role of  $t$ :** Away from the line  $y = -\frac{a}{b}x$ , as  $t$  increases, the functions will tend towards 1 as  $t$  goes to infinity, since the denominator in the exponential function increases with  $t$ .
3. **Comparison between  $u_1$  and  $v_1$ :** For  $D_1 < D_2$  away from the line  $y = -\frac{a}{b}x$ ,  $u_1$  will generally be larger than  $v_1$  for the same values of  $x, y, t$  (and vice-versa for  $D_1 > D_2$ ).
4. **Directional Dependence:** The direction given by  $ax + by = 0$  acts as a "ridge" or "peak" for both functions, with the maximum value of 1 along it. The functions decrease in value as one moves away from this line.

In conclusion, the line  $ax + by = 0$  is a special direction for the given functions where their value remains constant at 1 regardless of time. Away from this line, the functions exhibit the typical diffusion behavior, spreading and decreasing in value over time and space.

The described mechanisms allow us to elucidate the diffusion or dispersion of bromous acid ( $HBrO_2$ ) and bromide ions ( $Br^-$ ) over time and

space. Certainly, additional experimental set up is required to further determined if the line  $ax + by = 0$  is chemically plausible as an invariant ridge for both solutions regardless of the value of  $t$ .

## 8 Conclusion

Building upon the pioneering efforts of Belousov and Zhabotinsky and the subsequent refinements by Noyes and Field, our research brought to the fore unprecedented analytical solutions. We provided analyses in connection with the boundedness, regularity, and symmetries of solutions. Our approach to the Tanh-method and the ensuing exploration of traveling waves showcased the richness and depth of the Oregonator's solution space. Moreover, the foray into self-similar paradigms, the Hamilton-Jacobi equation, and the corresponding asymptotic solutions added new ideas for exploring further the oregonator model, possibly beyond the known oscillatory solutions.

Encouragingly, the mathematical tools and methodologies we refined may serve as robust platforms for future explorations concerning experimental works. Such works are mainly required for the definition of specific values for the involved constants and validation of the mathematical solutions.

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