Journal of Mathematical Chemistry 6(1991)359–375

NUCLEATION IN A BISTABLE BELOUSOV–ZHABOTINSKII SYSTEM

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Received 4 September 1990

Abstract

A new model of the Belousov–Zhabotinskii reaction is developed. It describes bistable behavior of the reaction. For this reaction–diffusion system existence results are proved. The critical radius of a nucleus is defined and studied by numerical methods.

1. Introduction

Nucleation and bistability are characteristic phenomena of many autocatalytical systems. Nitzan et al. [13] first described the nucleation of a new phase in a bistable one-variable system using a third-order reaction function. They showed the existence of a critical radius r_c, beyond which a nucleus of the new phase will grow on or will collapse if its radius is below r_c. These results are not directly applicable to the Belousov–Zhabotinskii reaction (BZR), whose kinetics are governed by maximum second-order reaction terms [4]. A model of the BZR reflecting the bistability of this reaction requires at least two variables.

Our aim is to discuss a model of bistability and nucleation in convection-free layers of BZ solutions in petri dishes. We consider the following subsystem of the full BZR in order to confine our model to two variables only, the concentrations of the autocatalyst $HBrO_2$ and the inhibitor Br^-:

$$BrO_3^- + 2H^+ + Br^- \longrightarrow HBrO_2 + HOBr \qquad \text{R1}$$

$$HBrO_2 + H^+ + Br^- \longrightarrow 2\,HOBr \qquad \text{R2}$$

$$BrO_3^- + H^+ + HBrO_2 + 2\,Me(red) \longrightarrow 2\,HBrO_2 + 2\,Me(ox) \qquad \text{R3}$$

$$2\,HBrO_2 \longrightarrow BrO_3^- + H^+ + HOBr \qquad \text{R4}$$

We neglect the concentrations of metal catalysts Me(red), Me(ox) and HOBr, and assume that the concentrations of BrO_3^- and H^+ are constant.

Additionally, we introduce a flow term φ_{Br^-}. This corresponds to the inhibitor release induced both by oxygen diffusing from the air into the liquid layer [10] and/or by light irradiation when the BZ system is photosensitive [9].

On the basis of this realistic flow term, the behavior of the system R1–R4 turns from monostability to bistability within a distinct region of φ_{Br^-}. In the region of bistability, the reaction–diffusion system performs transitions from one stable state to the other if the radius of the inducing nucleus exceeds a critical value r_c. The critical radius itself depends in the flow φ_{Br^-}. This relation $r_c = r_c(\varphi_{Br^-})$ is studied numerically. We found that the quantity r_c tends to infinity if the flow term tends to a certain value $\varphi_{Br^-}^{coex}$. If we take a higher value $\varphi > \varphi_{Br^-}^{coex}$, then we observe transitions to the other stable state.

2. The model

So, we start with the following system

$$\frac{\partial X}{\partial t} = d_x \frac{\partial^2 X}{\partial r^2} + k_3 A X - 2k_4 X^2 - k_2 X Y + k_1 A Y,$$

$$\frac{\partial Y}{\partial t} = d_y \frac{\partial^2 Y}{\partial r^2} - k_2 X Y - k_1 A Y + \varphi_{Br^-}, \qquad (1)$$

where $r \in \mathbb{R}$, $t > 0$. $X = [HBrO_2]$, $Y = [BrO_3^-]$, d_x, d_y are diffusion coefficients of $HBrO_2$ and Br^-, respectively, and k_i are the velocity constants. Table 1 contains the values of parameters.

Table 1

Values of parameters [3,8]

Parameter	Value	Unit
k_1	$2.1\ [H^+]^2$	$M^{-1}s^{-1}$
k_2	$10^5\ [H^+]$	$M^{-1}s^{-1}$
k_3	$45\ [H^+]$	$M^{-1}s^{-1}$
k_4	10^3	$M^{-1}s^{-1}$
φ	arbitrary	$M\ s^{-1}$
$[H^+]$	0.16	M
A	0.2	M
d_x	1.3×10^{-5}	cm^2s^{-1}
d_y	1.9×10^{-1}	cm^2s^{-1}

By the substitution

$$
\begin{aligned}
u_1 &:= 2k_4X/k_3A,\\
u_2 &:= k_2Y/k_3A,\\
D &:= 10^{-5}\,\mathrm{cm^2s^{-1}},\\
x &:= (k_3AD^{-1})^{1/2}r,\\
t' &:= k_3At,\\
\varphi &:= k_2/(k_3A)^2\,\varphi_{\mathrm{Br^-}},\\
m &:= k_1/k_3,\\
b &:= k_2/k_4,\\
q &:= 2k_1k_4/k_2k_3 = m/b,\\
d_1 &:= d_x/D,\\
d_2 &:= d_y/D,
\end{aligned}
$$

see [12], we obtain from (1) an equivalent dimensionless system of partial differential equatons. Let us consider this system on a bounded interval Ω, and let us establish this sytem with no flux boundary conditions and initial value. We then obtain

$$
\begin{aligned}
\frac{\partial u_1}{\partial t'} &= d_1\,\frac{\partial^2 u_1}{\partial x^2} + u_1(1-u_1-u_2)+qu_2\,,\\
\frac{\partial u_2}{\partial t'} &= d_2\,\frac{\partial^2 u_2}{\partial x^2} - bu_1u_2 - mu_2 + \varphi,
\end{aligned}
\tag{2}
$$

$x \in \Omega,\ t' > 0,\ \partial u_i/\partial n(\partial\Omega) = 0,\ u_i(0,x) = u_{0i}(x),\ i = 1, 2.$

3. The reaction system

Stationary solutions $u_s = (u_{s1}, u_{s2})$ of the corresponding reaction system

$$
\begin{aligned}
\frac{du_1}{dt'} &= u_1(1-u_1-u_2)+qu_2\,,\\
\frac{du_2}{dt'} &= -bu_1u_2 - mu_2 + \varphi
\end{aligned}
\tag{3}
$$

are solutions of the system

$$
\begin{aligned}
0 &= u_1(1-u_1-u_2)+qu_2\,,\\
0 &= -bu_1u_2 - mu_2 + \varphi.
\end{aligned}
\tag{4}
$$

The system (4) is equivalent to

$$u_2 = \varphi/(m + bu_1), \tag{5}$$

$$u_1^3 + u_1^2(m-b)/b + u_1(\varphi - m)/b - q\varphi/b = 0. \tag{6}$$

We are only interested in real, positive solutions $u_s^{(j)}$, $j = 1, 2, 3$. Regarding φ as a function of u_1: $\varphi = \varphi(u_1)$, from (6) we obtain the equivalent equation

$$\varphi(u_1) = u_1(1-u_1)(m+bu_1)/(u_1 - q). \tag{7}$$

Let us briefly discuss this function (7): Since $1 - q > 0$, φ tends to infinity for $u_1 \to q$. Moreover, φ vanishes at $u_1 = 1$, $u_1 = 0$, $u_1 = -m/b = -q$. Using parameter values of table 1, one obtains the positive local extrema of φ:

$$u_{s1_{max}} = 0.499063, \quad \varphi_{max} = 2.007756,$$

$$u_{s1_{min}} = 0.002257, \quad \varphi_{min} = 0.045723.$$

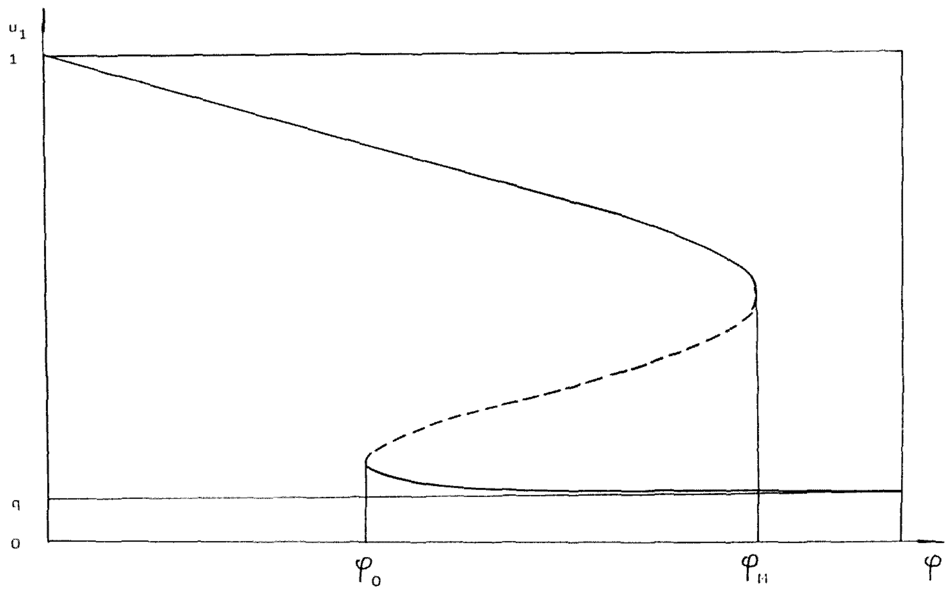

Fig. 1. Bistability diagram for u_{s1} with the parameters $m = 0.008$, $b = 8.0$, $q = 0.001$. The upper branch (full line) corresponds to $u_{s1}^{(3)}$, the middle branch (broken line) to $u_{s1}^{(2)}$, and the lower branch (full line) to $u_{s1}^{(1)}$.

In this way, we obtain the qualitative behaviour of (7) and therefore of (6), as shown in fig. 1. Let

$$u_{s1}^{(3)} \geq u_{s1}^{(2)} \geq u_{s1}^{(1)},$$

and $\varphi_0 := \varphi_{min}$, $\varphi_M := \varphi_{max}$. The stability behavior of $u_s^{(j)}$ can be determined easily:

LEMMA 3.1

(i) The equilibrium $u_s^{(1)}$ is asymptotically stable (in the sense of Lyapunov and with respect to system (3)), if $\varphi > \varphi_0$;

(ii) $u_s^{(2)}$ is unstable for all $\varphi_0 < \varphi < \varphi_M$;

(iii) $u_s^{(3)}$ is asymptotically stable for all $0 \le \varphi < \varphi_M$.

Proof

The linearization of (3) in u_s and substitution of (5) yield a (linear in φ) equation for the zero eigenvalue. This equation is equivalent to (7). Its extrema give the points where u_s changes its stability. Purely imaginary eigenvalues do not appear. □

Now assume there is given an initial value

$$u(0) = u_0 \in \mathbb{R}^2. \tag{8}$$

We shall prove that there exists a global solution of (3), (8) for some initial values u_0. It is clear that for every $u_0 \in \mathbb{R}^2$, the problem (3), (8) has a unique local solution.

Let

$$0 < q < 1,\ 0 < \varepsilon < \varphi/(m + b),$$

$$G_1 := \{q \le u_1 \le 1,\ \varepsilon \le u_2 \le \varphi/m\}.$$

THEOREM 3.2

Assume $u_0 \in G_1$. Then the solution $u(t')$ of (3), (8) exists for all $t' > 0$ and is bounded, and $u(t') \in G_1$ for all $t' \ge 0$.

Proof

Checking the vector field of (3) (see fig. 2) on the bounds of G_1 gives that there is no trajectory leaving G_1. Thus, the assertion is proved. □

Furthermore, the following theorem holds:

THEOREM 3.3

Closed trajectories do not exist in G_1.

Proof

Applying the Dulac criterion ([1], p. 120), we obtain by the Dulac function $B(u_1, u_2) = 1/u_1$:

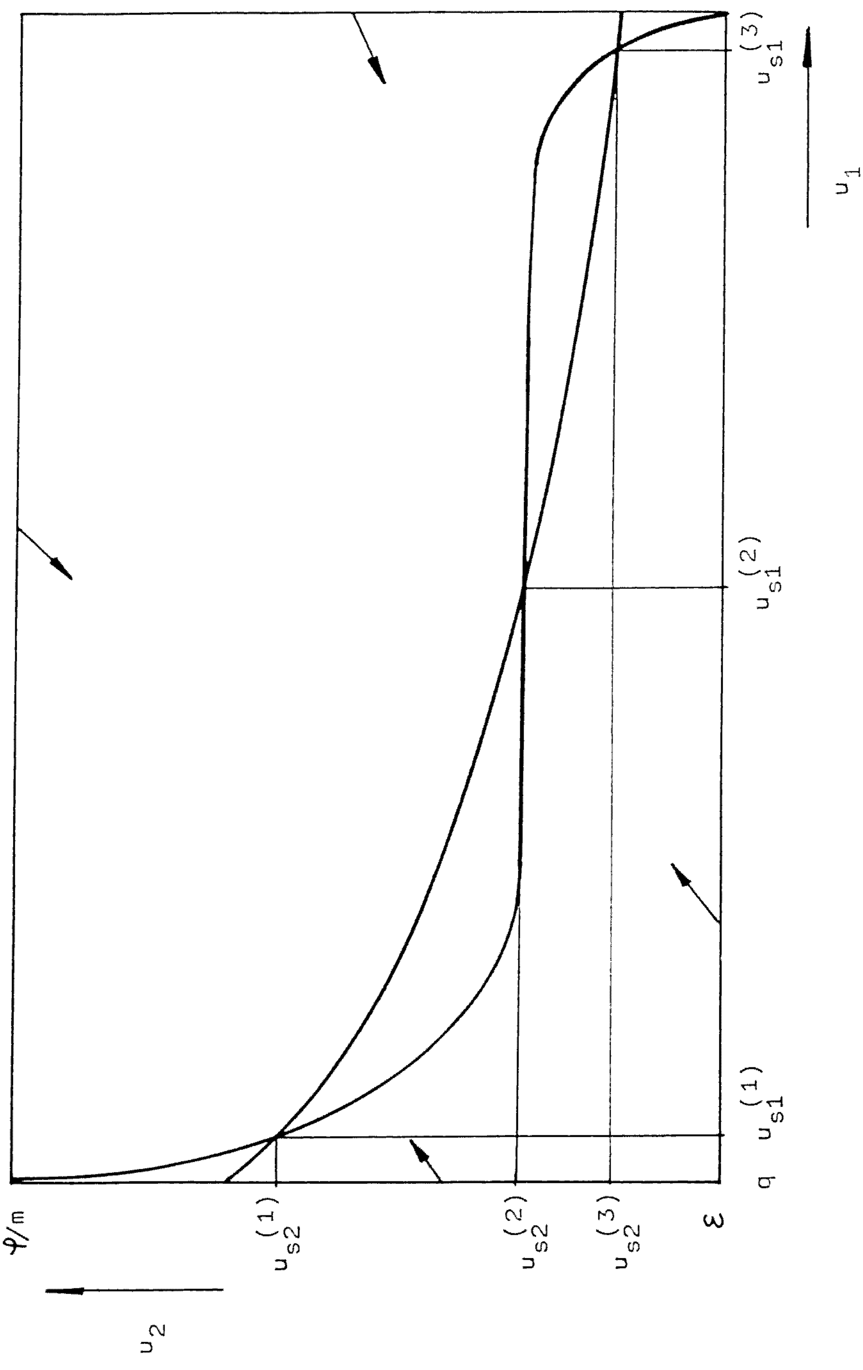

Fig. 2. The vector field of the system (3).

$$D := \frac{\partial}{\partial u_1}\big(B(u_1,u_2)f_1(u_1,u_2)\big) + \frac{\partial}{\partial u_2}\big(B(u_1,u_2)f_2(u_1,u_2)\big)$$
$$= -1 - qu_2/u_1^2 - b - m/u_1 < 0,$$

where $f = (f_1, f_2)$ is the reaction term in (3). This proves the assertion. □

COROLLARY 3.4

Let $u_0 \in G_1$, $u_0 \neq u_s^{(j)}$, $j = 1, 2, 3$. Then the solution $u(t'$ of (3), (8) converges either to $u_s^{(1)}$ or $u_s^{(3)}$ for $t' \to \infty$, and $u(t')$ tends to $u_s^{(2)}$ for $t' \to -\infty$.

Proof

The assertion follows from the Bendixon theorem, see e.g. [6]. □

4. Global existence of solutions

In this section, we shall investigate the global existence of solutions of problem (1). For this reason, we formulate (1) as an evolution problem in a convenient space X. Theorem 4.7 gives the existence result in X and in classical function spaces, too. Let us introduce the following definitions and notation.

The domain $\Omega \subset \mathbb{R}^n$, $n \leq 3$, is assumed to be an open smooth bounded connected set, $\partial\Omega \in \mathbb{C}^2$.

$$X := L^2(\Omega, R^2),\ \|u\|^2 = \int_\Omega \big((u_1(x))^2 + (u_2(x))^2\big)\,\mathrm{d}x,\quad u \in X,$$

$$H^k := W^{k,2}(\Omega, R^2),\ k = 1, 2, \ldots,$$

$$\|u\|_{H^k}^2 := \|u\|^2 + \sum_{j=1}^{n} \left\|\frac{\partial u}{\partial x_j}\right\|^2 + \ldots + \sum_{\substack{l=(l_1,\ldots,l_k):\\ \Sigma l_i = k}} \left\|\frac{\partial^k u}{\partial x_{l_1}\ldots\partial x_{l_k}}\right\|^2.$$

For a reference of the theory of the Sobolev spaces, see [14].

Let A be the linear operator $A : X \to X$, with $D(A) := \{(u_1, u_2) : u \in \mathbb{C}^\infty(\Omega)^\star$, $\partial u_i/\partial n(\partial\Omega) = 0\}$:

$$Au := -(d_1\Delta u_1,\ d_2\Delta u_2),$$

where $d_1, d_2 > 0$. We define the operator A to be the Friedrich extension of $\boldsymbol{A}$.

$^\star\mathbb{C}^\infty(\Omega, \mathbb{R}^2)$ consists of all functions whose derivatives admit a continuous prolongation to $\bar{\Omega}$.

The next lemma summarizes some simple but helpful properties of this operator A:

LEMMA 4.1

Let $d := \max(d_1, d_2)$. It holds that:

(i) $\langle (A + dId)u, u\rangle \le 2d \| u \|^2_{H^1}, \qquad u \in D(A).$

(ii) $\min(d_1, d_2) \| u \|^2_{H^1} \le \langle (A + dId)u, u\rangle, \quad u \in D(A).$

(iii) $D(A) \subset H^1$, and

$$\langle Au, v\rangle = \langle (d_1 u_1', d_2 u_2'), v'\rangle, \qquad u \in D(A),\ v \in H^1.$$

(iv) $D((A + dId)^{1/2}) = H^1$.

(v) The operator $A + dId$ is selfadjoint and positive.

(vi) The operator $-(A + dId)$ generates an analytic semigroup $\exp(-t(A + dId)) : X \to D(A)$, and

$$\exp(-t(A + dId)) \le c_1 \exp(-dt/2), \qquad t \ge 0. \tag{9}$$

Proof

(i) $\langle (A + dId)u, u\rangle \le d\langle \nabla u, \nabla u\rangle + d\langle u, u\rangle \le 2d \| u \|^2_{H^1}$.

(iii) See [11].

(iv) The assertion follows from

$$\langle A_d u, u\rangle = \langle A_d^{1/2} u, A_d^{1/2} u\rangle = \| A_d^{1/2} u \|.$$

(vi) Compare [5]. □

Set $A_d := A + dId$ with domain $D(A_d) := D(A)$. By

$$F(u) := \begin{pmatrix} u_1(1-u_1-u_2)+qu_2 \\ -bu_1u_2 - mu2 + \varphi \end{pmatrix}, \quad q, b, m, \varphi > 0,\ q < 1,$$

a nonlinear operator $F : H^1 \to X$ is defined.

Now, we may write (2) as an initial value problem

$$\frac{\mathrm{d}u}{\mathrm{d}t} + Au = F(u), \quad t > 0,$$

$$u(0) = u_0, \qquad u_0 \in X. \tag{10}$$

(Now, we shall write t instead of t'.)

We define a *solution of (10)* on $(0,T)$ to be a map $u \in \mathbb{C}^1((0,T),X) \cap \mathbb{C}([0,T),X)$, $u(t) \in D(A)$ for all $t \in (0,T)$ and some $T > 0$, and which solves (10).

We shall prove the unique solvability of problem (10) by investigating the modified system

$$\frac{\mathrm{d}u}{\mathrm{d}t} + Au = F_k(u), \quad t > 0,$$
$$u(0) = u_0, \qquad u_0 \in X. \tag{11}$$

Here, $F_k : X \to X$ is the operator

$$F_k(u) := \begin{pmatrix} u_{1k}(1 - u_{1k} - u_{2k}) + qu_2 \\ -bu_{1k}u_{2k} - mu_2 + \varphi \end{pmatrix},$$

and u_{ik} are the following projections:

$$u_{ik}(x) := \begin{cases} 0 & \text{if } 0 \geq u_i(x), \\ u_i(x) & \text{if } 0 \leq u_i(x) \leq k_i, \\ k_i & \text{if } k_i \leq u_i(x), \end{cases}$$

$i = 1, 2$, where k_i are some positive constants to be chosen later. Obviously, the mapping $u \to u_{ik}$ gives a pair (u_{1k}, u_{2k}), and u_{1k} (u_{2k}) is bounded by 0 and k_1 (k_2), respectively.

LEMMA 4.2

$F_k : X \to X$ is globally Lipshitzian.

Proof

$$\|F_k(u) - F_k(v)\|^2 = \int_\Omega ((u_{1k}(1 - u_{1k} - u_{2k}) + qu_2 - v_{1k}(1 - v_{1k} - v_{2k}) - qv)^2$$
$$+ (-bu_{1k}u_{2k} - mu_2 + bv_{1k}v_{2k} + mv_2)^2)^2 \mathrm{d}x$$
$$\leq 4 \int_\Omega ((u_{1k} - v_{1k})^2 + (v_{1k}^2 - u_{1k}^2) + (u_{1k}u_{2k} - v_{1k}v_{2k})^2$$
$$+ q^2(u_2 - v_2) + b^2(u_{1k}u_{2k} - v_{1k}v_{2k}) + m^2(u_2 - v_2)^2)\mathrm{d}x$$
$$= 4 \int_\Omega ((u_{1k} - v_{1k})^2 + (u_{1k} + v_{1k})^2(u_{1k} - v_{1k})^2 + q^2(u_2 - v_2)^2$$
$$+ m^2(u_2 - v_2)^2 + (1 + b^2)(u_{1k}u_{2k} - v_{1k}v_{2k})^2)\mathrm{d}x$$

$$\leq 4\int_\Omega ((1+4k_1^2+2k_2^2(1+b^2))(u_1-v_1)^2$$

$$+(2k_1^2(1+b^2)+q^2+m^2)(u_2-v_2)^2)\,dx$$

$$= c_{\mathrm{LIP}}^2\|u-v\|^2. \qquad \square$$

The next lemma is an easy consequence of Sobolev's embedding theorems:

LEMMA 4.3

Let $n \leq 3$, $u, v \in H^2$, $\| u - v \|_{H^1} \to 0$. Then,

$\| F_k(u) - F_k(v) \|_{H^1} \to 0.$

LEMMA 4.4

Let $T > 0$ be any positive number. There exists a unique solution $u(t)$ of (11) on $(0, T)$; moreover, $u \in \mathbb{C}((0, T), H^1)$.

Proof

First, we show that the integral equation

$$u(t) = \exp(-tA_d)u_0 + \int_0^t \exp(-(t-s)A_d)g(u(s))\,ds \tag{12}$$

has a unique solution $u \in \mathbb{C}([0, T), X)$ satisfying $u(0) = u_0 \in X$, where

$g(u) := F_k(u) + du.$

Consider the operator $G : \mathbb{C}([0, T), X) \to \mathbb{C}([0, T), X)$:

$$(Gu)(t) := \exp(-tA_d)u_0 + \int_0^t \exp(-(t-s)A_d)g(u(s))\,ds, \qquad t > 0.$$

Obviously, G maps $\mathbb{C}([0, T), X)$ into itself. Define $\|\cdot\|_p$ by

$$\|u\|_p := \sup_{s\in[0,T)} (\|u(s)\|\exp(-ps)), \qquad p > 0,$$

and equip $\mathbb{C}([0, T), X)$ with this norm. If $u, v \in \mathbb{C}([0, T), X)$, we conclude from (9):

$$\|(Gu - Gv)(t)\| = \| \int_0^t \exp(-(t-s)A_d)[g(u(s)) - g(v(s))]\,\mathrm{d}s \|$$
$$\leq (c_{\mathrm{LIP}} + d)/(d/2+p)c_1 \exp(pt)\|u-v\|_p .$$

In this way, we obtain

$$\|Gu - gv\|_p \leq c_1 (c_{\mathrm{LIP}} + d)/(d/2+p)\|u-v\|_p . \tag{13}$$

Now, we choose $p \gg 1$ such that $c_2 := c_1(c_{\mathrm{LIP}} + d)/(d/2 + p) < 1$, and so

$$\|Gu - Gv\|_p \leq c_2 \|u-v\|_p . \tag{14}$$

By the Banach fixed point theorem, there exists a unique fixed point u of G in $\mathbb{C}([0, T), X)$.

By lemma 4.3, it can be shown that $u \in \mathbb{C}((0, T), H^1)$. Now, eq. (12) gives $u \in \mathbb{C}^1((0, T), X)$. It follows by the standard argument of Gronwall's lemma that the solution is unique. □

LEMMA 4.5

Let $u_0 \geq 0$. Then, for the solution u of (11), it holds that

$$u(t) \geq 0 \quad \text{for all } t \geq 0.$$

Proof

After computing the scalar product with u_2^- and u_1^-, it is clear that

$$u_1^- \equiv u_2^- \equiv 0.$$

(Here, we use the notation $u^+(x) := \max(u(x), 0)$, $u^-(x) := \max(-u(x), 0)$.) □

Now, we are able to solve problem (11):

LEMMA 4.6

Assume $u_0 \geq 0$, $u_0 \in L^\infty(\Omega, \mathbb{R}^2)$. The solution u of (11) exists on $(0, \infty)$ and satisfies:

$$0 \leq u_1 \leq \max(1, \| u_{01} \|_\infty),$$

$$0 \leq u_2 \leq \max(\varphi/m, \| u_{02} \|_\infty). \tag{15}$$

Proof

Let u be the nonnegative unique solution of (11), $t \geq 0$. Choose the constants $k_1 := \max(1, \| u_{01} \|_\infty)$, $k_2 := \max(\varphi/m, \| u_{02} \|_\infty)$. By the test function $(u_2 - k_2)^+$ one obtains

$$\|(u_2 - k_2)^+(t)\|^2/2 = -d_2 \int_0^t \int_\Omega (\nabla(u_2 - k_2)^+)^2 \mathrm{d}x\,\mathrm{d}t + \varphi \int_0^t \int_\Omega (u_2 - k_2)^+ \mathrm{d}x\,\mathrm{d}t$$

$$+ \int_0^t \int_\Omega (u_2 - k_2)^+(-b u_{1k} u_{2k} - m u_2)\mathrm{d}x\,\mathrm{d}t$$

$$\leq -m \int_0^t \int_\Omega (u_2 - k_2)^+(u_2 - k_2 + k_2)\mathrm{d}x\,\mathrm{d}t + \varphi \int_0^t \int_\Omega (u_2 - k_2)^+ \mathrm{d}x\,\mathrm{d}t$$

$$\leq (-m k_2 + \varphi) \int_0^t \int_\Omega (u_2 - k_2)^+ \mathrm{d}x\,\mathrm{d}t$$

$$\leq 0.$$

Consequently, $(u_2(t) - k_2)^+ = 0$, and so $u_2(t) \leq k_2$. By the test function $(u_1(t) - k_1)^+$, we have:

$$-\|(u_1 - k_1)^+(t)\|^2/2 = -d_1 \int_0^t \int_\Omega (\nabla(u_1 - k_1)^+)^2 \mathrm{d}x\,\mathrm{d}t + q \int_0^t \int_\Omega (u_1 - k_1) u_2 \,\mathrm{d}x\,\mathrm{d}t$$

$$+ \int_0^t \int_\Omega (u_1 - k_1)^+(1 - u_{1k} - u_{2k}) u_{1k} \,\mathrm{d}x\,\mathrm{d}t$$

$$\leq \int_0^t \int_\Omega (u_1 - k_1)^+ u_{2k}(-u_{1k} + q)\mathrm{d}x\,\mathrm{d}t$$

$$\leq 0.$$

This gives $(u_1 - k_1)^+(t) = 0$, so $u_1(t) \leq k_1$. □

Now, we want to prove our main result:

THEOREM 4.7

Assume $u_0 \geq 0$, $u_0 \in L^\infty(\Omega, \mathbb{R}^2)$. Then there exists a unique solution u of the problem (10) on $(0, \infty)$ satisfying (15). Moreover, $u(t) \in \mathbb{C}^2(\bar{\Omega}, \mathbb{R}^2)$, $\mathrm{d}u/\mathrm{d}t(t) \in \mathbb{C}(\bar{\Omega}, \mathbb{R}^2)$, $t > 0$. This means the solution exists in the classical sense.

Proof

Let u be the solution of (11). If we choose $k_1 := \max(1, \| u_{01} \|_\infty)$, $k_2 := \max(\varphi/m, \| u_{02} \|_\infty)$, then by lemma 4.6 we obtain $u_{ik}(t) = u_i(t)$, $i = 1, 2$, that is, (15) holds. Further, we have $F_k(u) = F(u)$, and $u(t)$ is the solution of (10). Since $u_i(t) \leq k_i$, $t \in [0, T)$, $u_i(t)$ has a continuous prolongation to $(0, \infty)$, and

$$\sup_{t>0} \| u_i(t) \| \leq k_i, \quad i = 1, 2.$$

Consequently, u belongs to $L^\infty([0, \infty), X)$.

Using theorem 3.5.2 in [5], it follows that

$$\frac{\mathrm{d}u}{\mathrm{d}t}(t) \in H^1, \quad t > 0.$$

Further, for $u(t) \in H^2$ we have $F(u) \in H^1$, $t > 0$. In this way,

$$Au = -\frac{\mathrm{d}u}{\mathrm{d}t} + F(u) \in H^1,$$

and so $u(t) \in H^3$, $t > 0$. Now, since $u(t) \in H^3 \subseteq \mathbb{C}(\bar{\Omega})$, $F(u(t)) \in \mathbb{C}(\bar{\Omega})$ and

$$\frac{\mathrm{d}u}{\mathrm{d}t}(t) \in \mathbb{C}(\bar{\Omega}), \quad n/4 < 1,$$

i.e. $\mathrm{d}u/\mathrm{d}t(t) \in \mathbb{C}(\bar{\Omega})$. This yields

$$Au = -\frac{\mathrm{d}u}{\mathrm{d}t} + F(u) \in \mathbb{C}(\bar{\Omega}),$$

implying $u(t) \in \mathbb{C}(\bar{\Omega})$. Consequently,

$$\frac{\mathrm{d}u}{\mathrm{d}t}(t) \in \mathbb{C}(\bar{\Omega}).$$ □

COROLLARY 4.8

Let $u_0 \geq 0$, $u_{01} \leq 1$, $u_{02} \leq \varphi/m$. Then the solution u of (19) exists and it holds that

$$0 \leq u_1 \leq 1,$$

$$0 \leq u_2 \leq \varphi/m.$$

Let

$$G_2 := \{q \leq u_1 \leq 1,\ 0 \leq u_2 \leq \varphi/m\}.$$

Using the same method as mentioned above but another definition of u_{1k}, namely

$$u_{1k}(x) := \begin{cases} q & \text{if } q \geq u_1(x), \\ u_1(x) & \text{if } q \leq u_1(x) \leq 1, \\ 1 & \text{if } 1 \leq u_1(x), \end{cases}$$

we obtain quite similar results:

LEMMA 4.9

Let $u_0 \in G_2$ (respectively, G_1). Then the solution u of (10) exists and belongs to G_2 (respectively, G_1).

5. Critical radius

The aim of this section is the investigation of the critical radius of a nucleus. Such questions have been studied in the case of one reaction–diffusion equation only [2]. Here, we consider the case $n = 1$, $\Omega = (0, L)$.

DEFINITION 5.1

The quantity r_c is called *critical radius* with respect to (12) and the initial value

$$u_{01}(x) = \begin{cases} u_{s1}^{(3)} & \text{if } 0 \leq x \leq x_1, \\ u_{s1}^{(1)} & \text{if } x_1 < x \leq L, \end{cases}$$

$$u_{02}(x) = \begin{cases} u_{s2}^{(3)} & \text{if } 0 \leq x \leq x_1, \\ u_{s2}^{(1)} & \text{if } x_1 < x \leq L, \end{cases} \tag{16}$$

if there exists a solution u of (10) with the special initial value (16) having the following properties:

(i) if $x_1 > r_c$, $u(t)$ tends to $u_s^{(3)}$ as $t \to \infty$,

(ii) for $0 < x_1 < r_c$, $u(t)$ tends to $u_s^{(1)}$ as $t \to \infty$.

The problem (10) with initial value (16) was integrated by the Euler difference method. Observing the coexistence of two asymptotically stable equilibria $u_s^{(1)}$ and $u_s^{(3)}$, there arises the question: What happens if we increase φ? The front travels back, and it is possible to define an inverse critical radius r_c^{inv} in a natural way. Results of our numerical investigations are summarized in table 2.

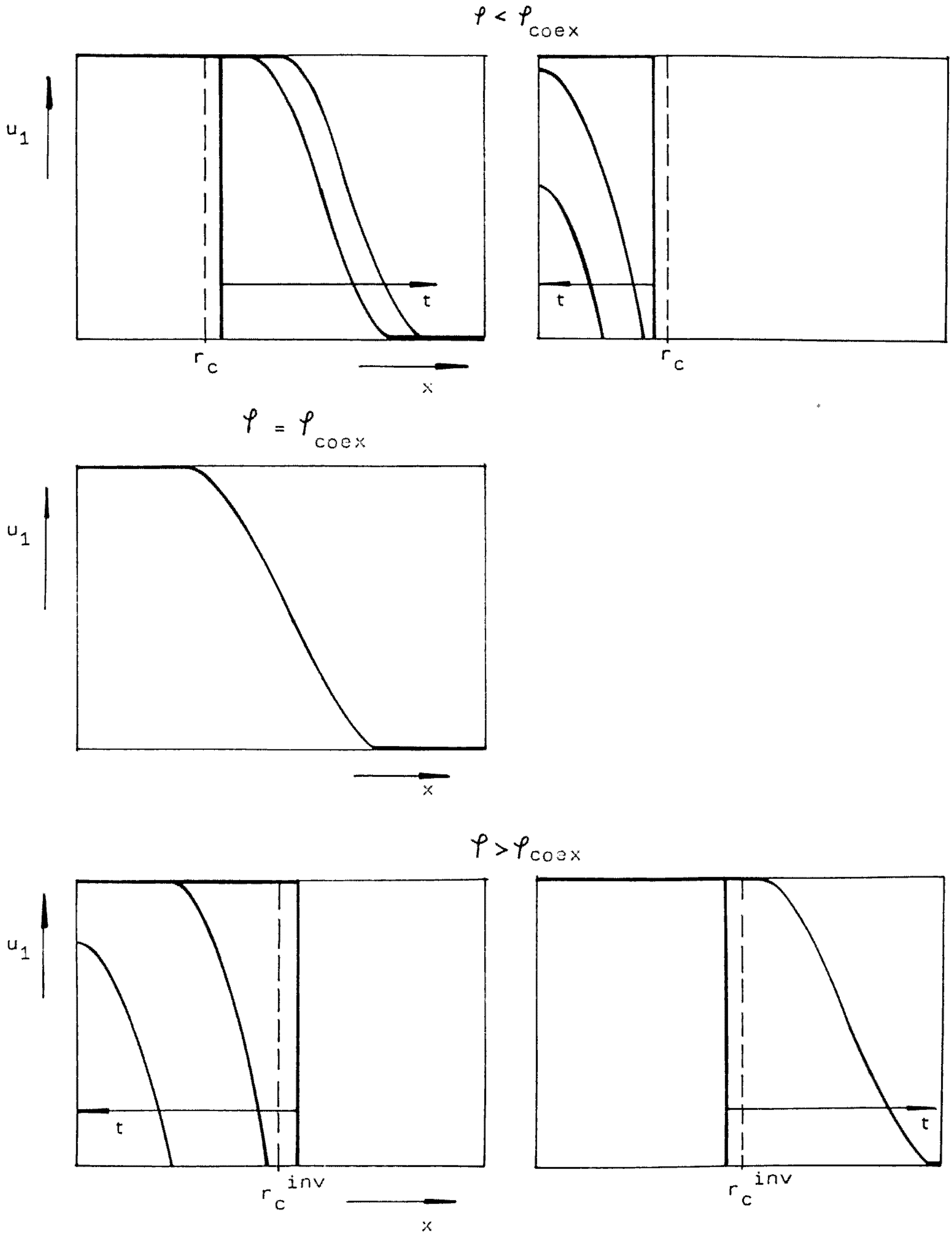

Fig. 3. The critical radius r_c and the inverse critical radius r_c^{inv}.

Table 2

The critical radius in dependence on φ

φ	r_c [dimensionless]	r_c [10^{-3} cm]
0.05	$\in (0.2, 0.3)$	$\in (0.5, 0.8)$
0.1	$\in (1.2, 1.4)$	$\in (3.1, 3.6)$
0.2	$\in (2.2, 2.4)$	$\in (5.7, 6.2)$
0.3	$\in (3.2, 3.4)$	$\in (8.3, 8.8)$
0.4	$\in (4.2, 4.4)$	$\in (10.9, 11.4)$
0.5	$\in (5.6, 5.8)$	$\in (14.6, 16.1)$
0.55	$\in (6.8, 7.4)$	$\in (17.7, 19.2)$
φ	r_c^{inv} [dimensionless]	r_c^{inv} [10^{-3} cm]
0.8	$\in (2.8, 3.2)$	$\in (7.3, 8.3)$
0.9	$\in (1.6, 2.0)$	$\in (4.2, 5.2)$
1.1	$\in (0.8, 1.0)$	$\in (2.1, 2.6)$
1.2	$\in (0.6, 0.8)$	$\in (1.6, 2.1)$

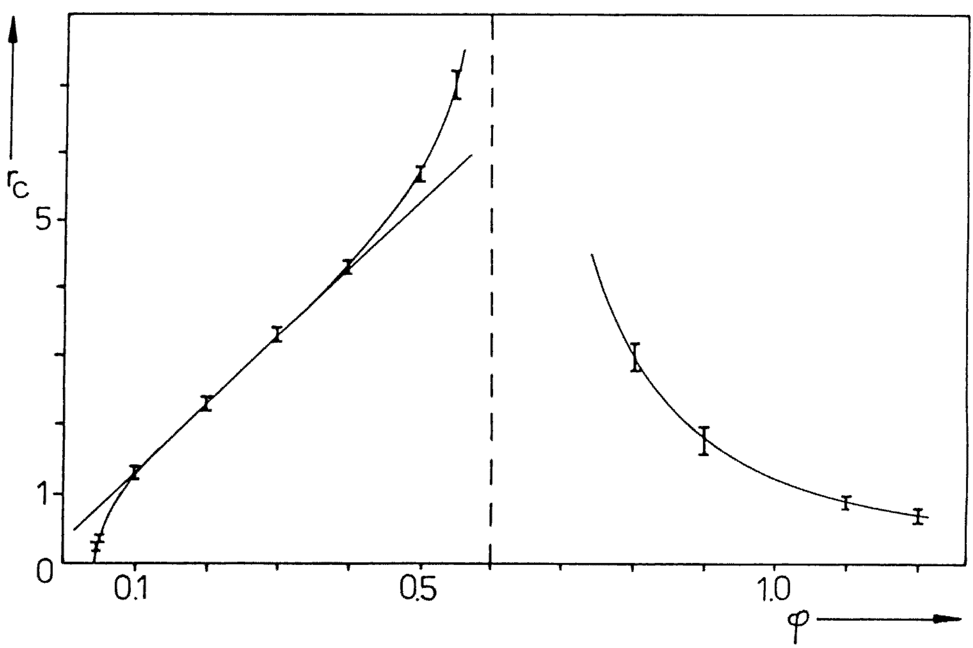

Fig. 4. Numerically determined values of critical radii r_c in dependence on φ.

6. Discussion

With φ nearby 0.6, the critical radius becomes infinite for transitions in both directions. In this case, we obtain coexistence of both phases $u_s^{(1)}$ and $u_s^{(3)}$, because we have a time-independent spatial separatrix (standing wave). We denote the corresponding flow value by φ_{coex}.

Note that for $\varphi < \varphi < \varphi_{coex}$, only transitions $u_s^{(1)} \to u_s^{(3)}$, and for $\varphi_{coex} < \varphi < \varphi_M$, only opposite transitions are possible.

The results about the magnitude of a nucleus have experimental importance if we realize the BZ system as described above. Including photosensitivity of oxygen, the reactions R1–R4 are valid if the reduction R5

$$\text{Me(ox)} + \text{organic reductants} \to \text{Me(red)} + h\,\text{Br}^- + \text{organic products} \qquad \text{R5}$$

does not release the inhibitor Br^-($h = 0$). Then the concentration of Me(ox) is not involved explicitly in the R1–R4 subset; thus it can be treated like an autonomous two-variable system as performed above.

Acknowledgements

The authors wish to thank Dr. L. Kuhnert, Dr. K.R. Schneider and Dr. K. Groeger for their interest in this work.

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