On the Brusselator Equation

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Abstract

We extend the generalized maximum principle of Lou and Ni \[1\] of elliptic equations to parabolic equations. By this result, we show that the solution of Brusselator equation has a global attractor and the size of it depends on the parameters $\alpha$, $\beta$. The "activation" and "depletion" is a well known terminology to biologists and chemists but it is not defined mathematically. According to our interpretations, we are able to show that the unique trivial steady state $(\alpha, \frac{\beta}{\alpha})$ plays the role as the threshold of initiation of this motion.

1 Introduction

The content of this article is from the author’s previous work [nee]. The Brusselator equation was introduced by Prigogine and Lefever \[1\]. It describes activation-depletion mechanism \[\] of a chemical (or biological chemical \[\], \[\]) reaction and it is a Turing system as well. This chemical reaction is an auto-catalytic reaction in which one of the reactant will generate itself as the reaction proceeds. The reaction is characterized as follows:

$$A \rightarrow X, \quad B + X \rightarrow C, \quad \cdots$$

The corresponding mathematical model is as follows:

$$
\begin{align*}
    u_t &= D\Delta u + \alpha - (1 + \beta)u + u^2v, \\
    v_t &= k\Delta v + \beta u - u^2v, \quad x \in \Omega; \\
\end{align*}
$$

with Neumann boundary condition

$$
\begin{align*}
    \frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0, \quad x \in \partial \Omega,
\end{align*}
$$

and initial data;

$$
\begin{align*}
    u_0 &= u(0, x), \\
    v_0 &= v(0, x).
\end{align*}
$$

This system attracts many researches on the subject of instability and the structure of the attractor (cf. \[\], \[\]) that induced by the parameters. In particular, You \[\] studied the existence of a global attractor for the semiflow solution of the extended Brusselator system of six equations in the $L^2$ phase space, which is a cubic-autocatalytic and partially reversible reaction-diffusion system with linear coupling between compartments. The method of grouping and re-scaling estimation is developed to prove the absorbing property and the asymptotic compactness of this reaction-diffusion systems. Furthermore, the author proved that the global attractor is an $(H, E)$ global attractor with the $L^1$ regularity and that the Hausdorff dimension and the fractal dimension of the global attractor are finite.

The behavior of the solutions is complicated because of many parameters. In revealing the behavior of the solutions, we found that the meanings of "activation" and "depletion" are not clear mathematically although they are well known terminologies for biologists or chemists. With the interpretation, we found, as Lemma 8, that the steady state $(\alpha, \frac{\beta}{\alpha})$ plays the role as the threshold of the mechanism of activation and depletion. Moreover, the occurrence of Hopf’s bifurcation then indicates the existence of time periodic solutions and thus, as lemma 8, the roles of activation and deletion change according to parameters $\alpha$ and $\beta$.

In this paper, we begin with the existence of time global solution. To this end, we first extend the generalized maximum principle of \[\] to parabolic equation. By this result, we are able to show that (1) has a global attractor and the radius of it depends on $\alpha$, $\beta$ and diffusion coefficients $D$ and $k$ as well. However, the parameters that affect the stability are $\alpha$ and $\beta$ but not the diffusion coefficients. We therefore study the asymptotic behavior corresponding to the diffusion coefficients.
2 Global Attractor

Throughout this article, \( u, v, \alpha \) and \( \beta \) stand for the concentrations of activators, substrates and other chemical substances that join the reaction, respectively. \( \lambda_i \) and \( \vartheta_j \) denote the \( i \)-th eigenvalue and the corresponding eigenfunction of \( \Delta \) on \( \Omega \) satisfying Neumann boundary conditions. To simplify the notation, we denote \( E_T = \{(x,t) | x \in \Omega \text{ and } t \in (0,T) \} \). For the purpose of completeness, we give the proof of the extended generalized maximum principle of parabolic type of equation from Lou and Ni [1].

Proposition 1 Let \( g \in C(\Omega \times (0,T) \times \mathbb{R}) \) and \( w(x,0) \geq 0 \).

(i) If \( w \in C^{2,1}(\Omega \times (0,T)) \cap C^{1,0}(\Omega \times [0,T]) \) satisfies

\[
-w_t + \Delta w + g(x,w) \geq 0 \quad \text{in } E_T, \quad \frac{\partial w}{\partial n} \leq 0, \quad \partial \Omega
\]  

and \( w(x,0) = \max_{(x,t) \in \Omega \times [0,T]} \max_{x \in \Omega \times [0,T]} w(x,t) \geq 0 \); then, \( g(x,0)w(x,0) \geq 0 \).

(ii) If \( w \in C^{2,1}(\Omega \times (0,T)) \cap C^{1,0}(\Omega \times [0,T]) \) satisfies

\[
-w_t + \Delta w + g(x,w) \leq 0 \quad \text{in } E_T, \quad \frac{\partial w}{\partial n} \geq 0, \quad \partial \Omega
\]  

and \( w(x,0) = \min_{(x,t) \in \Omega \times [0,T]} \max_{x \in \Omega \times [0,T]} w(x,t) \geq 0 \); then, \( g(x,0)w(x,0) \leq 0 \).

Proof. We will only prove (i), since (ii) can be derived similarly. Let \( (x_0,t_0) \) be an interior point of domain \( \Omega \times (0,T) \) such that \( w(x_0,t_0) = \max_{(x,t) \in \Omega \times [0,T]} w(x,t) \). From (4) \( g(x_0,t_0)w(x_0,t_0) \geq w_t(x_0,t_0) \Delta w(x_0,t_0) \geq 0 \).

To prove the case of the boundary point \( (x_0,t_0) \in \partial \Omega \times [0,T] \), we argue by contradiction (cf. [1]) and we assume that \( g(x_0,t_0)w(x_0,t_0) < 0 \) where \( w(x_0,t_0) = \max_{x \in \Omega \times [0,T]} w(x,t) \). By (4), \( g(x_0,t_0)w(x_0,t_0) + \Delta w(x_0,t_0)w(x_0,t_0) \geq w_t(x_0,t_0) \), we have \( w_t(x_0,t_0) \geq 0 \), thus, \( w \) is larger at earlier time. We derive a contradiction. Thus (i) is proved.

The behavior of the solution of (1) is complicated. However, restricting the diffusion coefficient to \( D=1 \), we can easily show that the solution has a global absorbing set in the neighborhood of the unique trivial steady state \( (0,0) \). By scaling, we can always adjust the parameter of equation (1). Without loss of generality, we study the following equations :

\[
\begin{align*}
\frac{u_t}{T} &= D \Delta u + \alpha(1+\beta)u + u^2 v \\
\frac{v_t}{T} &= \Delta v + \beta u - u^2 v \\
\end{align*}
\]

where \( x \in \Omega \).

We will discuss the asymptotic behavior of the solution due to \( D \) later. We denote

\[
F(\alpha,\beta,u,v) = \left( \frac{\alpha(1+\beta)u + u^2 v}{\beta u - u^2 v} \right). 
\]

Furthermore, we say that \( F(\alpha,\beta,u,v) \) is non-negative (non-positive) provided that each components of \( F \) is non-negative (non-positive). To derive the apriori estimate of the solution, we will start with the case that \( D=1 \) and then extend our result further to \( D \neq 0 \). We denote Banach space \( X=C(\Omega) \times C(\Omega) \) and \( B_r(p) \) to denote the ball of radius \( r \) centered at \( p \). Without loss of generality, we assume that \( \Omega \subset \mathbb{R}^d \) with \( \mu(\Omega)=1 \), where \( \mu(\cdot) \) is the measure of \( \mathbb{R}^d \).

Theorem 2 If \( u,v \in C(\Omega) \) are non-negative and the diffusion coefficient \(|D-1| \leq \varepsilon \), for some \( \varepsilon > 0 \), then (6) has a unique positive classical solution satisfying:

\[
\frac{\alpha}{1+\beta} \leq u \leq \frac{\beta(\beta+1)}{\alpha}, \quad \frac{\alpha \beta}{\alpha^2 + \beta(\beta+1)} \leq \frac{\beta(\beta+1)}{\alpha}. 
\]

Moreover, \( (u(t,x),v(t,x)) \in B_r(p) \subset X \) for all \( t \geq 0 \) where
\[
 r = \max \left\{ \frac{a \beta}{1+\beta}, \frac{\beta (\beta+1)}{a}, \frac{\beta (\beta+1)}{\alpha} \frac{\alpha}{\alpha^2 + \beta (\beta+1)} \right\} \tag{9}
\]

and \( p = (\alpha, \frac{\beta}{\alpha}) \).

Proof. We begin with \( D = 1 \), and let \( u(p_n) = \min_{\xi \in \Omega \times (0,T)} u(\xi) \); then, by (ii) of proposition 1, we have
\[
 0 \geq \alpha - (1+\beta)u(p_n) + u^2(p_n) \geq \alpha - (1+\beta)u(p_n)
\]
thus
\[
 0 \geq u(p_n) \geq \frac{\alpha}{1+\beta}. \tag{10}
\]

Let \( v(q_m) = \max_{\xi \in \Omega \times (0,T)} v(\xi) \); then, by (i) of proposition 1 and (10), we have
\[
 0 \leq v(q_m) \leq \frac{\beta (\beta+1)}{\alpha}. \tag{11}
\]

We define \( w = u + v \); then,
\[
 0 = -w_t + \Delta w + \alpha - u. \tag{12}
\]

Let \( w(r_m) = \max_{\xi \in \Omega \times (0,T)} w(\xi) \); then, by (i) of proposition 1, \( u(r_m) \leq \alpha \). Hence,
\[
 u(x,t) \leq w(x,t) \leq w(r_m) = u(r_m) + v(r_m) \leq \alpha + \frac{\beta (\beta+1)}{\alpha}. \tag{13}
\]

Let \( v(q_n) = \min_{\xi \in \Omega \times (0,T)} v(\xi) \); then, by (ii) of proposition 1, we have \( \beta u(q_n) \leq u^2(q_n) v(q_n) \). Hence,
\[
 v(x,t) \geq v(q_n) \geq \frac{\beta}{u(q_n)} \geq \frac{a \beta}{\alpha^2 + \beta (\beta+1)}. \tag{14}
\]

To attain the global solution, we let
\[
 L_D = \begin{pmatrix} D \Delta & 0 \\ 0 & \Delta \end{pmatrix},
\]
and \( U = (u,v), F(\alpha,\beta,u,v) = F(\alpha,\beta,U) \); then, (1) may rewrite as follows:
\[
 U_t = L_D U + F(\alpha,\beta,U) \tag{15}
\]

Since \( \Delta \) generates a contraction semi-group in \( C(\Omega) \), so does the direct sum \( L_D \). Thus the existence of unique local solution of equation (15) is established. By (8) and standard results of parabolic equation [], the solution of (6) is classical. Moreover, (8) implies that there is a global absorbing set in \( C^1((0,\infty),X) \cap C([0,\infty),X) \). This completes the proof.

The theorem reveals that the radius of the absorbing set depends on both the concentrations \( \alpha \) and \( \beta \). However, it is well known that the diffusion coefficient will affect the regularity of the solution. This motivates us to study the asymptotic behavior as \( D \to 0 \) in the next section.

3 The diffusion coefficient and asymptotic behavior

In previous section we explore the asymptotic behavior of the solution when \( D \) is near 1. We shall extend our result further and begin with the case when the diffusion coefficient \( D = 0 \). In this cases, equation (6) is reduced to:

\[
 \begin{cases} 
 u_t = u^2 v - (\beta+1)u + \alpha \\
 v_t = \Delta v - u v + \beta u 
 \end{cases} \quad \lambda \in \Omega; \tag{16}
\]
Lemma 3 If \(0 < u_0 < \beta + 1\) and \(u, v\) are positive then \(u\) blows up in finite time; furthermore; the solution \(v\) is bounded, \(0 \leq v < M_v\), for some constant \(M_v > 0\).

Proof. Again, we let \(X = C(\Omega) \times C(\Omega)\) and

\[
L = \begin{pmatrix}
-\beta - 1 & 0 \\
0 & \Delta
\end{pmatrix} = \begin{pmatrix}
L_1 & 0 \\
0 & L_2
\end{pmatrix}.
\]

Since \(L_1\) and \(L_2\) both generate contractive semi-groups on \(C(\Omega)\), so does \(L\). Thus the existence and uniqueness of local solution of equation (16) is established.

To show that the solution \(u\) of the first equation of (16) is unbounded, we will argue by contradiction and assume that \(u\) is bounded. In this case, we claim that \(v\) is bounded away from zero. It follows that \(v > m_v > 0\).

Furthermore, we let \(\gamma = \frac{\beta}{u(q)}\) and

\[
I_u = \int_{\Omega} u \, dx,
\]

then

\[
\frac{dI_u}{dt} = \int_{\Omega} u^2 v(\beta + 1) u \, dx \geq \int_{\Omega} u^2 v(\beta + 1) u \, dx.
\]

Let \(y(t)\) be the solution of

\[
y' = \gamma y^2 - (\beta + 1)y,
\]

then \(y\) blows-up in finite time and so does \(u\). This contradicts to our assumption that \(u\) is bounded.

By (17), \(v \geq m_v\) is bounded from below and \(v \equiv 0\) if \(\sup_{x} u = 0\). To prove that \(v\) is bounded above, we let \(v(q) = \max_{(x,t) \in E} v(x,t)\) and \(u(q) = \min_{(x,t) \in E} u(x,t)\); then, again by Proposition 1,

\[
u^2(v) v(\beta + 1) v \leq \beta u(v),
\]

thus

\[
v(q) \leq \frac{\beta}{u(q)}.
\]

Thus \(v\) is bounded from above if \(u(q) > 0\). To prove that \(u(q) > 0\), we apply the quadratic formula to the right hand side of \(u\); and by \(v\) is non-negative, we have

\[
r = \frac{(\beta + 1) \pm \sqrt{(\beta + 1)^2 - 4v^2\alpha}}{2v} > 0.
\]

The radius of the global absorbing set of \(v\) may be obtained directly from the Lyapunov function

\[
I_v = \frac{1}{2} \int_\Omega v^2 \, dx.
\]

We therefore omit the proof.
The solution \( u \) blows-up in finite time is a reasonable guess because of the nonlinearity of the reaction term, but on the contrary, blow-up occurs only when \( D=0 \).

**Lemma 4** If the diffusion coefficient \( D \neq 0 \) then the solution has a global attractor.

Proof. Let \( w = u + v \) then

\[
\frac{\partial}{\partial t} \int \omega \, dx = \int \omega \, \Delta u + \int \omega \, v + \int \omega \, \alpha.
\]

Integrating (19) over \( \Omega \) and deriving it with respect to \( t \), it yields

\[
\frac{\partial}{\partial t} \int \omega \, dx = \int \omega \, \Delta u + \int \omega \, v + \int \omega \, \alpha.
\]

By lemma 3, \( v \) is bounded therefore \( \int v \, dx \leq k \) for some constant \( k \). Let \( y(t) \) be the solution of

\[
y' = -y + k,
\]

then \( \int w \, dx \leq y \) and \( w \) has a global attractor hence \( u \) also has a global attractor.

### 4 Hopf’s bifurcation

The existence of global absorbing set leads to a nature question namely the stability of the steady states. We begin with the apriori estimate of the steady states solution of equation (1).

**Corollary 5** If \((u, v)\) is a positive steady states solution of (1) then \( \int u \, dx = \alpha \) and \( \int v \, dx \leq \frac{\beta}{\alpha'} \).

Proof. The steady states solution of equation (1) satisfies

\[
\begin{cases}
0 = D \Delta u + \alpha - (1 + \beta)u + u^2 v, \\
0 = \Delta v + \beta u - u^2 v; \\
\end{cases}
\quad x \in \Omega.
\]

The first result can be obtained directly from integrating (20). Integrating the second equation gives

\[
\int \beta u - u^2 v \, dx = 0,
\]

and the first gives

\[
\alpha - \int (\beta + 1)u - u^2 v \, dx = 0.
\]

The positivity of \( u, v \) and the Hölder inequality imply that

\[
(\int u \, dx) 12 \int v \, dx \leq \int u^2 v \, dx.
\]

Thus

\[
\int v \, dx \leq \frac{\beta}{\alpha'}.
\]

This completes the proof.

The previous results show that the steady states solution \( u \) can be written as \( \tilde{u} + \alpha \) where \( \tilde{u} \) satisfies \( \int \tilde{u} \, dx = 0 \).

The stability of steady states and the bifurcation of (\( \tilde{u} \)) can be found in many articles thus we will just give a brief proof here.
Theorem 6 The Hopf’s bifurcation of system (1) occurs at

$$\mu_j = \lambda_j \frac{\alpha^2 - \beta + 1 \pm \sqrt{(\alpha^2 - \beta + 1)^2 - 4\alpha^2}}{2D}. \quad (24)$$

The steady state is stable if $\alpha^2 < \beta - 1$ and unstable otherwise. In particular, Hopf’s bifurcation occurs if $\beta = \alpha^2 + 1$.

Proof. Linearizing (1) at $(\alpha, \frac{\beta}{\alpha})$ yields the following linear equations:

$$0 = D \Delta u + (\beta - 1)u + \alpha^2 v \quad (25)$$
$$0 = \Delta v - \beta u - \alpha^2 v.$$

Let

$$L = \begin{pmatrix} \beta - 1 & \alpha^2 \\ -\beta & -\alpha^2 \end{pmatrix};$$

then, the eigenvalue $\mu_j$ satisfies (24).

Note that for fixed $\alpha$, $\frac{d\mu_j}{d\beta} \neq 0$ and

$$(\alpha^2 - \beta + 1)^2 - 4\alpha^2 = (\alpha^2 - 1 - \beta)^2 - 4\beta.$$

Therefore, Hopf’s bifurcation occurs when $\beta = \alpha^2 - 1$.

5 The parameters and the behavior of the solution

In this section, we will first demonstrate how the parameters $\alpha, \beta$ and the behavior of the concentration of the substance are related. Without loss of generality, we assume $|\Omega|=1$ where $|\Omega|$ is the measure of domain $\Omega$. To clarify the terminologies "activation" and "depletion", we give the definition as follows:

Definition 7 A substance $u$ is activated if the concentration $\int_\Omega u \, dx$ of the corresponding substance is increasing; and depleted if its concentration is decreasing.

We denote by

in particular, $\phi_0(x) = 1$ and $\lambda_0 = 0$ and $\phi_j$ be the $j$th eigenfunction of Laplace with Neumann boundary condition.

Lemma 8 If $(u, v)$ is a positive solution of equation (1) then the following is true:

(i) If $\alpha \geq u, \beta \leq v$ then $\frac{dU}{dt} \geq 0$ and $\frac{dV}{dt} \leq 0$.

(ii) If $\alpha \leq u, \frac{\beta}{\alpha} \geq v$ then $\frac{dU}{dt} \leq 0$ and $\frac{dV}{dt} \geq 0$.

Proof. Multiplying $\phi_j$ to (1) and integrating over $\Omega$ yields

$$\begin{cases} 
\frac{dU_j}{dt} = \int_\Omega [\alpha(\Delta u + \beta + 1)u + u^2 v] \phi_j(x) dx \\
\frac{dV_j}{dt} = -\int_\Omega \beta u - u^2 v \phi_j(x) dx \end{cases}. \quad (26)$$

For $j=1$, the first equation of (26) satisfies
\[
\frac{dU_i}{dt} = \int_\Omega (\alpha - u) - \beta u + u^2 v dx
\]
(27)

Thus \(\alpha, V_{1t},\) and \(U_{1t}\) are related to each other.

Next, we will show that \(V_1\) is controlled by \(\beta\). Inserting inequality (23) to the second equation of (26) yields

\[
\frac{dV_1}{dt} \leq \left( \frac{\beta}{V_1} - 1 \right) \int_\Omega u^2 v dx.
\]

Thus \(v \geq \beta\) implies \(\frac{dV_1}{dt} \leq 0\) and hence \(\frac{dU_1}{dt} \geq 0\).

On the other hand, if \(\alpha < u\) then (27) implies that

\[
\frac{dU_1}{dt} \leq -\frac{dV_1}{dt}.
\]

From the second equation of (26) we have

\[
\frac{dV_1}{dt} \geq \int_\Omega u(\beta - av) dx.
\]

Thus if \(\frac{\beta}{a} > v\) then

\[
\frac{dV_1}{dt} \geq 0.
\]

The proof is completed.

From the previous lemma, we see how the parameters affect the behavior of the solution \(u, v\). In fact, the next result reveals the asymptotic behavior of the solution.

**Lemma 9** \((U_j, V_j) \to (0, 0)\) as \(j \to 1\).

Proof. For \(j > 1\), multiplying \(\varphi_j\) to (1) and integrating over \(\Omega\), we have

\[
\begin{cases}
\frac{dU_j}{dt} &= -(D\lambda_j + \beta + 1)U_j + \int_\Omega u^2 v \varphi_j(x) dx \\
\frac{dV_j}{dt} &= -\lambda_j V_j + \beta U_j - \int_\Omega u^2 v \varphi_j(x) dx
\end{cases}
\]
(28)

Let \(f_j(t) = \int_\Omega u^2 v \varphi_j(x) dx\); then, \(U_j, V_j\) has closed form

\[
\begin{align*}
U_j &= U_0 e^{-At} \int_0^t f_j(s) ds \\
V_j &= V_0 e^{-\lambda_j t} \int_0^t U_j(s) - f_j(s) ds
\end{align*}
\]
(29)

where \(A = D\lambda_j + \beta + 1\). By theorem 2, \(f_j\) is bounded. Therefore, \(U_j, V_j \to 0\) as \(t \to \infty\).
To the author’s knowledge, there are still many open problems involving this system of equations. For example, the structure of the blow-up set is not clear when $D=0$.

References