TRAVELING WAVES IN QUADRATIC AUTOCATALYTIC SYSTEMS WITH COMPLEXING AGENT

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Abstract. The quadratic autocatalytic reaction forms a key step in a number of chemical reaction systems, and traveling waves are observed in such systems. In this study, we investigate the effect of complexation reactions on traveling waves in the quadratic autocatalytic reaction system. More precisely, under the assumption that the complexation reaction is fast relative to the autocatalytic reaction, we show that the governing system is reduced to a two-component reaction-diffusion system with density-dependent diffusivity. Further, the numerical evidence suggests that for some parameter values, a traveling wave solution of this reduced two-component system is nonlinearly selected. This is contrast to that associated with the quadratic autocatalytic reaction (without complexation reactions).

Dedicated to Prof. Sze-Bi Hsu in appreciation of his inspiring ideas

1. Introduction. In this paper, we consider the model based on the quadratic autocatalytic step with complexation reactions

\[ \begin{align*}
A + B & \rightarrow 2B \quad \text{(rate: } k_0ab; \text{ autocatalysis step),} \\
S + B & \rightleftharpoons SB \quad \text{(rates: forward, } k^+sb; \text{ backward, } k^-c; \text{ complexation step).} 
\end{align*} \tag{1.1} \]

Here \( a, b, s \) and \( s \) are the concentrations of the reactant A, the autocatalyst B, the complexing agent S, and the complex SB, respectively, and \( k_0, k^+ \) and \( k^- \) are reaction rate constants. (1.1a) is the well-known quadratic reaction [1, 2], while the complexation reaction step (1.1b) indicates that the autocatalyst B undergoes the reaction with the complexing agent S to form the complex SB. The purpose of this paper is to study the effect of complexation reactions on the dynamics of the quadratic autocatalytic system, in particular the formation of traveling waves.

The governing equation

We first follow Merkin and Ševčíková [7] (also see [6, 8]) to state the governing equations associated with the reaction scheme (1.1). Let \( a, b, s \) and \( c \) be the
concentrations of A, B, S, and SB, respectively. Then the reaction-diffusion system corresponding to the reaction scheme (1.1) reads as follows:

\[
\begin{align*}
  a_t &= d_A a_{xx} - k_0 ab, \\
  b_t &= d_B b_{xx} + k_0 ab - (k^+ sb - k^- c), \\
  c_t &= (k^+ sb - k^- c), \\
  s + c &= \bar{S}_0.
\end{align*}
\]

(1.2)

Here \(d_A\) and \(d_B\) are the diffusion coefficients of A and B, respectively. The complex \(SB\) is assumed to have zero diffusivity since it is in general a large molecule. The final equation of system (1.2) represents the conservation of the complexing agent \(S\) with uniform initial concentration \(\bar{S}_0\). Following Merkin and Ševčíková [7], we assume that the reactant A is initially at uniform concentration and the catalyst B is locally introduced into the system. Hence the initial condition for (1.2) is given by

\[
\begin{align*}
  a(\cdot, 0) &= a_{ini}, \\
  b(\cdot, 0) &= b_{ini}p(\cdot), \\
  s(\cdot, 0) &= \bar{S}_0, \\
  c(\cdot, 0) &= 0
\end{align*}
\]

where \(a_{ini}\) and \(b_{ini}\) are constants, and \(p\) is a smooth function with compact support.

Now, introduce dimensionless quantities

\[
\begin{align*}
  \tilde{t} &= (k_0a_{ini})t, \\
  \tilde{x} &= \sqrt{\frac{k_0a_{ini}}{d_A}}x, \\
  d = \frac{d_B}{d_A}, \\
  \alpha &= \frac{k^-}{k_0a_{ini}}, \\
  K &= \frac{k^+ a_{ini}}{k^-}, \\
  S_0 &= \frac{\bar{S}_0}{a_{ini}}.
\end{align*}
\]

Then the original system (1.2) is transformed into the following system (dropping the bars for simplicity):

\[
\begin{align*}
  \begin{cases}
    a_t &= a_{xx} - ab, \\
    b_t &= d b_{xx} + ab - \alpha(K sb - c), \\
    c_t &= \alpha(K sb - c), \\
    s + c &= S_0,
  \end{cases}
\end{align*}
\]

(1.3)

with the initial data

\[
\begin{align*}
  a(\cdot, 0) &= 1, \\
  b(\cdot, 0) &= \frac{b_{ini}}{a_{ini}}p(\cdot), \\
  s(\cdot, 0) &= S_0, \\
  c(\cdot, 0) &= 0.
\end{align*}
\]

(1.4)

Merkin and Ševčíková [7] numerically showed that the solution of the initial problem (1.3)-(1.4) will evolve into a pair of diverging waves which propagate outward from the initial reaction zone. Due to the symmetry, we concentrate here only on the wave traveling to the right.

We give the definition of traveling wave solutions of (1.3). Thus, a traveling wave solution of system (1.3) is a nonnegative solution of system (1.3) of the form

\[
(\sigma(x, t), b(x, t), c(x, t)) = (A(z), B(z), C(z)), \quad z = x - vt,
\]

with \(v\) being the velocity of the wave. We also assume that

\[
(A(\cdot), B(\cdot), C(\cdot)) \to 0 \quad \text{for } z \to \pm \infty.
\]

Upon substituting the ansatz on \((A, B, C)\) into (1.3), we are led to the governing system for \((A, B, C)\) as follows:
\[
\begin{align*}
&A_{zz} + v A_z - AB = 0, \\
&dB_{zz} + v B_z + AB - \alpha (KSB - C) = 0, \\
&vC_z + \alpha (KSB - C) = 0, \\
&S + C = S_0,
\end{align*}
\] (1.5a)-(1.5d)

with the boundary condition

\[
(A, B, C)(-\infty) = (0, b_*, c_*), \quad (A, B, C)(+\infty) = (1, 0, 0),
\] (1.6)

where \(b_*\) and \(c_*\) are positive constants satisfying

\[
b_* + c_* = 1. \tag{1.7}
\]

We remark that the boundary condition for \((A, B, C)\) at \(+\infty\) is motivated by the initial data (1.4). Next, the condition \(b_* + c_* = 1\) can be obtained by adding the equations (1.5a)-(1.5c) and by integrating over \(\mathbb{R}\), which leads to the equality

\[
v(1 - b_*) - vc_* = 0.
\]

Remark: In fact, in [6, 7] a general family of autocatalysis reaction is considered with the reaction speed proportional to \(ab^n\) with \(n \geq 1\). In the case \(n > 1\), however, the linearization matrix at \((a, b) = (1, 0)\) is degenerated, so the theory of exponential dichotomy exploited in this paper cannot be straightforwardly used.

Fast complexation reaction

In general, complexation reaction are very fast as compared with the other reactions in the reaction system. Further, if the complexation reaction (1.1b) is very fast compared to the reaction (1.1a), its effect on the dynamics of (1.3) can be analyzed more simply. To see this, we formally derive a reduced system of (1.3). Indeed, if \(\alpha\) is very large, then the complexation reaction is in chemical equilibrium, that is,

\[
KSB - c = 0,
\]

which, with \(s + c = S_0\), gives

\[
c = \frac{\sigma b}{1 + K b}, \quad s = \frac{S_0}{1 + K b}, \tag{1.8}
\]

where \(\sigma = KS_0\). It then follows that

\[
b_t + c_t = \left(1 + \frac{\sigma}{(1 + K b)^2}\right)b_t := \frac{1}{g(b)} b_t.
\]

Combining this equation with (1.3) leads to the following reduced system

\[
\begin{align*}
\left\{ 
& a_t = a_{xx} - ab, \\
& \frac{1}{g(b)} b_t = db_{xx} + ab,
\end{align*}
\] (1.9)

with the initial data

\[
a(\cdot, 0) = 1, \quad b(\cdot, 0) = \frac{b_{ini}}{a_{ini}} p(\cdot). \tag{1.10}
\]

Here \(a_{ini}\), \(b_{ini}\), and \(p\) are defined as before.

Now, a traveling wave solution of system (1.9) is a nonnegative solution of system (1.9) of the form

\[
(a(x, t), b(x, t)) = (A(z), B(z)), \quad z = x - vt,
\]
with \( v \) being the velocity of the wave. Upon substituting the ansatz on \((A, B)\) into (1.9), we are led to the governing system for \((A, B)\) as follows:

\[
\begin{align*}
A_{zz} + vA_z - AB &= 0, \\
\frac{dB_{zz}}{g(B)} + vB_z + AB &= 0,
\end{align*}
\]

with the boundary condition

\[
(A, B)(-\infty) = (0, b_s), \quad (A, B)(+\infty) = (1, 0),
\]

where \( b_s \) is the unique positive root of the quadratic polynomial

\[
Q(b) := Kb^2 + (1 + \sigma - K)b - 1 = 0.
\]

To see that \( b_s \) is a zero of \( Q(b) \), one can use the condition (1.7) and the first equality in (1.8), from where, upon identifying \( b_s \) with \( b_s \), we obtain the equation \( Q(b_s) = 0 \). We also remark that when \( \sigma = 0 \), the traveling wave problem (1.11)-(1.12) corresponds to that for the quadratic autocatalytic reaction without complexation reactions. The traveling wave solutions for the latter case has been well studied [1, 2, 10].

**Outline of the paper**

The purpose of this paper is to show that for large \( \alpha \), a solution of traveling wave problem (1.5)-(1.6) is approximated well by that of traveling wave problem (1.11)-(1.12). This will be done in Sec. 2, and the result is given in Theorem 1. In Sec. 3, we will numerically argue that traveling waves of (1.9) are nonlinearly selected. In other words, for some parameter values, the minimal speed of traveling waves of (1.9) is larger than that determined by the linearized system of (1.11) around the unstable equilibrium \((1, 0)\). We make a crucial remark about this result. When \( \sigma = 0 \) which is equivalent to the absence of the complexation reaction step (1.1b), system (1.9) is reduced to the system determined by the quadratic reaction step (1.1a). It is known [1, 2] that a traveling wave solution of the system associated with the quadratic reaction step (1.1a) is always linearly selected. So the numerical evidence in Sec. 3 suggests that the complexation reaction step (1.1b) can have a significant effect on the dynamics of the system associated with the quadratic reaction step (1.1a).

2. **Traveling waves of system (1.3) with fast complexation reaction.** In this section, we discuss how to relate a solution of traveling wave problem (1.5)-(1.6) to that of traveling wave problem (1.11)-(1.12). For the reader’s convenience, we restate the traveling wave problem (1.5)-(1.6) as follows:

\[
\begin{align*}
\alpha'' + va' - ab &= 0, \\
db'' + vb' + ab - \alpha(Ksb - c) &= 0, \\
v'c + \alpha(Ksb - c) &= 0,
\end{align*}
\]

with the boundary conditions

\[
(a, b, c)(-\infty) = (0, b_s, c_s) \text{ and } (a, b, c)(+\infty) = (1, 0, 0),
\]

where for some \( S_0 > 0 \), \( s \) and \( c \) are subject to an additional constraint

\[
s + c = S_0,
\]
and the prime denotes the differentiation with respect to \( z \). Recall that \( b_s \) is the root of the following quadratic equation

\[
K b_s^2 + (1 + KS_0 - K)b_s - 1 = 0. \tag{2.4}
\]

Note that the boundary conditions for \( c \) at \( z = \pm \infty \) follows from those for \( b \) at \( z = \pm \infty \), and (2.1c) and (2.3).

### 2.1. A transformed system.

To see the relation between the problems (1.5)-(1.6) and (1.11)-(1.12), we first reformulate (1.5)-(1.6).

To proceed, set

\[ \eta = Ksb - c = KS_0b - (1 + Kb)c \]

where the second equality is obtained using the identity \( s + c = S_0 \). It follows from (2.5) and (2.2) that

\[ \eta(-\infty) = \eta(\infty) = 0. \tag{2.6} \]

Now, we represent the variable \( c \) in term of \( \eta \) and \( b \) in system (2.1). It follows from Eq. (2.5) that for \( \sigma = KS_0 \) we have

\[ c = \frac{\sigma b}{1 + Kb} - \frac{\eta}{1 + Kb}. \tag{2.7} \]

and hence that

\[ c' = \frac{\sigma b'}{(1 + Kb)^2} - \frac{\eta'}{1 + Kb} + \frac{K\eta}{(1 + Kb)^2}b'. \tag{2.8} \]

It follows that (2.1c) can be rewritten as

\[ -v \frac{\eta'}{1 + Kb} + \alpha \eta + \Phi_3(b, b', \eta) = 0, \tag{2.9} \]

where

\[ \Phi_3(b, b', \eta) := v \left( \frac{\sigma}{(1 + Kb)^2} + \frac{K\eta}{(1 + Kb)^2} \right)b'. \]

Using (2.8), and summing (2.1b) and (2.1c), we obtain the following equation for \( b \)

\[ db'' + v(b' + c') + ab = db'' + v \left( 1 + \frac{\sigma}{(1 + Kb)^2} \right)b' + ab + \Phi_20(b, b', \eta, \eta') = 0, \]

where

\[ \Phi_20(b, b', \eta, \eta') = -v \left( \frac{\eta}{1 + Kb} \right)' \tag{2.10} \]

As a result, we arrive at the following system of equations for \( a, b \), and \( \eta \):

\[
\begin{align*}
\alpha'' + \alpha' - ab &= 0, \tag{2.11a} \\
\frac{db''}{v \left( 1 + \frac{\sigma}{(1 + Kb)^2} \right)} b' + ab + \Phi_20(b, b', \eta, \eta') &= 0, \tag{2.11b} \\
-v \frac{\eta'}{1 + Kb} + \alpha \eta + \Phi_3(b, b', \eta) &= 0. \tag{2.11c}
\end{align*}
\]

In the formal asymptotic approximation, i.e. assuming \( \alpha = \infty \), Merkin and Ševčiková [7] neglect the term \( \Phi_20 \) in (2.11b), and do not take into account the
third equation, as in this limit \( \eta \equiv 0 \). In this approximation, one obtains a system for \( a = a_0 \) and \( b = b_0 \):

\[
\begin{align*}
\frac{d^2 a_0'}{dx^2} + va_0' - a_0b_0 &= 0, \\
\frac{db_0'}{dx} + \left(1 + \frac{\sigma}{(1 + Kb_0)^2}\right)b_0' + a_0b_0 &= 0.
\end{align*}
\] (2.12)

In [7], the numerical solutions for \( a_0 \) and \( b_0 \) have been found in the form of heteroclinic profiles, with \( a_0(\cdot) \) increasing and \( b_0(\cdot) \) decreasing. These profiles correspond to travelling wave solutions propagating with the speed \( v > 0 \).

2.2. **Use of the implicit function theorem.** Assuming the existence of heteroclinic solutions to system (2.12), we will use the implicit function theorem to prove that, for \( \alpha \) sufficiently large, the heteroclinic solutions to system (2.12) also exist and are continuous functions of the parameter \( \alpha^{-1} \). Due to technical reasons \( \alpha^{-1} \) will be denoted in the sequel by \( \varepsilon^2 \).

Recall a version of the implicit function theorem.

**Theorem A.** ([3, Theorem 2.3]) Suppose \( \Lambda, H, Z \) are Banach spaces, \( L \subset \Lambda, U \subset H \) are open sets, \( F : L \times U \to Z \) is continuously differentiable with respect to \( h, (\lambda_0, h_0) \in L \times U, F(\lambda_0, h_0) = 0 \) and \( D_h F(\lambda_0, h_0) \) has a bounded inverse. Then there is a neighborhood \( L_1 \times U_1 \subset L \times U \) of \((\lambda_0, h_0)\) and a function \( f : L_1 \to U_1 \), \( f(\lambda_0) = h_0 \) such that \( F(\lambda, h) = 0 \) for \((\lambda, h) \in L_1 \times U_1 \) if and only if \( h = f(\lambda) \). If additionally \( F \in C^k(\Lambda \times U, Z) \), \( k \geq 1 \), then \( f \in C^k(L_1, U_1) \).

Let us start from the analysis of the properties of (2.11c). Define

\[
q(\xi) = \frac{\alpha}{v}(1 + Kb(\xi)) + \frac{Kb'(\xi)}{1 + Kb(\xi)}
\] (2.13) and

\[
f(\xi) = -\frac{\sigma b'(\xi)}{1 + Kb(\xi)}.
\] (2.14)

(2.11c) can rewritten in the form:

\[
\eta'' - q(\xi)\eta + f = 0.
\] (2.15)

Using the method of variation of constants, we can write the general solution to (2.15) as

\[
\eta_*(\xi) = -\int_0^\xi \exp \left(\int_0^t q(\mu)\,d\mu\right) f(t)\,dt + \tilde{C} \exp \left(\int_0^\xi q(\mu)\,d\mu\right).
\] (2.16)

It is seen from (2.13) that for a given function \( b(\cdot) \) such that \( 1 + Kb(\cdot) > K_b > 0 \) for all \( \xi \in \mathbb{R} \), \( b'(\xi) \) uniformly bounded in \( \mathbb{R} \), and \( q(\xi) > q > 0 \) for \( \xi \in \mathbb{R} \). Next, supposing that \( b'(\xi) \to 0 \) for \( \xi \to \pm\infty \), we conclude that \( f(\xi) \to 0 \) for \( \xi \to \pm\infty \), so by taking

\[
\tilde{C} = \int_0^\infty \exp \left(\int_0^t q(\mu)\,d\mu\right) f(t)\,dt,
\]
we obtain a candidate for a solution to Eq. (2.15) satisfying the boundary conditions (2.6):

\[
\eta_*(\xi) = \exp \left(\int_0^\xi q(\mu)\,d\mu\right) \left[\int_0^\infty \exp \left(\int_0^t q(\mu)\,d\mu\right) f(t)\,dt\right]
\]
Proof. Consider the case $\xi \to \infty$. Then
\[
\left| \int_\xi^\infty \exp\left( - \int_\xi^t q(\mu) \, d\mu \right) f(t) \, dt \right| \leq \int_\xi^\infty \exp\left( - \int_\xi^t q(\mu) \, d\mu \right) |f(t)| \, dt \leq \frac{1}{\xi} \quad \forall \xi \to \infty.
\]
(2.18)

Now suppose that $\xi \to -\infty$. We have $\int_\xi^\infty = \int_{\xi/2}^\infty + \int_{\xi/2}^\infty$, hence denoting $\sup_{t \in (\xi, \infty)} |f(t)|, |f|^* = \sup_{t \in R} |f(t)|$, we conclude that
\[
\left| \int_\xi^\infty \exp\left( - \int_\xi^t q(\mu) \, d\mu \right) f(t) \, dt \right| \leq \exp\left( - \int_{\xi/2}^\infty q(\mu) \, d\mu \right) \int_{\xi/2}^\infty \exp\left( - \int_{\xi/2}^t q(\mu) \, d\mu \right) |f|^* \, dz
\]
\[
+ \int_{\xi/2}^\infty f(\xi) \exp\left( - \int_\xi^t q(\mu) \, d\mu \right) dt \leq \frac{1}{\xi} \left( \exp(-q(\xi)/2)|f|^* + f(\xi) \right).
\]
(2.19)

To prove the second part, we allow $\xi$ to tend to $\pm \infty$ in Eq. (2.15). Let $\xi \to -\infty$. Then
\[
|\eta'(\xi)| \leq q(\xi)|\eta(\xi)| + |f(\xi)| \leq \frac{q(\xi)}{\alpha} \left( \exp(-q(\xi)/2)|f|^* + f(\xi) \right),
\]
which shows that $\eta'(\xi) \to 0$ for $\xi \to -\infty$. Similarly, we show that $\eta'(\xi) \to 0$ for $\xi \to \infty$.

Let
\[
\tilde{q}(\xi) := \frac{q(\xi)}{\alpha} = \frac{1}{v} (1 + Kb(\xi)) + \frac{1}{\alpha} \frac{Kb'(\xi)}{1 + Kb(\xi)}.
\]
In fact, $\tilde{q}$ is also a function of $\alpha$, but we will denote this dependence explicitly below.

Lemma 2.2. Suppose that $\tilde{q}(\xi) > \tilde{q} > 0$ for $\xi \in \mathbb{R}$ and that $\|\tilde{q}\|_{C^1(\mathbb{R})} \leq C_q$, where $C_q$ does not depend on $\alpha$ for $\alpha \to \infty$. Suppose also that $\|f\|_{C^1(\mathbb{R})} < C_f$. Then
\[
\|\eta\|_{B_1} \leq \frac{1}{\alpha} C(\tilde{q}, f),
\]
(2.20)

where $C(\tilde{q}, f)$ does not depend on $\alpha$.

Proof. Let us note that $\tilde{q} = v^{-1}(1 + Kb) + O(\alpha^{-1})$ and $\eta$ satisfies the equation:
\[
\eta' - \alpha \tilde{q}(\xi) \eta + f = 0.
\]
(2.21)

As $\eta$ given by (2.17) is bounded and $\eta(\pm \infty) = 0$, it follows that there must exist $\xi_0 \in \mathbb{R}$, where $\eta(\xi_0) = 0$ and $\eta(\cdot)$ attains a (global) extremum. Thus
\[
\|\eta\|_{B_0} = |\eta(\xi_0)| = \frac{1}{\alpha} \left| \frac{f(\xi_0)}{\tilde{q}(\xi_0)} \right| \leq \frac{1}{\alpha} \left\| \frac{f}{\tilde{q}} \right\|_{B_0}.
\]
(2.22)

Taking the derivative of the left hand side of (2.21), we have
\[
\eta' - \alpha \tilde{q}' \eta - \alpha \tilde{q} \eta' + f' = 0,
\]
and so
\[ \eta_*' = \frac{\eta_*'}{\alpha q} - \tilde{q}\eta_*' + \frac{f'}{\alpha q}. \] (2.23)

As \( \eta_*'(\pm\infty) = 0 \), we can use the same arguments as in the case of \( \eta_* \), to conclude that there must exist \( \xi_1 \in \mathbb{R} \), such that \( \eta_*''(\xi_1) = 0 \) and \( \eta_*' \) attains a global extremum. Therefore
\[
\|\eta_*'\|_{B_0} = |\eta_*'(\xi_1)| = \left| \frac{\eta_*''(\xi_1)}{\alpha q(\xi_1)} - \frac{\tilde{q}(\xi_1)\eta_*'(\xi_1)}{\alpha q(\xi_1)} + \frac{f'(\xi_1)}{\alpha q(\xi_1)} \right|
\leq \left| \frac{\tilde{q}(\xi_1)\eta_*'(\xi_1)}{\alpha q(\xi_1)} \right| + \left| \frac{f'(\xi_1)}{\alpha q(\xi_1)} \right|
\leq \frac{1}{\alpha} \left( \left\| \frac{\tilde{q}}{q} \right\|_{B_0} \cdot \left\| \frac{f}{\tilde{q}} \right\|_{B_0} + \left\| \frac{f'}{\tilde{q}} \right\|_{B_0} \right),
\]
from which (2.20) follows. \( \square \)

We have thus shown that, if the functions \( b(\cdot) \in C^2(\mathbb{R}) \) satisfy the condition
\[ 1 + Kb(\xi) > K_0 > 0, \] (2.25)
then for
\[ \varepsilon^2 := \frac{1}{\alpha}, \] (2.26)
(2.11c) can be written in the form
\[ \eta(\xi) - \varepsilon^2 S(\varepsilon^2; b, b')(\xi) = 0, \] (2.27)
where
\[ S(\varepsilon^2; b, b')(\xi) := \varepsilon^{-2} \eta(\xi) = \varepsilon^{-2} \int_\xi^\infty \exp \left( - \int_t^\infty \varepsilon^{-2} \tilde{q}(\mu) d\mu \right) f(t) dt, \] (2.28)
with \( q(\xi) \) and \( f(\xi) \) replaced via (2.13) and (2.14).

Below we will use the implicit function theory in appropriate Banach spaces to show that for \( \alpha < \infty \) but sufficiently large, we can find solutions \( (a(\cdot; \alpha), b(\cdot; \alpha), \eta(\cdot; \alpha)) \) (depending on the parameter \( \alpha \)) to system (2.11), such that \( (a(\cdot; \alpha), b(\cdot; \alpha), \eta(\cdot; \alpha)) \to (a_0, b_0, 0) \) as \( \alpha \to \infty \) and such that \( (a(\pm\infty; \alpha), b(\pm\infty; \alpha)) \) satisfy the boundary conditions (2.2). Since system (2.12) is autonomous, if \( (a_0(\xi), b_0(\xi)) \) is a solution, then \( (a_0(\xi + \xi_0), b_0(\xi + \xi_0)) \) is also a solution for any \( \xi_0 \in \mathbb{R} \). So we can choose \( \xi_0 \) in such a way that
\[ a_0(0) = \frac{a_0(-\infty) + a_0(\infty)}{2}. \]
Such a condition will be also imposed on the solutions to system (2.1) for finite \( \alpha \), i.e. we assume that
\[ a(0) = \frac{a(-\infty) + a(\infty)}{2}. \] (2.29)

For \( b(\cdot) \) satisfying condition (2.25), in view of (2.27), system (2.11) can be written as
\[
\begin{cases}
\alpha'' + va' - ab = 0, \\
\left( 1 + \frac{\sigma}{1 + K b^2} \right) b' + ab + \varepsilon^2 \Phi_{20}(b, b', \eta, \eta') = 0,
\end{cases}
\] (2.30a)
(2.30b)
\[ \eta(\xi) - \varepsilon^2 S(\varepsilon^2; b(\xi), b'(\xi)) = 0, \] (2.30c)
where $S$ is defined in (2.28). Let us recall that by Lemma 2.2 $S$ stays bounded in the $C^3(\mathbb{R})$ norm as $\varepsilon \to 0$ for all $b$ bounded in the $C^2(\mathbb{R})$ norm and satisfying the condition (2.25) (see also [4]).

By integrating the sum of (2.30a) and (2.30b) from $-\infty$ to $z$, we arrive at the system

$$
\begin{aligned}
\begin{cases}
a'' + va' - ab = 0, \\
(a + db)' + v(a + b) - vb_s - \frac{v\sigma}{K}\left(\frac{1}{1 + Ka} \frac{1}{1 + Kb}ight) + \varepsilon^2\int_{-\infty}^{z} \Phi_2 d\xi = 0, \\
\eta(\xi) - \varepsilon^2 S(\varepsilon^2; b, b')(\xi) = 0.
\end{cases}
\end{aligned}
$$

(2.31a)

(2.31b)

(2.31c)

Assuming that $a(-\infty) = 0$, we obtain from (2.31b) that $b(-\infty) = b_s$. Next, taking into account (2.10) and (2.6) and supposing that $b(\infty) = 0$, we infer that $a(\infty) = 1$ only if $b_s$ is defined as a solution to Eq. (2.4). It thus follow that if $a(-\infty) = 0$ and $b(\infty) = 0$, then $b(-\infty) = b_s$ and $a(\infty) = 1$.

To have the boundary conditions preserved under the perturbation, we will define:

$$
a =: a_0 + a, \quad b =: b_0 + b,
$$

(2.32)

and consider the system of equations:

$$
\begin{aligned}
\begin{cases}
(a_0 + a)' + v(a_0 + a)'(b_0 + b) = 0, \\
((a_0 + a) + d(b_0 + b)' + v((a_0 + a) + (b_0 + b)) - vb_s - \frac{v\sigma}{K}\left(\frac{1}{1 + Ka} \frac{1}{1 + Kb}ight) + \varepsilon^2\int_{-\infty}^{z} \Phi_2 d\xi = 0, \\
\eta(\xi) - \varepsilon^2 S(\varepsilon^2; b_0 + b, b_0 + b')(\xi) = 0.
\end{cases}
\end{aligned}
$$

(2.33a)

(2.33b)

(2.33c)

Let us emphasize that as $a(-\infty) = a_0(-\infty) = 0$ and $a(\infty) = a_0(\infty) = 1$, we have $\hat{a}(-\infty) = \hat{a}(\infty) = 0$. Hence it follows from (2.29) that

$$
\hat{a}(0) = 0.
$$

(2.34)

We can thus define the solutions to system (2.33) as zeros of the mapping

$$
\hat{F}(\varepsilon, \hat{a}, \hat{b}, \eta) = F^\varepsilon(\hat{a}, \hat{b}, \eta) = \left(F^\varepsilon_1(\hat{a}, \hat{b}, \eta), F^\varepsilon_2(\hat{a}, \hat{b}, \eta), F^\varepsilon_3(\hat{a}, \hat{b}, \eta)\right),
$$

(2.35)

where $F^\varepsilon_1(\hat{a}, \hat{b}, \eta)$ and $F^\varepsilon_3(\hat{a}, \hat{b}, \eta)$ are equal to the left hand sides of (2.33a) and (2.33b), respectively, and $F^\varepsilon_3(\hat{a}, \hat{b}, \eta)$ is equal to the left hand side of (2.30c). We choose $\varepsilon \in \mathbb{R}$, $\hat{a} \in B_{20}$, $\hat{b} \in B_2$, $\eta \in B_1$, and $F^\varepsilon_1 : \mathbb{R} \times B_{20} \times B_2 \times B_1 \mapsto B_0$, $F^\varepsilon_2 : \mathbb{R} \times B_{20} \times B_2 \times B_1 \mapsto B_1$, and $F^\varepsilon_3 : \mathbb{R} \times B_{20} \times B_2 \times B_1 \mapsto B_2$. To satisfy the condition (2.34), we impose the condition $\hat{a}(0) = 0$ on functions belonging to the space $B_{20}$. Note, that we have moved the position of the variable $\varepsilon$ to the upper index to emphasize that it plays the role of a parameter.

As the spaces $B_i$, $i = 0, 1, 2$, we choose the spaces of $i$-th times differentiable functions defined on $\mathbb{R}$ with well defined limits at $\pm \infty$ equal to 0, and with well
defined limits of the derivatives (for \( i = 1, 2 \)) equal to 0. To be more precise, we adopt the following definition.

**Definition 1.** Let \( B_i(\mathbb{R}) \subseteq C^i(\mathbb{R}), \ i = 0, 1, 2 \), denote the space of functions \( u : \mathbb{R} \rightarrow \mathbb{R} \) such that:

1. \( \lim_{\xi \to \pm \infty} u(\xi) \) exists and are equal to 0;
2. \( \lim_{\xi \to \pm \infty} u^{(j)}(\xi) = 0 \) for \( 1 \leq j \leq i, \ i = 1, 2. \)

Then the space \( B_i, i = 0, 1, 2, \) is a Banach space under the norm:

\[
\|u\|_{B_i} := \sum_{k=0}^{i} \sup_{\xi \in \mathbb{R}} |u^k(\xi)|.
\]

Let \( B_{i0} \subseteq B_i \) denote the space of functions \( u : \mathbb{R} \rightarrow \mathbb{R} \) such that:

\[
u(0) = 0.\]  

(2.36)

**Remark** It is seen from the explicit form of the components of \( \hat{F} \) together with the analysis carried out in Lemmata 2.1 and 2.2 that the mapping (2.35) is well defined in some neighbourhood of the point \((\varepsilon, \tilde{a}, \tilde{b}, \eta) = (0, 0, 0, 0)\). It can be determined as the set

\[
\{\varepsilon : \varepsilon \in (-\varepsilon_0, \varepsilon_0)\} \times \left\{\tilde{a} : \|\tilde{a}\|_{B_{20}} < M_a\} \times \{\tilde{b} : \|\tilde{b}\|_{B_{2}} < M_b\} \times \{\eta : \|\eta\|_{B_1} < M_\eta\right\}.
\]

To be more precise, having fixed the numbers \( M_a, M_\eta \) and \( M_b \) (where \( M_b \) is, in particular, such that inequality (2.25) is satisfied for some \( K_b > 0 \)), we can find the number \( \varepsilon_0 > 0 \) sufficiently small, such that all the components of the mapping are well defined. Next, for a possibly decreased value of \( \varepsilon_0 \), all the components of the mapping are continuously Frechet differentiable with respect \((\tilde{a}, \tilde{b}, \eta)\). □

Let us denote

\[
(F_1, F_2, F_3) := (F_1^0, F_2^0, F_3^0).
\]

For \( \varepsilon^2 = 0 \), the triple \((\tilde{a}, \tilde{b}, \eta) = (0, 0, 0)\) satisfies system (2.33), so system

\[
F_1(\tilde{a}, \tilde{b}, \eta) = 0, \quad F_2(\tilde{a}, \tilde{b}, \eta) = 0, \quad F_3(\tilde{a}, \tilde{b}, \eta) = 0
\]

as well, and the Frechet derivative \( DF \) of the mapping \( F \) at the point \((\varepsilon, \tilde{a}, \tilde{b}, \eta) = (0, 0, 0, 0)\) with respect to \((\tilde{a}, \tilde{b}, \eta)\) is equal to

\[
(\tilde{a}, \tilde{b}, \eta) \mapsto DF[\tilde{a}, \tilde{b}, \eta] = \left(DF_1[\tilde{a}, \tilde{b}, \eta], DF_2[\tilde{a}, \tilde{b}, \eta], DF_3[\tilde{a}, \tilde{b}, \eta]\right),
\]

where

\[
\begin{align*}
DF_1[\tilde{a}, \tilde{b}, \eta] &= \tilde{a}'' + v\tilde{a}' - b_0\tilde{a} - na_0b_0\tilde{b}, \\
DF_2[\tilde{a}, \tilde{b}, \eta] &= (\tilde{a} + b\tilde{b})' + v(\tilde{a} + \tilde{b}) + v\sigma(1 + Kb_0)\tilde{b}, \\
DF_3[\tilde{a}, \tilde{b}, \eta] &= \eta.
\end{align*}
\]  

(2.37)

The system \( DF_1[\tilde{a}, \tilde{b}] = 0, \ DF_2[\tilde{a}, \tilde{b}] = 0 \) is satisfied by \((\tilde{a}, \tilde{b}) = (a_0', b_0')\). Due to the monotonicity of \( a_0(\cdot) \), we can however exclude this solution from the considered spaces due to the pinning condition (2.34) (implying \( \tilde{a} \in B_{20} \)).
To apply the implicit function theorem, we should consider the solvability of the system:

\[
\begin{align*}
DF_1[\tilde{a}, \tilde{b}, \tilde{\eta}] &= f_1 \in C^0(\mathbb{R}), \quad (2.38a) \\
DF_2[\tilde{a}, \tilde{b}, \tilde{\eta}] &= f_2 \in C^1(\mathbb{R}), \quad (2.38b) \\
DF_3[\tilde{a}, \tilde{b}, \tilde{\eta}] &= f_3 \in C^1(\mathbb{R}). \quad (2.38c)
\end{align*}
\]

To be more precise, we have to show that for any \((f_1, f_2, f_3) \in B_0 \times B_1 \times B_0\) there exists a unique (bounded) solution \((\tilde{a}, \tilde{b}, \tilde{\eta}) \in B_{20} \times B_2 \times B_1\) to system (2.38).

Eq. (2.38c) is obviously solvable for all \(f_3\) by the function \(\tilde{\eta} = f_3\). Thus we can confine ourselves to the system composed of (2.38a) and (2.38b). Let

\[ y := \tilde{a} + \tilde{b}. \]

It follows that the system composed of (2.38a) and (2.38b) can be written as:

\[
y' = -\frac{v}{d} y - \frac{v}{d} \frac{\sigma}{(1 + Kb_0)^2} y - v \left(1 - \frac{1}{d}\right) a + \frac{v}{d} \frac{\sigma}{(1 + Kb_0)^2} \tilde{a} + f_2, \\
\tilde{a}' = p, \\
p' = -vp + \frac{a_0 b_0}{d} y + \left(b_o - \frac{a_0 b_0}{d}\right) \tilde{a} + f_1.
\]

For \(Y := (y, \tilde{a}, p)^\top\), it can be written as

\[ Y' = A(\xi) Y + (f_2, 0, f_1)^\top, \]

where

\[
A(\xi) := \begin{pmatrix}
-\frac{v}{d} - \frac{v}{d} \frac{\sigma}{(1 + Kb_0(\xi))^2} & -v \left(1 - \frac{1}{d}\right) + \frac{v}{d} \frac{\sigma}{(1 + Kb_0(\xi))^2} & 0 \\
0 & \frac{v}{d} \frac{\sigma}{(1 + Kb_0(\xi))^2} & 1 \\
\frac{a_0(\xi)b_0(\xi)}{d} & b_0(\xi) - \frac{a_0(\xi)b_0(\xi)}{d} & -v
\end{pmatrix}.
\]

According to the boundary conditions satisfied by the functions \(a_0\) and \(b_0\), we have

\[
A(-\infty) := \begin{pmatrix}
-\frac{v}{d} - \frac{v}{d} \frac{\sigma}{(1 + K b_s)^2} & -v \left(1 - \frac{1}{d}\right) + \frac{v}{d} \frac{\sigma}{(1 + K b_s)^2} & 0 \\
0 & 0 & 1 \\
0 & b_s & -v
\end{pmatrix},
\]

and

\[
A(\infty) := \begin{pmatrix}
-\frac{v}{d} (1 + \sigma) & -v \left(1 - \frac{1}{d}\right) + \frac{v \sigma}{d} & 0 \\
0 & 0 & 1 \\
\frac{1}{d} & -\frac{1}{d} & -v
\end{pmatrix}.
\]

For \(v > 0\) and \(b_s > 0\), \(A(-\infty)\) has three real nonzero eigenvalues:

\[-\frac{v}{d} - \frac{v}{d} \frac{\sigma}{(1 + K b_s)^2} < 0, \quad -v - \sqrt{v^2 + 4b_s} < 0, \quad -v + \sqrt{v^2 + 4b_s} > 0.\]

For next, all the eigenvalues of \(A(\infty)\):

\[-\frac{v}{d} (1 + \sigma) + \frac{\sigma}{2} \left[\frac{v}{d} (1 + \sigma)\right]^2 - 4, \quad -\frac{v}{d} (1 + \sigma) - \frac{\sigma}{2} \left[\frac{v}{d} (1 + \sigma)\right]^2 - 4,\]
have negative real parts.

To use the implicit function theorem, we will apply the exponential dichotomy theory, in particular the results of [9] (see also [5]). Thus we should prove that the operator
\[(y, \tilde{a}, p)^\top \mapsto ((y, \tilde{a}, p)^\top)' - A(\xi)(y, \tilde{a}, p)^\top\] (2.39)
is invertible. To prove the invertibility, we will use [9, Lemma 4.2]. Obviously, the matrix \(A(\xi)\) is continuous, hence bounded since \(A(-\infty)\) and \(A(\infty)\) are bounded. Moreover, as the matrices \(A(-\infty)\) and \(A(\infty)\) have no eigenvalues with zero real part, then, according to Lemma 3.4 in [9], the system
\[Y' - A(\xi)Y = 0\] (2.40)
has an exponential dichotomy on both of the half lines. According to our analysis of the eigenvalues of the matrix \(A(\cdot)\), the sum of the dimensions of the stable and unstable manifolds for system (2.40) is equal to \((3 + 1) = 4\). Hence the operator \(Y \mapsto Y' - A(\xi)Y\) is Fredholm of index 1. Moreover, the system adjoint to the system \(Y' - A(\xi)Y = 0\), i.e. \(Z' + A'(\xi)Z = 0\), has no bounded solution, because the eigenvalues of the matrix \(A(\infty)\) are equal to minus eigenvalues of the matrix \(A(\infty)\). It follows that there exists at least one solution to system (2.40) bounded in the space \(C^1(\mathbb{R})\). This solution is unique in the space of functions satisfying the condition \(Y_2(0) = 0\). This condition can be achieved by adding a term \(cY_0\) with appropriate value of the constant \(c\). Here \(Y_0\) is the unique bounded solution to the homogeneous system \(Y' - A(\xi)Y = 0\) which is exactly equal to \((a_0(\cdot) + db_0(\cdot), a'_0(\cdot), a''_0(\cdot))\). (The uniqueness follows from the fact that there is only one non-negative eigenvalue of the matrix \(A(-\infty)\).) As \(f_1(\xi)\) and \(f_2(\xi)\) tend to 0 as \(\xi \to \pm\infty\), then it follows from system (2.40) that \(y(\pm\infty) = 0\) and \(\tilde{a}(\pm\infty) = 0\). In view of the implicit function theorem, the definition of \(Y\), (2.32) and the relation \(\varepsilon^2 = \alpha^{-1}\), we conclude that, for all \(\alpha > 0\) sufficiently large, there exists a unique solution to system (2.31): \((a(\cdot; \alpha), b(\cdot; \alpha), \eta(\cdot; \alpha)) \in B_2 \times B_{2\alpha} \times B_1\) such that, for all \(\xi \in \mathbb{R}\), \((a(\xi; \alpha), b(\xi; \alpha), \eta(\xi; \alpha)) \to (a_0(\xi), b_0(\xi), 0)\). Due to the definition of the spaces \(B_i\), \(i = 0, 1, 2\), the functions \(a(\cdot; \alpha), b(\cdot; \alpha)\) satisfy conditions (2.2).

Having the functions \(b(\cdot; \alpha)\) and \(b(\cdot; \alpha)\), we obtain by means of (2.7), the function \(c(\cdot; \alpha)\):
\[c = \frac{\sigma b}{1 + Kb} - \frac{\eta}{1 + Kb}\]

Finally, one can see that the components of the mapping \(F_\varepsilon\) are continuously differentiable with respect to \(\varepsilon\) in the considered open neighbourhood of the point \((\varepsilon, \tilde{a}, \tilde{b}, \eta)\). Thus using the final statement of Theorem A, we conclude that the following theorem is valid.

**Theorem 1.** Suppose that for \(\alpha = \infty\), system (2.1) has a solution \((a, b, c) = (a_0(\cdot), b_0(\cdot), c_0(\cdot))\) with \(a_0\) and \(b_0\) satisfying system (2.12) (with boundary conditions (2.2)) and \(c_0 = \frac{\sigma b_0}{1 + K b_0}\). Then, for all \(\alpha > 0\) sufficiently large, there exists a unique solution \((a(\cdot; \alpha), b(\cdot; \alpha), c(\cdot; \alpha))\) to system (2.1) such that \((a(\cdot; \alpha), b(\cdot; \alpha), c(\cdot; \alpha)) \to (a_0(\cdot), b_0(\cdot), c_0(\cdot))\) in the norm of the space \(B_{2\alpha} \times B_2 \times B_1\). Moreover,
\[\|a(\cdot; \alpha) - a_0(\cdot)\|_{C^2(\mathbb{R})} = O(\alpha^{-1}),\quad \|b(\cdot; \alpha) - b_0(\cdot)\|_{C^2(\mathbb{R})} = O(\alpha^{-1}),\quad \|c(\cdot; \alpha) - c_0(\cdot)\|_{C^1(\mathbb{R})} = O(\alpha^{-1}).\]
3. **A conjecture on nonlinear determinacy of traveling waves.** In this section, we will argue that traveling wave solutions of system (1.9) are nonlinearly selected. Note that Merkin and Ševčíková [7] have employed the direct numerical integration to the traveling wave problem (1.11)-(1.12) for some cases to support this phenomenon. Here our method is to first numerically compute the solution of the initial value problem (1.9)-(1.10), and then calculate the spreading speed.

For readers’ convenience, we restate the traveling wave problem (1.11)-(1.12) as follows:

\[
\begin{aligned}
A_{zz} + vA_z - AB &= 0, \\
\frac{dB}{dz} + \frac{v}{g(B)} B_z + AB &= 0,
\end{aligned}
\] (3.1a, 3.1b)

with the boundary condition

\[(A, B)(-\infty) = (0, b_s), \quad (A, B)(+\infty) = (1, 0),\] (3.2)

where the function \(g(\cdot)\) is defined before (1.9).

Now we derive the wave speed \(v_{\text{linear}}\) determined by the linearized system of the traveling wave problem (1.11)-(1.12) around the unstable equilibrium \((1, 0)\). Set \(g_0 = g(0)\) and \(v_{\text{linear}} = 2\sqrt{dg_0}\), and consider the quadratic polynomial

\[P_v(\lambda) := d\lambda^2 + \frac{v}{g_0} \lambda + 1.\]

It is seen that for \(v \geq v_{\text{linear}}\), the equation \(P(\lambda) = 0\) has two negative roots \(-\lambda_v\) and \(-\hat{\lambda}_v\), with \(0 < \lambda_v \leq \hat{\lambda}_v\), where the equality sign holds only for \(v = v_{\text{linear}}\). Next, the roots change their sign if \(v \mapsto -v\). Hence, for \(v \leq -v_{\text{linear}}, P(\lambda) = 0\) has two positive roots \(\lambda_v\) and \(\hat{\lambda}_v\). Finally, let us note that for \(v \in (-v_{\text{linear}}, v_{\text{linear}})\), the roots are conjugated complex numbers with nonzero imaginary part.

*In the sequel, we retain the notations \(\lambda_v\) and \(v_{\text{linear}}\).* In the following lemma, we will show that nonnegative solutions to problem problem (3.1)-(3.2) can exist only for \(v \geq 2\sqrt{dg_0}\).

**Lemma 3.1.** For \(v < v_{\text{linear}}\), there exists no nonnegative solutions of the problem (3.1)-(3.2).

**Proof.** Assume that \((A, B)\) is a nonnegative solutions of the problem (3.1)-(3.2). Linearising the above system around the equilibrium \((1, 0)\) leads to the linear system

\[
\begin{aligned}
A_{zz} + vA_z - B &= 0, \\
\frac{dB}{dz} + \frac{v}{g_0} B_z + \frac{1}{d} B &= 0.
\end{aligned}
\] (3.3a, 3.3b)

Note that as \(P(\lambda)\) is the characteristic polynomial of (3.3b), a solution of (3.3b) is a linear combination of \(e^{\lambda_v z}\) and \(e^{\hat{\lambda}_v z}\).

First, we consider the case that \(v \leq -v_{\text{linear}} = -2\sqrt{dg_0}\). Then both of \(\lambda_v\) and \(\hat{\lambda}_v\) are positive. This, together with Hartman-Grobman theorem [3], implies that the \(B\)-component \(B(z)\) of the solution \((A, B)\) of (3.1)-(3.2) is unbounded as \(z \to \infty\), which is a contradiction. Next, for the case that \(|v| < 2\sqrt{dg_0}, \lambda_v\) and \(\hat{\lambda}_v\) form a complex conjugate pair. This would imply that the \(B\)-component \(B(z)\) of the solution \((A, B)\) of (3.1)-(3.2) cannot be of a positive sign for \(z\) near infinity, a contradiction again. This completes the proof of this lemma. \(\square\)
Figure 1. Time-evolution of the solution \((A, B)\) of system (1.9) with \(L = 1600\). The initial data is that \(A_0(x) = 1\) \((0 \leq x \leq L)\), and \(B_0(x) = 0\) \((20 \leq x \leq L)\) and \(1\) \((0 \leq x < 20)\). Here the parameters are \(d = 2\), \(K = 2\), and \(\sigma = 4\).

Next we numerically investigate the propagation behavior of the solutions \((A, B)\) of system (1.9) in the large interval \(\Omega_L = [0, L]\) with the Neumann boundary conditions at \(x = 0\) and \(L\), and the initial conditions

\[
(A, B) (0, x) = (A_0, B_0) (x), \quad x \in [0, L],
\]

where the initial reactant \(A_0\) is at the uniform concentration 1 and the initial catalyst \(B_0\) is non-negative and of suitably compact support, as shown in Figure 1(a). The choice of the initial condition (3.4) is motivated by the requirement of experimental protocols. Then, as shown in Figure 1, the region of catalysts \(B\) expands uniformly into the region of reactants \(A\), and the whole domain \([0, L]\) is eventually occupied by catalysts after large time. Further, the spreading speed of catalysts becomes constant after large time. Such a spreading speed is denoted by \(v_m\). It is widely accepted that for monostable parabolic systems, the solution with the initial data of compact support will generate wavefronts which propagate outward from the initial reaction zone, whose spreading speed is consistent with the minimal speed of traveling wave solutions of the underlying system. Based this principle, we view \(v_m\) as the minimal speed of traveling wave solutions of the traveling wave problem (3.1)-(3.2). Then the term “nonlinearly selected” will correspond to the parameter \(\sigma\) for which \(v_m > v_{\text{linear}}\). We numerically find such values of \(\sigma\), as shown.
Figure 2. The dependence of wave speed $v_m$ on $\sigma$. The parameter $K = 2$ and the diffusivity parameter $d$ is 0.5, 1, 2 and 4 for panels (a), (b), (c) and (d), respectively.

Therefore, we can conclude that for some values of $\sigma$, traveling wave solutions of system (1.9) are nonlinearly selected.

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