Computational Study of Traveling Wave Solutions of Isothermal Chemical Systems

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Abstract. This article studies propagating traveling waves in a class of reaction-diffusion systems which model isothermal autocatalytic chemical reactions as well as microbial growth and competition in a flow reactor. In the context of isothermal autocatalytic systems, two different cases will be studied. The first is autocatalytic reaction of order $m$ without decay. The second is chemical reaction of order $m$ with a decay of order $n$, where $m$ and $n$ are positive integers and $m > n \geq 1$. A typical system in autocatalysis is $A + 2B \rightarrow 3B$ and $B \rightarrow C$ involving two chemical species, a reactant $A$ and an auto-catalyst $B$ and $C$ an inert chemical species.

The numerical computation gives more accurate estimates on minimum speed of traveling waves for autocatalytic reaction without decay, providing useful insight in the study of stability of traveling waves.

For autocatalytic reaction of order $m = 2$ with linear decay $n = 1$, which has a particular important role in chemical waves, it is shown numerically that there exist multiple traveling waves with 1, 2 and 3 peaks with certain choices of parameters.

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Key words: Isothermal chemical systems, microbial growth in a flow reactor, traveling wave, multiple peak solutions, minimum speed, existence, non-existence.

1 Introduction

In this paper we study two reaction-diffusion systems of the form

\[ \begin{align*}
(1) \quad u_t &= D_A u_{xx} - f(u, v), \\
& \quad v_t = D_B v_{xx} + f(u, v) - L(v),
\end{align*} \]

(1.1)

and

\[ \begin{align*}
(1I) \quad u_t &= D_A u_{xx} - f(u, v), \\
& \quad v_t = D_B v_{xx} + f(u, v),
\end{align*} \]

(1.2)

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where \( f \) is a \( C^1 \) function defined on \([0, \infty) \times [0, \infty)\), \( L \) a \( C^1 \) function defined on \([0, \infty) \times [0, \infty)\), with properties

\[
\begin{align*}
  f(u,0) &= f(0,v) = 0, \quad \text{and} \quad f(u,v) > 0 \quad \text{on} \quad (0, \infty) \times (0, \infty), \\
  L(0) &= 0 \quad \text{and} \quad L(v) > 0 \quad \text{on} \quad (0, \infty),
\end{align*}
\]

and \( D_A, D_B \) are positive constants representing the diffusion coefficients of two different species, which are in general unequal due to different molecular weights and/or sizes.

The particular feature we are interested in is (i) the existence of multiple traveling waves for (1.1), and estimate of minimum speed for (1.2). Without loss of generality, we shall assume in what follows that \( D_A = 1 \) and use \( d \) in place of \( D_B \), since the general case can be transformed to this one by a simple non-dimensional scaling.

Many interesting phenomena in population dynamics, bio-reactors and chemical reactions can be modeled by a system of the form as in (1.1). For example, a system modeling microbial growth and competition in a flow reactor was first studied in [2] and [23], where a special case is \( f(u,v) = F(u)v, \ L(v) = Kv, \ K \) a positive constant, and \( F(0) = 0 \) and \( F'(0) > 0 \). In that context, \( u \) is the density of nutrient and \( v \) the density of microbial population. \( L(v) \) is the death rate of microbial. Subsequent works with emphasis on traveling waves appeared later in [14] and [24].

Another interesting case arises from isothermal autocatalytic chemical reaction between two chemical spices \( A \) and \( B \) taking the form:

\[
A + mB \rightarrow (m+1)B \quad \text{with rate} \quad r[A][B]^m,
\]

where \( m \geq 1 \) is an integer and \( r > 0 \) is a rate constant. In that situation, \( f(u,v) = uv^m \) with \( u \) the concentration density of \( A \) and \( v \) the density of \( B \). If there is no decay, then \( L(v) = 0 \).

The resulting system is

\[
\begin{align*}
  u_t &= u_{xx} - uv^m, \\
  v_t &= dv_{xx} + uv^m, \\
\end{align*}
\]

after a simple non-dimensional transformation. The importance of autocatalytic chemical reaction in chemical waves, Turing pattern formation and real-world chain chemical reactions is well documented in literature. The global dynamics of the Cauchy problem of (1.3) was studied in [3, 16, 19, 20] in one and two dimensional cases using Renormalization Group method coupled with key a priori estimates. The existence and non-existence, as well as stability of traveling waves of (1.3) were investigated in [4–6, 17]. In particular, it was established in [4] that for any fixed boundary value of \((u,v) = (0,a_0), a_0 > 0, \) at \(-\infty, \) there exists \( C_* = C_*(d,a_0,m) \) such that there exists a traveling wave with speed \( C \) when \( C \geq C_* \). That is, the situation is in the classical mono-stable category.

The traveling wave problem for (I) is far more complex. For example, the system

\[
\begin{align*}
  u_t &= u_{xx} - uv^m, \\
  v_t &= dv_{xx} + uv^m - kv^m,
\end{align*}
\]
where \( m \geq 1 \) and \( k > 0 \) is a rate constant, were first studied in [24] for a special case and later in [14] for a general case when \( m = 1 \). Other related results appeared in [11, 12]. Whereas \( m > 1 \) case has been studied in [10, 25]. The results again are in the classical mono-stable category for existence of traveling waves.

But, for the system

\[
(IV) \begin{cases} 
  u_t = u_{xx} - uv^m, \\
  v_t = dv_{xx} + uv^m - kv,
\end{cases}
\]

where \( m > 1 \) and \( k > 0 \), the situation is totally different. The following results are proved recently by Qi and his collaborators, [7, 8, 21].

**Theorem 1.1.** Suppose \( m > 1 \) and \( k > 0 \) and the boundary value at \(-\infty\) is given as \((u, v) = (a_0, 0)\) with \( a_0 > 0 \).

(i) If \( d > 1 \) and \((d - 1)C^2 = k\), then there exists a traveling wave of (1.5) with speed \( C \) provided \( d \) is not far away from 1 and \( a_0 \) suitably large.

(ii) For any \( m > 1 \) and \( k > 0 \) and any \( a_0 > 0 \) fixed, there exists a traveling wave. Furthermore, the speed set for existence is a bounded interval.

(iii) For \( a_0 \gg 1 \), there exist multiple traveling waves with different speed. Moreover, the traveling wave solutions can be characterized as having exactly one, two, \( \cdots \), local maxima for the function \( w = u^{m-1}v \). The number of solutions goes to \( \infty \) as \( a_0 \to \infty \).

In spite of deep theoretical results obtained so far, there are a number of key issues which need to be addressed.

**Question 1:** What is the minimum speed for the system (1.3)?

The importance of this question is that for mono-stable type of problems, the experience of a single equation tells us it is the minimum speed traveling wave which is most relevant for the study of stability.

**Question 2:** What is the traveling wave solution structure for the system (1.5)?

The main purpose of the present work is to give an accurate estimate of minimum speed for (1.3) and to study the dependence of traveling wave solution structure for (1.5) on the boundary value at \(-\infty\).

The organization of the paper is that we present our numerical results on (III) in Section 2 and the detailed computational approach on (IV) in Section 3. We end the paper with brief discussion on the systems in Section 4.

### 2 The auto-catalytic system without decay

In this section, we study the system (III) with the purpose of using novel numerical scheme to get accurate estimate on minimum speed and how it depends on the diffusion coefficient \( d \).
**Travelling Wave Problem:** Given $C > 0$, let $(u(x, t), v(x, t)) = (\alpha(z), \beta(z))$, where $z = x - Ct$, find $(\alpha, \beta) \in [C^2(\mathbb{R})]^2$ that satisfies

\[
\begin{cases}
\alpha_{zz} + C\alpha_z = \alpha\beta^n, & \alpha \geq 0, \quad \forall z \in \mathbb{R}, \\
d\beta_{zz} + C\beta_z = -\alpha\beta^n, & \beta \geq 0, \quad \forall z \in \mathbb{R}, \\
\lim_{z \to \infty} (\alpha(z), \beta(z)) = (1, 0), \\
\lim_{z \to -\infty} (\alpha(z), \beta(z)) = (0, 1).
\end{cases}
\tag{2.1}
\]

Here $C > 0$ is the constant traveling speed. The boundary value at $-\infty$ is set to be $(0,1)$ because the general case of $(0, a_0)$ with $a_0 > 0$ can be reduced to the case by a simple scaling with speed $C(a_0) = a_0^{n/2}C(1)$. It is easy to see that $[\alpha_z + C\alpha + d\beta_z + C\beta]_z = 0$, so that there is a conservation law

\[
\alpha_z + d\beta_z + C(\alpha + \beta) = 1,
\]

which justifies the boundary condition at $x = \infty$ and enables us to reduce the order of traveling wave problem from four to three. Moreover, if $d = 1$, the conservation law above gives $\alpha = 1 - \beta$. The system is reduced to a classical mono-stable scalar equation

\[
\beta_{zz} + C\beta_z + \beta^n(1 - \beta) = 0.
\]

In general, $\alpha$ is monotone increasing, but $\beta$ is monotone decreasing before $\beta$ reaches zero. By first making a change of variables $y = Cz/d$ and then using $s = 1 - \beta$ as independent variable, the following 2nd order system is derived in [4]:

\[
\begin{align*}
PP' &= A(1 - s)^m - P &\forall s &\in [0,1], \\
PA' &= \kappa^2[P + s] - dA &\forall s &\in [0,1], \\
P(s) &> 0, A(s) > 0 &\forall s &\in (0,1), \\
P(0) &= 0, A(0) = 0.
\end{align*}
\tag{2.2}
\]

where $P(s)$ is $\beta_y(y)$ and $A(s) = d\alpha(y)/C^2$. $\kappa = d/C$. It is clear that $(A, P)$ is a traveling wave of (III) if and only if $P(s) \searrow 0$ as $s \nearrow 1$. The main result of [4] can be summarized as follows.

**Theorem 2.1.** Let the boundary condition of traveling wave at $-\infty$ be fixed as $(0,1)$.

1. Suppose $d < 1$ and $m \geq 2$. A unique (up to translation) traveling wave solution exists for (III) if $C \geq 4d/\sqrt{1 + 4d}$. On the other hand, there exists no solution for if $C \leq d/\sqrt{K(m)}$, where $K(m)$ is a constant, which increases with $m$. In particular, $K(1) = 1/4, K(2) = 2$.

2. Suppose $d \geq 1$ and $m \geq 1$. There exists a positive constant $C_{\text{min}}$ such that (III) admits a traveling wave if and only if $C \geq C_{\text{min}}$. In addition, $C_{\text{min}}$ is bounded by

\[
\sqrt{\frac{d}{K(m)}} \leq C_{\text{min}} \leq \sqrt{\frac{d}{K(m)}} \frac{1}{\sqrt{1 - (1 - \frac{d}{4})/\sqrt{4K(m) + 1}}}.
\]

\( m = 2, \ d = 0.1, \ C_{\text{min}} = 0.0989 \)
\( m = 2, \ d = 1.2, \ C_{\text{min}} = 0.7749 \)
\( m = 2.5, \ d = 1.2, \ C_{\text{min}} = 0.6345 \)

Figure 1: Three different cases where minimum speeds are determined and corresponding traveling wave solutions \( (A, P) \) shown in the graph.

Figure 2: We compare the numerically computed \( C_{\text{min}} \) with the lower bound, shown as blue line and upper bound, shown as blue “–” from Theorem 2.1 for \( d > 1 \) and \( d < 1 \), respectively. It is clear that for \( d > 1 \), it demonstrates a good match of theoretical result with numerical computation. But, for \( 0 < d < 1 \), the numerical results shows the minimum speed is far below that of theoretical result pointing out further refinement is needed to improve the estimate theoretically.

Remark 2.1. The above result was obtained using comparison with \( d = 1 \) case for \( d > 1 \) and therefore it is a sharp bound when \( 0 < d - 1 \ll 1 \). But, for \( d < 1 \), the result is shown by a direct proof and it deviates from the single equation case of \( d = 1 \) even for \( d \) close to 1.

The formulation in (2.2) of traveling wave problem as a second order ODE system in phase plane gives us an alternative way to design numerical schemes. Let

\[ P(s) = \lambda s + a_1 s^2, \quad A(s) = \lambda (1 + \lambda) s + b_1 s^2 \quad \text{for} \ 0 < s \ll 1, \]

simple computation shows that

\[ \lambda = \frac{\sqrt{4\kappa^2 + d^2} - d}{2}, \quad a_1 = \frac{b_1 (d + 2\lambda)}{\lambda (d - 1)}, \quad b = -\frac{m \lambda^2 (1 + \lambda)}{6\lambda^2 + 2\lambda d + 3\lambda + d}. \]
Figure 3: We also did Regression Analysis trying to catch the dependence of $C_{\text{min}}$ on $d$ analytically. By using a curve of the form $C_1 \sqrt{d} + C_2 + C_3/d + C_4/d^2$. The best fitting curve when $m = 2.5$ is $\sqrt{d}/2 - 1/5 + 1/(2d) - 1/(20d^2)$. The best fitting curve when $m = 2$ is $(2.5/3)/\sqrt{d}$.

Our numerical scheme has the following key ingredients:

(i) It uses the above asymptotic expansion at $s=0$ as initial input for $0 < s \ll 1$ and then use Matlab to compute the solution up to $s=1$.

(ii) The algorithm in Matlab is the explicit fourth-order Runge-Kutta method. The criterion to judge whether the resulting solution is a traveling wave is to check whether $P(s) > 0$ on $(0,1)$ and $|P(1)|$ is less than a preset upper bound of the order $10^{-6}$.

(iii) All results were checked and confirmed by using double-precision Mathematica.

We have done extensive computation for two cases, $m = 2$ and $m = 2.5$ to determine $C_{\text{min}}$ for various values of $d$. The method works well for wide range of $d$ value from $d$ fairly small such as $d = 0.1$ to rather big value of $d = 5$.

3 The auto-catalytic system with decay

In this section, we study how to use computation to reveal the complex solution structure of traveling wave solution to system (IV).

It is easy to verify that all equilibrium points of (IV) are in the form $(a,0)$ with $a \in \mathbb{R}$. Hence, any traveling wave $u(x,t) = u(x-ct)$, $v(x,t) = v(x-ct)$, with $c > 0$ as the speed, must link one equilibrium point $(a_0,0)$ at $x = -\infty$ to another one $(a_1,0)$ at $x = \infty$ with $a_1 > a_0 > 0$. Thus, we consider traveling wave problem

$$
\begin{align*}
&u'' + cu' = uv^m, & u' > 0, & \text{in } \mathbb{R}, \\
&d v'' + cv' = v - uv^m, & v' > 0, & \text{in } \mathbb{R}, \\
&u(-\infty) = h, & v(-\infty) = 0, & v(\infty) = 0, & u(\infty) < \infty.
\end{align*}
$$

(3.1)
The important implications of such a setting are (i) \( v \) has no monotonicity which is a strong contrast to the auto-catalytic chemical reaction without decay, for which some interesting results are proved in [3–5, 17], and (ii) there is no corresponding single equation to compare with. Indeed, it is not too hard to show that \( v \) is increasing coming out of \( x = -\infty \) and then starts to decrease and may oscillate a few times. Whereas \( u' > 0 \) in \( \mathbb{R} \) for a traveling wave. In addition, define

\[
x_1(c) := \sup \{ z \in \mathbb{R} \mid v' > 0 \text{ in } (-\infty, z) \}, \quad x_2(c) := \sup \{ z \in \mathbb{R} \mid v > 0 \text{ in } (-\infty, z) \}.
\]

For each constant \( c \geq 0 \), we consider the initial value problem, for \((u, v) = (u(x, c), v(x, c))\),

\[
\begin{align*}
&u'' + Cu' = uv''_+ \quad \text{in } \mathbb{R}, \\
&d v'' + Cv' - v = -uv''_+ \quad \text{in } \mathbb{R}, \\
&[u, v] = [h, e^{\lambda x}] + \mathcal{O}(1)e^{\mu x} \quad \text{as } x \to -\infty,
\end{align*}
\]

(3.3)

where \( \lambda \) is the positive root of \( \lambda^2 / d + c \lambda = 1 \) and \( v_+ := \max\{v, 0\} \). We denote

\[
\begin{align*}
A := & \{ C \geq 0 \mid x_2(C) < \infty \}, \\
B := & \{ C \geq 0 \mid x_2(C) = \infty, \lim_{x \to \infty} u(x, C) = \infty \}, \\
C := & \{ C \geq 0 \mid x_2(C) = \infty, \lim_{x \to \infty} u(x, C) < \infty \}.
\end{align*}
\]

(3.4)

The approach in [7] is to use speed \( C \) as a shooting parameter. In fact, the following is a summary of key technical results in [7].

**Lemma 3.1.** Suppose \( d, h > 0 \) are fixed. For each \( c \geq 0 \), problem (3.3), with \( \lambda = (\sqrt{C^2 + 4d} - C) / 2d \) and \( v_+ := \max\{v, 0\} \), admits a unique solution. The solution depends on \( c \) continuously and satisfies \( u' > 0 \) in \( \mathbb{R} \). In addition, \( x_1(C) < \infty, v'(x_1(C), c) = 0 > v''(x_1(C), C) \), and one and only one of the following holds:

1. \( x_2(C) < \infty \) and \( v(x_2(C), C) = 0 \);
2. \( x_2(C) = \infty \) and \( \lim_{x \to \infty} u(x, C) = \infty \);
3. \( x_2(C) = \infty \) and \( \lim_{x \to -\infty} u(x, C) < \infty \). In this case, \( \lim_{x \to -\infty} v(x, C) = 0 \), so \((C, u, v)\) solves (3.1).

Moreover, \( A \) and \( B \) are open, \( 0 \in A \), and \( |M, \infty) \subset B \) for some \( M \gg 1 \). Thus, \( C \) is non-empty and problem (3.1) admits a solution for some \( C > 0 \).

The work in [8] is on the case of \( h \gg 1 \). By make the following change of scale and variables:

\[
\epsilon = h^{-\frac{\nu}{d}}, \quad u = [1 + \epsilon a]h, \quad v = h^{-\frac{\nu}{d} - 1}b, \quad C = \epsilon e,
\]

(3.3) is transformed and the existence of traveling wave is equivalent to finding \((a, b, c) \in C^2(\mathbb{R}) \times C^2(\mathbb{R}) \times (0, \infty)\) which satisfy

\[
\begin{align*}
&a'' + \epsilon e a' = [1 + \epsilon a]b'' , \quad a' > 0, \quad \text{in } \mathbb{R}, \\
&db'' + \epsilon eb' = b - [1 + \epsilon a]b'' , \quad b > 0, \quad \text{in } \mathbb{R}, \\
&a(-\infty) = 0, \quad b(-\infty) = 0, \quad a(\infty) = 0, \quad b(\infty) < \infty.
\end{align*}
\]

(3.5)
To describe the main result of [8], we introduce notation

\[ G(s) = s^2 - \frac{2s^{m+1}}{m+1}, \quad \alpha = \frac{1}{m-1}, \quad M = \left( \frac{m+1}{2} \right)^\alpha, \]

\[ \sigma = 4 \int_0^M \sqrt{G(s)} \, ds, \quad \gamma = 2ad \int_0^M \frac{s^m ds}{\sqrt{G(s)}}, \]

where \( s_+ = \max\{s,0\} \). Our main result is the following:

**Theorem 3.1.** Let \( m > 1 \) and \( d > 0 \) be given constants.

1. There exist positive constants \( M_1, M_2, \) and \( M_3 \) that depend only on \( m \) and \( d \) such that for each \( \varepsilon > 0 \), (3.5) admits no solution if \( c \geq \max\{\sqrt{M_1/\varepsilon}, M_2\} \) or if \( c \leq \gamma - M_3\varepsilon \).

2. For each sufficiently small positive \( \varepsilon \) and each integer \( n \) satisfying \( 1 \leq n \leq \varepsilon^{-1/4} \), there exists a constant \( c_n = n\gamma \left[ 1 + O(\varepsilon + [n - 1]^2\varepsilon|\ln\varepsilon|) \right] \) such that when \( c = c_n \), the system (3.5) admits a solution, unique up to a translation. The solution is an \( n \)-peak solution in the sense that \( w := [1 + ea]^b \) admits exactly \( n \) local maxima and \( n - 1 \) interior local minima.

The numerical computation for (3.3) is to catch the corresponding traveling wave with one, two and three peaks of \( w \), respectively. The result not only verifies the mathematical proof, but also provides more detailed information about the solutions. But, the difficulty is that we need to integrate the solutions with high order nonlinearities over an extended interval. We use numerical analysis to verify theoretical results for various cases of \( c_n \) using Matlab, which implements explicit fourth-order Runge-Kutta method for the computation. To make sure the computation is accurate, we check the results by using the double precision build-in solver NDsolve from Mathematica.

Figs. 4(a)-4(b) represents the numerical result for (3.5) for 1-peak solution \( w = (1 + \varepsilon a)^b \) where \( \varepsilon = 0.00025, c = c_1 = \gamma = 6 \) and the integration interval is \([0,28]\). As shown in the figure, the solutions only have one peak on the \( b - b' \) phase plane.

Figs. 4(c)-4(d) is the results for (3.5) for 2-peak solution \( w = (1 + \varepsilon a)^b \), where \( \varepsilon = 0.00025, c = c_2 = 2\gamma = 12 \) and the integration interval is \([0,39]\).

Figs. 5(a)-5(b) is the results for (3.5) for 3-peak solution \( w = (1 + \varepsilon a)^b \), where \( \varepsilon = 0.00025, c = c_3 = 3\gamma = 18 \) and the integration interval is \([0,50]\). The three-peak solutions are as expected on the \( b - b' \) phase plane.

This Figs. 5(c)-5(d) shows the computation with \( \varepsilon = 0.00038, c = c_3 = 3, \gamma = 18 \) on the finite interval \([0,58]\). A small change of \( \varepsilon \) from the setting of Figs. 5(a)-5(b) results in 4-peak solution with the same speed. Moreover, Figs. 5(e) and 5(f) show in \( b - b' \) phase plane that small change in \( \varepsilon \) with same speed \( C \) gives different types of solutions.

### 4 Discussion

Numerical computation is a powerful tool in understanding complex solution structure of traveling wave problem in systems like (IV). This is our first endeavor in this direction.
The result is yielding good insight into the problem which provides good lead in our further analysis.

We shall do more computation in future and use more sophisticated algorithms to try to overcome a particular challenge which we did not elaborate in details, which is (IV) has positive solutions \((u,v)\) with \(v\) decaying to zero algebraically as \(x^{-1/2}\) and \(u\) growing to \(\infty\) also algebraically as \(x^{1/2}\). They are not traveling waves. How to distinguish traveling wave from such solutions proves to be a challenge for us right now.

Another direction we shall do computation is to study the buoyant instability when a fluid is involved in system (III) as in the famous iodate-arsenous-acid (IAA) reaction. When the fluid strength is increased, the original planar wave is destabilized, resulting cellular fingering. We shall use Hele-Shaw cell in two dimensional setting to approximate the full three dimensional Navies-Stokes equation.
(a) $\varepsilon = 0.00025, c = 18$

(b) $\varepsilon = 0.00025, c = 18$

(c) $\varepsilon = 0.00038, c = 18$

(d) $\varepsilon = 0.00038, c = 18$

(e) $\varepsilon = 0.0022, c = 12$ on the interval $[0,46]$

(f) $\varepsilon = 0.0023, c = 12$ on the interval $[0,55]$

Figure 5: Three- and Four-peak solutions.

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