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Traveling Fronts for Higher Order Autocatalytic Reaction-Diffusion Systems

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Abstract

This article investigates the existence of traveling fronts and their propagation speeds for the two component higher order autocatalytic reaction-diffusion systems with any diffusion coefficients. Our elementary analysis of the vector fields in the phase space gives the estimate of the minimal propagation speeds in terms of the order of autocatalysis and the diffusion coefficients.

Key Words: traveling fronts, propagation speed, autocatalytic reaction, phase space
AMS Classification:35K57,34C37

1 Introduction

Autocatalytic reaction-diffusion systems including the Brusselator [?], the Field-Noyes model [6] and the Gray-Scott model [?], have stimulated an extensive amount of theoretical studies on waves and patterns produced by chemical reactions (see for example, [12]). One of the basic elements responsible for chemical pattern formation is travelling waves which describe the development of chemical processes. The series of the papers by Needham at al.([2]-[5], [13]-[17]) studied extensively the traveling waves in autocatalytic reactions. Focant and Gallay [7] and Hosono and Kawahara [11] also discussed the traveling waves for the mixed order autocatalytic two component systems and their minimal propagation speeds. The similar type of traveling

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waves appears in the combustion problem and the speed of combustion waves were discussed by the several authors ([8], [22] and the references therein). This paper concerns traveling fronts and their speeds for the higher order autocatalytic reaction-diffusion system of the form:

$$\begin{cases} u_t = d_1 u_{xx} - k_1 u v^m, \\ v_t = d_2 v_{xx} + k_2 u v^m, \end{cases} \tag{1}$$

where u and v are concentrations of the reactant and the autocatalyst respectively, d_1 and d_2 are diffusion coefficients, and k_1 and k_2 are any positive constants. Without loss of generarlity, we may suppose $k_1 = k_2 = 1$.

Then, traveling front solutions for (1) are defined as follows. The nonnegative bounded functions of the form $(u(x,t), v(x,t)) = (U(z), V(z))$ with $z = x - ct$ are said to be traveling front solutions for (1) when they satisfy the equations

$$\begin{cases} d_1 U'' + cU' - UV^m = 0, \\ d_2 V'' + cV' + UV^m = 0, \end{cases} \tag{2}$$

with the boundary conditions

$$P_- \equiv (U(-\infty), V(-\infty)) = (\alpha, 1), \qquad P_+ \equiv (U(+\infty), V(+\infty)) = (1, 0). \tag{3}$$

Here $'$ denotes $\frac{d}{dz}$ and α is an unknown nonnegative constant to be determined.

By applying the comparison argument, Takase and Sleeman [21] already proved that there exists the minimal wave speed c^* such that traveling front solutions for (1) exist for each $c \geq c^*$. The purpose of this paper is to discuss the properties of the minimal wave speed c^*, especially the dependence of c^* on the parameters m, d_1 and d_2. The method of the proof employed here is the shooting argument which looks for the connection orbits of (2) and (3) in the 3-dim phase space. Throughout this paper, we always assume that $m > 1$ without notice.

In the next section, we present the preliminary results required for the later discussions. In section 3, we investigate the existence of traveling fronts for (1) and their minimal propagation speeds when $0 < d_1 < d_2$. In section 4, we study the same problem when $d_1 > d_2 > 0$.

2 The preliminary results

In this section, we begin by stating the properties of the traveling front solutions for (1), that is, the solutions of (2) and (3).

Proposition 1 ([3]) *Assume that there exists a traveling front solution $(U(z), V(z))$ for (1). Then it satisfies the followings for all $z \in R$.*

(i) $0 < U < 1, \quad 0 < V < 1.$

(ii) $0 < U' < +\infty, \quad -\infty < V' < 0.$

(iii) $$U + V - 1 \begin{cases} > 0, & \textit{for } d_1 < d_2, \\ = 0, & \textit{for } d_1 = d_2, \\ < 0, & \textit{for } d_1 > d_2. \end{cases}$$

(iv) $\lim_{z \to -\infty} (U(z), V(z) = (0, 1)$, *that is* $\alpha = 1$.

For the equal diffusion case: $d_1 = d_2 = 1$, we already had the following theorem.

Theorem 2 ([20]) *Assume that* $d_1 = d_2 = 1$. *Then, there exists some positive* c_1^* *such that only for each* $c \geq c_1^*$, (1) *has a unique monotone traveling front solution. Furthermore, the minimal speed* c_1^* *satisfies that*

$$\frac{2}{m(m+1)} \leq c_1^{*2} \leq \frac{2}{(m-1)m}. \tag{4}$$

For the extreme case: $d_1 = 0$, we may assume $d_2 = 1$ without loss of generality, and know the following result.

Theorem 3 ([10]) *Assume that* $d_1 = 0, d_2 = 1$. *Then, there exists* c_0^* *such that only for each* $c \geq c_0^*$, (1) *has a unique traveling front solution. Furthermore, the minimal speed* c_0^* *satisfies*

$$\frac{1}{m} < c_0^{*2} \leq \frac{1}{m-1}. \tag{5}$$

For another extreme case: $d_2 = 0$, we may assume $d_2 = 1$ without loss of generality, and easily have the following result.

Theorem 4 *Assume that* $d_2 = 0, d_2 = 1$. *Then, there exists a unique traveling front solution for* (1) *for each positive* c.

In the next two sections, on the basis of these results, we discuss the general case that the both diffusion coefficients are not zero.

3 The case $0 < d_1 < d_2$

For the case that $0 < d_1 < d_2$, the system (2) can be written as

$$\begin{cases} dU'' + cU' - UV^m = 0, \\ V'' + cV' + UV^m = 0, \end{cases} \tag{6}$$

by the change of the independent variable z and the parameter c, where $d = \frac{d_1}{d_2}$. The boundary conditions are specified by (3) with $\alpha = 0$.

Adding the above two equations and integrating the resulting equation, we have the relation $dU'+V'+c(U+V-1)=0$ with the aid of the boundary condition (3). Let $X=U+V-1$. Proposition 1 assures that X is positive when $0<d<1$. Then (6) is reduced to the first order system

$$\begin{cases} X' = -\dfrac{c}{d}X - (\dfrac{1}{d}-1)W, \\ V' = W, \\ W' = -cW - (1-V+X)V^m, \end{cases} \tag{7}$$

The boundary conditions are

$$\begin{aligned} (X(-\infty), V(-\infty), W(-\infty)) &= (0,1,0), \\ (X(+\infty), V(+\infty), W(+\infty)) &= (0,0,0). \end{aligned} \tag{8}$$

Introducing the new dependent variables by

$$q = V, \qquad p = \frac{1}{q}q', \tag{9}$$

we can write (7) as

$$\begin{cases} X' = -\dfrac{c}{d}X - (\dfrac{1}{d}-1)pq, \\ q' = pq, \\ p' = -cp(p+c) - (1-q+X)q^{m-1}, \end{cases} \tag{10}$$

where the singularity $(0,0,0)$ of (7) into two critical points $P_0=(0,0,0)$ and $P_c=(0,0,-c)$ in (10). Thus, (10) has three critical points $P_0=(0,0,0), P_c=(0,0,-c)$ and $P_1=(0,1,0)$. The property of these critical points are as follows. $P_1=(0,1,0)$ has the 1-dim unstable manifold which we denote by $\mathcal{U}_d$ and the 2-dim stable manifold. $P_0=(0,0,0)$ is a topologically stable node. $P_c=(0,0,-c)$ has the 2-dim stable manifold and the 1-dim unstable manifold.

Now our problem is finding an orbit of (10) connecting $P_1=(0,1,0)$ with $P_0=(0,0,0)$ or with $P_c=(0,0,-c)$, which lies entirely in $\Omega^+=\{(X,q,p): X>0, 0<q<1, p<0\}$. In order to discuss this problem, we need the further information for the case of $d=0$. The change of the variables (9) rewrite (6) with $d=0$ as

$$\begin{cases} q' = pq \\ p' = -cp(p+c) - (1-q-\dfrac{pq}{c})q^{m-1}, \end{cases} \tag{11}$$

which has three critical points $(0,0),(1,0)$ and $(0,-c)$. The proof of Theorem 3 assures that there exists a unique orbit of (11) connecting $(1,0)$ to $(0,-c)$ if $c=c_0^*$ and to $(0,0)$ if $c>c_0^*$. This orbit can be represented by

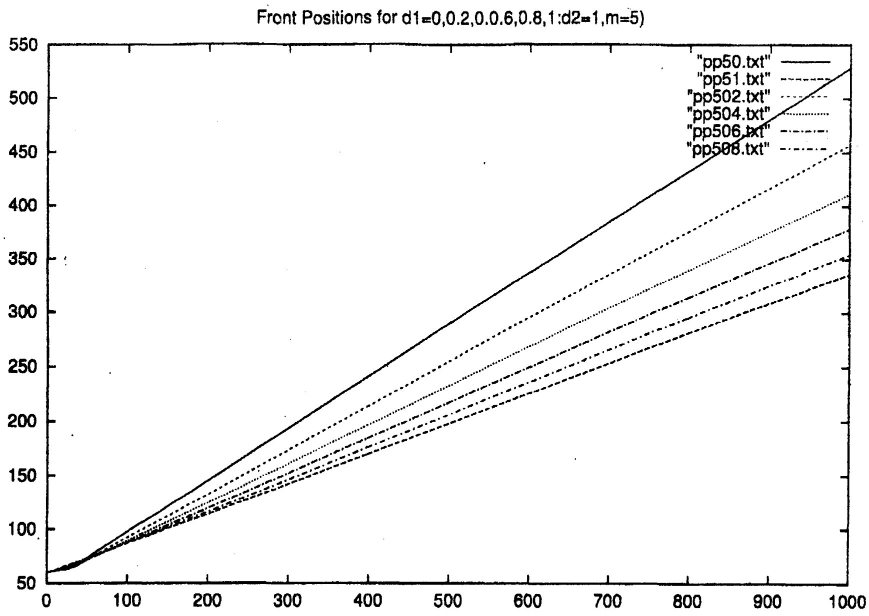

Fig. 1: The position of the front $x(t)$ of $u(x(t),t) = \frac{1}{2}$ $(0 \le t \le 1000)$ for $d = 0(\text{pp50}), 0.2(\text{pp502}), 0.4(\text{pp504}), 0.6(\text{pp506}), 0.8(\text{pp508}), 1.0(\text{pp51}), m = 5$.

$p = \psi_c(q) < 0$ for $0 < q < 1$, and it satisfies that $\psi_c(1) = 0$ for $c \ge c_0^*$, $\psi_{c_0^*(m)}(0) = c_0^*$, and $\psi_c(0) = 0$ for $c > c_0^*$. Let us define the regionΩ_1^+ by $\{(X,q,p) : 0 < X < -\frac{1}{c}\psi_c(q)q, 0 < q < 1, \psi_c(q) < p < 0\}$. By examining the vector field of (10) and the behavior of $\mathcal{U}_d$, we see

Lemma 5 *Assume that* $0 < d < 1$. *Then, for each* $c \ge c_0^*$, *there exists an orbit of* (10) *which connects* P_1 *with* P_0.

This lemma enables us to apply the Wazewski Theorem and we can prove the following lemma.

Lemma 6 *Assume that* $0 < d < 1$. *Then, there exists some positive constant* c_d^* *such that, for* $c = c_d^*$, (10) *has a unique orbit connecting* P_1 *with* P_c.

We have the monotone dependency of connection orbits of (10) with respect to the parameters c and d. In the following propositions, we assume that $0 < d, d' \le 1$.

Proposition 7 *Let* d *be fixed. Assume that for some* $c_1 > 0$, *there exists a connection orbit of* (10) *lying in* Ω^+. *Then, for each* $c \ge c_1$, *there exists a connection orbit of* (10) *lying in* Ω^+.

Proposition 8 *Let c be fixed positive. Assume that for some d', there exists a connection orbit of* (10) *lying in Ω^+. Then, for each $d \geq d'$, there exists a connection orbit of* (10) *lying in Ω^+.*

Lemma 6 and Proposition 7 assure the existence of a connection orbit of (10) only for each $c \geq c_d^*$, that is, c_d^* is the minimal wave speed. Furthermore, Proposition 8 asserts that $c_d^* \leq c_{d'}^*$ if $d \geq d'$. Combining these results, we obtain the following theorem.

Theorem 9 *Assume that $0 < d < 1$. Then, there exists some c_d^*, such that a traveling front solution for* (1) *exists uniquely only for each $c \geq c_d^*$. Furthermore, the minimal speed c_d^* is strictly monotone decreasing with respect to d, and it satisfies that $c_1^* < c_d^* < c_0^*$.*

Fig. 1 shows the numerical result of the propagation speeds of the traveling fronts obtained by solving the evolutional system (1) with the appropriate initial data of the step function type. This result illustrates numerically the last assertion of Theorem 9.

4 The case $d_1 > d_2 > 0$

For the case that $d_1 > d_2 > 0$, the system (2) can be written as

$$\begin{cases} U'' + cU' - UV^m = 0, \\ DV'' + cV' + UV^m = 0, \end{cases} \tag{12}$$

by the change of the independent variable z and the parameter c, where $D = \frac{1}{d} = \frac{d_2}{d_1} < 1$.

Put $X = U + V - 1$. Proposition 1 again assures that X is negative when $0 < D < 1$. Then (12) is reduced to the first order system

$$\begin{cases} X' &= -X - (1-D)W, \\ V' &= W, \\ W' &= -\dfrac{c}{D}W - \dfrac{1}{D}(1 - V + X)V^m. \end{cases} \tag{13}$$

The boundary conditions are (8). Let $D = \epsilon^2$, and replace c, $\dfrac{z}{\epsilon}$ and ϵW by ϵc, z and W respectively. Then (13) is written as

$$\begin{cases} X' &= -c\epsilon^2 X + (1-\epsilon^2)W, \\ V' &= W, \\ W' &= -cW - (1 - V + X)V^m. \end{cases} \tag{14}$$

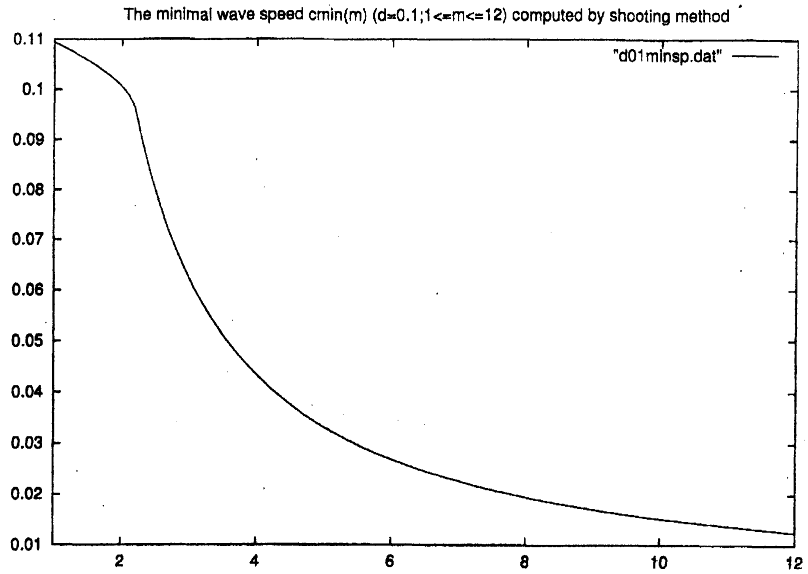

Fig. 2: The graph of $c_D^*(m)(D = 0.2)$ for $(1 \leq m \leq 12)$

Applying the change of the variables (9) to (14), we arrive at the following system which is the same as (10) with $\epsilon^2 = \frac{1}{d}$.

$$\begin{cases} X' = -c\epsilon^2 X + (1-\epsilon^2)pq, \\ q' \ = pq, \\ p' \ = -p(p+c) - (1-q+X)q^{m-1}. \end{cases} \tag{15}$$

Now our problem is finding an orbit of (10) connecting $P_1 = (0,1,0)$ with $P_0 = (0,0,0)$ or with $P_c = (0,0,-c)$, which lies entirely in $\Omega^- = \{(X,q,p) : X < 0, 0 < q < 1, p < 0\}$. Repeating the similar arguments in the section 3, we can prove the following theorem.

Theorem 10 *Assume that* $0 < D < 1$. *Then, there exists some* c_D^*, *such that a traveling front solution for* (1) *exists for each* $c \geq c_D^*$. *Furthermore, the minimal speed* c_D^* *satisfies that* $c_D^* < \sqrt{D}c_1^* = \sqrt{\frac{2D}{m(m-1)}}$.

FIg.2 shows that the minimal wave speed c_D^* is monotone decreasing with respect to the parameter m. This is obtained numerically by the shooting method which follows the unstable manifold of the critical point P_1 of (15).

5 Concluding remarks

We have discussed the propagation speeds of the chemical reaction fronts and give the estimate of the minimal speed in terms of the diffusion coefficients

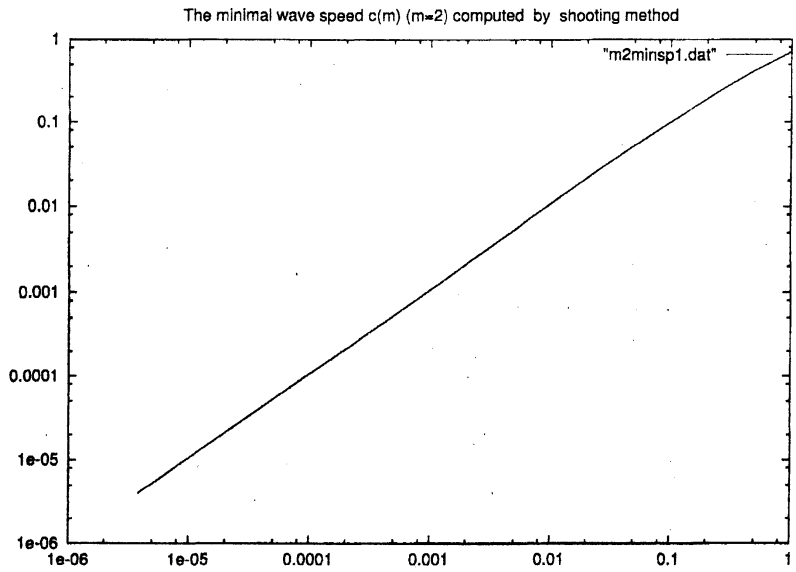

Fig. 3: The dependency of c_D^* on $\sqrt{D}$ (log-log scale)

and the order of autocatalytic reactions. When $0 < D < 1$, unfortunately we cannot have the estimate below of the minimal front speed c_D^*. Our numerical result shown in Fig.3 suggests that $c_D^* = \sqrt{D}\{\sigma(m) + o(\sqrt{D})\}$. The complete proofs of the results stated in this article will appear in the forthcoming paper.

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