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TRAVELLING FRONTS OF REACTION DIFFUSION SYSTEMS MODELING AUTO-CATALYSIS

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Abstract. In this paper, we demonstrate new methods to prove existence of travelling front solutions and better estimates of minimum travelling speed to reaction diffusion systems modelling cubic Auto-Catalysis chemical reactions $A+2B \to 3B$ involving two chemical species, a reactant A and an auto-catalyst B. Furthermore, we show the development of interface in the form of travelling fronts for quadratic Auto-Catalysis chemical reactions $A+B \to 2B$ when initial values are set up similar to an experiment involving Auto-Catalysis as a key step.

1. **Introduction.** In this paper we consider an isothermal autocatalytic chemical reaction step governed by either the cubic reaction relation

$$A + 2B \to 3B \qquad \text{with rate } \; kab^2,$$

where $k > 0$ is the reaction rate, and a and b are the concentrations of reactant A and auto-catalyst B, respectively, or the quadratic reactions relation

$$A + B \to 2B \qquad \text{with rate } \; kab.$$

Well-documented in the literature, the cubic reaction relation, or its quadratic Auto-Catalysis counterpart $A + B \to 2B$ appears in several im- portant models of real chemical reactions, e.g. almost isothermal flames in the carbon-sulphide-oxygen reaction (Voronkov & Semenov [13]), iodate- arsenous acid reactions (Saul & Showwalter [11]), hydroxylamine-nitrate re- actions (Gowland & Stedman [3]), as well as other applications.

Experimental observations demonstrate the existence of propagating chemical wave fronts in chemical systems for which either cubic-catalysis or quadratic Auto-Catalysis forms a key step ([6], [14]). These wavefronts, or travelling waves, arise due to the interaction of reaction and diffusion. Quite often when a quantity of auto-catalyst is added locally into an expanse of reactant, which is initially at uniform concentration, the ensuing reaction is observed to generate wavefronts which propagate outward from the initial reaction zone, consuming fresh reactant ahead of the wavefront as it propagates. This is the phenomenon to be addressed in this paper. For this purpose, we consider a one dimensional slab geometry and the following partial differential equations (PDEs) that govern mass concentration and molecular diffusion for the cubic reaction scheme:

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$$\frac{\partial a}{\partial t} = D_A \frac{\partial^2 a}{\partial x^2} - kab^2, \qquad \frac{\partial b}{\partial t} = D_B \frac{\partial^2 b}{\partial x^2} + kab^2,$$

where D_A and D_B are the constant diffusion rates of A and B, respectively. By introducing dimensionless parameters, dependent and independent variables the PDE system takes the dimensionless form

$$\begin{cases} \dfrac{\partial a}{\partial t} = \dfrac{\partial^2 a}{\partial x^2} - ab^2, & x \in \mathbb{R}, t > 0 \\ \dfrac{\partial b}{\partial t} = D\dfrac{\partial^2 b}{\partial x^2} + ab^2, & x \in \mathbb{R}, t > 0, \end{cases} \tag{1}$$

A similar consideration yields, for quadratic reaction scheme

$$\begin{cases} \dfrac{\partial a}{\partial t} = \dfrac{\partial^2 a}{\partial x^2} - ab, & x \in \mathbb{R}, t > 0 \\ \dfrac{\partial b}{\partial t} = D\dfrac{\partial^2 b}{\partial x^2} + ab, & x \in \mathbb{R}, t > 0, \\ a(x,0) = 1, \quad b(x,0) = g(x), & x \in \mathbb{R}, t = 0. \end{cases} \tag{2}$$

For the application of the above systems in complex fluids and combustion problems, see [6, 7, 8, 9]. The wave front propagating phenomenon corresponds to the following behavior of solutions to (1) ((2)): After certain time of initiation, there are two wave fronts expanding towards $x = \pm\infty$ at a certain speed v. In between the two fronts, the reactant is consumed so $a \approx 0$; since each unit of reactant consumed produces exactly one unit of auto-catalyst, one can expect that $b \approx 1$ inside the wave front. Outside the wave front, the reactant mixture is basically unstirred, so $a \approx 1$ and $b \approx 0$. Focusing on the right front one expects that $(a(x;t);b(x;t)) = (\alpha(z), \beta(z))$, where $z = x - vt$, and (α, β) solves the following system:

$$\begin{cases} \alpha_{zz} + v\alpha_z = \alpha\beta^2, & \alpha \geqslant 0 & \forall\, z \in \mathbb{R}, \\ D\beta_{zz} + v\beta_z = -\alpha\beta^2, & \beta \geqslant 0 & \forall\, z \in \mathbb{R}, \\ \lim_{z\to\infty}(\ \alpha(z), \beta(z)\ ) = (1,0), \\ \lim_{z\to-\infty}(\ \alpha(z), \beta(z)\ ) = (0,1). \end{cases} \tag{3}$$

Here $v > 0$ is the constant travelling speed.

Travelling Wave Problem: Given $v > 0$, find $(\alpha, \beta) \in [C^2(\mathbb{R})]^2$ that satisfies (3).

In this paper we study the existence and non-existence of the travelling waves, which can be generated from (1) with proper initial values. One of the most important questions in the study of (3) is the existence of minimum speed travelling wave and the estimate of the minimum speed v_{min}. In particular, for what range of v, in relation to D, does a travelling wave solution exist?

2. **Sharp estimates of minimum speed in cubic reaction.** In this section, we study the PDE system (1). The main purpose is to give a much improved estimate of minimum speed v_{min}.

Theorem 1. *Suppose $D < 1$. For the travelling wave problem (3),*

$$\text{there exists a unique (up to translation) solution if} \quad v > \frac{4D}{\sqrt{1+4D}};$$

$$\text{there does not exist any solution if} \quad v < \frac{D}{\sqrt{2}}.$$

Clearly the above result provides a pretty satisfying bound on the range of wave speeds. In particular, it shows that $v_{min}(D) \propto D$ for small D. One of the important issues in discussing existence and non-existence of travelling wave solution is whether the set of v of the speed for which existence holds is a single interval. While there are heuristic and numerical arguments in demonstrating that the set of admissible wave speed is an interval $[v_{min}, \infty)$, for the moment we can only supply a rigorous proof for the case $D > 1$.

Theorem 2. *Suppose $D > 1$. There exists a positive constant v_{min} that (3) admits a solution if and only if $v \geq v_{min}$. In addition, v_{min} satisfies the estimate*

$$\sqrt{\frac{D}{2}} \leqslant v_{min} \leqslant \sqrt{\frac{D}{1+1/D}}.$$

It is clear from Theorem 2 that in the special case of $D = 1$, (3) admits a solution if and only if $v \geq 1/\sqrt{2}$.

The corresponding traveling wave problem is to solve

$$\begin{cases} \alpha_{zz} + v\alpha_z = \alpha\beta^2, & \alpha \geqslant 0 \qquad \forall\, z \in \mathbb{R}, \\ D\beta_{zz} + v\beta_z = -\alpha\beta^2, & \beta \geqslant 0 \qquad \forall\, z \in \mathbb{R}, \\ \lim_{z\to\infty}(\ \alpha(z), \beta(z)\ ) = (1, 0), \\ \lim_{z\to-\infty}(\ \alpha(z), \beta(z)\ ) = (0, 1). \end{cases} \tag{4}$$

Suppose (v, α, β) solves (4). Then $[\alpha_z + v\alpha + D\beta_z + v\beta]_z = 0$, so that $\alpha_z + D\beta_z + v(\alpha + \beta)$ is a constant function. Using the boundary conditions, we find that

$$\alpha_z + D\beta_z + v(\alpha + \beta - 1) = 0 \qquad \text{on} \ \ \mathbb{R}.$$

With the new variable $w = \beta_z$, (4) is equivalent to the following third order ODEs system

$$\begin{cases} \alpha_z = v(1 - \alpha - \beta) - Dw, \\ \beta_z = w, \\ w_z = -D^{-1}(\alpha\beta^2 + vw), \\ \lim_{z\to\infty}(\alpha(z), \beta(z), w(z)) = (1, 0, 0), \\ \lim_{z\to-\infty}(\alpha(z), \beta(z), w(z)) = (0, 1, 0). \end{cases} \tag{5}$$

It is clear that in the (α, β, w) phase space, there are two equilibrium points: $(0, 1, 0)$ and $(1, 0, 0)$.

2.1. **A Scalar Equation.** First we review the existence of traveling wave of unit speed to the equation

$$u_{zz} + u_z = ku(1 - u)^n, \quad 0 \leqslant u \leqslant 1 \quad \text{on} \ \ \mathbb{R}, \ \ u(-\infty) = 0, \quad u(\infty) = 1. \tag{6}$$

Here $n \geqslant 1$ is a parameter and k is a positive constant. We seek upper bounds on k for the existence of a solution. Since a solution, if it exists, satisfies $u_z > 0$ on $\mathbb{R}$, we can write $u' = Q(u)$ and work on the (u, Q) phase plane. The resulting equation on the phase plane is

$$\begin{cases} QQ' + Q = ku(1-u)^n & \forall\, u \in [0,1], \\ Q(0) = 0, \quad Q > 0 \text{ on } (0,1). \end{cases} \tag{7}$$

There is a one-to-one correspondence between solutions to (6) and solutions to (7) satisfying the additional requirement $Q(1) = 0$.

Lemma 1. *For each $n \geqslant 1$ and $k > 0$, there exists a unique solution $Q = Q(n, k; \cdot)$ to (7). In addition, there exists a positive constant $K(n)$ such that $Q(n, k; 1) = 0$ if $k \in (0, K(n)]$ and $Q(n, K; 1) > 0$ if $k \in (K(n), \infty)$. Consequently, (7) admits a solution if and only if $k \in (0, K(n)]$.*

In addition, $K(n)$ is a strictly increasing function of n and $K(1) = \frac{1}{4}$, $K(2) =$ 2.

Proof. The existence of Q and K follows by the comparison principle. The exact value of $K(1)$ is calculated by a known fact that the function $K(1)u(1-u)$ is concave, so the minimum wave speed $v = 1$ satisfies $1 = 2\sqrt{K(1)}$; hence $K(1) = 1/4$. In the case $n = 2$, the exact solution is given by $Q = u(1-u)$, so $K(2) = 2$. We omit details, because it is a standard argument. $\square$

2.2. **New Setting—A Non-Autonomous 2×2 System.** Different from earlier work in [10], here we shall use a transformation to turn the third order autonomous system (5) into a second order non-autonomous system, using $u := 1 - \beta$ as the independent variable. This is allowed since for the solution of interest, $\beta_z < 0$, so $z \to 1 - \beta(z)$ has an inverse. To make the resulting system as simple as possible, we also scale the other variables. Hence, we introduce

$$u = 1 - \beta, \qquad A = \frac{D\alpha}{v^2}, \qquad y = \frac{vz}{D}, \qquad \kappa := \frac{D}{v}.$$

The system of differential equations (5) becomes:

$$\begin{cases} u_{yy} + u_y = A(1-u)^2 & \text{on } \mathbb{R}, \\ A_y = \kappa^2(u + u_y) - DA & \text{on } \mathbb{R}. \end{cases}$$

Since $u_y > 0$ for the solution of interest, we can use u as the independent variable. Introducing $P(u) = u_y$, we have an equivalent system of second order non-autonomous (singular) ODEs.

$$\begin{cases} PP' = A[1-u]^2 - P & \forall u \in [0,1], \\ PA' = \kappa^2[P + u] - DA & \forall u \in [0,1], \\ P(u) > 0,\ A(u) > 0 & \forall\, u \in (0,1), \\ P(0) = 0,\ A(0) = 0. \end{cases} \tag{8}$$

Lemma 2. *For every $D > 0$ and $\kappa > 0$, (8) admits a unique solution. In addition,*

$$P(u) = \lambda\, u + O(u^2), \quad A(u) = \lambda(1+\lambda)u + O(u^2) \qquad \text{as } u \searrow 0 \tag{9}$$

where

$$\lambda := \tfrac{1}{2}(\sqrt{4\kappa^2 + D^2} - D) \qquad \Big(\text{the only positive root to } \lambda(\lambda + D) = \kappa^2\Big).$$

Furthermore, $A'(u) > 0$ for all $u \in [0, 1)$ and there are only two possible cases:

(a) $P(1) > 0$*; there does not exist any travelling wave solution to (4).*

(b) $P(1) = 0$*; there exists a travelling wave solution to (4), unique up to translation.*

Proof. The lemma is very technical, and we refer the reader to [1] for details. □

2.3. **The Case $D \geqslant 1$.**

Lemma 3. *Suppose $D \geqslant 1$. Then $DA(u) \geqslant \kappa^2 u$ for all $u \in [0, 1]$. Consequently, there is no travelling wave solution to (4) when $\kappa^2 > 2D$, i.e., when $v < \sqrt{D/2}$.*

Proof. For the proof, see [1]. □

Lemma 4. *Suppose $D > 1$. Then,*

$$A(u) < \lambda(1 + \lambda)\, u, \qquad P(u) < \lambda\, u \quad \forall\, u \in (0, 1).$$

Consequently, there exists a traveling wave solution to (4) when $\lambda(\lambda + 1) \leq 2$, i.e. when

$$v \geq \sqrt{\frac{D}{1 + D^{-1}}}.$$

Proof. A higher order Taylor expansion near $u = 0$ shows that $A < \lambda(\lambda + 1)\, u$ and $P < \lambda\, u$ for all sufficient small positive u. Set

$$\hat{B} = \sup\{b \in (0, 1) \mid P(u) < \lambda\, u, \qquad A(u) < \lambda(1 + \lambda)u \quad \forall u \in (0, b)\}.$$

We show that $\hat{B} = 1$. Suppose on the contrary that $\hat{B} < 1$. Then either $P(\hat{B}) - \lambda\hat{B} = 0$ or $A(\hat{B}) - \lambda(1 + \lambda)\hat{B} = 0$. In $(0, \hat{B}]$,

$$\begin{aligned} P[A - \lambda(1 + \lambda)u]' &= \kappa^2(P + u) - DA - \lambda(1 + \lambda)P \\ &= \lambda(D + \lambda)(P + u) - DA - \lambda(1 + \lambda)P \\ &= -D[A - \lambda(1 + \lambda)u] + \lambda(D - 1)(P - \lambda u) \\ &\leq -D[A - \lambda(1 + \lambda)u]. \end{aligned}$$

Gronwall's inequality then implies that $A < \lambda(\lambda + 1)u$ on $(0, \hat{B}]$. Similarly, for all $u \in (0, \hat{B}]$,

$$\begin{aligned} P[P - \lambda u]' &= -(1 + \lambda)P + A(1 - u)^2 \\ &= -(1 + \lambda)(P - \lambda u) - \lambda(1 + \lambda)u + A(1 - u)^2 \\ &< -(1 + \lambda)(P - \lambda u). \end{aligned}$$

The Gronwall's inequality shows that $P < \lambda\, u$ on $(0, \hat{B}]$. We reach a contradiction. This proves that $\hat{B} = 1$; i.e. $P(u) < \lambda\, u$ and $A(u) < \lambda(1 + \lambda)u$ for all $u \in (0, 1)$.

Suppose $\lambda(1 + \lambda) \leq 2$. We can use comparison to show that $P(u) \leqslant Q(2, 2; u)$ for all $u \in [0, 1]$ so that $P(1) = 0$. Namely, there exists a travelling wave solution to (4). □

Proof of Theorem 2. The estimate of $v_{\min}$, when it exists, follows from the above two lemmas. For the proof of existence of $v_{\min}$, see [1].

2.4. **The case of $D < 1$.**

Lemma 5. *Suppose $D < 1$. Then $A > \kappa^2 u$ on $(0, 1)$. Consequently, when $\kappa^2 > 2$, i.e. $v < D/\sqrt{2}$, there is no travelling wave solution to (4).*

Proof. Direct calculation shows that

$$\begin{aligned} P[A - \kappa^2 u]' &= \kappa^2(P + u) - DA - \kappa^2 P = \kappa^2(1 - D)u - D(A - \kappa^2 u) \\ &> -D(A - \kappa^2 u) \quad \forall u \in (0, 1). \end{aligned}$$

Since $A = \lambda(1 + \lambda)u + O(u^2) > \kappa^2 u$, for all sufficiently small positive u, Gronwall's inequality gives $A > \kappa^2 u$ on $[0, 1)$.

One can show that $P(u) > Q(2, k^2; u)$ for all $u \in (0, 1)$ by first using an asymptotic expansion at $u = 0$ for $0 < u \le \epsilon$ and then a comparison principle for the differential equation in $(\epsilon, 1)$.

It then follows from Lemma 1 that when $\kappa^2 > 2$, we must have $P(1) \ge Q(2, k^2; 1) > 0$, i.e., there does not exists any solution to the travelling wave problem. □

To establish the existence of a solution, we need to find an upper bound of A. Although there is the estimate $A < \kappa^2(u + P)/D$ available for use, we are not satisfied with such an estimate since when D is very small, it is not sufficient to show that $v_{\min} = O(D)$. Hence, we seek another bound.

Lemma 6. *Suppose $D < 1$. Then $A(u)(1 - u) \le \lambda[P(u) + u] \qquad \forall\, u \in [0, 1)$.*

Proof. When $u = 0$, the two sides are equal. Computation shows, in $(0, 1]$,

$$\begin{aligned} & P[(1 - u)A - \lambda(P + u)]' \\ = \;& (1 - u)[\kappa^2(P + u) - DA] - \tfrac{1}{2}PA - \lambda A(1 - u)^2 \\ \le \;& -[D + \lambda(1 - u)][A(1 - u) - \lambda(P + u)] \\ + \;& (P + u)[(\kappa^2 - \lambda^2)(1 - u) - \lambda D] \\ = \;& -[D + \lambda(1 - u)][A(1 - u) - \lambda(P + u)] - \lambda D(P + u)[1 - (1 - u)] \\ \le \;& -[D + \lambda(1 - u)][A(1 - u) - \lambda(P + u)]. \end{aligned}$$

Here we have dropped the term $\frac{1}{2}P$ in the first inequality and used $\kappa^2 = \lambda(\lambda + D)$ in the second inequality. The assertion of the Lemma thus follows from the Gronwall's inequality. □

Proof of Theorem 1. The non-existence follows directly from Lemmas 5. We now prove the existence. Simple computation shows that $v \leqslant 4D/\sqrt{1 + 4D}$ is equivalent to $\lambda \leqslant 1/4$. We proceed to show that $P - u(1 - u)/2 \leqslant 0$ on $(0, 1)$. It is easy to verify, using result of Lemma 6, that

$$\begin{aligned} P[2P - u(1 - u)]' &= P(2u - 3) + 2A(1 - u)^2 \\ &\le P(2u - 3) + 2\lambda(P + u)(1 - u) \\ &= [u - 3/2 + \lambda(1 - u)][2P - u(1 - u)] \\ &\quad + u(1 - u)[2\lambda(1 - u) + \lambda(1 - u) + u - 3/2] \\ &< [u - 3/2 + \lambda(1 - u)][2P - u(1 - u)], \end{aligned}$$

since $\lambda \leq 1/4$ yields

$$\begin{aligned} & 2\lambda + \lambda(1-u) + u - 3/2 \\ \leq & \ 2\lambda + \lambda(1-u) + u - 3/2 \\ = & \ 2\lambda - 1/2 + (\lambda - 1)(1-u) \leq 0. \end{aligned}$$

Because $2P < u(1+u)$ for small u, the Gronwall's inequality shows that $P < u(1-u)/2$ on $(0,1)$. Thus $P(1) = 0$. This proves the existence, and completes the proof of the theorem. □

3. **Propagation of Local Disturbances in Quadratic Auto-Catalysis.** In this section, we study the quadratic system (2). The main purpose is to show that with a proper initial set-up, it generate wavefronts which propagate outward from the initial reaction zone, consuming fresh reactant ahead of the wavefront as it propagates.

Our basic assumption is the following:

(A1) $D \in (0, 1]$;
(A2) $u_0(x) = 1$ for all $x \in \mathbb{R}$;
(A3) v_0-a continuous non-negative function having compact support with $v_0(0) > 0$.

Our main result is the following:

Theorem 3. *Assume* **(A1)–(A3)** *and let* (u, v) *be the solution of (2). Set*

$$m(t) = 2t - 3(\log[3+t] - \log 3).$$

Then for each $t > 0$ *and* $x \in [-m(t), m(t)]$, $(u, v) \approx (0, 1)$ *in the following sense*

$$u(x,t) \leqslant e^{-\mu[m(t)-|x|]}, \qquad \Big|1 - v(x,t)\Big| \leqslant \frac{C}{\sqrt{1 + m(t) - |x|}}.$$

On the other-hand, when $x \in (-\infty, -m(t)] \cup [m(t), \infty)$, $(u, v) \approx (1, 0)$ *in the sense that*

$$\Big|1 - u(x,t)\Big| + v(x,t) \quad \leqslant \quad C\Big\{1 + |x| - m(t)\Big\} e^{m(t)-|x|}.$$

Whenever an auto-catalyst presents, the chemical reaction takes place very fast; as a result, the reactant is consumed quickly and therefore experiences an exponential decay (in time). The central issue here is to find the spreading speed of the auto-catalyst. Mathematically, by assuming D 2 (0; 1] (i.e. reactant diffuses no faster than the auto-catalyst does), we are able to find a good comparison to pin down the auto-catalyst's spreading speed. Due to the limit of the length, we shall not include the proof here, for the details see [2].

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