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The development of travelling waves in cubic auto-catalysis with different rates of diffusion

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Abstract

In this paper we study the isothermal auto-catalytic chemical reaction, $A + 2B \to 3B$ involving two chemical species A and B. Their diffusion coefficients, denoted by D_A and D_B, respectively, are unequal, which happens when the two chemical species have different molecular weights. The propagating reaction–diffusion waves that may develop from a local initial input of the auto-catalyst, B, are investigated in one spatial dimension. We show the existence of travelling wave solutions for all propagation speed $v \geq v_2^*$, with v_2^* a function of the ratio of the diffusion rates of the species A and B, representing the estimated minimum propagation speed. Our result improves significantly on the results of early works. In addition, we show the non-existence of travelling wave solutions when $v \leq v_2$, where v_2 depends on the ratio of the diffusion rates of the species A and B. We believe that our non-existence result is the first of the kind for equations of the isothermal auto-catalytic chemical reaction type. We also demonstrate similar results on the general isothermal auto-catalytic chemical reaction, $A + nB \to (n+1)B$, of n-th order with $n > 1$.

Keywords: Cubic auto-catalysis; Travelling wave; Minimum speed; Reaction–diffusion

1. Introduction

In this paper we consider the isothermal, auto-catalytic chemical reaction step which is governed by the cubic chemical reaction relation

$$A + 2B \to 3B \quad \text{with rate } kab^2. \tag{1.1}$$

Here, k is a positive rate constant, a and b are the concentrations of A and B, respectively. It is well documented in the literature that (1.1) has been used in several important models of real chemical reaction systems. For example, almost isothermal flames in the carbon–sulphide–oxygen reaction can be described in terms of the cubic auto-catalytic step (1.1) (Voronkov and Semenov [19]). It also provides a good model for both the iodate–arsenous acid reaction (Sauland Showalter [16]) and hydroxylamine–nitrate reaction (Gowland and Stedman [10]). For other applications, see also Aris et al. [1] and Sel'kov [17].

Experimental observations demonstrate that chemical systems for which cubic catalysis forms a key step can have propagating chemical wavefronts, when the reaction mixture is unstirred (see [11,21]). These wavefronts, or travelling waves, arise due to the interaction of reaction and diffusion. A typical situation which leads to the development of travelling waves is that which occurs when a quantity of the auto-catalyst, B, is added locally into an expanse of the reactant, A, which is initially at uniform concentration. The ensuing reaction is often observed to generate wavefronts, which propagate outward from the initial reaction zone, consuming fresh reactant A ahead of the wavefront as it propagates. This is the phenomenon that we address in the present paper. For simplicity, we shall discuss the one-dimensional slab geometry. The partial differential equations that govern mass concentration and molecular diffusion for the species A and B for the reaction scheme (1.1) are

$$\begin{aligned} \frac{\partial a}{\partial t} &= D_A \frac{\partial^2 a}{\partial x^2} - kab^2, \\ \frac{\partial b}{\partial t} &= D_B \frac{\partial^2 b}{\partial x^2} + kab^2, \end{aligned} \tag{1.2}$$

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where D_A and D_B are the constant diffusion rates of the reactant, A, and the auto-catalyst, B, respectively. The kinds of initial conditions, in accordance with the results of observed experiments, are

$$a(x,0) = a_0, \qquad b(x,0) = b_0 g(x), \tag{1.3}$$

where $g(x)$ is a given non-negative function of x with a maximum value of unity and compact support. Here a_0 and b_0 are the positive, constant initial concentration of A and maximum initial concentration of B respectively. In addition, we have the following boundary conditions:

$$a(x,t) \to a_0, \qquad b(x,t) \to 0 \quad \text{as } |x| \to \infty. \tag{1.4}$$

Introducing dimensionless variables

$$\alpha = \frac{a}{a_0}, \qquad \beta = \frac{b}{a_0}, \qquad \bar{t} = ka_0^2 t, \qquad \bar{x} = \left(\frac{ka_0^2}{D_A}\right)^{1/2} x,$$

and dropping overbars, the initial–boundary value problem (1.2)–(1.4) becomes

$$\begin{aligned} \frac{\partial \alpha}{\partial t} &= \frac{\partial^2 \alpha}{\partial x^2} - \alpha\beta^2, \\ \frac{\partial \beta}{\partial t} &= D\frac{\partial^2 \beta}{\partial x^2} + \alpha\beta^2, \end{aligned} \tag{1.5}$$

where $D = D_B/D_A$ and

$$\alpha(x,0) = 1, \qquad \beta(x,0) = \beta_0 g(x), \quad |x| < \infty. \tag{1.6}$$

The dimensionless parameter $\beta_0 = b_0/a_0$ is a measure of the maximum concentration of the initial input of the auto-catalyst, B, in relation to that of reactant A, whereas the dimensionless parameter, D, measures the rate of diffusion of the auto-catalyst, B, relative to that of the reactant A. The primary assumption of the present paper is $D \neq 1$, which arises when the chemical species involved have different molecular weights. In particular, enzyme reactions may involve large enzyme molecules and smaller substrate molecules, which can lead to very different rates of diffusion. Eq. (1.5) also arises in epidemiology, where α represents the population density of healthy individuals (see Bailey [3]) and β the population density of infected individuals. Again, when healthy individuals are significantly more or less mobile than the infected ones, D is very different from unity. When $D = 1$, the system can be reduced to a single equation, for which significant results and rich theory are established. We refer the reader to the works of Aronson and Weinberger [2], Chen and Guo [7], Fife and McLeod [8], Sattinger [15] and the excellent review paper by Xin [20] for detailed information.

An important part to the study of initial–boundary value problem (1.5) and (1.6) is the existence and non-existence of the travelling wave solutions, which may be generated from the initial–boundary value problem (1.5) and (1.6). We study these in this paper.

The equations which govern travelling wave solutions are obtained by looking for a solution of (1.5) in the form of $\alpha = a(x - vt), \beta = \beta(x - vt)$, which take the form, with

$$z = x - vt,$$

$$\begin{aligned} &\alpha_{zz} + v\alpha_z - \alpha\beta^2 = 0, \\ &D\beta_{zz} + v\beta_z + \alpha\beta^2 = 0, \end{aligned} \tag{1.7}$$

where $v > 0$ is the constant speed of propagation. Following the convention, in light of the scaling invariance of the equation under the transformation

$$u_\lambda(x,t) = \lambda u(\lambda x, \lambda^2 t), \quad \lambda > 0,$$

we consider the non-negative solution of (1.5) with $0 \le \alpha, \beta \le 1$. We make the following definition.

Definition 1.1. A travelling wave solution of (1.5) is a positive solution of (1.7) which satisfies the conditions $\alpha \to 1, \beta \to 0$ as $z \to \infty$ and $\alpha \to 0, \beta \to 1$ as $z \to -\infty$.

One of the most important questions in the study of (1.7) is that of the existence of a minimum speed travelling wave solution and the estimate of the minimum speed $v_{\min}$. In particular, a key question is: for what range of v, in relation to D, does a travelling wave solution exist?

The existence of travelling wave solutions to (1.5) and a related equation where the nonlinearity is $\alpha\beta$, instead of $\alpha\beta^2$,

$$\begin{aligned} \frac{\partial \alpha}{\partial t} &= \frac{\partial^2 \alpha}{\partial x^2} - \alpha\beta, \\ \frac{\partial \beta}{\partial t} &= D\frac{\partial^2 \beta}{\partial x^2} + \alpha\beta, \end{aligned} \tag{1.8}$$

is investigated extensively by Billingham, Merkin and Needham in a number of very important works (see [4,5,12–14]). A related work by Focant and Gallay [9] investigated the existence and stability of travelling waves when both the quadratic and cubic nonlinearities are present in the system. In particular, it was shown analytically in [4] that for both Eqs. (1.5) and (1.8), travelling wave solutions exist if

$$v > 2\sqrt{D}. \tag{1.9}$$

It was pointed out in [4] that, although the above result is optimal for the quadratic auto-catalysis (1.8), this is not the case for the cubic auto-catalysis (1.5). The authors then use other means, including numerical simulation, to provide a better estimates for $v_{\min}$.

The present work is very much stimulated by the pioneering works of Billingham, Merkin and Needham [4,5,12–14]. The main purpose of the present work is to show rigorously that the range of speed v for the existence of travelling wave solutions is considerably larger than the bound given in (1.9), making us a step closer to verifying analytically the bound given in [4] obtained by numerical simulation. For instance, it is shown in [4] numerically that $v_{\min} \sim 1.219D$ if $D \ll 1$, $v_{\min} \sim 0.862\sqrt{D}$ if $D \gg 1$. Our first result is as follows:

Theorem 1. *A unique travelling wave solution to (1.5) exists for*

$$v \ge \begin{cases} \sqrt{2D-1} & \text{if } D \ge 1, \\ \sqrt{D} & \text{if } D < 1. \end{cases}$$

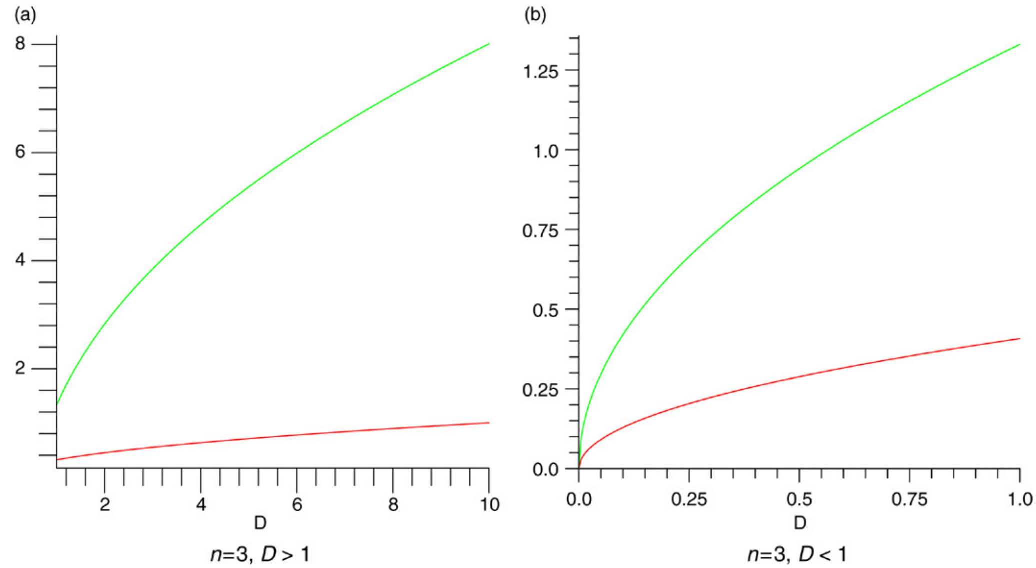

Fig. 1. Existence and non-existence curves.

Remark. The result of Theorem 1 comes out of more detailed analysis and better use of the structures of equations than in earlier works. The basic method is a variant of invariant region method as in [4].

On the other hand, we demonstrate that such solutions do not exist if v is relatively small. More precisely, we have

Theorem 2. *There exists no travelling wave solution for* (1.5) *if*

$$v \le \begin{cases} \sqrt{D/6} & \text{when } D \ge 1, \\ D/\sqrt{6} & \text{when } D < 1. \end{cases}$$

Remark. The authors of [4], on the basis of the results of asymptotic analysis and numerical simulation, conjectured that if $D \ll 1$, the travelling wave solution exists only in the range of $v = O(D)$. The above result provides a partial answer to that conjecture.

For the general n-th-order isothermal, auto-catalytic chemical reaction step which is governed by the chemical reaction relation

$$A + nB \to (n+1)B \quad \text{with rate } kab^n, \tag{1.10}$$

and $n > 1$, we can demonstrate both existence of a travelling wave solution if v is suitably large, and non-existence if v is relatively small. For this case, the governing equation, after proper scaling is

$$\begin{aligned} \frac{\partial \alpha}{\partial t} &= \frac{\partial^2 \alpha}{\partial x^2} - \alpha\beta^n, \\ \frac{\partial \beta}{\partial t} &= D\frac{\partial^2 \beta}{\partial x^2} + \alpha\beta^n, \end{aligned} \tag{1.11}$$

where $D = D_B/D_A$ and the initial value is as in (1.6).

Theorem 3. *A unique travelling wave solution exists for* (1.11) *if*

$$v \ge f(D) \equiv \begin{cases} 2\sqrt{D}\left(\frac{(n-1)(2D-1)}{D}\right)^{(n-1)/2} \Big/ n^{n/2} & \text{when } D \ge 1, \\ \sqrt{D}\sqrt{4(n-1)^{n-1}/n^n} & \text{when } D < 1. \end{cases}$$

There exists no travelling wave solution for (1.11) *if*

$$v \le g(D) \equiv \begin{cases} \sqrt{2D/(n+1)(n+2)} & \text{when } D \ge 1 \\ D\sqrt{2/(n+1)(n+2)} & \text{when } D < 1. \end{cases}$$

An illustration of the range of speeds of travelling waves for existence and non-existence is given in Fig. 1.

We note in passing the recent works studying the spatio-temporal profiles of L^1 initial values by Bricmont et al. [6] and the steady-state solutions of Shi and Wang [18].

The organization of this paper is as follows. In Section 2, we show existence for the cubic case (1.5) and (1.6). The non-existence of the cubic case is proved in Section 3. The general n-th-order case of (1.6)–(1.11) is dealt with in Section 4.

2. Existence of the cubic case

In this section, we show the existence of a travelling wave solution to (1.5) and prove Theorem 1.

It is easy to derive (see [4] or (2.2) below) that with the new variable $w = \beta_z$, the system (1.7) can be written as an equivalent third-order system:

$$\begin{aligned} \alpha_z &= v(1-\alpha-\beta) - Dw \\ \beta_z &= w \\ w_z &= -D^{-1}(\alpha\beta^2 + vw). \end{aligned} \tag{2.1}$$

It is clear that in the phase space of (2.1) there are two equilibrium points $(0, 1, 0)$ and $(1, 0, 0)$. We start by listing some basic properties of travelling wave solutions for which the proof can be found either in [4] or by elementary computation.

Proposition 1. *Suppose* (α, β) *is a travelling wave solution to* (1.5)*, then it has the following properties:*

(i) $\alpha_z > 0$, $\beta_z < 0$ *for all* $-\infty < z < \infty$.
(ii) $\alpha+\beta < 1$ *for all* $-\infty < z < \infty$ *if* $D < 1$, *while* $\alpha+\beta > 1$ *for all* $-\infty < z < \infty$ *if* $D > 1$.
(iii) $\alpha + D\beta = 1 + (D-1)e^{-vz}\int_{-\infty}^{z} v\beta e^{vs}\,ds$.
(iv) $\int_{-\infty}^{\infty}\alpha\beta^2 = v$.
(v) *The equilibrium point* $(0, 1, 0)$ *is a simple equilibrium point with a two-dimensional stable manifold and a one-dimensional unstable manifold. The eigenvalues and associated eigenvectors are*

$$\lambda_1 = -vD^{-1}, \qquad \mathbf{e}_{\lambda_1} = (0, -1, -\lambda_1)^T$$
$$\lambda_2 = -\frac{1}{2}\left(\sqrt{v^2+4}+v\right),$$
$$\mathbf{e}_{\lambda_2} = (\lambda_2(D\lambda_2+v), -1, -\lambda_2)^T$$
$$\lambda_3 = \frac{1}{2}\left(\sqrt{v^2+4}-v\right),$$
$$\mathbf{e}_{\lambda_3} = (\lambda_3(D\lambda_3+v), -1, -\lambda_3)^T.$$

(vi) *The equilibrium point* $(1, 0, 0)$ *is not a simple equilibrium point. It has a two-dimensional stable manifold and a one-dimensional center manifold. The eigenvalues and associated eigenvectors are*

$$\nu_1 = -v, \qquad \mathbf{e}_{\nu_1} = (1, 0, 0)^T$$
$$\nu_2 = vD^{-1}, \qquad \mathbf{e}_{\nu_2} = (0, -1, -vD^{-1})^T$$
$$\nu_3 = 0, \qquad \mathbf{e}_{\nu_3} = (1, -1, 0)^T.$$

Proof. All items except (iii) and (iv) have been proved in [4]. The proof of (iv) is straightforward, by direct integration of, say, the first equation of (1.7), and use of the boundary condition $\alpha \to 0$ as $z \to -\infty$ and $\alpha \to 1$ as $z \to \infty$. We now proceed to show (iii). By adding the two equations in (1.7), we get

$$(\alpha + D\beta)'' + v(\alpha+\beta)' = 0,$$

which upon an integration yields

$$(\alpha + D\beta)' + v(\alpha+\beta-1) = 0. \tag{2.2}$$

Multiplying the above equation by e^{vz} and integrating over $(-\infty, z)$ gives

$$(\alpha + D\beta)e^{vz} = e^{vz} + (D-1)\int_{-\infty}^{z} v\beta e^{vs}\,ds,$$

which is exactly (iii). This completes the proof of Proposition 1. □

Proof of Theorem 1. We start by considering the case of $D < 1$. Define the region R by

$$R = \left\{(\alpha, \beta, w) : 0 \le \alpha, 0 \le \alpha+\beta \le 1, 0 \le \beta \le 1, -\frac{v\beta}{2D} \le w \le 0\right\}.$$

It is clear that the travelling wave solution must come out of the unstable manifold of $(0, 1, 0)$ and by (v) of Proposition 1 go into R. This is because, by Proposition 1, along the unstable manifold,

$$\alpha = e^{\lambda_3 z}(D\lambda_3^2 + v\lambda_3), \qquad \beta - 1 = -e^{\lambda_3 z},$$

with

$$\lambda_3 = \frac{1}{2}\left(\sqrt{v^2+4}-v\right)$$

satisfying $\lambda_3^2 + v\lambda_3 = 1$. Hence,

$$\alpha+\beta-1 = e^{\lambda_3 z}(D\lambda_3^2 + v\lambda_3 - 1) < 0,$$

using the fact that $D < 1$. We proceed to show that all integral paths, once inside R, cannot get out. It suffices to prove that all such integral paths are directed strictly inside R at the faces of R, whilst they are directed into or along the surface of R at the edges. It is very easy to compute that on the face of $\alpha = 0$, $\alpha_z \ge 0$; on the face of $\beta = 1$, $\beta_z \le 0$, and $\beta > 0$ using the last condition of R. Therefore, we only need to establish the following facts:

(i) When $\alpha+\beta = 1$, $\alpha_z + \beta_z \le 0$,
(ii) When $w = -\frac{v\beta}{2D}$, $w_z + \frac{vw}{2D} \ge 0$.

(i) is readily verified using

$$\alpha_z + \beta_z = (1-D)w \le 0$$

when $\alpha+\beta = 1$. As for (ii),

$$w_z + \frac{vw}{2D} = -D^{-1}\left(\frac{vw}{2} + \alpha\beta^2\right) = -D^{-1}\left(-\frac{v^2}{4D} + \alpha\beta\right)\beta \ge 0,$$

since $\alpha+\beta \le 1$ implies $\alpha\beta \le 1/4$ and $v^2 \ge D$. This proves the case of $D < 1$.

When $D > 1$, suppose first that $v > \sqrt{2D-1}$; define the region R by

$$R = \left\{(\alpha, \beta, w) : 0 \le \alpha, 0 \le \alpha + c\beta \le 1, 0 \le \beta \le 1, -\frac{v\beta}{2D} \le w \le 0\right\}.$$

Here $c = D/(2D-1) - \epsilon$, with $\epsilon > 0$ arbitrarily small, satisfies $1/2 < c < 1$. At the face of $\alpha + c\beta = 1$,

$$\alpha_z + c\beta_z = v\beta(c-1) + (c-D)w < v\beta \times \left(c - 1 + \frac{D-c}{2D}\right) \le 0.$$

At the face of $w = -\frac{v\beta}{2D}$,

$$w_z + \frac{vw}{2D} = -D^{-1}\left(\frac{vw}{2D} + \alpha\beta^2\right) = -D^{-1}\left(\frac{v^2}{4D} + \alpha\beta\right)\beta \ge 0,$$

since $\alpha\beta \le \beta(1-c\beta) \le 1/4c$. The rest is the same as in $D < 1$. By continuity, R is invariant when $v = \sqrt{2D-1}$. This completes the proof of Theorem 1. □

Remark. If $D > 7/5$, we can prove a better estimate on the minimum speed v for which the travelling wave solution exists by using a more precise relation of α and β, property (iii) in Proposition 1.

Let

$$R = \left\{(\alpha, \beta, w) : 0 \le \alpha \le 1, 0 \le \beta \le 1, -\frac{v\beta}{3D} \le w \le 0\right\}.$$

We show that once the integral path, represented by the unstable manifold of (0, 1, 0), gets into R, it stays inside R when

$$v \ge \frac{3}{4}\sqrt{3D-1}. \tag{2.3}$$

This means that there is a unique travelling wave solution to (1.5) if

$$v \ge \frac{3}{4}\sqrt{3D-1}.$$

The only thing we need to show is that when $w = -\frac{v\beta}{3D}$, say at $z = z_0$, then $w_z + \frac{vw}{3D} \ge 0$ at the same point. Using the fact that $w + \frac{v\beta}{3D} \ge 0$ before the integral path hits the face, we obtain

$$\beta \ge \left(1 - \frac{1}{3D}\right) e^{-vz_0} \int_{-\infty}^{z_0} v\beta e^{vs}\, ds > 0.$$

This yields, in turn, at $z = z_0$,

$$\alpha \le 1 - D\beta + \frac{3D(D-1)}{3D-1}\beta, \quad \text{and} \quad \alpha\beta \le \frac{3D-1}{8D}.$$

One can now verify, using the above estimate of $\alpha\beta$, that

$$w_z + \frac{vw}{3D} \ge 0$$

at $z = z_0$.

3. Non-existence of the cubic case

In this section, we show the non-existence of a travelling wave solution to (1.5) when v is relatively small. The key to our approach is deriving integral identities involving α and β when (α, β) is a travelling wave solution.

First, we have

$$\int_{-\infty}^{\infty} (\alpha')^2\, dz + \int_{-\infty}^{\infty} \alpha^2\beta^2\, dz = \frac{v}{2}. \tag{3.1}$$

This is obtained by multiplying the first equation in (1.7) by α and integrating on R^1, taking into consideration $\alpha \to 1$ as $z \to \infty$ and $\alpha \to 0$ as $z \to -\infty$. Similarly, we get

$$D\int_{-\infty}^{\infty} (\beta')^2\, dz + \frac{v}{2} = \int_{-\infty}^{\infty} \alpha\beta^3 dz. \tag{3.2}$$

Multiplying the first equation in (1.7) by β and integrating on R^1, we obtain

$$-\int_{-\infty}^{\infty} \alpha'\beta'\, dz + v\int_{-\infty}^{\infty} \alpha'\beta\, dz - \int_{-\infty}^{\infty} \alpha\beta^3 = 0.$$

Similarly, multiplying the second equation in (1.7) by α and integrating on R^1, we have

$$-D\int_{-\infty}^{\infty} \alpha'\beta' dz + v\int_{-\infty}^{\infty} \alpha\beta' dz + \int_{-\infty}^{\infty} \alpha^2\beta^2 dz = 0.$$

By adding the above two identities, we obtain

$$-(D+1)\int_{-\infty}^{\infty} \alpha'\beta' dz = \int_{-\infty}^{\infty} \alpha\beta^3 - \int_{-\infty}^{\infty} \alpha^2\beta^2 dz$$
$$= \int_{-\infty}^{\infty} (\alpha')^2 dz + D\int_{-\infty}^{\infty} (\beta')^2 dz. \tag{3.3}$$

Here the last identity is a direct consequence of (3.1) and (3.2).

Proof of Theorem 2. The proof will be based on estimating the integral $\int_{-\infty}^{\infty} (\beta')^2\, dz$ in relation to D and v for a travelling wave solution. Our key estimate is

$$\frac{1}{12} \le v\int_{-\infty}^{\infty} (\beta')^2 dz < \min\left(\frac{1}{3}, \frac{D}{12}\right) \quad \text{if } D > 1. \tag{3.4}$$

Multiplying the second equation in (1.7) by β' and integrating on R^1, we have

$$v\int_{-\infty}^{\infty} (\beta')^2 dz = -\int_{-\infty}^{\infty} \beta'\alpha\beta^2 dz < -\int_{-\infty}^{\infty} \beta'\beta^2 dz = \frac{1}{3}. \tag{3.5}$$

Furthermore, using the fact that $\alpha' < -D\beta'$ when $D > 1$, we get

$$-\int_{-\infty}^{\infty} \beta'\alpha\beta^2 dz = \frac{1}{3}\int_{-\infty}^{\infty} \alpha'\beta^3 dz < \frac{D}{3}$$
$$\times \int_{-\infty}^{\infty} -\beta'\beta^3 dz = \frac{D}{12}. \tag{3.6}$$

But, since $\alpha > 1 - \beta$ when $D > 1$, and $\beta' < 0$,

$$-\int_{-\infty}^{\infty} \beta'\alpha\beta^2 dz > -\int_{-\infty}^{\infty} \beta'(1-\beta)\beta^2 dz = \frac{1}{12}. \tag{3.7}$$

The combination of (3.5)–(3.7) gives (3.4). Now, we can show the non-existence if $D > 1$. By (iv) of Proposition 1 and (3.2), we have

$$\frac{D}{12v} < D\int_{-\infty}^{\infty} (\beta')^2 dz < v/2,$$

therefore, $v > \sqrt{D/6}$ when $D > 1$.

When $D < 1$, the estimate we employ is

$$\frac{D}{12} \le v\int_{-\infty}^{\infty} (\beta')^2 dz < \frac{1}{12}, \tag{3.8}$$

which can be verified similarly as (3.4). The comparison of (3.2) and (3.8) yields

$$\frac{D^2}{12v} < D\int_{-\infty}^{\infty} (\beta')^2\, dz < v/2,$$

which implies immediately that $v > D/\sqrt{6}$. This completes the proof of Theorem 2. □

Remark. The non-existence bound can be improved significantly if, like in the proof of Theorem 1, we consider the travelling wave solution with the property $\beta' \ge -v\beta/2D$. Then it is easy to verify that

$$D\int_{-\infty}^{\infty} (\beta')^2 dz < \frac{v}{4}.$$

The same reasoning as in Theorem 2 would lead to the conclusion that there exists no travelling wave solution with the property $\beta' \geq -v\beta/2D$ if

$$v \leq \begin{cases} \sqrt{D/3} & \text{when } D \geq 1, \\ D/\sqrt{3} & \text{when } D < 1. \end{cases}$$

Likewise, no travelling wave solution with the property $\beta' \geq -v\beta/3D$ exists if

$$v \leq \begin{cases} \sqrt{D/2} & \text{when } D \geq 1, \\ D/\sqrt{2} & \text{when } D < 1. \end{cases}$$

It is interesting to note that, since the minimum speed of $D = 1$ case is $v = 1/\sqrt{2}$, the above expression looks very close to optimal, at least when D is close to one. But, we are unable to rigorously show the exact value of the minimum speed for the general case of $D \neq 1$. The answer is given in [4] using numerical simulation for both $D \ll 1$ and $D \gg 1$.

4. The n-th-order auto-catalysis

In this section, we demonstrate that the results that we proved in the previous two sections for cubic auto-catalysis can be generalized to the n-th-order auto-catalysis reaction whose governing equations are as in (1.11).

First, we observe that all properties listed in Proposition 1 are true except (iv), which should be replaced by

$$\int_{-\infty}^{\infty} \alpha\beta^n \mathrm{d}z = v.$$

Next, we list some integral identities which resemble that of the cubic case of $n = 2$:

$$\int_{-\infty}^{\infty} (\alpha')^2 \mathrm{d}z + \int_{-\infty}^{\infty} \alpha^2\beta^n \mathrm{d}z = \frac{v}{2}. \tag{4.1}$$

This is obtained by multiplying the first equation in (1.11) by α and integrating on R^1, taking into consideration $\alpha \to 1$ as $z \to \infty$ and $\alpha \to 0$ as $z \to -\infty$. Similarly, we get

$$D\int_{-\infty}^{\infty} (\beta')^2 \mathrm{d}z + \frac{v}{2} = \int_{-\infty}^{\infty} \alpha\beta^{n+1} \mathrm{d}z. \tag{4.2}$$

Multiplying the first equation in (1.11) by β and integrating on R^1, we have

$$-\int_{-\infty}^{\infty} \alpha'\beta' \mathrm{d}z + v\int_{-\infty}^{\infty} \alpha'\beta \mathrm{d}z - \int_{-\infty}^{\infty} \alpha\beta^{n+1} = 0.$$

Similarly, multiplying the second equation in (1.11) by α and integrating on R^1, we have

$$-D\int_{-\infty}^{\infty} \alpha'\beta' \mathrm{d}z + v\int_{-\infty}^{\infty} \alpha\beta' \mathrm{d}z + \int_{-\infty}^{\infty} \alpha^2\beta^n \mathrm{d}z = 0.$$

By adding the above two identities, we obtain

$$\begin{aligned} -(D+1)\int_{-\infty}^{\infty} \alpha'\beta' \mathrm{d}z &= \int_{-\infty}^{\infty} \alpha\beta^{n+1} - \int_{-\infty}^{\infty} \alpha^2\beta^n \mathrm{d}z \\ &= \int_{-\infty}^{\infty} (\alpha')^2 \mathrm{d}z + D\int_{-\infty}^{\infty} (\beta')^2 \mathrm{d}z. \end{aligned} \tag{4.3}$$

Here the last identity is a direct consequence of (4.1) and (4.2).

Proof of Theorem 3. The existence part can be proved exactly as in Theorem 1. We only need to note that if $D < 1$,

$$\alpha\beta^{n-1} \leq (1-\beta)\beta^{n-1} \leq \frac{(n-1)^{n-1}}{n^n}, \quad \text{since } \alpha \leq 1-\beta.$$

However for $D > 1$,

$$\alpha\beta^{n-1} \leq (1-c\beta)\beta^{n-1} \leq \frac{1}{n}\left(\frac{n-1}{nc}\right)^{n-1}, \quad \text{since } \alpha \leq 1-c\beta,$$

where $c = D/(2D-1)$.

The proof of non-existence will be based on estimating the integral $\int_{-\infty}^{\infty} (\beta')^2 \mathrm{d}z$ in relation to D and v for a travelling wave solution. Our key estimate is

$$\begin{aligned} \frac{1}{(n+1)(n+2)} &\leq v\int_{-\infty}^{\infty} (\beta')^2 \mathrm{d}z \\ &< \min\left(\frac{1}{n+1}, \frac{D}{(n+1)(n+2)}\right) \quad \text{if } D > 1. \end{aligned} \tag{4.4}$$

Multiplying the second equation in (1.11) by β' and integrating on R^1, we have

$$\begin{aligned} v\int_{-\infty}^{\infty} (\beta')^2 \mathrm{d}z &= -\int_{-\infty}^{\infty} \beta'\alpha\beta^n \mathrm{d}z < -\int_{-\infty}^{\infty} \beta'\beta^n \mathrm{d}z \\ &= \frac{1}{n+1}. \end{aligned} \tag{4.5}$$

Furthermore, using the fact that $\alpha' < -D\beta'$ when $D > 1$, we get

$$\begin{aligned} -\int_{-\infty}^{\infty} \beta'\alpha\beta^n \mathrm{d}z &= \frac{1}{n+1}\int_{-\infty}^{\infty} \alpha'\beta^{n+1} \mathrm{d}z < \frac{D}{n+1} \\ &\times \int_{-\infty}^{\infty} -\beta'\beta^{n+1} \mathrm{d}z = \frac{D}{(n+1)(n+2)}. \end{aligned} \tag{4.6}$$

But, since $\alpha > 1-\beta$ when $D > 1$,

$$\begin{aligned} -\int_{-\infty}^{\infty} \beta'\alpha\beta^n \mathrm{d}z &> -\int_{-\infty}^{\infty} \beta'(1-\beta)\beta^n \mathrm{d}z \\ &= \frac{1}{(n+1)(n+2)}. \end{aligned} \tag{4.7}$$

The combination of (4.5)–(4.7) gives (4.4). By (iv) of Proposition 1 and (4.2), we have

$$\frac{D}{(n+1)(n+2)v} < D\int_{-\infty}^{\infty} (\beta')^2 \mathrm{d}z < v/2,$$

and therefore,

$$v > \sqrt{\frac{2D}{(n+1)(n+2)}}$$

when $D > 1$.

When $D < 1$, the estimate we employ is

$$\frac{D}{(n+1)(n+2)} \leq v\int_{-\infty}^{\infty} (\beta')^2 \mathrm{d}z < \frac{1}{(n+1)(n+2)}, \tag{4.8}$$

which can be verified similarly to (4.4). The comparison of (4.2) and (4.8) yields

$$\frac{D^2}{(n+1)(n+2)v} < D\int_{-\infty}^{\infty}(\beta')^2 \mathrm{d}z < v/2,$$

which implies immediately that

$$v > D\sqrt{\frac{2}{(n+1)(n+2)}}.$$

This completes the proof of Theorem 3. □

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