The effects of coupling on chemical wave propagation in quadratic and cubic autocatalysis with decay

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The initiation of reaction-diffusion travelling waves in two regions coupled together by the linear diffusive interchange of an autocatalytic species is considered. In one region a purely autocatalytic production process (either quadratic or cubic) is assumed, while in the other region there are both autocatalytic and decay processes (either linear or quadratic). A perturbation analysis based on small initial inputs of the autocatalyst is presented. This indicates conditions under which travelling wave formation is possible as well as identifying two special cases which need further consideration, namely cubic autocatalysis in both regions with quadratic or linear decay in one region. The former case gives rise to a zero eigenvalue and the perturbation method has to be extended to include the higher order terms to resolve this case. The latter case requires a threshold on the initial input of autocatalyst and further information about this threshold is gained from a solution for strong coupling.

1. Introduction

In a previous paper [1] we considered the reaction-diffusion travelling waves that can develop in a coupled system involving simple isothermal autocatalytic (or chain-branching) kinetics. More specifically, we assumed that reactions took place in two separate and parallel regions, with, in region I, the reaction being given by quadratic autocatalysis

$$A + B \to 2B \quad \text{rate} \quad k_1 ab \tag{1a}$$

together with a linear decay (or termination) step

$$B \to C \quad \text{rate} \quad k_2 b \tag{1b}$$

(a and b are the concentrations of reactant A and autocatalyst B, the k_i are the rate constants and C is some inert product of reaction). The reaction in region II was just the quadratic autocatalytic production step (1a). The two regions were assumed to be coupled via a linear diffusive interchange of the autocatalytic species B. We took both regions to be infinite in extent and considered the propagation of

plane waves travelling parallel to each other. The waves were initiated through the simultaneous and localized input of some autocatalyst B into both regions.

We found that conditions for the initiation of travelling waves were independent of the magnitude of the local input of the autocatalyst B in the two regions, as described by the dimensionless parameters $\beta_0^{(i)}$ ($i = 1, 2$). However, these conditions did depend on the strength of the decay relative to the production step, given by the dimensionless parameter $k = k_2/k_1 a_0$ (where a_0 is the uniform initial concentration of reactant A), and the strength of the coupling between the two regions, characterized by the dimensionless parameter γ. In particular, we found that waves would form for all values of k when $\gamma < 1$, but required $k < (2\gamma - 1)/(\gamma - 1)$ when $\gamma > 1$. (Note that for the uncoupled system, travelling waves can develop in region I only when $k < 1$, [2].)

In a systematic analysis of this problem we identified the solution valid for small initial inputs of autocatalyst B, i.e. $\beta_0^{(i)} \ll 1$, as one which gave a clear insight into the nature of the solution of the general problem. Using this approach, we were able to identify the conditions on γ and k required for the initiation of reaction-diffusion travelling waves. These waves, which are the large time limit of the system, propagate with a constant speed v, their asymptotic wave speed, and are of permanent form, i.e. depend only on the single travelling co-ordinate $y = x - vt$. The small $\beta_0^{(i)}$ analysis also enabled us to determine the asymptotic wave speed v. In the present paper we use this approach to examine the conditions under which permanent-form travelling waves develop when, in region I, we have an autocatalytic production step, either quadratic (1a) or cubic.

$$\text{A} + 2\text{B} \rightarrow 3\text{B} \quad \text{rate} \quad k_3 ab^2 \tag{1c}$$

together with either a linear decay step (1b) or a quadratic decay step

$$\text{B} + \text{B} \rightarrow 2\text{C} \quad \text{rate} \quad k_4 b^2 . \tag{1d}$$

In region II we assume that there is still just an autocatalytic production step, either quadratic (1a) or cubic (1c). The coupling between the two regions is, in all cases, assumed to be via a linear diffusive interchange of autocatalyst B. (A schematic representation of the physical model is shown in fig. 1). The conditions under which travelling waves develop in region I, when not coupled to region II, have been treated in some detail by Merkin et al. [2] and Merkin and Needham [3,4].

The main purpose of our small $\beta_0^{(i)}$ analysis is to try to determine the conditions under which termination step in region I, characterized by the dimensionless parameter k, can inhibit (if at all) the formation of travelling waves in region II as the strength of the coupling between the two regions is varied. We find that we are able to do so for all but two cases, namely those which involve cubic autocatalysis in both regions I and II with either linear or quadratic decay steps in region I. In the former case we find that waves cannot be initiated for any values of γ and k for small initial inputs and there are threshold values for the $\beta_0^{(i)}$ to be overcome before wave formation could be achieved, (a similar situation was found in the uncoupled

I $A + nB \longrightarrow (n+1)B, (m, n = 1, 2)$

          $mB \longrightarrow C$

WAVES

COUPLING VIA B

WAVES

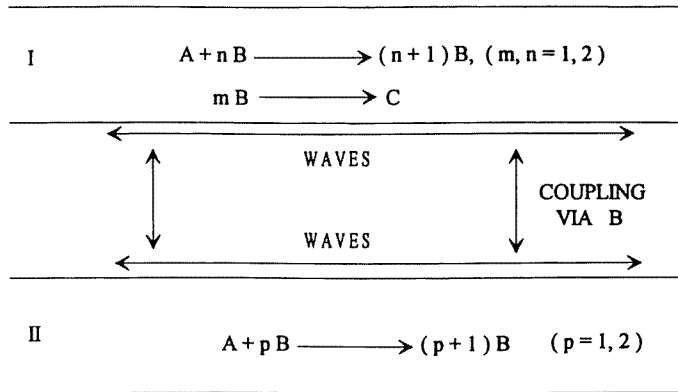II $A + pB \longrightarrow (p+1)B \quad (p = 1, 2)$

Fig. 1. A schematic representation of the physical model.

system, [3]). The latter gives rise to a zero eigenvalue and further considerations are required to determine the behaviour in this case.

We start by giving the dimensionless form of the equations for the initial-value problem. The appropriate non-dimensionalization, as well as some general a priori bounds, has already been given in [1].

2. Equations

From Merkin et al. [1] we have the following initial-value problem on $-\infty < x < \infty$, $t \geq 0$, for the dimensionless concentrations (α_1, β_1) in region I and (α_2, β_2) in region II of species A and B.

$$\frac{\partial \alpha_1}{\partial t} = \frac{\partial^2 \alpha_1}{\partial x^2} - \alpha_1 \beta_1^n, \tag{2a}$$

$$\frac{\partial \beta_1}{\partial t} = \frac{\partial^2 \beta_1}{\partial x^2} + \alpha_1 \beta_1^n - k\beta_1^m + \gamma(\beta_2 - \beta_1), \tag{2b}$$

$$\frac{\partial \alpha_2}{\partial t} = \frac{\partial^2 \alpha_2}{\partial x^2} - \alpha_2 \beta_2^p, \tag{2c}$$

$$\frac{\partial \beta_2}{\partial t} = \frac{\partial^2 \beta_2}{\partial x^2} + \alpha_2 \beta_2^p + \gamma(\beta_1 - \beta_2) \tag{2d}$$

(where $m, n, p = 1$ or 2). The initial and boundary conditions are

$$\alpha_i = 1, \quad \beta_i = \beta_0^{(i)} h_i(x) \quad \text{at} \quad t = 0, \quad -\infty < x < \infty, \tag{3a}$$

$$\alpha_i \to 1, \quad \beta_i \to 0 \quad \text{as} \quad |x| \to \infty \quad (t > 0) \tag{3b}$$

$(i = 1, 2)$, where

$$h_i(x) = \begin{cases} g_i(x), & |x| < \sigma, \\ 0, & |x| > \sigma, \end{cases}$$

and where the $g_i(x)$ are continuous and differentiable on $|x| < \sigma$ and have a maximum value of unity on this interval.

The physical situation modelled by eqs. (2) is that of relatively thin reaction zones (regions I and II) along which chemical species A and B are free to diffuse. The two regions are coupled through the transverse diffusion of the autocatalyst B, represented by a linear exchange term, the strength of which is characterized by the dimensionless parameter γ. A schematic description of the model is given in fig. 1 and is described in more detail in [1].

In [1] we established the a priori bounds for initial-value problem (2, 3):

$$0 \leqslant \alpha_i(x, t) \leqslant 1, \quad 0 \leqslant \beta_i(x, t) \leqslant 2 + \beta_0^{(1)} + \beta_0^{(2)} \tag{4}$$

$(i = 1, 2)$ on $-\infty < x < \infty$, $t \geqslant 0$. We were then able to use (4) to show that the initial-value problem (2, 3) had a unique global solution. These existence and uniqueness properties, as well as the boundedness of the solution, underpin our small $\beta_0^{(i)}$ solutions, which is what we discuss next.

3. Solution for $\beta_0^{(i)}$ small

Here we consider the solution of initial-value problem (2, 3) for $\beta_0^{(i)}$ small $(i = 1, 2)$. To do this we put $\beta_0^{(i)} = \epsilon B_0^{(i)}$ $(i = 1, 2)$ where $0 < \epsilon \ll 1$ and the $B_0^{(i)}$ are of $O(1)$ as $\epsilon \to 0$. We look for a solution by expanding

$$\alpha_i(x, t) = 1 + \epsilon^r A_i(x, t) + \dots, \quad \beta_i(x, t) = \epsilon B_i(x, t) + \dots \tag{5}$$

$(i = 1, 2)$ as $\epsilon \to 0$. Here $r = 1$ if any of $m, n, p = 1$ and $r = 2$ otherwise.

The equations for the B_i become decoupled from those for the A_i at leading order and it is these that we concentrate on. The form of the (linear) equations for the B_i depends on the nature of the reaction term and we start by considering quadratic autocatalysts $(p = 1)$ in region II.

(i) Quadratic autocatalysts in region II
Here eq. (2d) becomes at leading order, on using (5),

$$\frac{\partial B_2}{\partial t} = \frac{\partial^2 B_2}{\partial x^2} + \gamma B_1 + (1 - \gamma) B_2. \tag{6a}$$

We treat the cases of quadratic $(n = 1)$ and cubic $(n = 2)$ autocatalysis with linear $(m = 1)$ and quadratic $(m = 2)$ decay in region I separately. The case of quadratic autocatalysis and linear decay has already been treated fully in [1].

(a) Quadratic autocatalysis with quadratic decay

Here eq. (2b) becomes, at leading order,

$$\frac{\partial B_1}{\partial t} = \frac{\partial^2 B_1}{\partial x^2} + (1 - \gamma)B_1 + \gamma B_2 . \tag{6b}$$

To solve eqs. (6a, 6b), subject to the appropriate initial and boundary conditions derived directly from (3), we employ the same method as was used in [1]. We look for a solution by writing

$$B_1(x, t) = C_1 \, e^{\lambda t} \, u(x, t) , \quad B_2(x, t) = C_2 \, e^{\lambda t} \, u(x, t) , \tag{7}$$

where $u(x, t)$ satisfies the diffusion equation (i.e. $u_t = u_{xx}$) and where C_1 and C_2 are constants. The eigenvalues λ are then determined from the homogeneous linear equations

$$(\lambda - 1 + \gamma)C_1 - \gamma C_2 = 0 , \tag{8a}$$

$$-\gamma C_1 + (\lambda - 1 + \gamma)C_2 = 0 , \tag{8b}$$

giving the quadratic equation for λ

$$\lambda^2 - 2(1 - \gamma)\lambda + 1 - 2\gamma = 0 . \tag{9a}$$

It is straightforward to show that eq. (9a) has the roots

$$\lambda_+ = 1 , \quad \lambda_- = 1 - 2\gamma . \tag{9b}$$

From (9b) we can see that at least one eigenvalue λ_+ is positive for all parameter values and reveals an exponential growth in the B_i for x of $O(1)$ as $t \to \infty$. This leads to the expansion (5) becoming non-uniform with the growth in the B_i indicating wave formation for all values of k and γ. Moreover, we can use the argument presented in [1] to deduce that the asymptotic wave speed will be

$$v = \sqrt{2\lambda_+} = 2 . \tag{9c}$$

Thus, in this case, permanent-form travelling waves will be initiated for all values of k and γ and will ultimately travel with the same uniform wave speed given by (9c).

(b) Cubic autocatalysis with linear decay

Here eq. (2b) becomes, at leading order,

$$\frac{\partial B_1}{\partial t} = \frac{\partial^2 B_1}{\partial x^2} - (\gamma + k)B_1 + \gamma B_2 . \tag{10a}$$

Carrying out the same analysis as described above, we find that the equation for the eigenvalues λ is

$$\lambda^2 - (1 - k - 2\gamma)\lambda + (\gamma k - \gamma - k) = 0 . \tag{10b}$$

As above, we will have exponential growth in the B_i leading to wave formation if at least one of the eigenvalues is positive. Hence we need consider only

$$\lambda_+ = \tfrac{1}{2}\left(1 - 2\gamma - k + \sqrt{(1+k)^2 + 4\gamma^2}\right). \tag{10c}$$

It is relatively straightforward to show that $\lambda_+ = 0$ on the curve

$$\mathcal{C} = \left\{(\gamma, k): \gamma > 1, k = \frac{\gamma}{\gamma - 1}\right\} \tag{10d}$$

with $\lambda_+ > 0$ in the region in the (γ, k)-plane below the curve $\mathcal{C}$, i.e. waves will be initiated for all k when $\gamma \leqslant 1$ and for $k < \gamma/(\gamma - 1)$ when $\gamma > 1$. Moreover, their asymptotic wave speed will be given by

$$v = \left[2\left(1 - 2\gamma - k + \sqrt{(1+k)^2 + 4\gamma^2}\right)\right]^{1/2}. \tag{10e}$$

(c) Cubic autocatalysis with quadratic decay

Here, eq. (2b) becomes at leading order

$$\frac{\partial B_1}{\partial t} = \frac{\partial^2 B_1}{\partial x^2} + \gamma(B_2 - B_1) \tag{11a}$$

with the consequent equation for the eigenvalues

$$\lambda^2 - (1 - 2\gamma)\lambda - \gamma = 0. \tag{11b}$$

The largest root of eq. (11b) is

$$\lambda_+ = \tfrac{1}{2}\left(1 - 2\gamma + \sqrt{1 + 4\gamma^2}\right). \tag{11c}$$

Clearly $\lambda_+ > 0$ for all parameter values and hence wave formation is indicated for all values of k and γ, with asymptotic wave speed

$$v = \left[2\left(1 - 2\gamma + \sqrt{1 + 4\gamma^2}\right)\right]^{1/2}. \tag{11d}$$

We now go on to examine the case when there is a cubic autocatalytic production step $(p = 2)$ in region II.

(ii) Cubic autocatalysis in region II

Here, to leading order, eq. (2d) becomes, using (5),

$$\frac{\partial B_2}{\partial t} = \frac{\partial^2 B_2}{\partial x^2} + \gamma(B_1 - B_2). \tag{12}$$

We again treat the various cases of autocatalysis and decay in region I.

(a) Quadratic autocatalysis with linear decay

Here eq. (2b) becomes, at leading order

$$\frac{\partial B_1}{\partial t} = \frac{\partial^2 B_1}{\partial x^2} + (1 - k - \gamma)B_1 + \gamma B_2.$$ (13a)

On applying (7) in eqs. (12, 13a) we obtain the eigenvalue equation

$$\lambda^2 - (1 - k - 2\gamma)\lambda + \gamma(k - 1) = 0.$$ (13b)

It is straightforward to show that the largest eigenvalue λ_+ satisfies

$$\lambda_+ > 0 \quad \text{if} \quad k < 1,$$
$$\lambda_+ = 0 \quad \text{if} \quad k = 1,$$
$$\lambda_+ < 0 \quad \text{if} \quad k > 1,$$ (13c)

for all values of γ. (13c) shows that waves will be initiated when $k < 1$ while for $k > 1$ the system is asymptotically stable to small inputs of B independent of the strength of the coupling between the two regions. The zero eigenvalue $\lambda_+ = 0$ when $k = 1$ needs further discussion. Also, for $k < 1$, the asymptotic wave speed will be

$$v = \left[2\left(1 - k - 2\gamma + \sqrt{(1 - k)^2 + 4\gamma^2} \right) \right]^{1/2}.$$ (13d)

(b) quadratic autocatalysis with quadratic decay

Here eq. (2b) becomes, at leading order,

$$\frac{\partial B_1}{\partial t} = \frac{\partial^2 B_1}{\partial x^2} + (1 - \gamma)B_1 - \gamma B_2$$ (14a)

with, via (7), the corresponding eigenvalue equation

$$\lambda^2 - (1 - 2\gamma)\lambda - \gamma = 0,$$ (14b)

which gives

$$\lambda_+ = \tfrac{1}{2}\left((1 - 2\gamma) + \sqrt{1 + 4\gamma^2} \right).$$ (14c)

(14c) shows that $\lambda_+ > 0$ for all $\gamma > 0$ and hence wave formation is indicated for all values of k and γ. This case is essentially the same as part i(c) above with the asymptotic wave speed given by (11d).

(c) Cubic autocatalysis with linear decay

Here eq. (2b) becomes, at leading order,

$$\frac{\partial B_1}{\partial t} = \frac{\partial^2 B_1}{\partial x^2} - (k + \gamma)B_1 + \gamma B_2,$$ (15a)

leading to the eigenvalue equation

$$\lambda^2 + (k + 2\gamma)\lambda + \gamma k = 0.$$ (15b)

Equation (15b) gives for the largest root λ_+

$$\lambda_+ = \tfrac{1}{2}\left[-(k + 2\gamma) + \sqrt{k^2 + 4\gamma^2} \right] < 0$$ (15c)

for all $k > 0, \gamma > 0$.

In this case the system is always asymptotically stable to small initial inputs of autocatalyst B, returning to its unreacted state ($\alpha \equiv 1$, $\beta \equiv 0$) for t large. Thus we expect that there will be some threshold value on $\beta_0^{(i)}$ for wave initiation. It could also be the case that wave formation does not take place for any values of $\beta_0^{(i)}$. However, for the uncoupled system we have shown [3] that there is a finite value of the input parameter β_0 above which waves are initiated and we would expect a similar situation to apply here. Further consideration to this point will be given below.

(d) Cubic autocatalysis with quadratic decay

Equation (2b) becomes, at leading order,

$$\frac{\partial B_1}{\partial t} = \frac{\partial^2 B_1}{\partial x^2} + \gamma(B_2 - B_1).$$ (16a)

This, together with eq. (12), leads to a zero eigenvalue case, i.e.

$$\lambda_+ = 0$$ (16b)

for all parameter values. No conclusion as to whether waves are formed can be drawn from this small $\beta_0^{(i)}$ analysis and further considerations are needed.

(iii) Zero eigenvalue case

Here we consider the case of cubic autocatalysis in both regions I and II with a quadratic decay step in region I. We look for a solution for $\beta_0^{(i)}$ small by expanding via (5), and now retaining the terms of $O(\epsilon)$ in eqs. (2b, 2d). We obtain

$$\frac{\partial B_1}{\partial t} = \frac{\partial^2 B_1}{\partial x^2} + \gamma(B_2 - B_1) + \epsilon(1 - k)B_1^2,$$ (17a)

$$\frac{\partial B_2}{\partial t} = \frac{\partial^2 B_2}{\partial x^2} + \gamma(B_1 - B_2) + \epsilon B_2^2.$$ (17b)

It is convenient at this stage to introduce the functions

$$p(x, t) = \tfrac{1}{2}(B_1 + B_2), \quad q(x, t) = \tfrac{1}{2}(B_2 - B_1).$$ (18a)

When (18a) is applied to eqs. (17), we obtain

$$\frac{\partial p}{\partial t} = \frac{\partial^2 p}{\partial x^2} + \frac{\epsilon}{2}\left[(2 - k)q^2 + (2 - k)p^2 + 2kpq \right],$$ (18b)

$$\frac{\partial q}{\partial t} = \frac{\partial^2 q}{\partial x^2} - 2\gamma q + \frac{\epsilon}{2} \left[kp^2 + kq^2 + 2(2-k)pq \right] . \tag{18c}$$

We look for a solution of eqs. (18) by expanding

$$p(x, t) = p_0(x, t) + \epsilon p_1(x, t) + \dots , \tag{19a}$$

$$q(x, t) = q_0(x, t) + \epsilon q_1(x, t) + \dots . \tag{19b}$$

At leading order $p_0(x, t)$ satisfies a diffusion equation with solution

$$p_0(x, t) = \int_{-\infty}^{\infty} \hat{p}_0(s) \, e^{-s^2 t + isx} \, ds , \tag{20a}$$

while $q_0(x, t)$ satisfies the equation

$$\frac{\partial q_0}{\partial t} = \frac{\partial^2 q_0}{\partial x^2} - 2\gamma q_0 . \tag{20b}$$

Equation (20b) has a solution in the form

$$q_0(x, t) = e^{-2\gamma t} \int_{-\infty}^{\infty} \hat{q}_0(s) \, e^{-s^2 t + isx} \, ds . \tag{20c}$$

Here $\hat{p}_0$ and $\hat{q}_0$ are the Fourier transforms of the initial values of p_0 and q_0, derived in an obvious way from (3).

For our present purposes it is the behaviour of p_0 and q_0 for t large that is of interest. We find that $\eta = x/t^{1/2}$ is the appropriate variable to use and then, with η of $O(1)$ and t large, we have

$$p_0(\eta, t) \sim \hat{p}_0(0)t^{-1/2} \, e^{-\eta^2/4} , \tag{21a}$$

$$q_0(\eta, t) \sim \hat{q}_0(0)t^{-1/2} \, e^{-2\gamma t} \, e^{-\eta^2/4} . \tag{21b}$$

We are now in a position to discuss the terms of $O(\epsilon)$. Again we require only the behaviour as $t \to \infty$. Using (21) and noting that q_0 is exponentially small for t large and η of $O(1)$, we find that p_1 and q_1 are of the form

$$p_1 = F_1(\eta) + O(t^{-1}) , \quad q_1 = t^{-1}G_1(\eta) + o(t^{-1}) , \tag{22}$$

where

$$G_1 = \frac{k}{4\gamma} \hat{p}_0(0)^2 \exp(-\eta^2/2) \tag{23a}$$

and where F_1 satisfies the equation

$$F_1'' + \tfrac{1}{2}\eta F_1' = -\tfrac{1}{2}(2-k)\hat{p}_0(0)^2 \exp(-\eta^2/2) \tag{23b}$$

(where primes denote differentiation with respect to η). Equation (23b) has the solution

$$F_1 = -\sqrt{\frac{\pi}{2}}(2-k)\hat{p}_0(0)^2 \int_\eta^\infty \exp(-s^2/4)\,\text{erfc}(s/2)\,ds + A_1\,\text{erfc}(\eta/2)\,, \quad (23c)$$

where the constant A_1 is indeterminate at this stage.

From (21) and (23) we then have, for t large,

$$p(\eta, t) \sim \hat{p}_0(0)\frac{e^{-\eta^2/4}}{t^{1/2}} + \epsilon F_1(\eta) + \dots\,, \quad (24a)$$

$$q(\eta, t) \sim \hat{q}_0(0)\frac{e^{-2\gamma t}}{t^{1/2}}e^{-\eta^2/4} + \epsilon\frac{G_1(\eta)}{t} + \dots\,. \quad (24b)$$

Since $F_1(\eta)$ and $G_1(\eta)$ are bounded functions of η, a non-uniformity arises in expansions (19) as $t \to \infty$. This requires an outer region in which the appropriate scalings are

$$X = \epsilon x\,, \quad \tau = \epsilon^2 t\,, \quad (25a)$$

with

$$p(x, \tau) = \epsilon P(X, \tau)\,, \quad q(x, \tau) = \epsilon^3 Q(X, \tau)\,. \quad (25b)$$

Substituting (25) into eqs. (18) gives, at leading order,

$$\frac{\partial P}{\partial \tau} = \frac{\partial^2 P}{\partial X^2} + \left(1 - \frac{k}{2}\right)P^2\,, \quad (26a)$$

$$Q = \frac{k}{4\gamma}P^2 \quad (26b)$$

subject, on matching with (24), to

$$P(X, \tau) \sim \hat{p}_0(0)\tau^{-1/2}\exp(-X^2/4\tau) \quad \text{as} \quad \tau \to 0^+$$

with the matching of Q following automatically.

We now consider eqs. (26). For $k > 2$ it is straightforward to show using the comparison theorem for scalar parabolic operators [5] (comparing with the function $\phi = 2/(2-k)\tau$ that

$$|P(X, \tau)| \leqslant C\tau^{-1} \quad \text{as} \quad \tau \to \infty \quad (27a)$$

for some constant $C > 0$ and independent of X. This then implies, from (26b), that

$$|Q(X, \tau)| \leqslant \frac{kC^2}{4\gamma}\tau^{-2} \quad \text{as} \quad \tau \to \infty\,. \quad (27b)$$

Hence, when $k > 2$, the expansion remains uniform with the α_i and β_i returning to their unreacted states as $\tau \to \infty$ and travelling waves are not initiated.

For $k < 2$, eq. (26a) is of the Fujita-type, (see, for example, Levine [6]) and has a finite-time pointwise blowup. Thus wave formation is indicated in the case when

$k < 2$. (The finite-time blowup introduces further non-uniformities into the expansion as the solution is controlled by the a priori bounds (4).)

The above discussion applies also to the critical $k = 1$ case when there is quadratic autocatalysis with linear decay in region I, as identified above. The equations arising from expansion (5) are the same to $O(\epsilon)$ (with $k = 1$) for this case. Thus, in this critical case, travelling wave initiation is suggested, but on the much larger $O(\epsilon^{-2})$ time scale.

The small $\beta_0^{(i)}$ analysis of this section has identified two cases where further discussion is necessary, namely where there is cubic autocatalysis in both regions I and II and with linear and quadratic decay steps in region I. In the former case a threshold on the local input of autocatalyst B is suggested, while in the latter an extended two-time scale analysis suggests wave formation on the longer $O(\epsilon^{-2})$ time scale only for $k < 2$. Further information about these two special cases can be obtained from their solution for strong coupling, which is what we address next.

4. Solution for $\gamma \gg 1$

The basic structure for the general case has already been treated in [1], where a multiple-scales approach was used to obtain a solution for γ large. This treatment shows that, at leading order,

$$\alpha_1 = A_1(x, t), \quad \alpha_2 = A_2(x, t), \tag{28a}$$

and that β_1 and β_2 become equal on the short $O(\gamma^{-1})$ time scale with

$$\beta_1(x, t) = \beta_2(x, t) = B_1(x, t). \tag{28b}$$

The equations satisfied by the functions A_1 and A_2 are then the same as those satisfied by α_1 and α_2 (with (28b) used for β_1 and β_2) while B_1 satisfies an equation in which the kinetics are "averaged" over the two regions. This leads to, for the two cases we wish to consider (cubic autocatalysis in regions I and II with either linear or quadratic decay in region I),

$$\frac{\partial A_1}{\partial t} = \frac{\partial^2 A_1}{\partial x^2} - A_1 B_1^2, \tag{29a}$$

$$\frac{\partial A_2}{\partial t} = \frac{\partial^2 A_2}{\partial x^2} - A_2 B_1^2 \tag{29b}$$

together with, for linear decay in region I,

$$\frac{\partial B_1}{\partial t} = \frac{\partial^2 B_1}{\partial x^2} + \tfrac{1}{2}(A_1 B_1^2 + A_2 B_1^2 - kB_1) \tag{29c}$$

and, for quadratic decay in region I,

$$\frac{\partial B_1}{\partial t} = \frac{\partial^2 B_1}{\partial x^2} + \tfrac{1}{2}B_1^2(A_1 + A_2 - k) \,. \tag{29d}$$

The initial conditions are

$$A_1(x,0) = 1 \,, \quad A_2(x,0) = 1 \,, \tag{30a}$$

$$B_1(x,0) = \tfrac{1}{2}\left[\beta_0^{(1)}h_1(x) + \beta_0^{(2)}h_2(x)\right] \,. \tag{30b}$$

It is readily shown, by subtracting eqs. (29a, b) and using (30a), that

$$A_1(x,t) = A_2(x,t) \tag{31}$$

with eqs. (29c) and (29d) then becoming, respectively,

$$\frac{\partial B_1}{\partial t} = \frac{\partial^2 B_1}{\partial x^2} + A_1 B_1^2 - \frac{k}{2} B_1 \tag{32a}$$

and

$$\frac{\partial B_1}{\partial t} = \frac{\partial^2 B_1}{\partial x^2} + A_1 B_1^2 - \frac{k}{2} B_1^2 \,. \tag{32b}$$

The system is then given by eq. (29a) together with either eq. (32a) or (32b).

Taking the linear decay case first. Equations (29a, 32a) have already been treated in some detail in [3] where it was shown that travelling waves are initiated only when $k \leqslant 0.093$ and that, when this is the case, there is a (finite) threshold on the input of B for waves to form, with a lower bound on this threshold being, in the present case, $(\beta_0^{(1)} + \beta_0^{(2)}) > k$. The existence of a threshold on the $\beta_0^{(i)}$ was suggested by the small $\beta_0^{(i)}$ analysis of the previous section.

Turning to the case of quadratic decay, eqs. (29a, 32b) have been discussed in some detail in [4] where it is shown that waves can be initiated for all $k < 2$, with there being no threshold on the input of B for this to occur. The small $\beta_0^{(i)}$ analysis in the previous section was unable to determine whether waves would be initiated or not in the critical $k = 2$. The present analysis shows that travelling waves are not initiated in this critical case, at least in the limit of γ large.

5. Discussion

As in our previous studies of uncoupled systems [2,3,4,7], considerable differences exist in the basic mechanisms of travelling wave formation between quadratic autocatalysis and cubic autocatalysis. We found this to be the case here. Considering first the case when there is purely quadratic autocatalysis in region II, we found that when there is the relatively weak quadratic decay step in region I waves are formed regardless of how strong this decay strength is and how strong the coupling between the two regions is, for both quadratic and cubic autocatalytic production

in region I. In this case the production of autocatalyst B in region II and its subsequent diffusive transfer to region I is always sufficient to overcome the loss of B in region I.

Travelling waves can still form in region I when this has the relatively stronger linear decay step, but now there are restrictions on the parameters γ and k for this process to take place, at least from small initial inputs of B. For weak coupling ($\gamma \leqslant 1$) waves form no matter how strong the decay step but for stronger coupling between the two regions there is an upper bound on k beyond which wave formation in inhibited, with this threshold value of k being slightly higher for quadratic autocatalysis in region I. A further advantage of the small input analysis was that it suggested a value for the asymptotic wave speed. The situation for this case is summarized in table 1.

We have already seen from our previous work on uncoupled systems [3,4,7] that cubic autocatalysis is a much less vigorous production mechanism than quadratic autocatalysis and consequently any decay process can have a more substantial effect on the initiation of travelling waves. This is also seen in the present context. In all cases there are restrictions on the decay rate and coupling parameters for wave initiation. When cubic autocatalytic production is coupled to the more vigorous quadratic autocatalytic production the effect of the linear termination step is to limit the range of values of k but not those of γ over which waves are formed.

However, when there is cubic autocatalytic production in both regions, the effect of the decay step is much more pronounced, leading to no wave formation at all for small inputs of B when there is a strong linear decay. The weaker quadratic decay step gave a zero eigenvalue and our initial approach was inconclusive. A further refinement of the method for this case, examining the effect of the higher order terms, showed that waves would be initiated for $k < 2$ but on a much longer time scale than in the previous cases. The situation is summarized in table 2.

Table 1
Quadratic autocatalysis ($p = 1$) in region II together with various autocatalytic and decay steps in region I. Wave speed v calculated from the largest eigenvalue λ_+ via $v = 2\sqrt{\lambda_+}$.

Reaction in I	Waves formed	Wave speed, $v = 2\sqrt{\lambda_+}$
Quadratic with linear decay $n = 1, m = 1$	all $k, \gamma \leqslant 1$ $k < \dfrac{2\gamma - 1}{\gamma - 1}, \gamma > 1$	$\left[2\left(2 - 2\gamma - k + \sqrt{k^2 + 4\gamma^2}\right)\right]^{1/2}$
Quadratic with quadratic decay $n = 1, m = 2$	all k and γ	2
Cubic with linear decay $n = 2, m = 1$	all $k, \gamma \leqslant 1$ $k < \dfrac{\gamma}{\gamma - 1}, \gamma > 1$	$\left[2\left(1 - 2\gamma - k + \sqrt{(1 + k)^2 + 4\gamma^2}\right)\right]^{1/2}$
Cubic with quadratic decay $n = 2, m = 2$	all k and γ	$\left[2\left(1 - 2\gamma + \sqrt{1 + 4\gamma^2}\right)\right]^{1/2}$

Table 2

Quadratic autocatalysis ($p = 2$) in region II, together with various autocatalytic and decay steps in region I. Wave speed v (where given) calculated from the largest eigenvalue λ_+ via $v = 2\sqrt{\lambda_+}$.

Reaction in I	Waves formed	Wave speed, $v = 2\sqrt{\lambda_+}$
Quadratic with linear decay $n = 1, m = 1$	$k < 1$ for all γ	$\left[2\left(1 - k - 2\gamma + \sqrt{(1-k)^2 + 4\gamma^2} \right) \right]^{1/2}$
Quadratic with quadratic decay $n = 1, m = 2$	all k and γ	$\left[2\left(1 - 2\gamma + \sqrt{1 + 4\gamma^2} \right) \right]^{1/2}$
Cubic with linear decay $n = 2, m = 1$	threshold on β_0	$\lambda_+ = \frac{1}{2}\left(\sqrt{k^2 + 4\gamma^2} - k - 2\gamma \right) < 0$
Cubic with quadratic decay $n = 2, m = 2$	$(\lambda_+ = 0)$ $k < 2$ for all γ	–

To gain further insight into the behaviour of the solution in these two cases, we considered the solution for large γ. The enabled the system to be reduced to cases treated previously [3,4] and thus conclusions drawn. It confirmed the $k < 2$ condition for quadratic autocatalysis as well as excluding critical value $k = 2$, which our small $\beta_0^{(i)}$ analysis was unable to resolve. For linear decay it showed that there was a finite threshold on the $\beta_0^{(i)}$ for wave formation and also suggested that this would occur only for very restricted values of k.

Finally, we should note that, even in the region R_- (say) in the (γ, k) plane where both eigenvalues are negative and the unreacted state in locally stable, travelling wave formation for finite amplitude inputs of B is not precluded, i.e. there could still be some threshold on the $\beta_0^{(i)}$. This cannot be decided by our small $\beta_0^{(i)}$ theory. One way or resolving this is to determine the region R_T in the (γ, k) plane where permanent-form travelling wave solutions exist. Thresholds on the $\beta_0^{(i)}$ should then be expected in the intersection of R_- and R_T, and in the remainder of R_- global asymptotic stability of the unreacted state should be expected. For the case examined in detail in [1] (i.e. quadratic autocatalysis in both regions with linear decay in one), it was shown that the region in the (γ, k) plane in which at least, one of the eigenvalues of the small input analysis was strictly positive was precisely that region in which waves were initiated for all inputs, the unreacted state being globally asymptotic stable outside this region. Thus the small input analysis gave the conditions for wave formation that applied in the general problem.

Throughout we have assumed that the coupling between the two regions is achieved via the autocatalyst B. The situation where the two regions are coupled through the reactant A has been treated by Metcalf et al. [8] and Merkin et al. [9], with distinct differences with the present case being found.

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