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The development of travelling waves in a simple isothermal chemical system with general orders of autocatalysis and decay

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We examine the possibility of generating a propagating chemical wave front when a local input of an autocatalyst B is introduced into a uniform concentration of a reactant A. The autocatalysis is assumed to be of order m, so that $A \rightarrow B$ at a rate $k_1\,[A][B]^m$, while the autocatalyst decays to an inert product C at a rate of order n, $B \rightarrow C$, rate $k_2[B]^n$. The situation is examined for m, $n \geqslant 1$ and emphasis placed on obtaining threshold criteria for the development of reaction–diffusion fronts.

1. Introduction

Autocatalysis or chain-branching has been seen to play a key role in a number of chemical reactions, and it has been usual, in the reaction–diffusion context, to model this process by isothermal quadratic autocatalysis. Here the chemical reaction is represented schematically by

$$A + B \rightarrow 2B, \quad \text{rate } k_q\, ab, \tag{1a}$$

where a and b are the concentrations of reactant A and autocatalyst B respectively. This then leads to a consideration of the much-studied Fisher–Kolmogorov equation (see, for example, Fisher 1937; Kolmogorov *et al.* 1937; Aronson 1978; Fife 1978; Bramson 1983). This basic problem has arisen in other contexts; the original motivation (Fisher 1937) was to explain the advance of an advantageous gene through a population. It has also been proposed as a model for other biological and biochemical systems, many of which are described in the recent book by Murray (1989). In the chemical context, kinetic scheme (1*a*) has been suggested as a mechanism for certain isothermal gas-phase reactions (for example, Voronkov & Semenov 1939; Dixon-Lewis & Williams 1977; Gray 1988).

More recently Hanna *et al.* (1982) and Saul & Showalter (1984) have shown that certain liquid-phase reactions can be adequately described by the cubic autocatalytic rate law

$$A + 2B \rightarrow 3B, \quad \text{rate } k_c\, ab^2. \tag{1b}$$

The reaction–diffusion equations arising from this kinetic scheme (as well as the case when there is assumed to be a mixture of both quadratic and cubic autocatalysis) have been examined by Gray *et al.* (1990). Further work on travelling waves with cubic autocatalysis has been reported by Billingham & Needham (1991*a*), with an extensive study of both quadratic and cubic autocatalysis when the diffusion coefficients of species A and B are significantly different being described in Billingham & Needham (1991*b*, *c*, *d*).

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Recently the present authors have treated the case when the autocatalyst B is assumed not to be indefinitely stable, but decays to an inert product of reaction C either linearly,

$$B \rightarrow C, \quad \text{rate } \bar{k}_1\, b, \tag{2a}$$

or has a quadratic termination step

$$B + B \rightarrow C, \quad \text{rate } \bar{k}_q\, b^2 \tag{2b}$$

(Merkin *et al.* 1989; Merkin & Needham 1990, 1991). These detailed studies revealed that there are distinct and important differences in the conditions for the initiation of reaction–diffusion travelling waves, and in the structure of such waves, depending on the type of autocatalytic reaction scheme (either (1*a*) or (1*b*)) and decay rate (either (2*a*) or (2*b*)) considered.

This work brought out clearly the need for a careful appraisal of the actual chemical kinetics that should be used in modelling these processes. In nearly all cases of practical interest the full chain-branching or autocatalytic reaction is not given by just a single reaction step of the type given in (1*a*) or (1*b*), but involves many simple reactions. An attempt is then made to describe the complex overall mechanism in terms of a single reaction step by lumping or empirically fitting data. With this in mind, there is no reason to suppose that all such systems would be described by reaction rates proportional to just integer powers of the autocatalyst concentration. It is the purpose of this paper to relax this constraint and to examine the initiation and propagation of reaction–diffusion travelling waves for more general autocatalytic schemes

$$A + mB \rightarrow (m+1)\,B, \quad \text{rate } k_1 a b^m, \tag{3a}$$

and allowing for autocatalyst decay via

$$B \rightarrow C, \quad \text{rate } k_2\, b^n, \tag{3b}$$

where m and n are general (not necessarily integer) powers subject only to the restriction that $m, n \geqslant 1$. We shall, however, assume that reactant A and autocatalyst B have equal diffusion coefficients. The case $m = 1$, $n = 1$ is discussed in Merkin *et al.* (1989) and has been considered as a model for the spread of infectious disease (with the diffusion coefficient of A in this case being zero) by Kermack & McKendrick (1927) and Kendall (1965). The further cases $m = 2$, $n = 1$ and $n = 2$ are discussed in Merkin & Needham (1990) and $m = 1$, $n = 2$ in Merkin & Needham (1991).

Reaction schemes (3) lead to reaction–diffusion equations, which in dimensionless form and for plane geometry, are

$$\left.\begin{aligned} \partial\alpha/\partial t &= \partial^2\alpha/\partial x^2 - \alpha\beta^m, \quad (4a)\\ \partial\beta/\partial t &= \partial^2\beta/\partial x^2 + \alpha\beta^m - \kappa\beta^n, \quad (4b)\end{aligned}\right\} -\infty < x < \infty, \quad t \geqslant 0$$

subject to the initial conditions

$$\alpha \equiv 1, \quad \beta = \begin{cases} \beta_0 g(x), & |x| \leqslant \sigma, \\ 0, & |x| > \sigma, \end{cases} \quad \text{at } t = 0, \tag{5a}$$

where $g(x)$ is a positive, continuous function of x in $|x| \leqslant \sigma$, with $\max\{g(x)\} = 1$. In addition we have boundary conditions

$$\alpha \rightarrow 1, \quad \beta \rightarrow 0 \quad \text{as} \quad |x| \rightarrow \infty \quad \text{for} \quad t \geqslant 0. \tag{5b}$$

The non-dimensionalization of the original equations follows that used by the present authors in the above mentioned papers. The functions α and β are the dimensionless concentrations of species A and B respectively. The parameter $\kappa = k_2/k_1\, a_0^{1+m-n}$ (where a_0 is the initial uniform concentration of A) can be regarded as a chain-branching factor and represents the relative strength of the decay rate to the autocatalytic production step, the parameter β_0 represents the maximum value of the initial input of autocatalyst B relative to A.

In the previous cases much useful information about the conditions under which travelling waves can develop was obtained from two simplified versions of the full initial-value problem (4), (5), namely the well-stirred analogue of this problem and the solution for β_0 small. Consequently, this is where we start the present discussion.

2. The well-stirred analogue

The well-stirred analogue of the initial-value problem (4), (5) is

$$\mathrm{d}\alpha/\mathrm{d}t = -\alpha\beta^m, \quad \mathrm{d}\beta/\mathrm{d}t = \alpha\beta^m - \kappa\beta^n, \tag{6}$$

subject to $\alpha(0) = 1$, $\beta(0) = \beta_0$, in $\alpha \geqslant 0$, $\beta \geqslant 0$.

There are three cases to consider, depending on the sign of $m-n$. We start with the case $m = n$. Here the equation for the trajectories of the system in the (α, β) phase plane is

$$\mathrm{d}\beta/\mathrm{d}\alpha = (\kappa - \alpha)/\alpha, \quad \beta = \beta_0 \quad \text{when} \quad \alpha = 1. \tag{7\,a, b}$$

Equation (7a) is the same equation as discussed in Merkin *et al.* (1989) (for the case $m = n = 1$) and in Merkin & Needham (1990) (for the case $m = n = 2$) and the argument for a general index follows directly that given previously. From this we can deduce that we can expect no travelling wave to form for $\kappa \geqslant 1$, with there being a 'trigger' mechanism (independent of the magnitude of β_0) in the production of β for the initiation of a travelling wave only when $\kappa < 1$. Further, we expect that, at the rear of any such wave formed, α would tend to some non-zero constant α_s.

Next consider the case $m < n$. We note first that for $n-m = 1$, the equation for the integral paths in the phase plane reduces to

$$\mathrm{d}\beta/\mathrm{d}\alpha = \kappa\beta/\alpha - 1, \quad \beta = \beta_0 \quad \text{at} \quad \alpha = 1, \tag{8}$$

which is the same as that considered in Merkin & Needham (1991) for the case $m = 1$, $n = 2$. Here we found a 'trigger' mechanism for the initiation of a travelling wave for all values of κ and β_0. We also found that all trajectories in the positive quadrant of the (α, β) phase plane approached the origin, i.e. $\beta \to 0$ as $\alpha \to 0$ for all κ and β_0, the particular way in which this limit is approached depending on the value of κ, suggesting that α would become zero at the rear of the reaction–diffusion wave.

Similar behaviour is found for general values of m and n $(m < n)$, where the corresponding equation for the integral paths is

$$\mathrm{d}\beta/\mathrm{d}\alpha = (\kappa\beta^{n-m} - \alpha)/\alpha, \quad \beta = \beta_0 \quad \text{at} \quad \alpha = 1. \tag{9\,a, b}$$

The phase portrait of equation (9a) in the quadrant $\alpha, \beta > 0$ is readily obtained by a consideration of isoclines, and it is found to have precisely the same qualitative form as that of equation (8). Hence we still find a 'trigger' mechanism for the initiation of a travelling wave for all values of κ and β_0 and that all trajectories approach the origin. However, the way in which this limit is approached is different

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to the previous case; now we find that the behaviour of β for small α depends on whether $n-m>1$ or $n-m<1$, with, as $\alpha \to 0$,

$$\beta \sim (\kappa M)^{-1/M}(-\ln \alpha)^{-1/M}, \quad M = n-m-1>0 \tag{10a}$$

$$\beta \sim (\alpha/\kappa)^{-1/N}, \quad N = n-m>0,\ N<1. \tag{10b}$$

Finally, we consider the case $m>n$. Here the equation for the trajectories in the (α, β) phase plane is

$$\mathrm{d}\beta/\mathrm{d}\alpha = (\kappa - \alpha\beta^{m-n})/\alpha\beta^{m-n}. \tag{11}$$

The case $m=2$, $n=1$ has been discussed in Merkin & Needham (1990) and similar considerations apply for general m and n. The horizontal and vertical isoclines of equation (11) are given by $\beta = (\kappa/\alpha)^{1/m-n}$ and $\alpha = 0$, $\beta = 0$ respectively, so that

$$\frac{\mathrm{d}\beta}{\mathrm{d}\alpha}\begin{cases} <0 & \text{in} \quad \beta > (\kappa/\alpha)^{1/m-n}, \\ >0 & \text{in} \quad \beta < (\kappa/\alpha)^{1/m-n}. \end{cases} \tag{12}$$

Hence each integral path will start at large α, when it is asymptotic from above to the curve $\beta = (\kappa/\alpha)^{1/m-n}$. Then, as α decreases, β grows until it reaches a maximum at the horizontal isocline, from which it then decreases to zero at a finite value of α. Now the particular trajectory that we require is the one that starts with $\beta = \beta_0$ at $\alpha = 1$. So that if $\beta_0 < \kappa^{1/m-n}$, this trajectory starts below the horizontal isocline and β decreases monotonically to zero at $\alpha = \alpha_s$ (say), $\alpha_s \neq 0$. However, if $\beta_0 > \kappa^{1/m-n}$, this trajectory starts above the horizontal isocline and β begins by increasing before finally decreasing to zero at $\alpha = \alpha_s$. Hence we must have

$$\beta_0 > \kappa^{1/m-n} \tag{13}$$

to 'trigger' the production of B, which suggests that, in the full reaction-diffusion system, (13) will supply a lower bound on the value of β_0 required for the initiation of a travelling wave.

To summarize, the well-stirred analogue examined in this section indicates that for $m, n \geqslant 1$ we have the following cases.

(i) $m=n$. A travelling wave will be initiated in the reaction–diffusion system (4), (5) if and only if $\kappa < 1$, with no restriction on $\beta_0 > 0$.

(ii) $m<n$. A travelling wave will be initiated in the reaction–diffusion problem (4), (5) for all κ, $\beta_0 > 0$.

(iii) $m>n$. A travelling wave will not be initiated in the reaction–diffusion problem (4), (5) unless $\beta_0 > \kappa^{1/m-n}$, irrespective of any additional conditions on κ alone.

The above cases are further substantiated and modified by considering the solution of the full initial-value problem (4), (5) with $\beta_0 \ll 1$.

3. Solution for small β_0

To obtain a solution of the initial-value problem (4), (5) valid for $\beta_0 \ll 1$, we put

$$\alpha = 1 + \beta_0^m A(x,t), \quad \beta = \beta_0 B(x,t), \tag{14a}$$

with $A(x,t)$, $B(x,t)$ of $O(1)$ as $\beta_0 \to 0$. On substituting (14a) into equations (4), we find that we need consider only equation (4b), which becomes, on neglecting the small, $O(\beta_0^m)$, contribution to α,

$$\partial B/\partial t = \partial^2 B/\partial x^2 + \beta_0^{m-1} B^m - \kappa \beta_0^{n-1} B^n. \tag{14b}$$

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Equation (14*b*) has to be solved subject to initial and boundary conditions derived directly from (5).

There are special cases to consider before we discuss equation (14*b*) for general values of m and n. First, take the case $m = 1$, $n > 1$. Here the term of $O(\beta_0^{n-1})$ can be neglected at leading order, and we find that, for $t \gg 1$,

$$B(x,t) \sim B_0(\mathrm{i}x/2t)\mathrm{e}^{t}\,\mathrm{e}^{-x^2/4t}/t^{\frac{1}{2}}, \tag{15}$$

where $B_0(\cdot)$ is the Fourier transform of $g(x)$ and is a bounded function. This shows that for x of $O(1)$ the growth in B is exponential for all κ with the solution then being unstable, and suggests the formation of a reaction–diffusion wave for all values of κ no matter how small the initial input of autocatalyst. Moreover, analysis of the asymptotic form (15) in a moving frame of reference, as given in detail in Merkin & Needham (1989), shows that two diverging wave fronts with exponential profile and speed $v_0 = \pm 2$ propagate outwards into the unreacted state, indicating that this wave speed is independent of κ and equal to the Fisher–Kolmogorov wave speed.

Next, consider the case $n = 1$, $m > 1$. Here the term of $O(\beta_0^{m-1})$ can be neglected at leading order, with then

$$B(x,t) \sim B_0(\mathrm{i}x/2t)\,\mathrm{e}^{-\kappa t}\,\mathrm{e}^{-x^2/4t}/t^{\frac{1}{2}} \tag{16}$$

for $t \gg 1$. In this case $B(x,t) \to 0$ uniformly in x as $t \to \infty$ and the solution is stable. Hence there is no build up in the concentration of the autocatalyst and no wave will form for small initial inputs. This is in line with the conjecture from the previous section (inequality (13)).

Now take $m = n = 1$. Here both reaction terms in equation (14*b*) are included at leading order, with then

$$B(x,t) \sim B_0(\mathrm{i}x/2t)\,\mathrm{e}^{(1-\kappa)t}\,\mathrm{e}^{-x^2/4t}/t^{\frac{1}{2}}, \tag{17}$$

for t large. Here there is a build up in autocatalyst concentration only for $\kappa < 1$, which is the condition for the initiation of a travelling wave found by Merkin *et al.* (1989). As also reported in Merkin *et al.* (1989), (17) indicates that, with $\kappa < 1$, the initiated travelling waves will ultimately propagate with speed $\pm 2\surd(1-\kappa)$.

For general values of $m > 1$ and $n > 1$, both reaction terms in equation (14*b*) are omitted at leading order, leading to a diffusion equation to be solved for $B(x,t)$, giving, for $t \gg 1$,

$$B(x,t) \sim B_0(\mathrm{i}x/2t)\,\mathrm{e}^{-x^2/4t}/t^{\frac{1}{2}}. \tag{18}$$

In this case we must consider whether this leading-order diffusion approximation remains a uniform approximation to equation (14*b*) as $t \to \infty$, since all the reaction terms in (14*b*) have been neglected at this stage. We can achieve this by computing the ratio of the magnitude of the terms retained in equation (14*b*) to those neglected, via (18), for $t \gg 1$. It is readily seen that, for $m, n > 3$, the leading-order term does remain as a uniform approximation to (14*b*) as $t \to \infty$, and we can infer directly from (18) that, in this case, $B(x,t) \to 0$ uniformly in x as $t \to \infty$ through diffusion. Thus for $m,n > 3$ a travelling wave does not develop for small initial inputs of the autocatalyst.

However, for $1 < n < 3$ or $1 < m < 3$, a non-uniformity does develop in the solution of the leading-order problem for t large. There are three cases to consider.

(i) $1 < m < 3$, $n > m > 1$. Here it is the term of $O(\beta_0^{m-1})$ in equation (14*b*) that first

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becomes comparable with the retained terms, when t is of $O(\beta_0^{-2(m-1)/(3-m)})$ and x of $O(\beta_0^{-(m-1)/(3-m)})$. We then put

$$t = \beta_0^{-2(m-1)/(3-m)}\,\tau, \quad x = \beta_0^{-(m-1)/(3-m)}\,X, \quad B = \hat{B}\beta_0^{(m-1)/(3-m)}, \tag{19a}$$

with equation (14b) becoming, at leading order,

$$\partial\hat{B}/\partial\tau = \partial^2\hat{B}/\partial X^2 + \hat{B}^m, \quad |X| \geqslant 0, \quad \tau > 0, \tag{19b}$$

which must be solved subject to matching with (18) as $\tau \to 0$. Now, with $1 < m < 3$, the solution of this initial-value problem has a pointwise blow-up at finite $\tau > 0$ (Bandle & Levine 1989; Levine 1990). At this stage the small β_0 theory fails. However, this local blow-up leads to a rapid rise in the concentration of the autocatalyst from initially small values, indicating the formation of a reaction–diffusion wave on a timescale t of $O(\beta_0^{-2(m-1)/(3-m)})$.

(ii) $1 < n < 3$, $m > n > 1$. Here it is the term of $O(\beta_0^{n-1})$ in equation (14b) which first becomes comparable with the retained diffusion terms. This occurs on a timescale of $O(\beta_0^{-2(n-1)/(3-n)})$ and x of $O(\beta_0^{-(n-1)/(3-n)})$. On writing

$$t = \beta_0^{-2(n-1)/(3-n)}\,\tau, \quad x = \beta_0^{-(n-1)/(3-n)}\,X, \quad B = \beta_0^{(n-1)/(3-n)}\,\hat{B}. \tag{20a}$$

equation (14b) becomes, at leading order,

$$\partial\hat{B}/\partial\tau = \partial^2\hat{B}/\partial X^2 - \kappa\hat{B}^n, \quad |X| \geqslant 0, \quad \tau > 0, \tag{20b}$$

which again has to be solved subject to matching with (18) as $\tau \to 0$. It is readily shown via the comparison theorem for scalar parabolic operators (see, for example, Britton 1986) that the solution of this initial-value problem has $\hat{B}(X,\tau) \to 0$ as $\tau \to \infty$ uniformly in X, and hence no reaction–diffusion wave can form in this case.

(iii) $1 < m = n < 3$. In this case, both reaction terms in (14b) are of the same order, and become comparable with the retained diffusion terms when t is of $O(\beta_0^{-2(m-1)/(3-m)})$. The appropriate re-scaling on this long timescale is as in (19a), in terms of which equation (14b) becomes,

$$\partial\hat{B}/\partial\tau = \partial^2\hat{B}/\partial X^2 + (1-\kappa)\hat{B}^m, \quad |X| > 0, \quad \tau > 0, \tag{21}$$

again to be solved subject to matching with (18) as $\tau \to 0$. For $\kappa > 1$ it can be shown, again via a comparison theorem, that $\hat{B}(X,\tau) \to 0$ as $\tau \to \infty$ uniformly in X, and so no reaction–diffusion wave is initiated. However, for $\kappa < 1$, the initial-value problem has local point-wise finite-time blow-up and this indicates the onset of wave formation over a timescale of $O(\beta_0^{-2(m-1)/(3-m)})$. The case $\kappa = 1$ requires further consideration which is not presented here. An analysis of this critical case reveals that wave formation does not occur at $\kappa = 1$.

In the above analysis, we have not discussed the cases when $m = 3$, $n > 3$ or $n = 3$, $m > 3$. These are critical cases in the sense that the approach we have used above is not sufficiently refined to distinguish whether these cases result in a non-uniformity in the leading-order diffusion approximation as $t \to \infty$. However, these cases can be considered using a multiple scales approach on equation (14b) (Needham & Merkin 1991). This shows that finite-time blow-up occurs for $m = 3$, $n > 3$, which indicates reaction–diffusion wave formation, but over a much longer timescale, of $O(\exp(\beta_0^{-1}))$. However, for $n = 3$, $m > 3$, $B(x,t)$ decays to zero over the same long timescale, and a reaction–diffusion wave is not initiated.

The situation with the various cases is summarized in figure 1. We can draw some

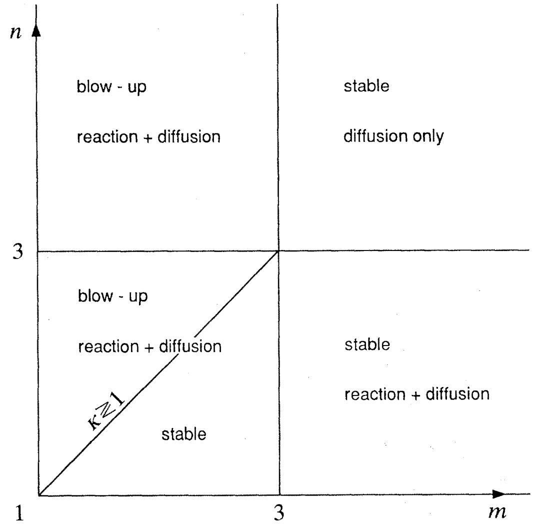

Figure 1. The behaviour of the small β_0 solution (§3) with respect to the autocatalysis exponent m and decay rate exponent n.

conclusions from this small β_0 theory. In particular, it indicates how the effect of diffusion may modify conclusions drawn from the well-stirred analogue treated in §2. We have seen that for $1 \leqslant n \leqslant 3$ and for $1 \leqslant m \leqslant 3$ the ultimate long time behaviour is dictated by the reaction terms and hence the well-stirred analogue is in agreement with the small β_0 theory, providing an accurate qualitative guide to the question of wave formation in the full system. However, for n, $m > 3$ with β_0 sufficiently small, diffusion dominates for all t and, not surprisingly, the well-stirred analogue fails to account accurately for the final outcome of the system. The well-stirred analogue indicates a threshold on β_0 for the formation of a travelling wave occurring only for $n < m$, this being a reaction-dominated threshold. However, the present small β_0 theory has shown that there is, in fact, a threshold on β_0 for all n, $m > 3$, with this being diffusion dominated.

4. Permanent form travelling waves

Here we examine the properties of permanent form travelling waves which can develop from the initial-value problem (4), (5). It is readily shown that any such wave necessarily has a constant propagation speed V_0. Also, by symmetry, we need consider only right-moving waves, in which case we have $V_0 > 0$. A permanent form travelling wave generated in the initial-value problem (4), (5) can therefore be defined by the following.

Definition. A unit travelling wave is a non-trivial ($\alpha \not\equiv 1, \beta \not\equiv 0$) wave of permanent form, travelling with constant speed $V_0 > 0$ and having uniform conditions $\alpha \rightarrow 1$, $\beta \rightarrow 0$ ahead of the wave and uniform conditions behind the wave. Throughout the wave α, β must satisfy equations (4) with $\alpha \geqslant 0$, $\beta \geqslant 0$.

The existence of a unit travelling wave then requires a non-trivial, non-negative solution of the ordinary differential equations,

$$\left.\begin{aligned} \alpha_{yy} + V_0 \alpha_y - \alpha\beta^m &= 0 \\ \beta_{yy} + V_0 \beta_y + \alpha\beta^m - \kappa\beta^n &= 0 \end{aligned}\right\} -\infty < y < \infty, \qquad (22\,a, b)$$

where $y = x - V_0 t$. Ahead of the wave we have,

$$\alpha \to 1, \quad \beta \to 0 \quad \text{as} \quad y \to \infty, \tag{23a}$$

while behind the wave,

$$\alpha \to \alpha_s, \quad \beta \to 0 \quad \text{as} \quad y \to -\infty \tag{23b}$$

for some $\alpha_s \geqslant 0$ (which may depend upon κ and V_0).

We first establish some overall properties of unit travelling waves, which hold for all n, $m \geqslant 1$. In what follows, proofs are given only for results which do not follow directly from similar results in Merkin *et al.* (1989), Merkin & Needham (1990), or Billingham & Needham (1991*b*).

(i) *Properties for n, $m \geqslant 1$*

*R*1. In a unit travelling wave $\alpha(y) > 0$ and $\beta(y) > 0$ for all $-\infty < y < \infty$. □

*R*2. In a unit travelling wave $\alpha_s < \alpha(y) < 1$ and $0 < \alpha(y) + \beta(y) < 1$ for all $-\infty < y < \infty$. □

*R*3. In a unit travelling wave $\alpha(y)$ is strictly monotone increasing.

Proof. Let $\alpha(y)$, $\beta(y)$ be a unit travelling wave. Suppose $\alpha_y(y)$ has more than one zero in $-\infty < y < \infty$. Let y_n and y_{n+1} be two consecutive zeros of α_y with $y_n < y_{n+1}$. Then, using equation (22*a*) and *R*1, we have that $\alpha_{yy}(y_{n+1}) > 0$ and hence $\alpha_y(y) < 0$ for all $y_n < y < y_{n+1}$. Thus $\alpha_{yy}(y_n) \leqslant 0$. However, from equation (22*a*) and *R*1 we obtain $\alpha_{yy}(y_n) > 0$. This leads to a contradiction and we conclude that $\alpha_y(y)$ has at most one zero for $-\infty < y < \infty$. Suppose now that $\alpha_y(y)$ has exactly one zero in $-\infty < y < \infty$ at $y = y_0$. Since $\alpha_y(y_0) = 0$, equation (22*a*) and *R*1 show that $\alpha_{yy}(y_0) > 0$, and hence $\alpha_y(y) < 0$ for all $-\infty < y < y_0$. Therefore, on integrating α_y with respect to y on the range $-\infty < y < y^*$, we obtain, on using (23*b*),

$$\int_{-\infty}^{y^*} \alpha_y \, dy = \alpha(y^*) - \alpha_s < 0,$$

for any $-\infty < y^* < y_0$, which violates *R*2. Thus we conclude that $\alpha_y(y) \neq 0$ for any $-\infty < y < \infty$. Condition (23*a*, *b*) and *R*2 then imply that $\alpha(y)$ is strictly monotone increasing for $-\infty < y < \infty$, as required. □

We now develop results specific to the three cases.

(ii) *Properties for $n = m \geqslant 1$*

*R*4. The existence of a unit travelling wave requires $\kappa < 1$. □

*R*5. In a unit travelling wave, $\beta(y)$ has a unique turning-point, which is a local maximum. □

*R*6. In a unit travelling wave, $\alpha_s < \kappa$. □

*R*7. In a unit travelling wave, $\beta(y) < (1 - \kappa)$. □

With regard to the existence of unit travelling waves, it is readily shown using formal asymptotic methods that for each $0 < \kappa < 1$, there exists a unique solution to the boundary-value problem (22), (23) for each V_0 sufficiently large. Moreover, it is clear that this boundary-value problem has no solution when $V_0 = 0$. This indicates that there must exist a $V^*(\kappa, m)$ such that, for any fixed $0 < \kappa < 1$, there will be a unique unit travelling wave solution for each $V_0 \geqslant V^*$. We have been unable this far to support this conjecture with a rigorous proof; however, numerical solutions of (22), (23) are strongly supportive of the result. We note that for the case $n = m = 1$, as discussed in Merkin *et al.* (1989), it was shown that $V^*(\kappa; 1) = 2\surd(1-\kappa)$ for $0 < \kappa < 1$. Also, it is readily shown that for fixed $0 < \kappa < 1$, $\alpha_s(V_0, \kappa; m) \to \alpha_s^\infty(\kappa)$ as $V_0 \to \infty$, where $\alpha_s^\infty(\kappa)$ is the smaller of the two positive zeros of the function $F(\alpha_s) = 1 - \alpha_s + \kappa \ln \alpha_s$. We can obtain the limiting forms of $\alpha_s^\infty(\kappa)$ as,

$$\alpha_s^\infty(\kappa) \sim \begin{cases} e^{-1/\kappa}(1 + e^{-1/\kappa}\kappa^{-1}) & \text{as} \quad \kappa \to 0^+, \\ 1 - (1-\kappa) + \ldots & \text{as} \quad \kappa \to 1^-. \end{cases}$$

(iii) *Properties for* $n > m \geqslant 1$

*R*8. In a unit travelling wave, $\beta(y)$ has a unique turning point which is a local maximum. □

*R*9. A unit travelling wave has $\alpha_s = 0$. □

*R*10. A unit travelling wave has,

$$\beta(y) < \begin{cases} \kappa^{-1/(n-m)}, & \kappa > 1, \\ 1, & \kappa \leqslant 1. \end{cases}$$

Proof. We note that *R*1 and conditions (23) show that $\beta(y)$ achieves its maximum value, β_{max}, say, on $-\infty < y < \infty$ at a local maximum at $y = y^*$, say, where $\beta_{yy}(y^*) \leqslant 0$, $\beta_y(y^*) = 0$. From (22*b*) it then follows that,

$$\beta_{max}^m\{\alpha(y^*) - \kappa\beta_{max}^{n-m}\} \geqslant 0.$$

However, $\beta_{max}^m > 0$ via *R*1, and so,

$$\beta_{max} \leqslant [\alpha(y^*)/\kappa]^{(1/n-m)} < \kappa^{-1/(n-m)}$$

via *R*2. Also from *R*2, $\beta_{max} < 1$, and the result follows. □

In this case it may be shown rigorously (following directly the re-normalization approach in Merkin & Needham (1991) for $n = 2$, $m = 1$) that a unique unit travelling wave exists for each $\kappa > 0$ and at each V_0 sufficiently large. Again it is readily shown that no unit travelling wave exists at $V_0 = 0$. This leads us to again conjecture that there exists a $V^*(\kappa; m, n)$ such that, for any $\kappa > 0$, there is a unique unit travelling wave for each $V_0 \geqslant V^*(\kappa; m, n)$. In the particular case when $m = 1$, we have $V^*(\kappa, 1, n) \equiv 2$ which is the Fisher–Kolmogorov minimum wave speed.

(iv) *Properties for* $m > n \geqslant 1$

*R*11. The existence of a unit travelling wave requires, $\kappa < P^P/(P+1)^{P+1}$, where $P = m - n$. When this condition is satisfied a unit travelling wave has $\beta^-(\kappa) < \beta_{max}(y) < \beta^+(\kappa)$ where $\beta^-(\kappa)$, $\beta^+(\kappa)$ are the two positive roots of the equation $\psi^P(\psi - 1) + \kappa = 0$.

Proof. In a unit travelling wave, since $\beta(y) \to 0$ as $|y| \to \infty$, $\beta(y)$ achieves its maximum at one or more points in $-\infty < y < \infty$. Let $y = y_s$ be one such point, then,

$$\beta(y_s) = \beta_{max} > 0, \quad \beta_y(y_s) = 0, \quad \beta_{yy}(y_s) \leqslant 0. \tag{24a}$$

Also, from equation (22*b*), we have,

$$\beta_{yy}(y_s) = \beta_{max}^n\{\kappa - \alpha(y_s)\,\beta_{max}^P\} \leqslant 0, \tag{24b}$$

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where $P = m-n > 0$. Hence via (24*a*, *b*) we find that,

$$\alpha(y_s) \geqslant \kappa\beta_{\max}^{-P}. \tag{24 c}$$

On combining (24*c*) with *R*2 we obtain,

$$\beta_{\max}^{P}\{\beta_{\max}-1\}+\kappa < 0. \tag{25}$$

Thus a unit travelling wave exists only if the inequality (25) has a non-empty solution set. It is readily seen that this is the case only when $\kappa < P^P/(P+1)^{P+1}$, in which case the equation $\psi^P(\psi-1)+\kappa = 0$ has precisely two positive zeros. The result then follows directly. □

We note first that in this case, the range of values of κ ($0 < \kappa < \kappa_P \equiv P^P/(1+P)^{1+P}$) for which a unit travelling wave can exist is much more restricted than in either of the two previous cases. In particular $\kappa_P \sim e^{-1}/P$ as $P \to \infty$, and the range of values of κ over which travelling waves are possible shrinks rapidly to zero with increasing P. We note further that for the case $m = 2$, $n = 1$ (i.e. $P = 1$), which has been studied in detail by Merkin & Needham (1990), the bound $\kappa_1 = \frac{1}{4}$ was found to provide only a relatively weak upper bound, with unit travelling waves actually existing only for $\kappa < 0.0465$. This suggest that for $P > 1$, the upper bound κ_P may still be relatively weak, with the range of κ over which travelling waves actually exist shrinking to zero faster than $O(P^{-1})$ as $P \to \infty$.

As found in Merkin & Needham (1990), for each value of κ for which travelling waves exist, numerical computations reveal that there are two values $V_1(\kappa, P)$, $V_2(\kappa, P)$ (with $V_1 > V_2$) such that a unique unit travelling wave exists for each $V_0 = V_2$ and $V_0 \geqslant V_1$. At the maximum value of κ for which unit travelling waves exist, $V_1 = V_2$, and the two branches come together. The existence of these two branches of unit travelling waves in this case could be substantiated further by examining the asymptotic solutions of (22), (23) for $0 < \kappa \ll 1$, following Merkin & Needham (1990).

5. The initial-value problem

Here we examine the overall properties of the full initial-value problem (4), (5). We first establish *a priori* bounds on the solution. In what follows, for convenience, we will refer to the initial-value problem (4), (5) as IVP.

*I*1. Let $\alpha(x,t)$, $\beta(x,t)$ be a solution of IVP for $t \in [0, T]$ and any $T > 0$. Then

$$0 \leqslant \alpha(x,t) < 1, \quad 0 \leqslant \beta(x,t) < 1+\beta_0$$

for all $(x,t) \in (-\infty, \infty) \times [0, T]$.

Proof. (*a*) To establish the left-hand inequalities, we apply theorem 14.11 from Smoller (1983). Using this it readily follows that the region $R \subset \mathbb{R}^2$, with $R = \{(\alpha, \beta)^T : \alpha, \beta \geqslant 0\}$, is a positively invariant region for equations (4). Since in IVP, $(\alpha(x,0), \beta(x,0))^T \in R$ for all $x \in (-\infty, \infty)$, the results follow directly.

(*b*) To establish the right-hand inequalities, we use the maximum principle for scalar parabolic operators (see, for example, Protter & Weinberger 1967; Britton 1986; Smoller 1983). From equations (4) and part (*a*), we have,

$$\alpha_t - \alpha_{xx} \leqslant 0, \quad (\alpha+\beta)_t - (\alpha+\beta)_{xx} \leqslant 0 \tag{26}$$

for all $(x,t) \in (-\infty, \infty) \times (0, T]$. Initial and boundary conditions (5) together with (26) and the strong maximum principle imply directly that $\alpha(x,t) < 1$ and $\alpha(x,t)+$

$\beta(x,t) < 1+\beta_0$ for all $(x,t) \in (-\infty, \infty) \times (0, T]$. On using part (*a*) again we have $\beta(x,t) < 1+\beta_0$ for all $(x,t) \in (-\infty, \infty) \times (0, T]$, as required.

We are now in a position to establish the following.

*I*2. IVP has a unique global solution.

Proof. We first rewrite IVP in terms of $A \equiv \alpha - 1$ and $B \equiv \beta$ to obtain,

$$\left.\begin{aligned} &\boldsymbol{U}_t = \boldsymbol{U}_{xx} + \boldsymbol{F}(\boldsymbol{U}), \; -\infty < x < \infty, \; t > 0, \\ &\boldsymbol{U}(x,0) = \boldsymbol{h}(x), \; -\infty < x < \infty, \\ &\boldsymbol{U}(x,t) \to \boldsymbol{0} \quad \text{as} \quad |x| \to \infty, \quad t \geqslant 0, \end{aligned}\right\} \overline{\text{IVP}}$$

where $\boldsymbol{U} = (A, B)^{\mathrm{T}}$, $\boldsymbol{F}(\boldsymbol{U}) = (-(A+1)B^m, (A+1)B^m - \kappa B^n)^{\mathrm{T}}$ and $\boldsymbol{h}(x) = (0, h(x))^{\mathrm{T}}$ with $h(x)$ given by (5*a*).

From *I*1, we observe that any solution of $\overline{\text{IVP}}$ for $t \in [0, T]$ and any $T > 0$, is *a priori* bounded in the L_∞ – norm, with, $\|\boldsymbol{U}(\cdot, t)\|_\infty \leqslant 2 + \beta_0$ for all $t \in [0, T]$. We now apply theorem 14.4 of Smoller (1983), with the admissible Banach space $BC_0 = \{w(x) : \mathbb{R} \to \mathbb{R} : w(x)$ is bounded and uniformly continuous with $|w(x)| \to 0$ as $|x| \to \infty\}$. Clearly $\boldsymbol{h}(x) \in BC_0$, and it then follows that there exists a solution of $\overline{\text{IVP}}$ in $0 \leqslant t \leqslant T$ for any $T > 0$, which gives global existence. Moreover, for each $t \geqslant 0$, $\boldsymbol{U}(x,t) \in BC_0$. Uniqueness follows directly from lemma 14.3 of Smoller (1983). □

We note that *I*1 and *I*2 demonstrate that the solution of IVP does not blow-up in finite-time or as $t \to \infty$ (in $\|\cdot\|_\infty$). We next establish the following threshold criterion on the input parameter β_0.

*I*3. Let $\alpha(x,t)$, $\beta(x,t)$ be the solution of IVP. Then for $m > 3$ there exists a $C(m) > 0$ such that when $\beta_0 \leqslant \sigma^{-2/m-1} C(m)$, $\alpha(x,t) \to 1$, $\beta(x,t) \to 0$ as $t \to \infty$, uniformly in x.

Proof. This follows from Needham & Merkin (1991). We only outline the proof here. For each $m > 3$, we can construct a similarity solution to the equation,

$$L[U] \equiv U_t - U_{xx} - U^m = 0, \; t > 0, \; -\infty < x < \infty,$$

of the form,

$$U(x,t) = (t+\sigma^2)^{-1/m-1} F_m(x[t+\sigma^2]^{-\frac{1}{2}}), \; |x|, \; t \geqslant 0, \tag{27a}$$

where $F_m(y)$ is a bounded, positive and even function of y, with $F_m(y) \to 0$ as $y \to \infty$ through terms exponentially small in y. In additions $F_m(y)$ is monotone decreasing in $y > 0$. At $t = 0$, the solution (27*a*) reduces to,

$$U(x,0) = \sigma^{-2/m-1} F_m(|x|/\sigma), \; -\infty < x < \infty. \tag{27b}$$

Thus using the above properties of $F_m(\cdot)$, we observe that, $\beta(x,0) \leqslant U(x,0)$, provided that $\beta_0 \leqslant \sigma^{-2/m-1} F_m(1)$. Moreover, $L[U] = 0$, $L[\beta] \leqslant 0$, $-\infty < x < \infty$, $t > 0$ using *I*1. An application of the comparison theorem for scalar parabolic operators then leads to, $\beta(x,t) < U(x,t)$, $-\infty < x < \infty$, $t > 0$. However, $U(x,t) \to 0$ as $t \to \infty$ uniformly in x, hence (since $\beta(x,t) \geqslant 0$ via *I*1), $\beta(x,t) \to 0$ as $t \to \infty$ uniformly in x as required. The result on $\alpha(x,t)$ then follows by considering the equation for $w \equiv \alpha + \beta - 1$. We note finally that $C(m) \leqslant F_m(1)$. □

We remark that the above proof fails when $m \leqslant 3$ due to the non-existence of the similarity solution (27*a*) in this range of m. In fact, all solutions of $L[U] = 0$ with non-negative initial conditions (except $U \equiv 0$) blow-up (in $\|\cdot\|_\infty$) in finite time for $m \leqslant 3$ (see, for example, the review of Levine 1990).

We now consider the three cases $n = m$, $n > m$ and $n < m$ separately.

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(i) IVP *with* $n = m \geqslant 1$

*I*4. The development of a permanent-form unit travelling wave in IVP as $t \to \infty$ requires $\kappa < 1$.

Proof. Follows from *R*4.

*I*5. Let $\alpha(x,t)$, $\beta(x,t)$ be the solution of IVP, then, for $\kappa \geqslant 1$,

$$\alpha(x,t) \sim \begin{cases} 1+O(t^{-\frac{1}{2}}), & 1 \leqslant m \leqslant 3, \\ 1+O(t^{-1/m-1}), & m > 3, \end{cases} \quad \text{as} \quad t \to \infty, \; -\infty < x < \infty, \tag{28a}$$

and

$$\beta(x,t) < \begin{cases} \beta_0/\{1+\beta_0^{m-1}(\kappa-1)(m-1)\,t\}^{1/m-1}, & m > 1, \\ \beta_0\,e^{-(\kappa-1)t}, & m = 1, \end{cases} \tag{28b}$$

for all $t > 0$, $-\infty < x < \infty$.

Proof. The proof follows Merkin & Needham (1990) and Needham (1991). For (28*b*) we use the scalar comparison theorem for parabolic operators, applied to the operator $L[U] \equiv U_t - U_{xx} - (1-\kappa)\,U^m$, together with the *a priori* bounds of *I*1. Estimate (28*a*) follows by considering the equation for $w \equiv \alpha+\beta-1$, following Needham (1991). □

Thus, with $\kappa > 1$, we have that $\beta(x,t) \to 0$ and $\alpha(x,t) \to 1$, uniformly in x, as $t \to \infty$. In this case, the unreacted state $\alpha \equiv 1$, $\beta \equiv 0$ is globally asymptotically stable with respect to initial disturbances in β with compact support.

(ii) IVP *with* $m > n \geqslant 1$

We first define $F(t)$ to be the unique solution to the initial-value problem,

$$F_t = F^n[F^{m-n} - \kappa], \quad F(0) = \beta_0, \quad t > 0.$$

It is readily shown that for $0 < \beta_0 < \kappa^{1/m-n}$, $F(t)$ is monotone decreasing in t, with,

$$F(t) \sim \begin{cases} O(t^{-1/(n-1)}), & n > 1, \\ O(e^{-\kappa t}), & n = 1, \end{cases} \tag{29}$$

as $t \to \infty$. This leads us to,

*I*6. Let $\alpha(x,t)$, $\beta(x,t)$ be the solution of IVP, then, with $\beta_0 < \kappa^{1/(m-n)}$, $\beta(x,t) < F(t)$ for all $t > 0$, $-\infty < x < \infty$, whilst,

$$\alpha(x,t) \sim \begin{cases} 1+O(t^{-\frac{1}{2}}), & 1 \leqslant n \leqslant 3, \\ 1+O(t^{-1/(n-1)}), & n > 3, \end{cases} \tag{30}$$

as $t \to \infty$, $-\infty < x < \infty$.

Proof. This follows Merkin & Needham (1990) and Needham (1991). We use the scalar comparison theorem for the parabolic operator $L[U] \equiv U_t - U_{xx} - U^m + \kappa U^n$ together with *I*1. The estimate (30) follows from considering the equation for $w \equiv \alpha+\beta-1$, as in Needham (1991). □

For this case we have, finally, the following.

*I*7. The development of a permanent-form unit travelling wave from IVP requires, $\kappa < P^P/(P+1)^{P+1}$ and $\beta_0 > \kappa^{1/P}$, where $P = m-n$.

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Proof. Follows directly from $R11$ and $I6$.

Thus, in this case, the formation of a permanent-form unit travelling wave in IVP requires κ to be sufficiently small and in addition, β_0 to exceed the threshold $\kappa^{1/P}$.

(iii) IVP *with* $n > m \geqslant 1$

Define $G(t)$ to be the unique solution of the initial-value problem,

$$G_t = G^m[1-\kappa G^{n-m}], \quad G(0) = \beta_0, \quad t > 0.$$

For all $\beta_0 > 0$, $G(t)$ is monotone in t with, $G(t) \to \kappa^{-1/(n-m)}$ as $t \to \infty$. We can now use $G(t)$ in the following.

$I8$. Let $\alpha(x,t)$ $\beta(x,t)$ be the solution of IVP, then, $\beta(x,t) < G(t)$ for all $t \geqslant 0$, $-\infty < x < \infty$.

Proof. Follows from the scalar comparison theorem for the parabolic operator $L[U] \equiv U_t - U_{xx} - (U^m - \kappa U^n)$ and $I1$. □

We have been unable to obtain any further information in this case, although for the case $m = 1$, $n = 2$, it has been shown in Merkin & Needham (1991) that wave formation occurs for any κ, $\beta_0 > 0$. For $1 \leqslant m \leqslant 3$, it is indicated in §§2 and 3 that this may still be the case. However, $I3$ introduces a threshold on β_0 for $m > 3$.

6. Discussion

We now summarize the information obtained in the previous sections to give an overall picture of wave formation in the initial-value problem (4), (5). We consider the three cases $n = m$, $m > n$ and $m < n$ separately.

(i) $n = m \geqslant 1$. For $m \leqslant 3$, we have seen in §§4, 5 that wave formation cannot occur for $\kappa \geqslant 1$ for any $\beta_0 > 0$. However, for $\kappa < 1$ the results of §§2, 3 suggest that wave formation occurs for all $\beta_0 > 0$. With $m > 3$, an additional threshold is introduced, with wave formation being inhibited when $\beta_0 \leqslant \sigma^{-2/(m-1)}\,C(m)$ for any $\kappa > 0$.

(ii) $m > n \geqslant 1$. For $m \leqslant 3$ we see from §4 that wave formation cannot occur for $\kappa \geqslant P^p/(P+1)^{p+1}$ $(P = m-n)$, whilst in §§2, 3, and 5 it is shown that wave formation requires $\beta_0 > \kappa^{1/P}$. With $m > 3$ we again have the additional restriction that wave formation is inhibited when $\beta_0 \leqslant \sigma^{-2/(m-1)}\,C(m)$.

(iii) $n > m \geqslant 1$. With $m \leqslant 3$, §§4, 5 provide no restriction on κ and β_0 for wave formation. Indeed, the $\beta_0 \ll 1$ theory of §3 and the well-stirred analogue of §2 indicate that wave formation occurs for all κ, $\beta_0 > 0$. Again for $m > 3$, the threshold $\beta_0 > \sigma^{-2/(m-1)}\,C(m)$ is now required for wave formation.

We finally remark that a threshold on the chain-branching factor κ is present in all cases *except* when $n > m \geqslant 1$. When this threshold is satisfied an additional threshold on the catalyst input parameter β_0 is present in all cases *only* when $m > 3$ (even when $\kappa = 0$ and termination is absent). However, for $m > n$, a threshold is present on β_0 for all $m > 1$.

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