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Multistability, oscillations and travelling waves in a product-feedback autocatalator model. II The initiation and propagation of travelling waves

BY S. M. COLLIER[1], J. H. MERKIN[1] AND S. K. SCOTT[2]

[1] *Department of Applied Mathematics, and* [2] *School of Chemistry, University of Leeds, Leeds LS2 9JT, U.K.*

Contents

The initiation and propagation of reaction diffusion travelling waves in a model product-feedback autocatalator kinetic scheme, for which the well-stirred (spatially homogeneous) case has been considered previously in detail, in discussed. *A priori* bounds and general properties are obtained for the initial-value problem. These are extended by numerical solutions of the initial-value problem in the three, previously identified expanding, contracting and reduced cases. In the reduced case, the concentrations attained at the rear of the wave are seen to depend on the existence and temporal stability of a non-trivial steady state of the system. In the contracting case, a constant non-zero value is achieved by the concentration of reactant A, while the concentrations of autocatalyst B and reactant C are pulse-like and tend to zero at long times. In the expanding case, a propagating wave front is seen, but now the concentrations behind the wave can grow in time. The permanent form travelling wave equations are then treated. General properties of their solutions are obtained and asymptotic solutions, valid for large initial concentrations of reactant A, are derived in all three cases.

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1. Introduction

In a recent paper (part I, Collier *et al.* (1992) we considered a modified version of the C-feedback autocatalator of Peng *et al.* (1990), namely the reaction scheme

$$\mathrm{P+C \rightarrow A+C}, \quad \text{rate} = k_0 p_0 c, \tag{1a}$$

$$\mathrm{A+2B \rightarrow 3B}, \quad \text{rate} = k_1 ab^2, \tag{1b}$$

$$\mathrm{B \rightarrow C}, \quad \text{rate} = k_2 b, \tag{1c}$$

$$\mathrm{C \rightarrow D}, \quad \text{rate} = k_3 c, \tag{1d}$$

where a, b and c are the concentrations of the reactants A, B and C respectively, p_0 is the (constant) concentration of the precursor P and the k_i are the rate constants.

Previously, we considered the well-stirred model in some detail. However, our main aim is to treat scheme (1) in the reaction-diffusion context. We have already identified the need to have a thorough understanding of the well-stirred system before undertaking a discussion of the reaction-diffusion model (Merkin & Needham 1990; Needham & Merkin 1991), and this was dealt with in part I. We are now in a position to treat this case, the dimensionless equations for which are, from part I, for planar geometry

$$\frac{\partial x}{\partial t} = \frac{\partial^2 x}{\partial r^2} + \mu z - xy^2, \tag{2a}$$

$$\frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial r^2} + xy^2 - y, \tag{2b}$$

$$\frac{\partial z}{\partial t} = \frac{\partial^2 y}{\partial r^2} + y - \gamma z, \tag{2c}$$

subject to the initial and boundary conditions

$$\left.\begin{aligned} x &= x_1, \\ y &= \begin{cases} y_0 g(r), & |r| < \sigma, \\ 0, & |r| > \sigma, \end{cases} \\ z &= 0, \end{aligned}\right\} \quad \text{at} \quad t = 0, \tag{3a}$$

$$x \rightarrow x_1, \quad y \rightarrow 0, \quad z \rightarrow 0 \quad \text{as} \quad |r| \rightarrow \infty, \tag{3b}$$

where $x_1, y_0, \mu = k_0 p_0/k_2$ and $\gamma = k_3/k_2$ are constants, and where x, y and z are the dimensionless concentrations of the reactants A, B and C respectively. $g(r)$ is a positive continuous function of r on $|r| < \sigma$ with a maximum value of unity.

In the well-stirred case (part I) we identified three distinct cases, depending on the sign of $\mu - \gamma$, which we referred to as

(*a*) $\mu > \gamma$ the 'expanding' case,

(*b*) $\mu < \gamma$ the 'contracting' case,

(*c*) $\mu = \gamma$ the 'reduced' case.

In the reduced case we found the possibility of multiple stationary states with saddle-node and Hopf bifurcations (both supercritical and subcritical). The limit cycles formed at the Hopf bifurcations were seen to break up at homoclinic orbit

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bifurcations. For the other two cases, there was only one possible stationary state, namely the trivial state $x = x_s$, $y = z = 0$ which was shown to be a stable node for all parameter values. In the 'contracting' case this stationary state was approached for large time (with the value of x_s depending on the initial conditions as well as on the parameters μ and γ). However, for the 'expanding' case the solution grew in time, in the sense that the total concentration $x+y+z \to \infty$ as $t \to \infty$. Finite periods of oscillatory behaviour were found in both cases, particularly when $|\mu-\gamma|$ was small and these could be identified in terms of known behaviour in the reduced case.

We start the discussion of the corresponding reaction-diffusion case by obtaining some general properties of the initial-value problem.

2. General properties of the initial-value problem

(*a*) *Special case* $\mu = 0$

This case has, in effect, already been discussed fully by Merkin & Needham (1990) and to obtain the equations treated in that paper we put

$$x = x_1 \bar{x}, \quad y = x_1 \bar{y}, \quad z = x_1 \bar{z}, \quad \bar{r} = x_1 r, \quad \bar{t} = x_1^2 t.$$

Equations (2) then become (with $\mu = 0$)

$$\frac{\partial \bar{x}}{\partial \bar{t}} = \frac{\partial^2 \bar{x}}{\partial \bar{r}^2} - \bar{x}\bar{y}^2, \tag{4a}$$

$$\frac{\partial \bar{y}}{\partial \bar{t}} = \frac{\partial^2 \bar{y}}{\partial \bar{r}^2} + \bar{x}\bar{y}^2 - \frac{1}{x_1^2}\bar{y}. \tag{4b}$$

(The equation for $\bar{z}$ becomes uncoupled from the equations for $\bar{x}$ and $\bar{y}$ and need not be considered.) The initial and boundary conditions are

$$\left.\begin{aligned} &\bar{x} = 1, \quad \bar{y} = \frac{y_0}{x_1} g(\bar{r}) \quad && \text{at} \quad t = 0, \\ &\bar{x} \to 1, \quad \bar{y} \to 0 && \text{as} \quad |\bar{r}| \to \infty. \end{aligned}\right\} \tag{4c}$$

From Merkin and Needham we know that this system can develop propagating reaction–diffusion waves only if $1/x_1^2 \leqslant \nu_0 \sim 0.0465$, i.e. only if $x_1 \geqslant 4.64$. Also, from result I8 in Merkin and Needham, we have a lower bound on y_0 for these waves to be formed, namely that $y_0 > x_1^{-1}$.

(*b*) *A priori bounds*

It is relatively straightforward to show, using the corollary to theorem 14.7 in Smoller (1983) and the discussion following this, that

$$\{x, y, z : x \geqslant 0, y \geqslant 0, z \geqslant 0\} \tag{5}$$

is an invariant set for the system (2), (3).

By adding equations (2) we have that the total concentration $\xi = x+y+z$ satisfies the equation

$$\frac{\partial \xi}{\partial t} = \frac{\partial^2 \xi}{\partial r^2} + (\mu - \gamma) z. \tag{6a}$$

It then follows, using (5) and the scalar maximum principle for parabolic operators

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(see, for example, Fife 1979) that, for the contracting and reduced cases, i.e. $\mu-\gamma \leqslant 0$,

$$0 \leqslant \xi \leqslant x_1+y_0, \quad t \geqslant 0, -\infty < r < \infty. \tag{6b}$$

Then, again from (5) we have that

$$\{x, y, z: x \geqslant 0, y \geqslant 0, z \geqslant 0, 0 \leqslant x+y+z \leqslant x_1+y_0\} \tag{6c}$$

and is an invariant set for the system (2), (3) when $\mu-\gamma \leqslant 0$. The existence of the *a priori* bound given by the bounded invariant set (6*c*) then guarantees the global existence and uniqueness of the solution in this case (Smoller 1983).

As would be expected from the well-stirred system, the expanding case, $\mu > \gamma$, appears not to be bounded above. However, we can get an estimate for the growth rate of the total concentration ξ, if we consider the linear parabolic operator

$$L[\psi] = \psi_t - \nabla^2\psi - (\mu-\mu)\,\psi. \tag{7a}$$

Now $L[\xi] = -(\mu-\gamma)(x+y) \leqslant 0$ from (6*c*), while, for the function $u(t) = (x_1+y_0)\,\mathrm{e}^{(\mu-\gamma)t}$, $L[u] = 0$. Also,

$$\xi(r,0) = x_1+y_0\,g(r) \leqslant x_1+y_0 = u(0).$$

Hence by the scalar comparison theorem for parabolic operators (Britton 1986)

$$\xi(r,t) \leqslant (x_1+y_0)\,\mathrm{e}^{(\mu-\gamma)t}, \quad -\infty < r < \infty, \quad t \geqslant 0. \tag{7b}$$

This gives an upper bound in the growth rate of the total concentration ξ.

Then, via (5) and since x, y and z are all individually less than ξ,

$$(x,y,z) \leqslant (x_1+y_0)\,\mathrm{e}^{(\mu-\gamma)t}, \quad -\infty < r < \infty, \quad t \geqslant 0. \tag{7c}$$

For $(\mu-\gamma) > 0$ (7*c*) gives an upper bound on the growth rate in the concentrations of the individual species A, B and C.

Furthermore, if we put $v = x_1 - \xi$, then

$$v_t - \nabla^2 v = -(\mu-\gamma)\,z \leqslant 0 \tag{8a}$$

on $-\infty < r < \infty$, $t \geqslant 0$ for $(\mu-\gamma) > 0$. Hence, again by the maximum principle, $v \leqslant 0$ giving

$$x+y+z \geqslant x_1 \quad \text{for} \quad -\infty < r < \infty, \quad t \geqslant 0. \tag{8b}$$

Combining results (7*b*) and (8*b*) we obtain the bound

$$x_1 \leqslant \xi \leqslant (x_1+y_0)\,\mathrm{e}^{(\mu-\gamma)t} \tag{8c}$$

for $t \geqslant 0$, $-\infty < r < \infty$ when $(\mu-\gamma) > 0$.

Next we return to the case $(\mu-\gamma) \leqslant 0$ and consider the operator

$$M[\psi] = \psi_t - \nabla^2\psi + \psi - (x_1+y_0)\,\psi^2. \tag{9a}$$

Now $M[y] = (x-(x_1+y_0))\,y^2 \leqslant 0$ (from (6*c*)) and, with

$$w = \frac{y_0}{(x_1+y_0)\,y_0 + [1-(x_1+y_0)\,y_0]\,\mathrm{e}^t}, \tag{9b}$$

$M[w] = 0$. Also, $y(r,0) = y_0\,g(r) \leqslant y_0 = w(0)$. Then, again by the scalar comparison theorem,

$$y(r,t) \leqslant \frac{y_0}{(x_1+y_0)\,y_0 + [1-(x_1+y_0)\,y_0]\,\mathrm{e}^t} \quad -\infty < r < \infty, \quad t \geqslant 0. \tag{9c}$$

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Equation (9*c*) shows that, if $(x_1+y_0)y_0<1$, $y\rightarrow 0$ uniformly in r as $t\rightarrow\infty$, and hence a necessary condition for the initiation of a travelling wave when $\mu-\gamma\leqslant 0$ is that

$$x_1 \geqslant (1-y_0^2)/y_0. \tag{10}$$

Clearly, for positive values of the parameters, this gives no restriction on x_1 for $y_0>1$ and for x_1 large and y_0 small gives $x_1>y_0^{-1}$.

We can gain further insight into the conditions under which reaction–diffusion travelling waves are initiated by considering the solution for y_0 small, which is what we do next.

(*c*) *Solution for y_0 small*

First assume that x_1 is $O(1)$, then to obtain a solution valid for $y_0 \ll 1$, we put

$$x = x_1+y_0 X, \quad y = y_0 Y, \quad z = y_0 Z. \tag{11}$$

At leading order, equation (2*b*) becomes

$$\frac{\partial Y}{\partial t} = \frac{\partial^2 Y}{\partial r^2} - Y, \tag{12a}$$

which has the solution satisfying the initial and boundary conditions derived from (3)

$$Y(r,t) = \frac{\mathrm{e}^{-t}}{2\sqrt{(\pi t)}}\int_{-\infty}^{\infty} \bar{g}(s)\,\mathrm{e}^{-s^2 t}\,\mathrm{e}^{-isr}\,\mathrm{d}s, \tag{12b}$$

where

$$\bar{g}(s) = \int_{-\sigma}^{\sigma} g(r)\,\mathrm{e}^{irs}\,\mathrm{d}r$$

is the Fourier transform of $g(r)$. For $t \gg 1$, (12*b*) gives

$$Y(r,t) \sim \frac{\mathrm{e}^{-t}}{2\sqrt{(\pi t)}}\bar{g}\left(\frac{ir}{2t}\right)\mathrm{e}^{-r^2/4t}. \tag{12c}$$

Expression (12*c*) shows that $Y(r,t)\rightarrow 0$ uniformly in r as $t\rightarrow\infty$.

A consideration of the equations for X and Z then shows that X is of $O(t^{-1/2})$, and that Z is of $O(\mathrm{e}^{-t})$ for $\gamma>1$, of $O(t\,\mathrm{e}^{-t})$ for $\gamma=1$ and of $O(\mathrm{e}^{-\gamma t})$ for $\gamma<1$, uniformly in r as $t\rightarrow\infty$. Hence no waves can be initiated in this case with the system returning uniformly to its unreacted state. This analysis suggests that, for x_1 of $O(1)$, there will be some threshold value of y_0, $y_{0,\min}$ (say), below which travelling waves will not develop for any value of x_1.

Next consider the case x_1 large. Inequality (10) suggests that the above conclusion could be modified when x_1 is of $O(y_0^{-1})$ and to discuss this case we put $\bar{x}_1 = x_1 y_0$, with $\bar{x}_1$ of $O(1)$ for $y_0 \ll 1$. We still use the scaling as given by (11), and it is again the equation for Y which is the important one. This is now, at leading order,

$$\frac{\partial Y}{\partial t} = \frac{\partial^2 Y}{\partial r^2} + \bar{x}_1^2 Y^2 - Y \tag{13a}$$

to be solved subject to initial and boundary conditions

$$Y = \begin{cases} g(r), & |r|<\sigma, \\ 0, & |r|>\sigma, \end{cases} \quad \text{at} \quad t=0, \quad Y\rightarrow 0 \quad \text{as} \quad |r|\rightarrow\infty. \tag{13b}$$

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To discuss equation (13) we start by considering the linear operator $L_1[\psi] = \psi_t - \psi_{rr} + \psi$. Then

$$L_1[0] = 0 \leqslant L_1[Y] = \bar{x}_1 Y^2. \tag{14a}$$

Hence, by the strong comparison theorem for scalar parabolic operators,

$$Y(r,t) > 0 \quad \text{on} \quad -\infty < r < \infty, \quad t > 0. \tag{14b}$$

Next we consider the operator $N[\psi] = \psi_t - \psi_{rr} - \bar{x}_1 \psi^2 + \psi$ and the function $\bar{Y}(t) = [\bar{x}_1 + (1-\bar{x}_1)\,\mathrm{e}^t]^{-1}$. Then $N[Y] = 0 = N[\bar{Y}]$ and $Y(r,0) \leqslant \bar{Y}(0)$.

Hence, $\bar{Y}$ is a supersolution for equation (13), giving the result

$$0 < Y(r,t) < \frac{1}{\bar{x}_1 + (1-\bar{x}_1)\,\mathrm{e}^t} \quad \text{on} \quad -\infty < r < \infty, \quad t > 0. \tag{15a}$$

For $\bar{x}_1 < 1$, (15) shows that $Y(r,t) \to 0$ uniformly in r as $t \to \infty$. Hence, a necessary condition for the growth in the concentrations of the reactants from initially small values and hence for the initiation of travelling waves is $\bar{x}_1 \geqslant 1$ i.e.

$$x_1 \geqslant y_0^{-1}, \quad y_0 \ll 1. \tag{15b}$$

Furthermore, $Y_0 = (3/2\bar{x}_1)\,\mathrm{sech}^2\,(\tfrac{1}{2}r)$ is a fixed point for equation (13a) and hence the solution with any initial function such that $g(r) \leqslant Y_0(r)$ on $|r| < \sigma$, will be bounded above by $Y_0(r)$, i.e.

$$0 < Y(r,t) \leqslant \frac{3}{2\bar{x}_1}\,\mathrm{sech}^2\,(\tfrac{1}{2}r) \quad \text{for} \quad -\infty < r < \infty, \quad t > 0. \tag{16a}$$

In particular, since we are taking $g(r) \leqslant 1$ on $|r| < \sigma$, a necessary condition for $Y(r,t)$ to grow in t (leading to the possible initiation of travelling waves) is that

$$x_1 > \frac{3}{2y_0}\,\mathrm{sech}^2\,(\tfrac{1}{2}\sigma) \tag{16b}$$

for y_0 small.

It is worth noting that the above theory applies to all three cases, and that 'threshold' values of x_1 and y_0 necessary for the development of large time behaviour, which is not just a return to the unreacted state, applies equally well to the expanding case ($\mu - \gamma > 0$), as to the contracting and reduced cases ($\mu - \gamma \leqslant 0$).

We also know that for $\bar{x}_1$ large (formally by a rescaling of r and t) that equation (13c) reduces to a Fujita-type that has been studied extensively, see, for example, the review article by Levine (1990). In this limiting case, the solution has a finite-time pointwise blowup. This suggests that for sufficiently large values of x_1, equation (13a) will also have such a finite-time blowup leading to the large increase in Y required to initiate the formation of waves. Note that, from *a priori* bound (6c), the y cannot grow indefinitely in the cases $\mu - \gamma \leqslant 0$.

(d) *Solution for small σ*

Further insight into the mechanism by which the travelling waves are formed can be gained by examining the solution of equations (2), (3) for small σ. A consideration of equations (2) and conditions (3a) suggests that the initial development occurs on a short timescale of $O(\sigma^2)$ and is confined to a lateral extent of $O(\sigma)$. Then on putting

$$\rho = r/\sigma, \quad \tau = t/\sigma^2, \tag{17}$$

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and assuming that x_1 and y_0 are both of $O(1)$ for the present, equations (2) and (3) become

$$\frac{\partial x}{\partial \tau} = \frac{\partial^2 x}{\partial \rho^2} + \sigma^2(\mu z - xy^2), \tag{18a}$$

$$\frac{\partial y}{\partial \tau} = \frac{\partial^2 y}{\partial \rho^2} + \sigma^2(xy^2 - y), \tag{18b}$$

$$\frac{\partial z}{\partial \tau} = \frac{\partial^2 z}{\partial \rho^2} + \sigma^2(y - \gamma z), \tag{18c}$$

subject to the conditions

$$x = x_1, \quad z = 0, \quad y = \begin{cases} y_0\, g(\rho), & |\rho| < 1, \\ 0, & |\rho| > 1, \end{cases} \quad \text{at} \quad t = 0, \tag{19a}$$

$$x \to x_1, \quad y \to 0, \quad z \to 0 \quad \text{as} \quad |\rho| \to \infty. \tag{19b}$$

At leading order, x, y and z all satisfy diffusion equations with solutions

$$x = x_1, \tag{20a}$$

$$z = 0, \tag{20b}$$

$$y = \frac{y_0}{2\surd(\pi\tau)} \int_{-\infty}^{\infty} \bar{g}(s)\, \mathrm{e}^{-s^2\tau}\, \mathrm{e}^{-\mathrm{i}s\rho}\, \mathrm{d}s, \tag{20c}$$

where $\bar{g}(s)$ is the Fourier transform of $g(\rho)$. From (20c) we find that

$$y \sim \frac{y_0}{2\surd(\pi\tau)} \bar{g}\left(\frac{\mathrm{i}\rho}{2\tau}\right) \mathrm{e}^{-\rho^2/4\tau} \tag{21}$$

as $\tau \to \infty$, uniformly in ρ.

The perturbations, $\bar{x}$ and $\bar{z}$ to the leading order solutions for x and z given by (20a, b) are both $O(\sigma^2)$ and satisfy the equations

$$\frac{\partial \bar{x}}{\partial \tau} = \frac{\partial^2 \bar{x}}{\partial \rho^2} - x_1 y^2, \tag{22a}$$

$$\frac{\partial \bar{z}}{\partial \tau} = \frac{\partial^2 \bar{z}}{\partial \rho^2} + y, \tag{22b}$$

with y as given by (20c), (21). The solution of equation (22) is given simply by

$$\bar{z}(\rho, \tau) = \tau y(\rho, \tau) \tag{22c}$$

so that z is of $O(\sigma^2 \tau^{1/2})$ uniformly in ρ for τ large.

If we now return to equation (18b) we see that the reaction terms neglected are to leading order, for τ large, of $O(\sigma^2\tau^{-1/2})$ whereas the terms retained are of $O(\tau^{-3/2})$. These will become comparable and the reaction start to make a significant contribution to the behaviour of the solution when τ is of $O(\sigma^{-2})$, with then ρ of $O(\sigma^{-1})$ and y and z both being small, of $O(\sigma)$. This suggests that the next stage in the time development occurs when t and r are both of $O(1)$, and with

$$x = x_1 + \sigma X, \quad y = \sigma Y, \quad z = \sigma Z. \tag{23a}$$

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Equations (2) become

$$\frac{\partial X}{\partial t} = \frac{\partial^2 X}{\partial r^2} + \mu Z - x_1 \sigma Y, \tag{23b}$$

$$\frac{\partial Y}{\partial t} = \frac{\partial^2 Y}{\partial r^2} + x_1 \sigma Y^2 - Y, \tag{23c}$$

$$\frac{\partial Z}{\partial t} = \frac{\partial^2 Z}{\partial r^2} + Y - \gamma Z. \tag{23d}$$

For x_1 of $O(1)$ equation (23*c*) reduces to equation (12*a*) as $\sigma \to 0$, and has a solution, $Y(r,t)$, given by (12*b*), such that $Y(r,t) \to 0$ uniformly in r as $t \to \infty$. Then, equations (23*b*) and (23*c*) show that, to leading order in σ, both $X(r,t) \to 0$ and $Z(r,t) \to 0$ uniformly in r as $t \to 0$.

The situation is now clear for a small initial input of autocatalyst B, characterized by $\sigma \ll 1$, x_1, y_0 of $O(1)$. There is an initial diffusive spread of B on the short, $O(\sigma^2)$, timescale, with the concentration of A remaining constant, and a small increase (of $O(\sigma)$) from an initially zero value in the concentration of C. On the longer, $O(1)$, timescale, the consuming reaction (1*c*) then becomes dominant and removes all the autocatalyst B before it can be produced via steps (1*a*, *b*). The concentrations of reactants A and C then return to their initial unreacted states through diffusion. In this case no travelling waves are initiated.

This situation will not apply when we make the initial input of B larger, either by increasing x_1 or by increasing y_0. The first case follows directly from equation (23*c*). For with x_1 large, of $O(\sigma^{-1})$, this equation now is in the form given by equation (13*a*), the behaviour of which has already been discussed.

The second case arises when y_0 is of $O(\sigma^{-1})$, then with $y_0 = \bar{y}_0/\sigma$, the total input of autocatalyst B is

$$y_0 \int_{-\sigma}^{\sigma} g(r)\,\mathrm{d}r = \bar{y}_0 \int_{-1}^{1} g(\rho)\,\mathrm{d}\rho, \tag{24a}$$

which remains of $O(1)$. This suggests putting $y = \sigma^{-1} Y$ and with $x = x_1$, of $O(1)$, to leading order equation (18*b*) becomes

$$\frac{\partial Y}{\partial \tau} = \frac{\partial^2 Y}{\partial \rho^2} + x_1 Y^2 - \sigma Y. \tag{24b}$$

The leading order solution to this equation for σ small has a finite-time blowup (Levine 1990), which suggests the formation of waves in this case on the shorter $O(\sigma^2)$ timescale.

We have established various necessary conditions for the initiation of travelling waves (more strictly, the conditions for the growth in reactant concentrations from initially small inputs required for the formation of such waves). For y_0 small, i.e. small inputs of autocatalyst B, we require the initial concentration of reactant A to be large, i.e. of $O(y_0^{-1})$, as given by inequalities (15*b*), (16*b*). The reason for this can be seen from reaction scheme (1). For growth in the concentration of B we require the autocatalytic production rate via step (1*b*) to be at least comparable with the decay step (1*c*), i.e. $k_1 x_1 y_0^2 \sim k_2 y_0$ and hence x_1 to be of $O(y_0^{-1})$.

For x_1 and y_0 both of $O(1)$, we have established a necessary condition (10) for the initiation of waves only in the case $(\mu - \gamma) \leqslant 0$, with the concentrations of the reactants remaining bounded throughout. For the case $(\mu - \gamma) > 0$ we have been

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unable to obtain such a bound, only a limit on the growth rate of the reactant concentrations being found. The question as to whether permanent-form travelling waves are initiated in this case, or whether the concentrations grow indefinitely in time (as they could in the well-stirred system, part I) is not clear at this stage.

For small inputs characterized by the parameter σ we again need large initial concentrations of A or B for the possibility of wave formation. More specifically, we need either x_1 or y_0 (or both) to be of $O(\sigma^{-1})$.

To proceed further, and to see if, and under what conditions, travelling waves can be initiated, we need to solve equations (2), (3) numerically.

3. Numerical solutions of the initial-value problem

The method we used to solve the initial-value problem (2, 3) numerically was essentially that described in Merkin & Needham (1989), with only minor changes being needed to accommodate the third equation. We took representative values of μ and γ to illustrate the various cases that can arise in the behaviour of the well-stirred system. Throughout we took $\sigma = 1$.

We started by examining the threshold values necessary for the initiation of non-trivial large time behaviour. The work in the previous section gives estimates for the lower bounds (10) and (16*b*), (which is, for $\sigma = 1$, $x_1 y_0 = 1.180$) on x_1 and y_0 for such behaviour. In all the cases considered which were below these bounds we found that, as expected, the solution returned to its unreacted state, quickly for y and z, and more slowly (by diffusion) for x. We also found that for values of x_1 and y_0 which were a little greater than the suggested lower bounds, again the solution returned to its unreacted state for t large. This suggests that the actual lower bounds on x_1 and y_0 could well be somewhat greater than those estimated above.

(*a*) *Reduced case* ($\mu = \gamma$)

Here we can identify x_1, the initial concentration of A, with the initial value c_0 in the well-stirred system. The reason for this will become apparent when we come to consider the equations for the permanent-form travelling waves. However, we can note in passing that the sum $\xi = x+y+z$ satisfies the diffusion equation in this case, with then $\xi \sim x_1 + O(t^{-1/2})$ as $t \to \infty$ uniformly in r and the correspondence between x_1 and the total initial concentration c_0 in the well-stirred system becomes clear. We then have the behaviour for the steady state

$$x_s = \frac{1}{2\mu}(\mu x_1 - [\mu^2 x_1^2 - 4\mu(\mu+1)]^{1/2}), \quad y_s = \frac{1}{x_s}, \tag{25a}$$

$$2\sqrt{\left(\frac{\mu+1}{\mu}\right)} < x_1 \leqslant \frac{(\mu+1)(\sqrt{(2+\mu)}-1)}{\mu} + \frac{1}{(\sqrt{(2+\mu)}-1)}, \quad \text{unstable node},$$

$$\frac{(\mu+1)(\sqrt{(2+\mu)}-1)}{\mu} + \frac{1}{(\sqrt{(2+\mu)}-1)} < x_1 < \frac{2-\mu}{\sqrt{(1-\mu)}} + \frac{\sqrt{(1-\mu)}}{\mu}, \quad \text{unstable focus},$$

$$\frac{2-\mu}{\sqrt{(1-\mu)}} + \frac{\sqrt{(1-\mu)}}{\mu} < x_1 < \frac{(\mu+1)(\sqrt{(2+\mu)}+1)}{\mu} + \frac{1}{(\sqrt{(2+\mu)}+1)}, \quad \text{stable focus},$$

$$\frac{(\mu+1)(\sqrt{(2+\mu)}+1)}{\mu} + \frac{1}{(\sqrt{(2+\mu)}+1)} \leqslant x_1, \quad \text{stable node}.$$

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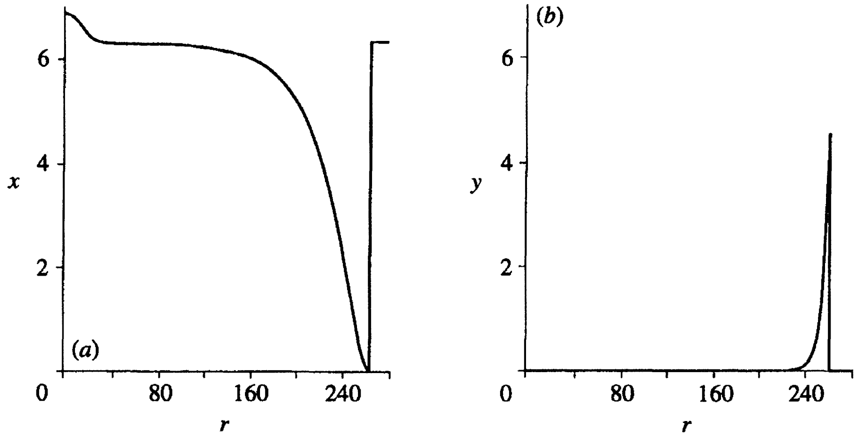

Figure 1. Concentration profiles for (a) x and (b) y, at large time, showing the emergence of a reaction-diffusion travelling wave, obtained from a numerical solution of the initial value problem (2), (3) for the reduced case $\mu = \gamma = 0.12$, $x_1 = 6.3$.

The other non-trivial steady state, corresponding to the other root in (25a) is always a saddle. These two steady states exist only for

$$x_1^2 > \frac{4(\mu+1)}{\mu}, \quad \text{or} \quad \mu > \frac{4}{x_1^2-4}. \tag{25b}$$

The trivial state

$$x = x_1, \quad y = 0 \tag{25c}$$

is always a stable node for all parameter values.

We fixed the value of μ at $\mu = 0.12$ and took $y_0 = 1.0$ throughout, and obtained numerical solutions for increasing values of x_1, each in the ranges:

(i) $0 < x_1 < 6.11010$, only stationary state (25c) exists and for $x_1 > 6.11010$, stationary state (25a) is

(ii) $6.11010 < x_1 < 6.44098$, unstable node,

(iii) $6.44098 < x_1 < 9.35006$, unstable focus

(iv) $9.35006 < x_1 < 9.82145$, unstable focus surrounded by a stable limit cycle

(v) $9.82145 < x_1 < 23.33003$, stable focus,

(vi) $23.33003 < x_1$, stable node.

We started by taking values of $x_1 < 6.11010$ and for all the initial inputs y_0 tried, we found that no travelling wave was generated, with the concentration y rapidly decreasing to zero with the concentration x returning more slowly (by diffusion) to its original unreacted state. This behaviour was also observed in both the contracting and expanding cases.

We then took values of x_1 in each of the different steady state behaviour regions (ii)–(vi) given above. The situation is illustrated in figures 1–3, where we give concentration profiles x and y at large values of t, taken to be sufficiently large for the travelling wave structure to have emerged fully in the numerical results.

In figure 1 we give results for $x_1 = 6.3$ ($x_s = 2.38243$, $y_s = 0.41974$, unstable node). Here a definite travelling wave structure has emerged with a drop in the concentration x to (almost) zero before it rises again at the rear of the wave to the constant value x_1. The trough in the concentration x corresponds to a pulse in an otherwise (almost) zero concentration y.

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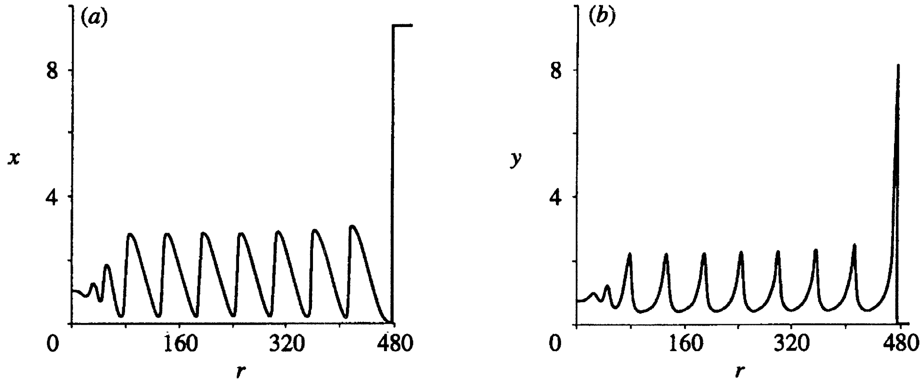

Figure 2. Concentration profiles for (*a*) x and (*b*) y, at large time, showing the emergence of a reaction-diffusion travelling wave, obtained from a numerical solution of the initial value problem (2), (3) for the reduced case $\mu = \gamma = 0.12$, $x_1 = 9.3667$.

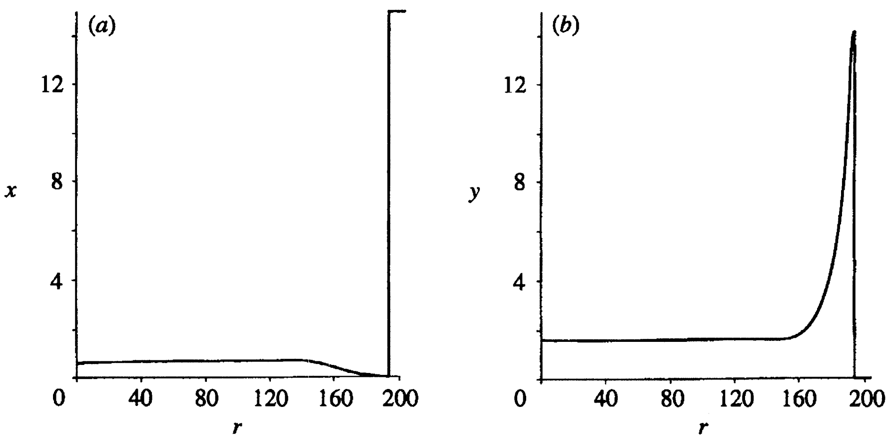

Figure 3. Concentration profiles for (*a*) x and (*b*) y, at large time, showing the emergence of a reaction-diffusion travelling wave, obtained from a numerical solution of the initial value problem (2), (3) for the reduced case $\mu = \gamma = 0.12$, $x_1 = 15.0$.

A similar situation arises for $x_1 = 7.0$ ($x_s = 1.79217$, $y_s = 0.55798$, unstable focus) with the concentration profiles of x and y for large times being almost identical to those shown in figure 1. The main difference between these two cases is that now the rise in x at the rear of the trough takes place over a slightly larger lengthscale. In both cases we found that the propagating wavefronts had a constant speed (at least to within the accuracy of the numerical scheme) for sufficiently large t.

For $x_1 = 9.36666$ (figure 2), a stable limit cycle exists in the well-stirred system and this is manifested by the emergence of a regular wave train in both x and y at the rear of the propagating reaction-diffusion front. Again we found that for sufficiently large times the reaction-diffusion front travelled with a constant speed and that each of the waves in the wave train at the rear of the propagating front also travelled with the same constant speed, once they had reached their asymptotic form. The situation at large times is then that the reaction-diffusion front propagates with a uniform speed followed by a regular wave train, stationary relative to the front. There is a region near the origin where waves are continually being generated; these grow in amplitude and period and propagate forwards to join the wave train at its rear. We

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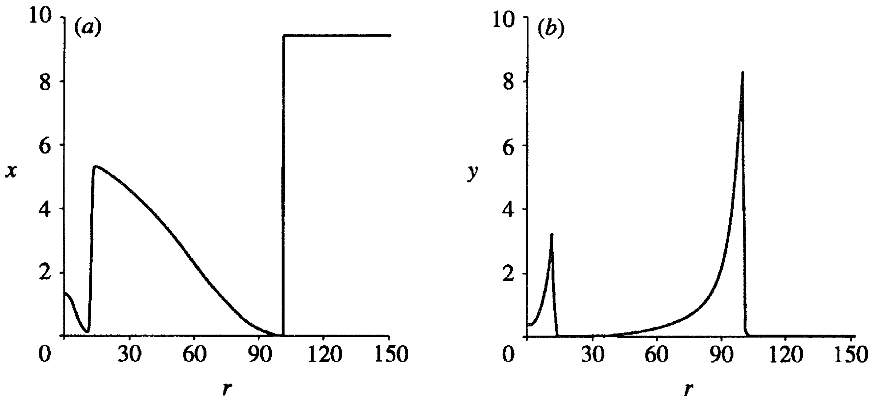

Figure 4. Concentration profiles for (*a*) x and (*b*) y, at large time, showing the emergence of a reaction-diffusion travelling wave, obtained from a numerical solution of the initial value problem (2), (3) for the contracting case $\mu = 0.12$, $\gamma = 0.15$, $x_1 = 9.3667$.

also compared the amplitude and period (adjusted by the constant wave speed) of the waves in this wave train and they were found to agree with the corresponding amplitude and period of the time-traces in the well-stirred system.

For $x_1 = 15.0$ ($x_s = 0.60543$, $y_s = 1.53745$, stable focus), shown in figure 3 and for $x_1 = 27.0$ ($x_s = 0.35022$, $y_s = 2.85533$, stable node) where the large time concentration profiles for x and y (not shown) are very similar to those shown in figure 3, the situation is different. Here a constant velocity travelling wave emerges and there is still a rapid fall in the concentration x in the wave with a corresponding rapid rise in the concentration y. However, at the rear of the wave, x and y now approach their (stable) non-trivial stationary states, as given by (25*a*), and do not return to their initial concentrations.

An interesting feature of these results is that the formation of a constant velocity travelling wave for large times requires the existence of the non-trivial stationary state (25*a*) even in those cases where this is unstable and the concentrations at the rear of the wave returns to their unreacted states. This results in the propagation of a dip in concentration of reactant A in an otherwise uniform distribution with a corresponding pulse in the concentration of the autocatalyst B.

(*b*) *Contracting case* ($\mu < \gamma$)

Here we again took $\mu = 0.12$ and now put $\gamma = 0.15$, and considered three cases for x_1, corresponding in the previous (reduced) case to unstable and stable stationary states, and to the existence of stable limit cycles. The results are shown in figures 4 and 5.

We started by considering the case $x_1 = 7.0$ and we found that the large time concentration profiles are very similar to those for the reduced case. It is observed that again a constant velocity propagating reaction-diffusion front is formed in which there is a drop in the concentration x to (almost) zero, before a rise to a constant non-zero value at the rear of the wave. This value is less than the original concentration x_1. The concentration y behaves as in the reduced case, being (almost) zero everywhere apart from in the pulse which again corresponds to the trough in the concentration x.

In figure 4, we give results for $x_1 = 9.36666$ to compare with figure 2. Again wave-like behaviour is produced at the rear of the wave, as in the reduced case. The

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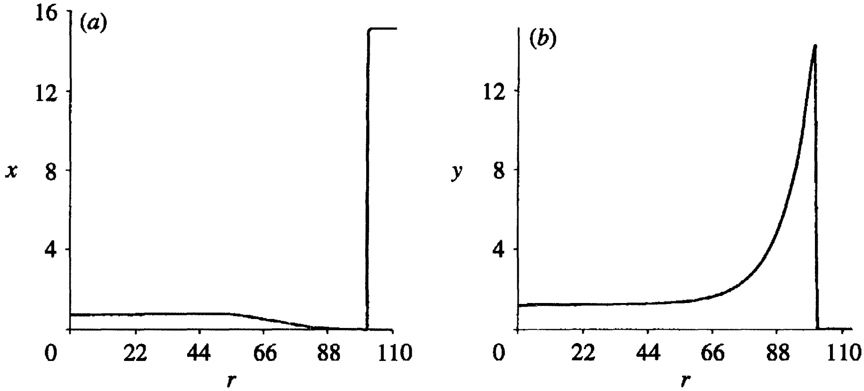

Figure 5. Concentration profiles for (*a*) x and (*b*) y, at large time, showing the emergence of a reaction-diffusion travelling wave, obtained from a numerical solution of the initial value problem (2), (3) for the contracting case $\mu = 0.12$, $\gamma = 0.15$, $x_1 = 15.0$.

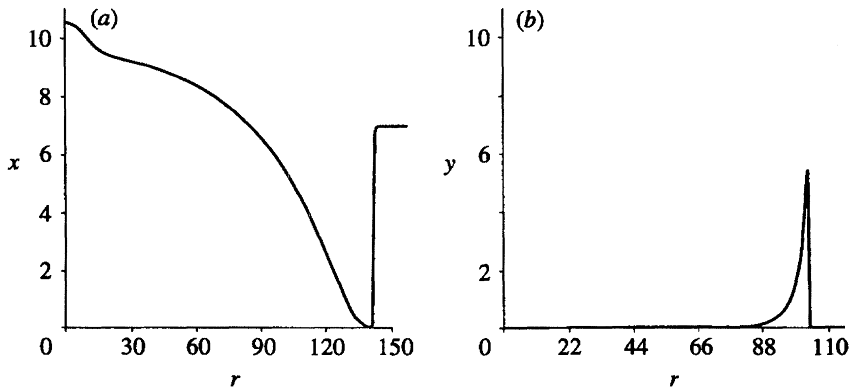

Figure 6. Concentration profiles for (*a*) x and (*b*) y, at large time, showing the emergence of a reaction-diffusion travelling wave, obtained from a numerical solution of the initial value problem (2), (3) for the expanding case, $\mu = 0.12$, $\gamma = 0.09$, $x_1 = 7.0$.

difference between the two cases is that now a regular wave train is not seen, with the oscillatory response dying out at large times.

In figure 5, we show results for $x_1 = 15.0$ (to compare with figure 3). The behaviour of the concentrations x and y is similar to that for the reduced case, but now x and y do not both approach non-zero stationary states at the rear of the wave but the concentration y falls slowly and uniformly to zero, producing a pulse-like wave form. The concentration x approaches a small but non-zero value at the rear of the wave.

(*c*) *Expanding case* ($\mu > \gamma$)

For this case we again kept $\mu = 0.12$, but now we took $\gamma = 0.09$, and considered the three different cases described in §3*b* above.

In figure 6, for $x_1 = 7.0$, there is again a constant velocity propagating front, but now the loss of the stationary state at the rear of the wave corresponds to a slow (and again almost uniform) increase in the concentration x with the concentration y remaining zero except in the pulse which corresponds to the trough in the concentration x.

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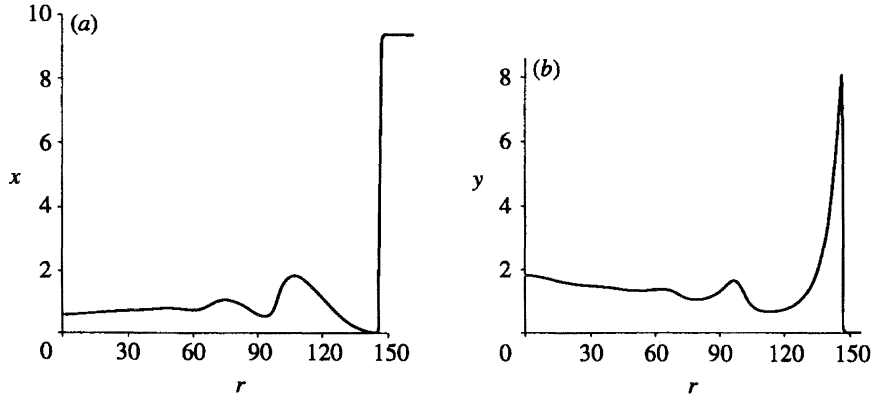

Figure 7. Concentration profiles for (*a*) x and (*b*) y, at large time, showing the emergence of a reaction-diffusion travelling wave, obtained from a numerical solution of the initial value problem (2), (3) for the expanding case $\mu = 0.12$, $\gamma = 0.09$, $x_1 = 9.3667$.

In figure 7, we show results for $x_1 = 9.36666$ (to compare with figure 2). Again we observe wave-like at the rear of the propagating front, but these eventually die out in both concentrations x and y. Finally we considered the case $x_1 = 15.0$. The behaviour here is very much as in the contracting case, the stationary state (25*a*) is not attained.

In both the expanding and contracting case a well-defined wave-front structure emerges at large times, in which there is a sharp drop (to almost zero) in the concentration x and a sharp rise in the concentration y. It is in the behaviour at the rear of the wave, where the only possible stationary state is the trivial one (25*c*), that differences between the two cases are seen. In the contracting case, x rises to a constant non-zero value, less than x_1, the concentration ahead of the wave, while y falls to (and remains at) zero. In the expanding case there are two possibilities depending on the value of x_1. Either, concentration x increases almost uniformly with time, with y falling to (and remaining at) zero (e.g. for $x_1 = 7.0$). Alternatively, concentration x falls uniformly to zero, while concentration y increases uniformly with time (e.g. for $x_1 = 15.0$).

4. Permanent form travelling waves

In this section we discuss the behaviour of the permanent form travelling wave which we have seen above can arise in the solution of the initial-value problem (2), (3) for large time. We introduce a travelling coordinate $s = r - v_0 t$, where v_0 is the (constant) wave speed of the propagating wave, $v_0 > 0$. Equations (2*a*–*c*) then become

$$\frac{\mathrm{d}^2 x}{\mathrm{d}s^2} + v_0 \frac{\mathrm{d}x}{\mathrm{d}s} + \mu z - xy^2 = 0, \tag{26a}$$

$$\frac{\mathrm{d}^2 y}{\mathrm{d}s^2} + v_0 \frac{\mathrm{d}y}{\mathrm{d}s} + xy^2 - y = 0, \tag{26b}$$

$$\frac{\mathrm{d}^2 z}{\mathrm{d}s^2} + v_0 \frac{\mathrm{d}z}{\mathrm{d}s} + y - \gamma z = 0, \tag{26c}$$

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subject to the boundary conditions that

$$x \to x_1, \quad y \to 0, \quad z \to 0 \quad \text{as} \quad s \to \infty \tag{27}$$

and that the conditions are uniform as $s \to -\infty$ at the rear of the wave.

Thus we require a non-trivial non-negative solution (i.e. $x \not\equiv x_1$, y, $z \not\equiv 0$) with $v_0 > 0$ of equations (26) satisfying the appropriate boundary conditions. We note that this leads directly to the requirement that $y(s) > 0$ on $-\infty < s < \infty$, established using essentially the same method (for an equivalent result) given by Billingham & Needham (1991*a*) and Merkin *et al.* (1993). Now assume that z is zero at a finite value s_0 of s, i.e. $z(s_0) = 0$. Then, since $z(s)$ is non-negative, $z'(s_0) = 0$ and z must have a local minimum at s_0. However, from equation (26*c*), $z''(s_0) = -y(s_0) < 0$, which gives a contradiction. Hence $z(s) > 0$ in $-\infty < s < \infty$. By using this result, and a similar argument, we can establish from equation (26*a*) that $x(s) > 0$ on $-\infty < s < \infty$, giving the result

$$x > 0, \quad y > 0, \quad z > 0 \quad \text{on} \quad -\infty < s < \infty. \tag{28}$$

We now examine the condition to be applied at the rear of the wave in more detail. An examination of equations (26) shows that, in general, we must have

$$x \to x_e, \quad y \to 0, \quad z \to 0 \quad \text{as} \quad s \to -\infty, \tag{29}$$

where x_e is a constant and will depend on the parameters of the system. If we now apply

$$\int_{-\infty}^{\infty} \ldots \mathrm{d}s \quad \text{to} \quad (26\,b,\, c)$$

we obtain, using (27) and (29)

$$\int_{-\infty}^{\infty} xy^2 \,\mathrm{d}s = \int_{-\infty}^{\infty} y \,\mathrm{d}s = \gamma \int_{-\infty}^{\infty} z \,\mathrm{d}s. \tag{30a}$$

Applying the same to equation (26*a*), and using (29) and (30*a*), then gives

$$v_0(x_1 - x_e) = (\gamma - \mu) \int_{-\infty}^{\infty} z \,\mathrm{d}s. \tag{30b}$$

Now via (28) the integral in (30*b*) is positive and hence:

$$x_e < x_1 \quad \text{for the contracting case,} \quad \mu < \gamma,$$
$$x_e > x_1 \quad \text{for the expanding case,} \quad \mu > \gamma.$$

(the former case was observed in the numerical results). The reduced case, $\mu = \gamma$, needs further consideration and this is what we examine next.

(*a*) *Reduced case*, $\mu = \gamma$

(i) *Boundary conditions*

On adding equations (26) we find that $\xi = x + y + z$ satisfies the equation, with $\mu = \gamma$,

$$\xi'' + v_0 \xi' = 0, \tag{31a}$$

$$\xi \to x_1 \quad \text{as} \quad s \to \infty, \quad \xi \quad \text{bounded as} \quad s \to -\infty. \tag{31b}$$

The solution of (31*a*, *b*) is simply

$$\xi = x_1, \tag{31c}$$

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with (26a, b) then becoming

$$x''+v_0 x'+\mu(x_1-x-y)-xy^2=0, \tag{32a}$$

$$y''+v_0 y'+xy^2-y=0, \tag{32b}$$

subject to boundary conditions (27) and either

$$x \to x_1, \quad y \to 0 \quad \text{as} \quad s \to -\infty \tag{33a}$$

or

$$x \to x_s, \quad y \to y_s \quad \text{as} \quad s \to -\infty, \tag{33b}$$

where (x_s, y_s) is given by (25a). It is condition (31c) that enables us to identify x_1 with the initial value c_0 in the well-stirred system (part I), as noted earlier, thus leading to stationary states (25a).

Boundary condition (33a) arises naturally from (30b). The extra boundary condition (33b) arises from the reduction of the order of the system, and is not in violation of (30) as the infinite integrals involved in this relation are no longer convergent.

The boundary conditions satisfied at the rear of the wave require further discussion. On putting $x = x_s+X$, $y = y_s+Y$, where X and Y are small as $s \to -\infty$, we obtain linear equations for X and Y which have a solution in the form

$$X = A\,e^{\lambda t}, \quad Y = B\,e^{\lambda t}, \tag{34a}$$

where the eigenvalue λ is given by the quartic equation

$$\lambda^4+2v_0\lambda^3+(v_0^2+2x_s y_s-1-\mu-y_s^2)\lambda^2 + v_0(2x_s y_s-1-\mu-y_s^2)\lambda+y_s^2(1+\mu)+\mu-2\mu x_s y_s = 0. \tag{34b}$$

We require equation (34b) to have roots which are positive (or have positive real part). It is straightforward to show that, when (x_s, y_s) is given by the trivial state (25c), equation (34b) has the required solutions

$$\lambda = \tfrac{1}{2}(\surd(v_0^2+4)-v_0), \quad \tfrac{1}{2}(\surd(v_0^2+4\mu)-v_0) \tag{35}$$

for all values of μ.

When (x_s, y_s) is given by (25a), equation (34b) can be expressed in the form

$$\lambda^4+2v_0\lambda^3+(\mathrm{Tr}+v_0^2)\lambda^2+v_0\,\mathrm{Tr}\,\lambda+\Delta = 0, \tag{36}$$

where Tr and Δ are the trace and determinant respectively of the jacobian of the well-stirred system corresponding to the stationary state (25a). These are given in part I, where it was shown that $\Delta > 0$ for all values of μ and x_1 for which stationary state (25a) exists. Moreover, it is clear that equation (36) cannot have solutions of the required form when $\mathrm{Tr} \geqslant 0$, i.e. when stationary state (25a) is unstable. Hence, a necessary condition for this stationary state to be attained at the rear of the wave is that $\mathrm{Tr} < 0$, i.e. (25a) is temporally stable. Thus the only condition that can be satisfied at the rear of the wave when (25a) is unstable is the trivial state (25c).

(ii) *General properties*

We now establish properties of the solutions of equations (26) subject to boundary conditions (29) and (33a) or (33b). We have already noted in (28) that $x > 0$, $y > 0$ on $-\infty < s < \infty$ and it is straightforward to deduce that

$$x < x_1, \quad y < x_1, \quad x+y < x_1 \quad \text{on} \quad -\infty < s < \infty. \tag{37}$$

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To establish the first of these inequalities, we note first that $x_s, y_s \leqslant x_1$ and hence, if there is an interval of s over which $x > x_1$ then x will have at least one local maximum on this interval. Suppose that x attains such a local maximum at $s = s_1$ (say), with then $x'(s_1) = 0$, $x''(s_1) \leqslant 0$, $x(s_1) > x_1$. However, from equation (32 *a*)

$$x''(s_1) = x(s_1)\,y(s_1)^2 + \mu(x(s_1) + y(s_1) - x_1) > 0 \tag{38}$$

by (28) and the hypothesis. This is a contradiction and we can conclude that $x < x_1$ on $-\infty < s < \infty$.

On putting $\psi = x + y$ and adding equations (32 *a*, *b*) we obtain

$$\psi'' + v_0\,\psi' + \mu(x_1 - \psi) - y = 0. \tag{39}$$

Noting that $x_s + y_s < x_1$, a similar argument then shows that $\psi < x_1$ on $-\infty < s < \infty$. The inequality $y < x_1$ then follows directly.

We can obtain a bound on the maximum value of $y(s)$ when boundary conditions (27) and (33 *a*) apply, by first noting that y will have at least one local maximum on $-\infty < s < \infty$. Suppose one such local maximum occurs at $s = s_2$ (say), at which point $y'(s_2) = 0$, $y''(s_2) \leqslant 0$, $y(s_2) = y_m$. Then, from equation (32 *b*),

$$y''(s_2) = y_m(1 - x(s_2)\,y_m) \leqslant 0 \tag{40a}$$

from which it follows that

$$x(s_2) \geqslant 1/y_m. \tag{40b}$$

Then, from inequality (37), we have

$$x_1 \geqslant x(s_2) + y_m \geqslant \frac{1}{y_m} + y_m. \tag{40c}$$

Rearranging (40 *c*) gives the condition that

$$y_m \leqslant \tfrac{1}{2}(x_1 + \surd(x_1^2 - 4)). \tag{41}$$

Expression (41) requires $x_1 \geqslant 2$, and hence a necessary condition for the existence of a solution of equations (32) is that $x_1 \geqslant 2$, which is the necessary condition for the existence of stationary state (25 *c*) and suggests, together with the evidence from the numerical solutions, that non-trivial solutions of equations (32) exist only when stationary state (25 *a*) exists.

(iii) *Solution for x_1 large*

Further information about the nature of the solution of equations (32) can be obtained by considering the solution valid for x_1 large. To start we put

$$x = x_1 X, \quad y = x_1 Y, \quad v_0 = x_1 \bar{v}, \quad \bar{s} = x_1 s, \tag{42a}$$

with equations (32) becoming

$$X'' + \bar{v}X' - XY^2 + \mu x_1^{-2}(1 - X - Y) = 0, \tag{42b}$$

$$Y'' + \bar{v}Y' + XY^2 - x_1^{-2}\,Y = 0, \tag{42c}$$

satisfying

$$X \to 1, \quad Y \to 0 \quad \text{as} \quad \bar{s} \to \infty, \tag{42d}$$

where primes denote differentiation with respect to $\bar{s}$. The boundary conditions at the rear of the wave are relaxed at this stage.

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Equations (42b, c) suggest looking for a solution valid for x_1 large by expanding

$$\left.\begin{aligned}\bar{X}(\bar{s};x_1) &= X_0(\bar{s})+x_1^{-2}X_1(\bar{s})+\dots,\\ \bar{Y}(\bar{s};x_1) &= Y_0(\bar{s})+x_1^{-2}Y_1(\bar{s})+\dots,\\ \bar{v} &= \bar{v}_0+x_1^{-2}\bar{v}_1+\dots.\end{aligned}\right\} \tag{43}$$

At leading order we obtain the equations

$$X_0''+\bar{v}_0X_0'-X_0Y_0^2=0, \tag{44a}$$

$$Y_0''+\bar{v}_0Y_0'+X_0Y_0^2=0, \tag{44b}$$

with

$$X_0\to 1,\quad Y_0\to 0\quad \text{as}\quad \bar{s}\to\infty. \tag{44c}$$

By adding equations (44a, b) and using boundary condition (44c) and the requirement that the solution not be exponentially large as $\bar{s}\to-\infty$ (to be able to match to further regions at the rear of the wave), we obtain

$$X_0+Y_0=1. \tag{45a}$$

Equations (44a, b) then have the solution

$$X_0=\frac{e^{\bar{v}_0\bar{s}}}{1+e^{\bar{v}_0\bar{s}}},\quad Y_0=\frac{1}{1+e^{\bar{v}_0\bar{s}}},\quad \bar{v}_0=\frac{1}{\sqrt{2}}, \tag{45b}$$

which is the solution for the cubic-Fisher problem (Saul & Showalter 1984; Gray *et al.* 1990).

The particular choice of solution given by (45b) requires some comment. It has been shown by Billingham & Needham (1991b) that equations (44) with condition (45a) have a solution for all $\bar{v}_0\geqslant 1/\sqrt{2}$. However, all solutions for $\bar{v}_0>1/\sqrt{2}$ have only algebraic decay at the front of the wave with the solution given by (45b) being the only one with exponential decay as $\bar{s}\to\infty$. Now our original initial-value problem (2), (3) has initial data for y with compact support and, to match onto this form at the front of the wave, the decay rate in y must be exponential there, leading to solution (45b).

Before proceeding to the higher order terms, we note that this leading order solution has a non-uniformity, since (45b) implies that $x\to 0$, $y\to x_1$ as $\bar{s}\to-\infty$ and boundary conditions (33) are not satisfied.

At $O(x_1^{-2})$ we obtain, using (45a),

$$X_1''+\bar{v}_0X_1'-2X_0Y_0Y_1-Y_0^2X_1=-\bar{v}_1X_0', \tag{46a}$$

$$Y_1''+\bar{v}_0Y_1'+2X_0Y_0Y_1+Y_0^2X_1=-\bar{v}_1Y_0'+Y_0, \tag{46b}$$

subject to

$$X_1\to 0,\quad Y_1\to 0\quad \text{as}\quad \bar{s}\to\infty. \tag{46c}$$

By adding equations (46a, b) and using (45a) we find that $\psi_1=X_1+Y_1$ satisfies

$$V_1''+\bar{v}_0\psi_1=Y_0. \tag{47a}$$

The required solution is, on using (45b),

$$\psi_1=\frac{1}{\bar{v}_0^2}[\bar{v}_0\bar{s}-\log(1+e^{\bar{v}_0\bar{s}})(1+e^{-\bar{v}_0\bar{s}})]. \tag{47b}$$

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Solution (47 *b*) show that

$$\psi_1 \sim \frac{1}{\bar{v}_0^2}(\bar{v}_0\,\bar{s}-1)+O(\mathrm{e}^{\bar{v}_0\bar{s}}) \quad \text{as} \quad s\to-\infty. \tag{47c}$$

A further consideration of equations (46 *a*, *b*) then shows that

$$Y_1 \sim \frac{1}{\bar{v}_0^2}(\bar{v}_0\,\bar{s}-1)+\ldots, \quad \text{as} \quad \bar{s}\to-\infty \tag{48}$$

with X_1 being exponentially small as $\bar{s}\to-\infty$.

Before leaving this thin region at the front of the wave, where s is of $O(x_1^{-1})$, we note that equation (46 *a*) becomes

$$X_1''+\bar{v}_0 X_1'-(1-X_0)(1-3X_0)\,X_1 = 2X_0(1-X_0)\,\psi_1-\bar{v}_1 X_0', \tag{49a}$$

with ψ_1 given by (47 *b*). Now equation (49 *a*) has a complementary function X_0', and to obtain a solution of this equation which has $X_1\to 0$ as $\bar{s}\to\infty$ and is not exponentially large as $\bar{s}\to-\infty$, we require that the consistency condition

$$\int_{-\infty}^{\infty}(\bar{v}_1 X_0'-2X_0(1-X_0)\,\psi_1)\,X_0'\,\mathrm{e}^{\bar{v}_0\bar{s}}\,\mathrm{d}\bar{s} = 0 \tag{49b}$$

be satisfied. This condition determines $\bar{v}_1$, and, after performing the necessary integrations, we find that

$$\bar{v}_1 = -3/2\bar{v}_0^3. \tag{49c}$$

Hence the asymptotic form of the wave speed is

$$v_0 = \frac{x_1}{\surd 2}\left(1-\frac{6}{x_1^2}+\ldots\right) \quad \text{as} \quad x_1\to\infty. \tag{49d}$$

Finally, we note that the solution up to $O(x_1^{-2})$ does not involve the parameter μ. This first appears in the solution at $O(x_1^{-4})$ where we find that

$$X_2 \sim \frac{-\mu\bar{s}}{\bar{v}_0} \quad \text{as} \quad \bar{s}\to-\infty. \tag{50}$$

From (42 *a*), (45 *b*) and (48) we have that

$$y \sim x_1\left(1+\frac{s}{\bar{v}_0}x_1^{-1}+\ldots\right) \tag{51a}$$

at the rear of this region at the front of the wave. Equation (51 *a*) suggests that a further region is required in which s is of $O(x_1)$. To proceed we start by assuming that the parameter μ is of $O(1)$, with (50), (51 *a*) and (32 *a*) then suggesting that we put

$$x = x_1^{-1}U, \quad y = x_1 V, \quad \zeta = x_1^{-1}s \quad (\zeta<0). \tag{51b}$$

On applying (51 *b*), equations (32) become

$$\mu(1-V)-UV^2+x_1^{-2}(\bar{v}U'-\mu U)+x_1^{-3}\,U'' = 0, \tag{52a}$$

$$\bar{v}V'+UV^2-V+x_1^{-2}\,V'' = 0, \tag{52b}$$

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where primes now denote differentiation with respect to ζ. The matching conditions are that

$$U \sim -\mu\zeta/\bar{v}_0, \tag{52c}$$

$$V \sim 1+\zeta/\bar{v}_0+\dots, \tag{52d}$$

as $\zeta \to 0^-$.

Equations (52) suggest looking for a solution by expanding in powers of x_1^{-1}. It is straightforward to show that the leading order terms (U_0, V_0) are given by

$$U_0 = \frac{\mu(\mu+1)[1-\exp((\mu+1)\,\zeta/\bar{v}_0)]}{[\mu+\exp((\mu+1)\,\zeta/\bar{v}_0)]^2}, \tag{53a}$$

$$V_0 = \frac{1}{(\mu+1)}[\mu+\exp((\mu+1)\,\zeta/\bar{v}_0)]. \tag{53b}$$

As $\zeta \to -\infty$, $U_0 \to \dfrac{\mu+1}{\mu}$, $V_0 \to \dfrac{\mu}{\mu+1}$, so that

$$x \to x_1^{-1}\left(\frac{\mu+1}{\mu}\right), \quad y \to x_1\left(\frac{\mu}{\mu+1}\right) \tag{54}$$

at the rear of the wave. We can see that (54) is the asymptotic form of the non-trivial stationary state (25a) for large x_1 and hence, in this case it is this stationary state which is attained at the rear of the wave.

The structure of the permanent-form travelling wave for x_1 large and μ of $O(1)$ is now clear. There is a thin region at the front of the wave, of thickness $O(x_1^{-1})$, in which the concentration of A decreases and that of B increases, reaching a maximum value of $O(x_1)$. There is then a further, much thicker region, of thickness $O(x_1)$ in which the concentration of A remains small, of $O(x_1^{-1})$ while the concentration of B decreases but still remains large, of $O(x_1)$, with the non-trivial stationary state (25a) being achieved at the rear of the wave.

We have shown in part I that, when x_1 is large and μ is of $O(1)$, stationary state (25a) is stable. However, this is not the case when μ is small, and in particular there is a Hopf bifurcation (corresponding to a change in stability of (25a)) when $\mu = x_1^{-1}+O(x_1^{-2})$. This suggests that we also need to consider the case when μ is of $O(x_1^{-1})$. To do this we put

$$\bar{\mu} = \mu x_1 \tag{55a}$$

where now $\bar{\mu}$ is of $O(1)$. The solution in the region at the front of the wave, as given by (45a, b), (47b) and(48) is not affected by this (though (50) will be).

We still require a region in which s is of $O(x_1)$, and in which transformation (51b) applies, with the modification that now

$$x = x_1^{-2}\,U. \tag{55b}$$

Equations (32) become, on applying (51b) and (55)

$$\bar{\mu}(1-V)-UV^2+x_1^{-2}\bar{v}U'-\bar{\mu}x_1^{-3}U+x_1^{-4}U'' = 0, \tag{56a}$$

$$\bar{v}V'-V+x_1^{-1}UV^2+x_1^{-2}V'' = 0. \tag{56b}$$

The matching conditions are still given by (52c, d), with $\bar{\mu}$ replacing μ in (52c). The leading order terms (U_0, V_0) are now given by

$$U_0 = \bar{\mu}(1-\mathrm{e}^{\zeta/\bar{v}_0})\,\mathrm{e}^{-2\zeta/\bar{v}_0}, \tag{57a}$$

$$V_0 = \mathrm{e}^{\zeta/\bar{v}_0}. \tag{57b}$$

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Equation (57) shows that $V_0 \to 0$, whereas U_0 becomes exponentially large as $\zeta \to \infty$. To obtain further information about this non-uniformity we need to consider (U_1, V_1), the terms of $O(x_1^{-1})$. We find that

$$V_1 = \bar{\mu}\left(1 + \frac{\zeta}{\bar{v}_0}\,e^{\zeta/\bar{v}_0}\right), \tag{58a}$$

$$U_1 = -\bar{\mu}^2\,e^{-2\zeta/\bar{v}_0}\left(1+\frac{\zeta}{\bar{v}_0}\,e^{\zeta/\bar{v}_0}\right)(2e^{-\zeta/\bar{v}_0}-1). \tag{58b}$$

From (58) we have that

$$x \sim x_1^{-2}\bar{\mu}\,e^{-2\zeta/\hat{v}_0}\left(1 - 2\bar{\mu}\frac{e^{-\zeta/\bar{v}_0}}{x_1} + \dots\right), \tag{59a}$$

$$y \sim \bar{\mu} + \dots, \tag{59b}$$

as $\zeta \to -\infty$. (59) suggests that we require a further region in which

$$\zeta = \bar{v}_0 \log\left(\frac{\bar{\mu}}{x_1}\right) + \bar{\zeta} \tag{60}$$

and in which we leave x and y unscaled. Equations (32) then become, at leading order,

$$\bar{v}_0\,x' + \bar{\mu} - xy^2 = 0, \tag{61a}$$

$$\bar{v}_0\,y' + xy^2 - y = 0, \tag{61b}$$

where primes now denote differentiation with respect to $\bar{\zeta}$. The matching condition is, from (59)

$$x \sim \frac{e^{-2\bar{\zeta}/\bar{v}_0}}{\bar{\mu}}(1 - 2\,e^{-\bar{\zeta}/\bar{v}_0} + \dots), \quad y \sim \bar{\mu}\,e^{\bar{\zeta}/\bar{v}_0}(1 + e^{-\bar{\zeta}/\bar{v}_0} + \dots). \tag{61c}$$

Equations (61) have been discussed in some detail by Merkin *et al.* (1987) where it was shown that

$$x \to \frac{1}{\bar{\mu}}, \quad y \to \bar{\mu} \quad \text{as} \quad \bar{\zeta} \to -\infty \quad \text{for} \quad \bar{\mu} > 1. \tag{62a}$$

(62a) corresponds to the non-trivial state (25a) in the limit as $x_1 \to \infty$, $\bar{\mu} = \mu x_1$ of $O(1)$. Thus for $\bar{\mu} > 1$, i.e. $\mu > x_1^{-1}$, stationary state (25a) is stable and this is the stationary state attained at the rear of the wave. For μ in the range $1 > \bar{\mu} > \mu_c = 0.90032$, the solution of equations (61) approaches a stable limit cycle as $\bar{\zeta} \to -\infty$ (through a Hopf bifurcation at $\bar{\mu} = 1$). This corresponds to the appearance of a travelling wave train at the rear of the reaction-diffusion front. For $\bar{\mu} < \mu_c$,

$$x \sim \frac{-\bar{\mu}}{\bar{v}_0}\bar{\zeta} + \dots, \quad y \to 0 \quad \text{as} \quad \bar{\zeta} \to -\infty \tag{62b}$$

(with y being exponentially small for $\bar{\zeta}$ large).

A further region is then required, in which y is exponentially small and in which

$$x = x_1\,\bar{U}, \quad s = \bar{v}_0\,x_1 \log(2\bar{\mu}^2/x_1) + x_1^2\,\sigma. \tag{63}$$

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By using (63) equation (32*a*) becomes

$$\bar{v}\bar{U}' + \bar{\mu}(1-\bar{U}) + x_1^{-3}\,\bar{U}'' = 0 \tag{64a}$$

(where primes denote differentiation with respect to σ). The matching condition on $\bar{U}$ is, from (62*b*)

$$\bar{U} \sim \frac{-\bar{\mu}}{\bar{v}_0}\sigma + \ldots \quad \text{as} \quad \sigma \to 0^-. \tag{64b}$$

The required solution for the leading order term $\bar{U}_0$ in an expansion in inverse powers of x_1 is

$$\bar{U}_0 = 1 - \mathrm{e}^{(\bar{\mu}/\bar{v}_0)\sigma} \tag{64c}$$

and shows that $\bar{U}_0 \to 1$, i.e. $x \to x_1$, at the rear of the wave. Thus, in the case when $\bar{\mu} < \mu_c$, i.e. $\mu < \mu_c x_1^{-1}$ and the non-trivial stationary state (25*a*) is unstable and there is no further stable attractor in the system, it is the trivial stationary state, i.e. $x = x_1$, $y = 0$, which is approached at the rear of the wave.

(*b*) *Expanding* ($\mu > \gamma$) *and contracting* ($\mu < \gamma$) *cases*

(i) *General properties*

We have already seen that the only boundary conditions that can be satisfied in these cases are (27) and (29). We start by obtaining conditions on the total concentration $\zeta = x+y+z$. By adding equations (26) and integrating, we find that

$$\frac{\mathrm{d}\xi}{\mathrm{d}s} = -(\mu-\gamma)\,\mathrm{e}^{-v_0 s}\int_{-\infty}^{s} \mathrm{e}^{-v_0 \bar{s}}\, z(\bar{s})\,\mathrm{d}\bar{s}. \tag{65}$$

Now, from (28), ξ' must be of one sign, negative for $\mu > \gamma$ (expanding case) and positive for $\mu < \gamma$ (contracting case). Thus the total concentration increases monotonically through the wave in the expanding case and decreasing monotonically through the wave in the contracting case.

Furthermore (65) shows that on $-\infty < s < \infty$,

$$x_1 \leqslant x+y+z \leqslant x_e \quad \text{in the expanding case,} \tag{66a}$$

$$x_e \leqslant x+y+z \leqslant x_1 \quad \text{in the contracting case.} \tag{66b}$$

Then, using (28), x, y and z individually satisfy the right-hand inequalities in (66), i.e.

$$0 \leqslant (x,y,z) \leqslant x_e \quad \text{in the expanding case,} \tag{67a}$$

$$0 \leqslant (x,y,z) \leqslant x_1 \quad \text{in the contracting case.} \tag{67b}$$

Since $y \to 0$ as $|s| \to \infty$ and (29) holds, y achieves its maximum on $-\infty < s < \infty$. Suppose that y has a maximum y_m at $s = t_1$, then $y'(t_1) = 0$, $y''(t_1) \leqslant 0$, with equation (26*b*) giving

$$y''(t_1) = y_m(1 - y_m\, x(t_1)) \leqslant 0. \tag{68a}$$

Hence, $x(t_1) \geqslant 1/y_m$ and since for the contracting case $x(t_1) + y_m + z(t_1) \leqslant x_1$ and $z(t_1) > 0$, we obtain the same bound on y_m, namely

$$y_m \leqslant \tfrac{1}{2}(x_1 + \surd(x_1^2 - 4)) \tag{68b}$$

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as for the reduced case, noting that this again requires $x_1 \geqslant 2$. For the expanding case, we now have $x(t_1)+y_m+z(t_1) \leqslant x_e$ (and $z(t_1) \geqslant 0$). This gives the bound

$$y_m \leqslant \tfrac{1}{2}(x_e+\surd(x_e^2-4)) \tag{68c}$$

for the expanding case. Note that this requires $x_e \geqslant 2$ which suggests (since here $x_1 < x_e$) a higher value of x_1 is required for the existence of a solution of equations (26) in this case.

Also, since $z \to 0$ as $|s| \to \infty$, z achieves its maximum z_m (say) at $x = t_2$ on $-\infty < s < \infty$, where $z'(t_2) = 0$, $z''(t_2) \leqslant 0$. Equation (26*c*) then gives

$$z''(t_2) = \gamma z_m - y(t_2) \leqslant 0, \tag{69a}$$

which gives $\gamma z_m \leqslant y(t_2) \leqslant y_m$, and hence

$$z_m \leqslant \frac{1}{2\gamma}(x_1+\surd(x_1^2-4)) \tag{69b}$$

for the contracting case and

$$z_m \leqslant \frac{1}{2\gamma}(x_e+\surd(x_e^2-4)) \tag{69c}$$

for the expanding case. Conditions (69*b*, *c*) give stronger inequalities on z_m than (67) for $\gamma > 1$, whereas for $\gamma < 1$, they give a stronger result only when $x_1^2 \leqslant 1/\gamma(1-\gamma)$.

(ii) *Solution for large* x_1

Finally, we obtain a solution of equations (26) valid for x_1 large. We consider only the case when μ and γ are both of $O(1)$. We start, as in the reduced case, in a region of thickness $O(x_1^{-1})$ at the front of the wave, where we scale

$$x = x_1 X, \quad y = x_1 Y, \quad z = x_1 Z, \quad \bar{s} = x_1 s, \quad v_0 = x_1 \bar{v}. \tag{70}$$

When (70) is substituted into equations (26) and a solution sought by expanding in powers of x_1^{-2} the leading order terms in X and Y are as given by (45*b*) for the reduced case. Equation (26*c*) gives for the leading order term Z_0

$$Z_0'' + \bar{v}_0 Z_0' = 0 \tag{71a}$$

subject to
$$Z_0 \to 0 \quad \text{as} \quad \bar{s} \to \infty \tag{71b}$$

and Z_0 not exponentially large as $\bar{s} \to -\infty$. The solution is

$$Z_0 \equiv 0. \tag{71c}$$

At $O(x_1^{-2})$, we obtain, from equation (26*c*)

$$Z_1'' + \bar{v}_0 Z_1 + Y_0 = 0, \tag{72a}$$

with solution

$$Z_1 = \frac{1}{\bar{v}_0^2}[(1+\mathrm{e}^{-\bar{v}_0 \bar{s}}) \log(1+\mathrm{e}^{\bar{v}_0 \bar{s}}) - \bar{v}_0 \bar{s}] \tag{72b}$$

which shows that $Z_1 \to 0$ as $\bar{s} \to \infty$, while

$$Z_1 \sim \frac{1}{\bar{v}_0^2}(-\bar{v}_0 \bar{s} + 1) \tag{72c}$$

as $s \to -\infty$.

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The behaviour of X_1 and Y_1 as $\bar{s}\to-\infty$ is, as in the reduced case, given by (48). This then suggests a further region, of thickness $O(x_1)$ is required in which we put

$$x = x_1^{-1}U, \quad y = x_1 V, \quad z = x_1 W, \quad \zeta = x_1^{-1}s, \tag{73}$$

with equations (26) giving

$$\mu W - UV^2 + x_1^{-2}\bar{v}_0 U' + x_1^{-4}U'' = 0, \tag{74a}$$

$$\bar{v}_0 V' + UV^2 - V + x_1^{-2}V'' = 0, \tag{74b}$$

$$\bar{v}_0 W' + V - \gamma W + x_1^{-2}W'' = 0 \tag{74c}$$

(where primes now denote differentiation with respect to ζ). Equations (74) are to be solved subject to the matching conditions that

$$U = O(\zeta), \quad V = 1 + \frac{\zeta}{\bar{v}_0} + \dots, \quad W = \frac{-\zeta}{\bar{v}_0} + \dots, \quad \text{as} \quad \zeta \to 0^-. \tag{75}$$

A solution of equations (74) is sought by expanding in powers of x_1^{-2}, the leading order terms can be shown, after some algebra, to be

$$V_0 = \frac{1}{\bar{v}_0(\lambda_1-\lambda_2)}[(1-\bar{v}_0\lambda_2)\,e^{\lambda_1\zeta} + (\bar{v}_0\lambda_1 - 1)\,e^{\lambda_2\zeta}], \tag{76a}$$

$$W_0 = \frac{1}{\bar{v}_0(\lambda_1-\lambda_2)}[e^{\lambda_2\zeta} - e^{\lambda_1\zeta}], \tag{76b}$$

$$U_0 = \frac{\mu\bar{v}_0(\lambda_1-\lambda_2)(e^{\lambda_2\zeta}-e^{\lambda_1\zeta}))}{[(\bar{v}_0\lambda_1-1)\,e^{\lambda_2\zeta} + (1-\bar{v}_0\lambda_2)\,e^{\lambda_1\zeta}]^2}, \tag{76c}$$

where

$$\lambda_1 = \frac{1}{2\bar{v}_0}[1+\gamma+\surd((1-\gamma)^2+4\mu)], \quad \lambda_2 = \frac{1}{2\bar{v}_0}[1+\gamma-\surd((1-\gamma)^2+4\mu)].$$

Note that λ_1 and λ_2 are both real, $\lambda_1 > 0$ and $\lambda_2 < \lambda_1$.

We now have two cases to consider depending on whether $\mu < \gamma$ or $\mu > \gamma$. In the first case ($\mu < \gamma$), $\lambda_2 > 0$ and then V_0, $W_0 \to 0$ as $\zeta \to -\infty$, while $U_0 \to \infty$, more specifically

$$U_0 \sim \frac{\mu\bar{v}_0(\lambda_1-\lambda_2)}{(\bar{v}_0\lambda_1-1)^2}\,e^{-\lambda_2\zeta}, \tag{77a}$$

$$V_0 \sim \frac{(\bar{v}_0\lambda_1-1)}{\bar{v}_0(\lambda_1-\lambda_2)}\,e^{\lambda_2\zeta}, \quad W_0 \sim \frac{e^{\lambda_2\zeta}}{\bar{v}_0(\lambda_1-\lambda_2)} \tag{77b}$$

as $\zeta \to -\infty$.

To continue, we examine the behaviour of the terms of $O(x_1^{-2})$. We find that V_1 and W_1 are both of $O(e^{-\lambda_2\zeta})$, while U_1 is of $O(e^{-3\lambda_2\zeta})$ as $\zeta \to -\infty$. This suggests that we require a shift of origin in ζ, namely

$$\zeta = \frac{1}{2\lambda_2}\log(x_1^{-2}) + \bar{\zeta}, \tag{78}$$

with then from (77) and (78) x, y and z all being of $O(1)$ when $\bar{\zeta}$ is of $O(1)$.

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Hence, for the contracting case ($\mu < \gamma$), we have a final region in which x, y and z are unscaled, the wave speed is $v_0 = x_1/\sqrt{2}$ from (45*b*) and (70), and the independent variable given by (78). This leads to the equations at leading order

$$\bar{v}_0 x' + \mu z - xy^2 = 0, \tag{79a}$$

$$\bar{v}_0 y' + xy^2 - y = 0, \tag{79b}$$

$$\bar{v}_0 z' + y - \gamma z = 0, \tag{79c}$$

with

$$x \sim \frac{\mu \bar{v}_0(\lambda_1 - \lambda_2)}{(\bar{v}_0 \lambda_1 - 1)^2} \mathrm{e}^{-\lambda_2 \bar{\zeta}},$$

$$y \sim \frac{(\bar{v}_0 \lambda_1 - 1)}{\bar{v}_0(\lambda_1 - \lambda_2)} \mathrm{e}^{\lambda_2 \bar{\zeta}}, \quad z \sim \frac{\mathrm{e}^{\lambda_2 \bar{\zeta}}}{\bar{v}_0(\lambda_1 - \lambda_2)} \tag{79d}$$

as $\bar{\zeta} \to \infty$.

Equations (79) are essentially the equations for the well-stirred system treated in part I, where it was shown that $y \to 0$, $z \to 0$ while $x \to x_e$, an $O(1)$ constant value, as $\bar{\zeta} \to -\infty$. The value of x_e cannot be determined directly from this analysis, but can be obtained by numerical integration for specific values of μ and γ. (This was also illustrated in part I.) The main point to note, however, is that even though the concentration of reactant A is large (of $O(x_1)$) ahead of the wave, it falls to a much smaller, $O(1)$, value at the rear of the wave, while the concentrations of species B and C both undergo large, $O(x_1)$, excursions in the reaction-diffusion wave. This can be seen in the numerical results for the contracting case, particularly in figure 5.

For the expanding case, $\mu > \gamma$, $\lambda_2 < 0$ and now, $U_0 \to 0$, while $V_0 \to \infty$ and $W_0 \to \infty$ as $\zeta \to -\infty$, with their specific forms given by (77). The shift of origin given by (78) is still required, with equations (79) resulting. Now these have to be solved in the expanding case subject to large initial values of y and z and a small initial value of x. This problem was addressed specifically in part I. From part I it follows that x undergoes a small increase before decaying to zero and both y and z decrease at first before finally increasing as $\bar{\zeta} \to -\infty$. This behaviour was seen in the numerical results for the expanding case.

The wave structure for large x_1 is now clear in both cases. In the contracting case the concentrations y and z are pulse-like, being zero outside the wave, though achieving large $O(x_1)$, maxima within the wave. The concentration x undergoes a sharp fall from x_1 ahead of the wave to a small, $O(x_1^{-1})$ value, before rising again to a constant value, considerably smaller than its initial value. This structure is similar to that for the reduced case when the stationary state (25*a*) is unstable, except that there x approaches x_1 at the rear of the wave.

In the expanding case a permanent-form travelling wave, in which the concentrations of all three chemical species approach constant values at the rear of the wave and remain at these values after the wave has passed, is not observed. In this case there is still a constant velocity propagating front structure in which x falls sharply from its large value ahead of the front and in which y and z rise sharply to $O(x_1)$ values. This frontal structure has a constant form for large time, being dependent only on the travelling coordinate s. However, after this reaction-diffusion front has passed the concentration x dies away to zero while concentrations y and z increase, with this taking place on a long, $O(x_1)$, lengthscale.

The structure in the initial part of the wave is the same in all cases being given by (44), (45) and is essentially the same as for the cubic-Fisher problem. This is to be

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expected from reaction scheme (1), where, for x_1, large, it will be the cubic autocatalytic reaction (1 *b*) which will predominate. Only when the concentrations of B and C have increased and that of A fallen in the wave will the effects of the other reaction steps be felt.

5. Conclusions

The combined analyses of the previous paper (part I) and the preceding sections have provided a detailed understanding of the reaction-diffusion events that can be supported by the present model scheme. Three distinct types of permanent-form travelling waves have been observed for the special, reduced case (with $\mu = \gamma$). These are: a pulse in which the system is disturbed locally from its trivial (unreacted) state but recovers to that same state in the post-wave region; a front that connects the trivial state to a different (reacted) steady state in the post-wave region and; a front that then sets up a periodic wavetrain corresponding to local oscillations about the (unstable) reacted state. The fronts in these case differ from classic Fisher–Kolmogorov fronts in that they involve saddle–saddle rather than saddle–node connections.

A necessary condition for the existence of a permanent-form, constant velocity travelling wave solution of the reaction-diffusion system is the existence of the non-trivial steady state solution (25*a*) of the corresponding well-stirred system. In terms of the initial concentration of reactant A, which is the only intermediate present ahead of the front initially, this requires $x_1 > 2$ and $\mu > 4/(x_1^2-4)$, as determined in part I. The non-trivial state (25*a*) is not required to be stable. If this state is stable, the system can settle uniformly and asymptotically onto this after the passage of the front. If the non-trivial state is unstable, but surrounded by a stable limit cycle born from a supercritical Hopf bifurcation in the corresponding well-stirred system, a wavetrain is established behind the front. In the absence of a stable attractor in the vicinity of the reacted, non-trivial state, there is a recovery wave as the system returns to the unreacted state at sufficiently long time.

The conditions for a wavetrain are intimately linked to the conditions for the existence of a stable limit cycle in the well-stirred case. Stable limit cycles are born at points of supercritical Hopf bifurcations and are extinguished via homoclinic orbit formation. The loci of these events in the $\mu - c_0$ parameter plane, equivalent to the $\mu - x_1$ parameter plane here, have been determined in part I. For large x_1, the condition for the existence of wavetrain solutions can be obtained analytically, with $0.90032 < \mu x_1 < 1$.

In addition to the existence of the non-trivial steady state, there is a critical initiation condition on the concentration of the autocatalyst, y_0, for the establishment of permanent-form travelling waves. For large x_1, a lower bound on this critical initiation is $y_0 > x_1^{-1}$. In the same limit of large x_1, the reaction-diffusion front has, to leading order, the characteristics of a cubic Fisher–Kolmogorov front, with dimensionless velocity $v_0 = x_1/\sqrt{2}$.

For the contracting case, with $\mu < \gamma$ but with $\mu - \gamma$ small, similar permanent-form travelling waves are established under similar conditions: both in terms of the existence of (quasi) steady or oscillatory non-trivial states and of the critical initiation condition. In this case, there is an additional region at long times in which the system finally evolves to the only true steady state, with $x \to x_e$, $y \to 0$ and $z \to 0$, where $x_e \leqslant x_1$ is some final concentration of reactant A (determined numerically from the equations for the well-stirred system).

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In the expanding case, for which the total concentration $\xi = x+y+z$, increases monotonically in time, the behaviour at long times after the front either has $x \to \infty$ and $y \to 0$ or $x \to 0$ and $y \to \infty$, depending on the parameter values and the initial conditions. Estimates for the maximum concentrations of y and z achieved in the reaction-diffusion front have been obtained for all three cases, equations (68) and (69), in the limit of large x_1.

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