

Propagating reaction–diffusion waves in a simple isothermal quadratic autocatalytic chemical system

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Abstract. The propagating reaction–diffusion waves that develop in the isothermal autocatalytic system $A + B \rightarrow 2B$ from a local initial input of reactant B are considered. A solution valid for a small initial input of B is obtained first, and this is augmented by numerical solutions of the general problem. These show that, asymptotically, the reaction–diffusion wave propagates with the minimum, physically acceptable, wave speed. The large-time solution for the general case is then discussed and it is shown that ahead of the reaction–diffusion front is a weak diffusion-controlled region. It is the matching between these two regions that fixes the wave speed, so that the speed of propagation of the reaction–diffusion front is controlled by the rate at which B can spread forward by diffusion.

1. Introduction

We consider the isothermal quadratic autocatalytic reaction



where a and b are the concentrations of the species A and B and k_1 is the rate constant. In particular we discuss the reaction–diffusion waves that can be set up by this simple reaction. To this end we consider the situation of an initial infinite expanse of reactant A into which an amount of reactant B is introduced in some local region. A and B react via (1) setting up concentration gradients and from this initial region reaction-diffusion waves propagate outwards. We treat only the case of one-dimensional slab geometry (with co-ordinate x) and, by symmetry, we need only consider the region $x > 0$.

We find that to determine the large-time behaviour we need to look for travelling-wave solutions of an equation for b of the form

$$\frac{\partial b}{\partial t} = \frac{\partial^2 b}{\partial x^2} + b(1 - b). \quad (2)$$

This problem has a long history; it was proposed originally by Fisher, [1], as a model for the advance of an advantageous gene. Later the same equation has arisen in laminar flame propagation (see, for example, [2] and [3]), and in neurophysiology [4, 5, 6]. Kolmogorov et al. [7] showed that equation (2) possesses a travelling-wave solution which propagates with a uniform velocity v_0 with the necessary condition that $v_0 \geq 2$. Later it was shown by McKean [8] that from a step-function initial distribution the solution of (2) evolved into a wave propagating with the minimal velocity $v_0 = 2$, a result derived also by Rosen [9], though his argument required the application of a particular biological constraint. The result given in [8] has been extended by Bramson [10, 11] who showed that the position of the front $x = m(t)$

was, in our notation, given by

$$m(t) = 2t - \frac{3}{2} \log t + O(1), \quad (3)$$

for t (time) large.

The arguments given in [8, 10, 11] are in terms of Brownian Motion and, though mathematically thoroughly rigorous, are somewhat complex. It is the intention in this paper to present a very much simpler argument which also arrives at result (3) and which brings out more clearly the mechanism by which the reaction–diffusion wave is propagated in the context of the simple isothermal autocatalytic reaction (1). We show, in this particular situation, that ahead of the reaction–diffusion front is a very weak diffusion-controlled region. Hence we see that it is necessary for a small amount of reactant B (we show that, in fact, this is exponentially small) to first diffuse into this region ahead of the reaction–diffusion front, to initiate the reaction with A. This then allows the autocatalytic reaction (1) to develop which then enables the reaction–diffusion wave to propagate forward with a speed which is controlled by the ability of B to diffuse ahead of it. We feel that this gives a better insight into the basic mechanism behind the propagation of the wave in our chemical context and is worth presenting for that reason.

2. Equations

The equations for the species A and B, reacting via (1), are

$$\frac{\partial a}{\partial \bar{t}} = D \frac{\partial^2 a}{\partial \bar{x}^2} - k_1 ab, \quad (4a)$$

$$\frac{\partial b}{\partial \bar{t}} = D \frac{\partial^2 b}{\partial \bar{x}^2} + k_1 ab, \quad (4b)$$

where we have assumed equal diffusion coefficients for A and B and where \bar{x} and \bar{t} are space and time variables respectively.

The type of chemical reactions which are modelled by the kinetic scheme (1) generally involve species A and B which have a comparable molecular size. For reactions involving such molecules little variation is found between their diffusion rates and it is then plausible to consider the species A and B as having equal diffusion coefficients, as a first approximation. However, it should be noted that the kinetic scheme (1), with some modifications, does have similarities with biological mechanisms, for example enzyme reactions, where the molecular size and hence the diffusion rates of the species A and B could differ considerably. The modifications arising from differing diffusion coefficients are discussed in Billingham and Needham [12]. The initial conditions are

$$\begin{aligned} a &= a_0, & -\infty < x < \infty, \\ b &= \begin{cases} b_0 g(\bar{x}), & |x| < l \\ 0, & |x| > l \end{cases} \end{aligned} \quad (5)$$

where $g(\bar{x})$ is some given smooth symmetric function of \bar{x} , and a_0 and b_0 are positive

constants. Equations (4) are made non-dimensional by putting

$$t = k_1 a_0 \bar{t}, \quad x = \left(\frac{k_1 a_0}{D} \right)^{1/2} \bar{x}, \quad a = a_0 \alpha, \quad b = a_0 \beta, \quad (6)$$

after which (4) and (5) become

$$\frac{\partial \alpha}{\partial t} = \frac{\partial^2 \alpha}{\partial x^2} - \alpha \beta, \quad (7a)$$

$$\frac{\partial \beta}{\partial t} = \frac{\partial^2 \beta}{\partial x^2} + \alpha \beta, \quad (7b)$$

and

$$\alpha = 1, \quad \text{all } x, \quad (8)$$

$$\beta = \begin{cases} \beta_0 g(x), & |x| < \lambda \\ 0, & |x| > \lambda \end{cases},$$

where the non-dimensional parameters $\beta_0 = b_0/a_0$ (a measure of the initial concentration of B relative to A) and $\lambda = (k_1 a_0 t^2/D)^{1/2}$. Note that in (6) we have used $(k_1 a_0)^{-1}$ which is representative of the time scale of reaction (1) and we have kept the imposed length scale in the initial conditions (8) through the parameter λ .

We begin by looking at the solution for small β_0 , which we shall find brings out all the salient features of the general solution. We then go on to look at the general solution when t is large, and, in particular, at the reaction–diffusion wave. We complete the work by giving some numerical solutions of equations (7), which confirm the analysis.

3. Solution for small β_0

To obtain a solution of equations (7) valid for $\beta_0 \ll 1$ we expand

$$\alpha = 1 + \beta_0 A_1(x, t) + \dots, \quad \beta = \beta_0 B_1(x, t) + \dots, \quad (9)$$

where A_1 and B_1 satisfy the equations

$$\frac{\partial A_1}{\partial t} = \frac{\partial^2 A_1}{\partial x^2} - B_1, \quad (10a)$$

$$\frac{\partial B_1}{\partial t} = \frac{\partial^2 B_1}{\partial x^2} + B_1, \quad (10b)$$

subject to

$$A_1 = 0, \quad B_1 = \begin{cases} g(x), & |x| < \lambda \\ 0, & |x| > \lambda \end{cases} \quad \text{at } t = 0.$$

The solution for B_1 can be written as

$$B_1 = e^t \int_{-\infty}^{\infty} \bar{B}(s) e^{isx - s^2 t} ds, \quad (11a)$$

where $\bar{B}(s) = (1/2\pi) \int_{-\lambda}^{\lambda} g(u) e^{-ius} du$, which is an analytic function of the complex variable s for all $|s| < \infty$. Then using (11a) in equation (10a) we obtain

$$A_1 = (1 - e^t) \int_{-\infty}^{\infty} \bar{B}(s) e^{isx - s^2 t} ds. \quad (11b)$$

(11a) shows that even with a small initial input, the concentration of B increases rapidly with the assumption behind (9) of small β soon becoming invalid. There is also, from (11b), a consequent depletion of A.

It is instructive to examine the behaviour of B_1 for $t \gg 1$. From (11a) it follows that

$$B_1(x, t) \sim \sqrt{\pi} \frac{\bar{B}\left(\frac{ix}{2t}\right) e^t e^{-x^2/4t}}{\sqrt{t}} + \dots, \quad (12)$$

as $t \rightarrow \infty$ for all local initial conditions of the type considered. Now, if we write the exponent in (12) as $E = (x^2/4t) - t = (x^2 - 4t^2)/4t$ and consider lines of constant exponential phase ϵ_0 (say), then these are given by $x^2 = 4t^2 + 4\epsilon_0 t$. So that with $t > 0$ in the (x, t) plane these lines become parallel and propagate with the same speed $v_0 = \pm 2$ at $t \rightarrow \infty$. This indicates the formation of travelling waves with asymptotic speeds $v_0 = \pm 2$. Following the right-moving wave we introduce the co-ordinate $y = x - 2t$, and then the exponent E may be written as

$$E = \frac{y(y + 4t)}{4t}. \quad (13)$$

From (13) we can see that there are two cases to consider. First, when y is of $O(1)$, (13) gives $E = y + O(t^{-1})$, so that (12) becomes

$$B_1(x, t) \sim \sqrt{\pi} \frac{\bar{B}(i) e^{-y}}{\sqrt{t}} + \dots, \quad (14a)$$

in which both diffusion and reaction effects are contributing, and B_1 is algebraically small, of $O(t^{-1/2})$. However, (14a) does not hold when both y and t are large, in which case both terms in (13) must be retained with (12) becoming

$$B_1(x, t) \sim \sqrt{\pi} \bar{B}\left(i\left(\frac{y + 2t}{2t}\right)\right) \frac{e^{-y - y^2/4t}}{\sqrt{t}} + \dots, \quad (14b)$$

showing that here diffusion is the predominant effect. Moreover, this region is also very weak, with B_1 now exponentially small, of $O(e^{-2\sqrt{t}/\sqrt{t}})$. Thus, ahead of the reaction-diffusion front, there is a very weak diffusing region.

We use this information from the small β_0 solution with local initial conditions to discuss the general solution of equations (7) when t is large. Before doing so, however, we obtain numerical solutions of equations (7), which show the formation of reaction-diffusion waves.

4. Numerical solution

To solve equations (7) numerically, we take a form for $g(x)$ which is symmetric about $x = 0$ so that the solution will also be symmetric. Hence we need consider the region $x \geq 0$, applying the boundary condition $\partial\alpha/\partial x = \partial\beta/\partial x = 0$ at $x = 0$. There will be another symmetrically disposed solution in $x \leq 0$. The numerical scheme used is a modified Crank–Nicolson method. We first write the t -derivatives in terms of forward differences and average the other quantities over the step from t to $t + \Delta t$. This results in a pair of coupled nonlinear ordinary differential equations in x which we solve by replacing the x -derivatives by central differences, giving the two sets of algebraic equations

$$u_{j+1} - 2u_j + u_{j-1} - \frac{h^2}{2} u_j v_j - \frac{2h^2}{\Delta t} (u_j - 2\alpha_{1j}) = 0, \tag{15a}$$

$$v_{j+1} - 2v_j + v_{j-1} + \frac{h^2}{2} u_j v_j - \frac{2h^2}{\Delta t} (v_j - 2\beta_{1j}) = 0, \tag{15b}$$

$j = 0, 1, 2, \dots, N$, where $u_j = \alpha_{1j} + \alpha_{2j}$, $v_j = \beta_{1j} + \beta_{2j}$ (suffices 1 and 2 refer to values at t and $t + \Delta t$ respectively), and where h is the step length in the x -direction. The outer boundary conditions give $u_{N+1} = 2$, $v_{N+1} = 0$, and from the symmetry condition we have $u_{-1} = u_1$, $v_{-1} = v_1$ which leads to an obvious modification to equations (15) for $j = 0$.

Equations (15) are solved iteratively using the Newton–Raphson method. Starting with initial estimates for the u_j and v_j a better estimate for the u_j is first calculated from (15a). These new values are then used in (15b) to calculate a better estimate for the v_j . This procedure is repeated until a converged solution is obtained, which was deemed to have been reached when the difference between two successive iterates was everywhere less than 10^{-6} . The scheme was found to converge easily, using as initial estimates the values of u_j and v_j at the previous time step, taking typically just 3 for 4 iterations for convergence. At each stage of the Newton iteration we need to solve a set of $(N + 1)$ linear equations given in terms of a tridiagonal matrix. To invert this matrix we used Choleski decomposition [13], which was found to be computationally very efficient; such an efficient procedure being required because of the large number of algebraic equations involved at each time step.

To start the calculation initial conditions (8) were used and the solution advanced in steps at Δt . A check was kept on the size of the error introduced by differencing in the t -direction by covering the step from t to $t + \Delta t$ in first one and then two steps and calculating the maximum difference between these two solutions. If this was greater than 5.10^{-5} , the step size was halved and the process repeated. This procedure was also used as a test to double the step Δt if it was found that this maximum difference was less than 5.10^{-6} at the previous step (i.e. 0.1 of the accuracy criterion). At each stage, the values of α and β as calculated by the two step integration were used as initial values for the next step in the solution and were the values outputted. In this way we could be confident of the accuracy of our solution as t increased. A step size in the x -direction of $h = 0.1$ was used throughout. Some trial runs were made with $h = 0.05$ and these showed that with $h = 0.1$ we could achieve the required accuracy. Because of the development of the reaction–diffusion wave for large t , we had to apply the outer boundary condition at a large distance and we took $N = 1500$ (i.e. the outer boundary condition was applied at $x = 150$). This was found to give sufficient space for the reaction–diffusion wave to develop fully.

Results are presented taking for $g(x)$ the ‘top-hat’ profile

$$g(x) = \begin{cases} 1, & |x| < \lambda \\ 0, & |x| > \lambda \end{cases}$$

An alternative form, $g(x) = e^{-x^2/\lambda^2}$, was also tried, and apart from the first few steps in the calculation the results for the two cases are virtually indistinguishable. This initial condition gave a discontinuity at $x = \lambda$ which required the use of a small initial starting value for Δt ($\Delta t = 0.000625$), but after a few steps this could be increased (as described above) and for most of the calculation a step of $\Delta t = 0.32$ was found to achieve the prescribed accuracy. With the smooth form $g(x) = e^{-x^2/\lambda^2}$ no such trouble was encountered at the start.

As t increases, a reaction-diffusion wave is set up. This is illustrated in Figure 1 where we plot profiles of α and β at $t = 65$, for the case $\lambda = \beta_0 = 1$. This picture is typical of the reaction-diffusion waves seen at the other values of t (and with other choices of β_0 and λ as well as for $g(x)$). There is a small (and decreasing with t) residue of the initial input of B seen in β near $x = 0$ (whereas α quickly decays to zero here). This is followed by a long region where $\beta = 1$ and $\alpha = 0$ (the species A and B are in their fully reacted states). Finally there is a front where α and β change rapidly to their outer unreacted values. It should be noted that in this front we find that the condition $\alpha + \beta = 1$ is quickly attained (to well within the accuracy of the numerical scheme) even though α and β themselves evolve much more slowly to their final asymptotic values.

Also of interest is the speed of propagation of the wave. To fix the position of the front, at each step we calculated x_m the value of x where $\partial\alpha/\partial x$ took its maximum value. Graphs of x_m against t are shown in Figure 2 for the typical case $\beta_0 = 1$, $\lambda = 1$ and for the cases $\lambda = 10$, $\beta_0 = 10$ (for which the input of B was 100 times that for the typical case) and for $\beta_0 = 0.1$,

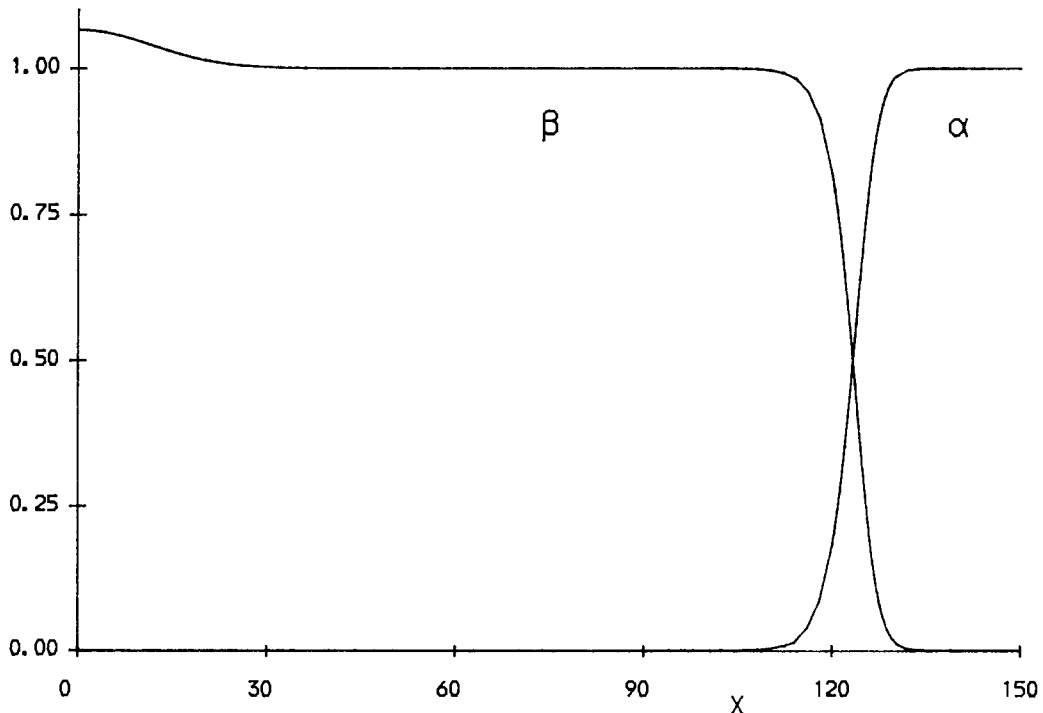


Fig. 1. The reaction-diffusion wave: profiles of α and β at $t = 65$ for $\lambda = 1$, $\beta_0 = 1$.

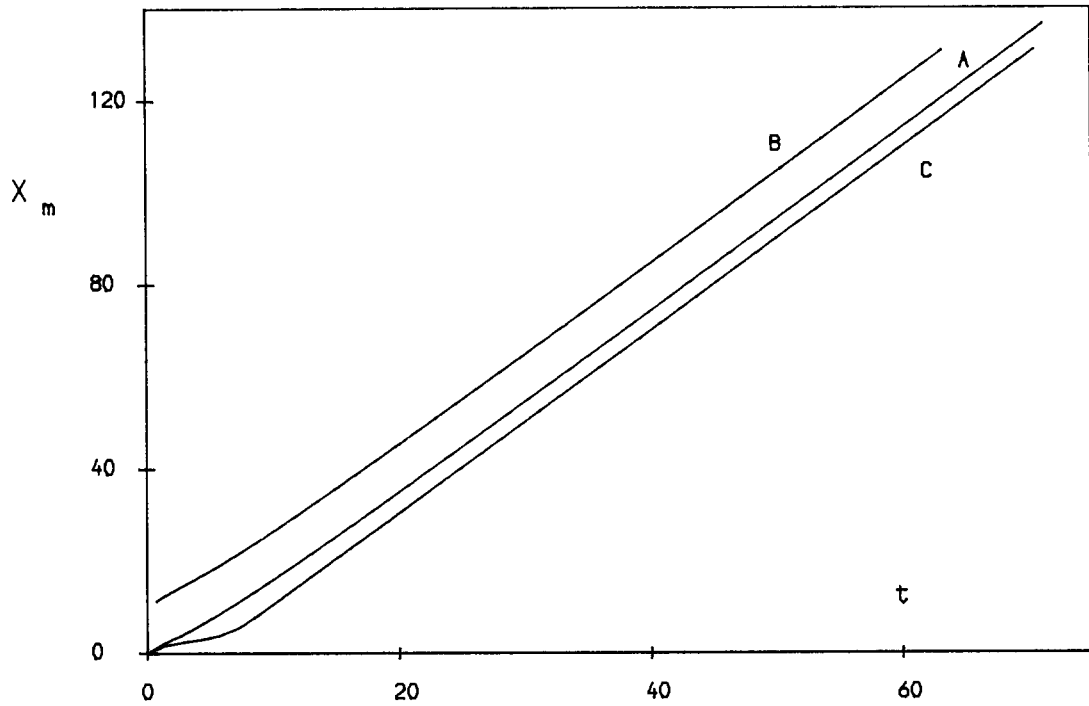


Fig. 2. The position of the reaction–diffusion front x_m plotted against t , for the cases (a) $\lambda = 1, \beta_0 = 1$, (b) $\lambda = 10, \beta_0 = 10$ and (c) $\lambda = 0.1, \beta_0 = 0.1$.

$\lambda = 0.1$ (input of B is 0.01 that of the typical case). In each of the three cases (with very different initial amounts of B) we can see that the curves approach a straight line with the same gradient. In fact, the position of the front is insensitive to the initial input of B (as was found for other choices of λ and β_0) and that for large times, the speed of propagation of this front always approached the same asymptotic value, i.e. $\Delta x_m / \Delta t \rightarrow 2$ as t increased. The next step is to discuss the structure of this reaction–diffusion wave.

5. Reaction–diffusion wave, large-time solution

Here we look for a solution of equations (7) valid for large t , the main feature of which, as we have seen from the numerical solutions is a propagating reaction–diffusion wave and it is the structure of this wave that we discuss first. As a preliminary we note that $\omega = \alpha + \beta$ satisfies the diffusion equation

$$\frac{\partial \omega}{\partial t} = \frac{\partial^2 \omega}{\partial x^2}, \tag{16}$$

which, together with the initial condition $\omega = 1 + \beta_0 g(x)$ can be solved to obtain

$$\omega = 1 + \frac{\beta_0}{2\sqrt{\pi t}} \int_{-\lambda}^{\lambda} g(\xi) e^{-(x-\xi)^2/4t} d\xi. \tag{17}$$

We now look for an asymptotic of equations (7) as $t \rightarrow \infty$, the leading term of which is a

permanent-form travelling wave moving with a speed $v(t)$ (>0). We introduce the travelling co-ordinate,

$$y = x - v(t). \quad (18)$$

With $\omega(x, t)$ given by (17), equations (7) reduce to a single equation for α , namely

$$\frac{\partial \alpha}{\partial t} = \frac{\partial^2 \alpha}{\partial y^2} + \frac{dv}{dt} \frac{\partial \alpha}{\partial y} - \alpha(\omega - \alpha). \quad (19a)$$

As $t \rightarrow \infty$ we require α to approach a permanent-form steady solution in terms of the variable y , that is $\alpha(y, t) \rightarrow \alpha_0(y)$ as $t \rightarrow \infty$ with y of $O(1)$. Thus α_0 must satisfy the equation

$$\frac{d^2 \alpha_0}{dy^2} + \frac{dv}{dt} \frac{d\alpha_0}{dy} - \alpha_0(1 - \alpha_0) = 0 \quad (19b)$$

on noting that from (17), $\omega \rightarrow 1$ as $t \rightarrow \infty$ with y fixed for any $v(t) > 0$. The solution of equation (19b) must be independent of t and this is possible only if $\lim_{t \rightarrow \infty} dv/dt$ is independent of t , so that $dv/dt \rightarrow v_0$ as $t \rightarrow \infty$, where v_0 is a constant. Thus $v \sim v_0 t + \dots$ as $t \rightarrow \infty$. With this form for $v(t)$, ω is $1 + O(t^{-1/2} \exp(-v_0^2 t/4))$ for t large and y of $O(1)$, and, as we shall show that the perturbations to α and β separately are only algebraically small in t , we can, to this approximation put $\alpha + \beta = 1$ (this was borne out by the numerical solutions). Thus we can simplify equation (19a) to

$$\frac{\partial^2 \alpha}{\partial y^2} + \frac{dv}{dt} \frac{\partial \alpha}{\partial y} - \alpha(1 - \alpha) = \frac{\partial \alpha}{\partial t}. \quad (19)$$

At leading order $\alpha = \alpha_0(y)$, where α_0 satisfies the ordinary differential equation

$$\alpha_0'' + v_0 \alpha_0' - \alpha_0(1 - \alpha_0) = 0, \quad (20a)$$

subject to the boundary conditions

$$\alpha_0 \rightarrow 1 \quad \text{as } y \rightarrow \infty, \quad \alpha_0 \rightarrow 0 \quad \text{as } y \rightarrow -\infty. \quad (20b)$$

(primes denote differentiation with respect to y). Using (20b) it follows from (20a) that, as $y \rightarrow \infty$,

$$\alpha_0 \sim 1 - (A_0 e^{-\lambda_1 y} + B_0 e^{-\lambda_2 y}) + \dots, \quad (21)$$

where A_0 and B_0 are constants and where the λ_i are given by

$$\lambda_i = \frac{1}{2}(v_0 \pm \sqrt{v_0^2 - 4}) \quad (i = 1, 2), \quad (22)$$

with $\lambda_2 \geq \lambda_1$. Hence a physically acceptable solution is possible for all $v_0 \geq 2$. (For $v_0 < 2$ the solution is damped oscillatory, giving rise to physically unacceptable negative values for β). As $y \rightarrow -\infty$, $\alpha_0 \sim C_0 e^{\mu y} + \dots$, $\mu = \frac{1}{2}(\sqrt{v_0^2 + 4} - v_0)$ and we obtain a physically acceptable solution of equation (20a) which satisfies boundary conditions (20b), and hence the

leading-order equation for the front does not fix the speed of propagation. A result described by Britton [15] and Rosen [9] uses a biological constraint to neglect the smaller of the eigenvalues (22) and hence one is then able to determine a unique solution for the front from the leading-order problem. There is no such a priori reason for doing so in our isothermal chemical context and we now develop a consistent asymptotic theory on the assumption that the wave travels with the minimum possible speed $v_0 = 2$. We then indicate where this theory would break down if we were to take $v_0 > 2$. With $v_0 = 2$, (21) and (22) lead to

$$\alpha_0 \sim 1 - (A_0 y + B_0) e^{-y} + \dots, \tag{23}$$

as $y \rightarrow \infty$. The leading-order problem is now unique up to a shift in the origin of y , and A_0 and B_0 will be known from a (numerical) integration of the equations.

We take an expansion for α and v in the form

$$\alpha(y, t) = \alpha_0(y) + t^{-1} \alpha_1(y) + \dots, \quad \frac{dv}{dt} = 2 + v_1 t^{-1} + \dots. \tag{24}$$

The equation for the leading-order term is (20a) subject to (20b) with $v_0 = 2$, and the equation at $O(t^{-1})$ is

$$\alpha_1'' + 2\alpha_1' - (1 - 2\alpha_0)\alpha_1 = -v_1 \alpha_0', \tag{25}$$

subject to the boundary conditions

$$\alpha_1 \rightarrow 0 \quad \text{as } y \rightarrow \infty, \quad \text{and as } y \rightarrow -\infty. \tag{26}$$

As $y \rightarrow \infty$ the solution of equation (25) behaves like

$$\alpha_1 \sim -v_1 \left[\frac{A_0}{6} y^3 + \frac{(B_0 - A_0)}{2} y^2 \right] e^{-y} + (A_1 y + B_1) e^{-y} + \dots.$$

The expansion can be continued in this way: at $O(t^{-2})$ we find that

$$\alpha_2 \sim \left(\frac{A_0 v_1}{120} (1 - v_1) y^5 + \dots \right) e^{-y} + \dots \quad \text{as } y \rightarrow \infty.$$

At this stage in the expansion the behaviour of the solution for y large involves the exponential e^{-y} together with successively higher powers of y . So we expect this solution to break down when y is large, which suggests the need for a further outer expansion in which diffusion plays the major role. This was seen in the small β_0 , when the solution develops from local initial conditions, solution described in Section 3 and can also be seen from equation (7b) for β . For with $\alpha = 1 - \beta$ and β small (y large) equation (7b) becomes, using (18) with $v_0 = 2$, approximately,

$$\frac{\partial \beta}{\partial t} = \frac{\partial^2 \beta}{\partial y^2} + 2 \frac{\partial \beta}{\partial y} + \beta. \tag{27}$$

Equation (27) has a solution of the form $\beta = e^{-y} g(y, t)$ where g satisfies the diffusion equation whose solution involves terms in $e^{-y^2/4t}$ for y large.

The above suggests that in this outer region we write

$$\alpha = 1 + e^{-y} t^{1/2} f(\eta, t), \quad \eta = y/t^{1/2}, \quad (28)$$

where η is of $O(1)$, i.e. y is large, of $O(t^{1/2})$. The solution in this outer region must match with the solution for the inner (front) region. Hence, using (23) and (26),

$$f \sim -\left(A_0 \eta + v_1 A_0 \frac{\eta^3}{6} + \dots\right) - t^{-1/2} \left(B_0 + v_1 \frac{(B_0 - A_0)}{2} \eta^2 + \dots\right) + \dots, \quad (29)$$

for $\eta \ll 1$. Equation (19) becomes, using (28),

$$\frac{\partial^2 f}{\partial \eta^2} + \frac{\eta}{2} \frac{\partial f}{\partial \eta} - (v_1 + \frac{1}{2})f + v_1 t^{-1/2} \frac{\partial f}{\partial \eta} - t \frac{\partial f}{\partial t} + \text{e.s.t.} = 0, \quad (30)$$

where e.s.t. stands for terms which are exponentially small in y .

We look for a solution of equation (30) by expanding,

$$f(\eta, t) = f_0(\eta) + t^{-1/2} f_1(\eta) + \dots \quad (31)$$

f_0 satisfies the equation

$$f_0'' + \frac{\eta}{2} f_0' - (v_1 + \frac{1}{2})f_0 = 0, \quad (32)$$

(primes now denote differentiation with respect to η), subject to

$$f_0 \rightarrow 0 \quad \text{as } \eta \rightarrow \infty, \quad (33)$$

$$f_0 \sim -A_0 \eta \left(1 + v_1 \frac{\eta^2}{6} + \dots\right), \quad \eta \ll 1.$$

The solution of equation (32) which has $f_0 = -A_0 \eta + \dots$ for η small can be written in terms of confluent hypergeometric functions [14] as

$$f_0 = -A_0 \eta e^{-\eta^2/4} {}_1F_1\left(\frac{3}{2} + v_1; \frac{3}{2}; \frac{\eta^2}{4}\right). \quad (34)$$

Now, in general, the confluent hypergeometric function ${}_1F_1(\frac{3}{2} + v_1; \frac{3}{2}; \frac{1}{4}\eta^2)$ is exponentially large for η large, being of $O(\eta^{2v_1} e^{\eta^2/4})$, and hence f_0 will be algebraic at infinity unless the series terminates, which it does when $\frac{3}{2} + v_1 = -k$ ($k = 0, 1, 2, \dots$). Taking the smallest of these gives

$$v_1 = -\frac{3}{2}, \quad f_0 = -A_0 \eta e^{-\eta^2/4}. \quad (35)$$

We can then go on to check that this form for f_0 agrees with (33) for η small.

Hence we have shown that $dv/dt = 2 - 3/(2t) + \dots$ for t large, from which it follows that

$$v = 2t - \frac{3}{2} \log t + C_0 + \dots, \quad (36)$$

where C_0 is a constant of $O(1)$ which cannot be determined from the asymptotic expansion and represents an $O(1)$ shift in origin in t . We should expect this arbitrariness in the solution as the system is autonomous and arises because some of the detail of the small time behaviour of the solution is lost in this asymptotic solution. Result (36) is, in our notation, the same result derived by Bramson [10, 11] (stated previously in the introduction as (3)). Here we have derived the same result from a simple argument, and it arises from the requirement of matching the reaction–diffusion front region to a very weak diffusion-controlled region ahead of it. The argument given by Bramson is in terms of Brownian motion and is much more involved than the present one.

It now remains to see why this asymptotic solution requires the particular choice $v_0 = 2$. For, if $v_0 > 2$ then $\alpha_0 \sim 1 - A_0 e^{-\lambda_1 y} + \dots$ where λ_1 is the smaller of the roots given by (22), and now the higher-order terms in the expansion with y large involve the term $e^{-\lambda_1 y}$ multiplied by increasing integer powers of y (rather than y^2 as in the previous case). Then to match with an outer solution (in which, since this is diffusion dominated, the independent variable must still be $\eta = y/t^{1/2}$) an expansion in powers of $t^{-1/2}$ is required. The $O(t^{-1/2})$ term, α_1 , still satisfies equation (25) but now,

$$\alpha_1 \sim \left(\frac{v_1 \lambda_1}{2\lambda - v_0} \right) A_0 y e^{-\lambda_1 y} + A_1 e^{-\lambda_1 y} + \dots \quad \text{as } y \rightarrow \infty.$$

For the outer solution we have then $\alpha = 1 + e^{-\lambda_1 y} \bar{f}(\eta, t)$ where \bar{f} satisfies the equation

$$\frac{\partial \bar{f}}{\partial \eta} (v_0 - 2\lambda_1) + t^{-1/2} \left(\frac{\partial^2 \bar{f}}{\partial \eta^2} + \frac{\eta}{2} \frac{\partial \bar{f}}{\partial \eta} - t \frac{\partial \bar{f}}{\partial t} \right) + \text{e.s.t.} = 0, \tag{37a}$$

with

$$\bar{f} \sim -A_0 \left[1 - \left(\frac{v_1 \lambda_1}{2\lambda_1 - v_0} \right) \eta + \dots \right] + \dots, \quad \eta \ll 1. \tag{37b}$$

The only possibility for a solution of equation (37a) which matches with (37b) is if $v_0 = 2\lambda_1$, which we can see from (22) implies that $v_0 = 2$, and the previous formulation must be followed.

Finally we look briefly at the behaviour for x of $O(1)$. An examination of equations (7) reveals that the decay of B to its uniform state will be algebraic, while A must be used up much more quickly, dying away exponentially. This is also confirmed by the numerical results (a typical situation is shown in Fig. 1). Here β is given by expression (17) when approximated for $t \gg 1$ (with $\alpha \ll \beta$, $\alpha + \beta \approx \beta$) so that

$$\beta = 1 + t^{-1/2} \left[\left(\frac{\beta_0}{2\sqrt{\pi}} \int_{-\lambda}^{\lambda} g(\xi) d\xi \right) + \dots \right]. \tag{38}$$

For α we write

$$\alpha = e^{-(1-\sigma^2)t} t^m F(x, t), \tag{39}$$

where $\sigma(0 < \sigma < 1)$ and m are to be determined. Putting $\beta = 1 + t^{-1/2} G(x, t)$ where $G(x, t)$ is given by (17) and at leading order for t large by (38), equation (7a) becomes

$$\frac{\partial^2 F}{\partial x^2} - \sigma^2 F - \frac{FG}{t^{1/2}} - \frac{m}{t} F = \frac{\partial F}{\partial t}. \tag{40}$$

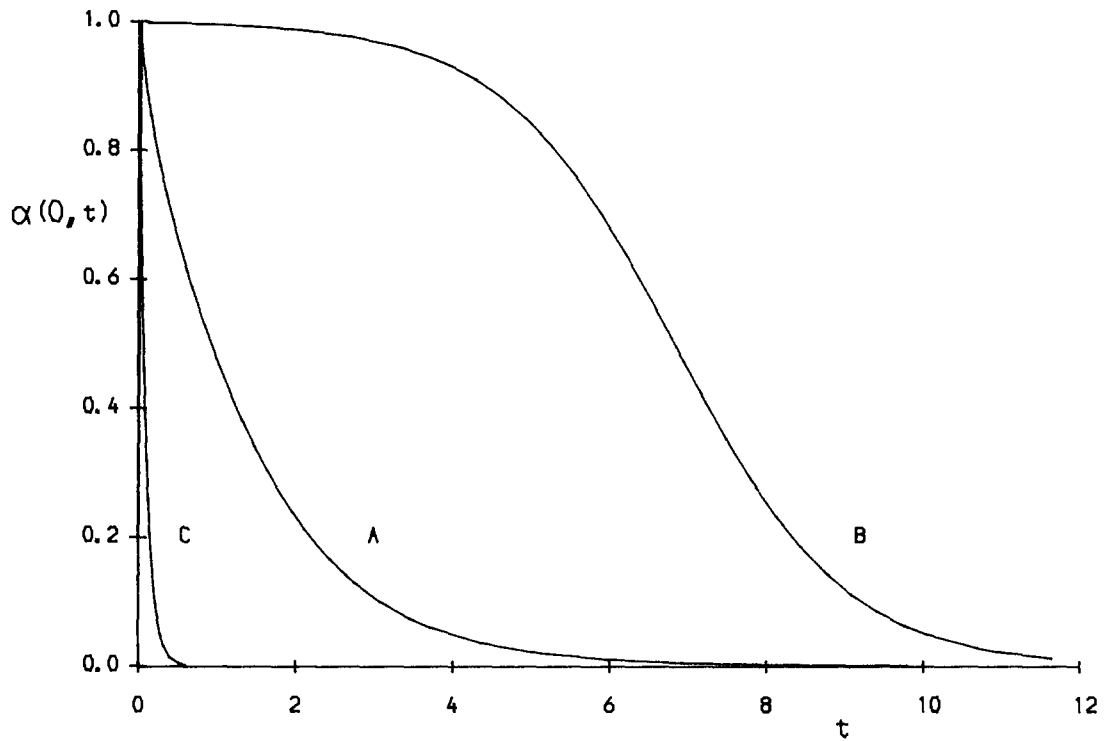


Fig. 3. Graphs of $\alpha(0, t)$ for the three cases (a) $\lambda = 1, \beta_0 = 1$, (b) $\lambda = 10, \beta_0 = 10$ and (c) $\lambda = 0.1, \beta_0 = 0.1$.

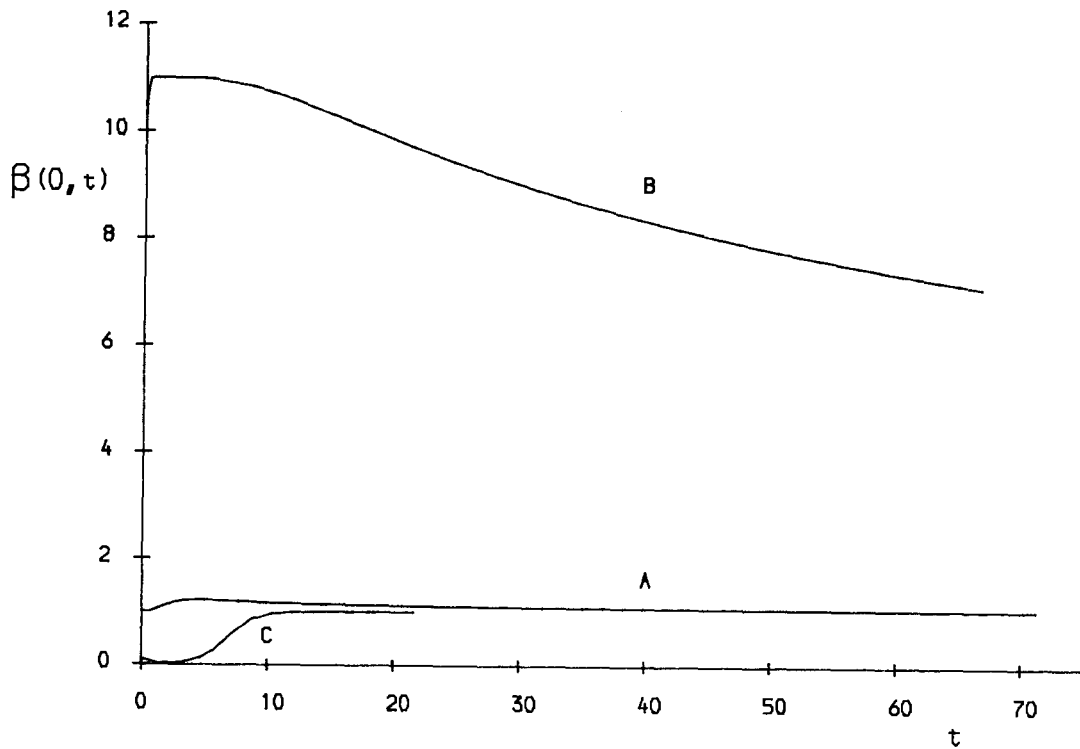


Fig. 4. Graphs of $\beta(0, t)$ for the three cases (a) $\lambda = 1, \beta_0 = 1$, (b) $\lambda = 10, \beta_0 = 10$ and (c) $\lambda = 0.1, \beta_0 = 0.1$.

At leading order, the solution of equation (40) (taken to be symmetric about $x = 0$) is $F = K_0 \cosh \sigma x$ (where K_0 is an arbitrary constant). So for x large $\alpha \sim K_0 e^{-(1-\sigma^2)t} t^m e^{\sigma x} + \dots$. Writing this in terms of y and using (36) gives $\alpha \sim \bar{K}_0 e^{-(1-\sigma^2-2\sigma)t} t^{m-3\sigma/2} e^{\sigma y} + \dots$. Matching with the solution from the reaction–diffusion wave as $y \rightarrow -\infty$ gives $\sigma = \sqrt{2} - 1$ and $m = \frac{3}{2}(\sqrt{2} - 1)$ so that $\alpha \sim \bar{K}_0 e^{\mu y}$, where μ is as given earlier with $v_0 = 2$. Hence when x is of $O(1)$, α is of $O(t^{\frac{3}{2}(\sqrt{2}-1)} e^{-2(\sqrt{2}-1)t})$ for t large.

The difference in the behaviour of α and β for x of $O(1)$ can be seen in Figs 3 and 4 where we plot graphs of $\alpha(0, t)$ and $\beta(0, t)$ for the three cases described earlier, namely for $\lambda = 1$, $\beta_0 = 1$; $\lambda = 0.1$, $\beta_0 = 0.1$ and $\lambda = 10$, $\beta_0 = 10$. Figure 3 shows that the greater the initial input of B, the sooner α is reacted away to zero and that, once started, this is a rapid reaction (with very small amounts of B ($\beta_0 = 0.1$, $\lambda = 0.1$) there is a short initiation period prior to the reaction getting started). In all cases all of the A is used up over a relatively short time scale.

Figure 4 shows that the behaviour of β is quite different. There is an initial adjustment due to the presence of A but when all of this has been used up, the concentration gradient in β can spread out only by diffusion. As this is a slow process, β tends to its asymptotic value ($\beta(0, t) \rightarrow 1$ as $t \rightarrow \infty$) only very slowly, in line with (38) where $\beta - 1$ is $O(t^{-1/2})$ for t large.

6. Conclusion

The propagating reaction–diffusion wave should properly be seen as the large-time solution for an initial-value problem. When it is looked at in this way, there must ultimately be a unique propagation speed arising from some given set of initial conditions. The asymptotic theory then shows that the wave will travel with the minimum possible speed for all local initial conditions of the type (5) (as is also confirmed by the numerical solutions). By just considering the reaction–diffusion front in isolation, we are unable to predict its propagation speed. As the wave propagates through the medium it quickly uses up all of reactant A, but leaves behind a small and slowly-decaying residue of reactant B.

The asymptotic theory shows that ahead of the wave there is a very weak diffusive region and it is of interest to see how this arises from the interaction of the process. At the outset B is introduced only into some local region, with there being no B (and hence no reaction with A) outside this region. This sets up concentration gradients on which diffusion can operate, while where B is plentiful this reacts with A. Meanwhile the region where B is present has spread out further by diffusion so the reaction can also start here as well. Hence the reactive zone spreads out, leaving behind a region where eventually all the A has been used up. A reaction–diffusion wave is then seen, pushing ahead of it a weak diffusive region, this being needed to trigger the reaction. So the speed of propagation of the reaction–diffusion wave is ultimately controlled by the rate at which B can spread forward by diffusion.

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