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The Evolution of Travelling Waves in Reaction-Diffusion Equations with Monotone Decreasing Diffusivity. II. Abruptly Vanishing Diffusivity

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The evolution of travelling waves in reaction–diffusion equations with monotone decreasing diffusivity. II. Abruptly vanishing diffusivity

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In this paper we continue our study of some of the qualitative features of chemical polymerization processes by considering a reaction–diffusion equation for the chemical concentration in which the diffusivity vanishes abruptly at a finite concentration. The effect of this diffusivity cut-off is to create two distinct process zones; in one there is both reaction and diffusion and in the other there is only reaction. These zones are separated by an interface across which there is a jump in concentration gradient. Our analysis is focused on both the initial development of this interface and the large time evolution of the system into a travelling wave form. Some distinct differences from our previous analysis of smoothly vanishing diffusivity are found.

1. Introduction

In part I (Needham & King 1995) of this work we were concerned with the effects of concentration dependent diffusivity, which vanished smoothly at a finite concentration, on the solutions to a class of reaction–diffusion equations. These equations are of some interest as they give a qualitative description of some features of the chemical process of polymerization. Our major interest here is to model, in a simple manner, the increasing entanglement of long-chain molecules as the polymer concentration increases. This entanglement causes a reduction in the mobility of the nascent polymer matrix which is represented by a decreasing diffusivity with a cut-off at a finite concentration. A number of experimental and theoretical studies of this phenomena were reviewed in part I, to which reference should be made.

We now turn our attention to the other canonical type of diffusivity cut-off; one that happens abruptly. From the statistical mechanics viewpoint (Doi & Edwards 1986) this corresponds to regarding the loss of diffusivity in the polymer as a phase change, akin to the sudden freezing of water as the temperature reduces below a threshold value. In the experimental literature known to us, the results available do not seem to be readily capable of distinguishing between smooth and abrupt cut-off in diffusivity. We shall show later in this work that an abrupt diffusivity cut-off causes a far more marked jump in the flux of chemical either side of the moving interface between reaction and reaction–diffusion zones. This jump is an order of

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magnitude larger in general than in the smoothly vanishing diffusivity case and, as such, may be subject to experimental observation.

The structure of this paper is similar to that of part I. We begin by formulating the reaction–diffusion equation as an integral conservation law and proceed to derive appropriate conditions that hold at the moving interface. Some *a priori* bounds and existence results on the concentration and displacement of the interface are also given, together with a lower bound on the time taken for the concentration to reach its cut-off level. The initial development of the interface from this critical level is then considered and reaction rates and data types that allow both singular and slow frontal motion are identified. The large time behaviour of the system is next shown to allow the propagation of travelling waves with a speed equal to or above a certain minimum. By considering asymptotic corrections to the travelling wave forms we show that, for a wide class of initial data, the minimum speed wave is selected. Finally a numerical method is developed that solves the moving boundary problem and confirms the asymptotic structure we have developed.

2. Conservation laws and differential equations

As a model for the polymer reaction process described in the introduction, we consider a scalar reaction–diffusion process in one space dimension for the variable u, which we may regard as the concentration of the autocatalytic chemical species (polymer). The dimensionless integral conservation law governing the evolution of u in x (space) and t (time) is then given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{x_1}^{x_2} u\,\mathrm{d}x = [F_x(u)]_{x_1}^{x_2} + \int_{x_1}^{x_2} R(u)\,\mathrm{d}x \tag{2.1}$$

for any $x_2 > x_1 \geqslant 0$ and $t > 0$. The derivation of (2.1) follows directly that given in part I. As in part I, we impose the following conditions on $R(u)$, namely,

$$\left.\begin{aligned}
&R(u)\in C^1(-\infty,\infty),\\
&R(0)=R(1)=0,\\
&R'(0)=1,\quad R'(1)<0,\\
&R(u)>0,\quad u\in(0,1),\quad R(u)<0,\quad u\in(1,\infty),\\
&R(u)\leqslant u,\quad u\in[0,1],
\end{aligned}\right\} \tag{2.2a–c}$$

with $u \equiv 0$ being the unreacted state and $u \equiv 1$ being the fully reacted state. However, the nature of the flux function $F(u)$ is constructed to model the effect of a rapid reduction in the diffusivity of u when $u \sim \tilde{u}_c(>0)$, with $\tilde{u}_c$ being a critical concentration corresponding to the 'locking' of the polymer molecules. We adopt the form

$$F(u) = \begin{cases} u, & u \leqslant \tilde{u}_c,\\ \tilde{u}_c, & u > \tilde{u}_c, \end{cases} \tag{2.3}$$

which leads to a diffusivity $D(u) \equiv F'(u)$ given by

$$D(u) = \begin{cases} 1, & u < \tilde{u}_c,\\ 0, & u > \tilde{u}_c, \end{cases} \tag{2.4}$$

with $D(\cdot)$ being undefined at $u = \tilde{u}_c$. In terms of polymer reactions, we also make the restriction

$$0 < \tilde{u}_c < 1, \tag{2.5}$$

which ensures that the diffusivity of the polymer drops to zero before the reaction is completed.

As in part I we examine the initial-boundary value problem which arises when a localized quantity of u is introduced initially into the otherwise unreacting state $u \equiv 0$. Thus we must solve equation (2.1) in $x, t > 0$ subject to

$$u(x,0) = \begin{cases} u_0\, g(x), & 0 \leqslant x \leqslant \sigma, \\ 0, & x > \sigma, \end{cases} \tag{2.6a}$$

$$u_x(0,t) = 0, \quad t > 0, \tag{2.6b}$$

$$u(x,t) \to 0 \quad \text{as} \quad x \to \infty, \quad t > 0. \tag{2.6c}$$

The function $g(x)$ is positive, analytic and monotone decreasing in $0 \leqslant x \leqslant \sigma$ with $g(\sigma) = 0$ and $g(0) = 1$. The dimensionless parameter σ measures the support of the initial data, while u_0 is the maximum input concentration of u, which for the polymer problem has

$$0 < u_0 < \tilde{u}_c. \tag{2.7}$$

As in part I we consider solutions $u(x,t)$ to the initial-boundary value problem (2.1), (2.6) on $D_T = \{(x,t) \in \mathbb{R}^2 : 0 < x < \infty, 0 < t \leqslant T\}$, which have $u(x,t)$ continuous on $\bar{D}_T$, while u_t, u_x, u_{xx} exist and are continuous in D_T except along simple differentiable curves $x = s(t)$, say, upon which $u = \tilde{u}_c$. However, we require that the limits of u_t, u_{xx}, u_x exist as points on such curves are approached from either side. We denote this class of functions on D_T as $C_p[D_T]$, and refer to this as the class of piecewise-classical solutions to (2.1), (2.6) on D_T.

3. Piecewise-classical solutions

Let $u(x,t)$ be a piecewise-classical solution to (2.1), (2.6) on D_T, and define

$$D_+ = \{(x,t) \in D_T : u(x,t) > \tilde{u}_c\},$$
$$D_- = \{(x,t) \in D_T : u(x,t) < \tilde{u}_c\},$$

with C denoting the common boundary of $D_\pm$. It is then clear that $u(x,t)$ satisfies the partial differential equations

$$u_t = u_{xx} + R(u), \quad (x,t) \in D_-, \tag{3.1a}$$

$$u_t = R(u), \quad (x,t) \in D_+, \tag{3.1b}$$

while across C (which we describe by $x = s(t)$) the integral conservation law (2.1) must be satisfied. On taking $x_+ \in D_+$ and $x_- \in D_-$ we obtain from (2.1)

$$\int_{x_-}^{s(t)} u_t \,\mathrm{d}x + \int_{s(t)}^{x_+} u_t \,\mathrm{d}x + \dot{s}[u(x,t)]_{s^-}^{s^+} = -u_x(x_-,t) + \int_{x_-}^{x_+} R(u)\,\mathrm{d}x, \tag{3.2}$$

where we have put $x_+ > x_-$, without loss of generality. After taking the limits $x_+ \to s^+, x_- \to s^-$ in (3.2), and noting that $u \in C_p[D_T]$, we arrive at the condition

$$u_x|_{C^-} = 0, \tag{3.3}$$

where $C^\pm$ denotes the limits on approaching C from $D_\pm$ respectively. Condition (3.3) must be satisfied simultaneously with

$$u|_{C^+} = u|_{C^-} = \tilde{u}_c, \tag{3.4}$$

at $x = s(t)$.

We now follow part I in looking for a piecewise-classical solution to the initial-boundary value problem (2.1), (2.6) in three distinct domains.

Domain A, $0 \leqslant x < \infty$, $0 \leqslant t < t_c$

$$u_t = u_{xx} + R(u), \quad 0 \leqslant u < \tilde{u}_c, \tag{3.5a}$$

$$u(x,0) = \begin{cases} u_0 g(x), & 0 \leqslant x \leqslant \sigma, \\ 0, & x > \sigma, \end{cases} \tag{3.5b}$$

$$u_x(0,t) = 0, \quad 0 < t < t_c, \tag{3.5c}$$

$$u(x,t) \to 0 \quad \text{as} \quad x \to \infty, \quad 0 \leqslant t < t_c. \tag{3.5d}$$

Domain B, $0 \leqslant x < s(t)$, $t > t_c$

$$u_t = R(u), \quad u > \tilde{u}_c, \tag{3.6a}$$

$$u(x,t) \to \tilde{u}_c \quad \text{as} \quad x \to s^-(t), \quad t > t_c. \tag{3.6b}$$

Domain C, $x \geqslant s(t)$, $t > t_c$

$$u_t = u_{xx} + R(u), \quad 0 \leqslant u < u_c, \tag{3.7a}$$

$$\left.\begin{aligned} u(s(t),t) &= \tilde{u}_c, \\ u_x(s(t),t) &= 0, \\ u(x,t) &\to 0 \quad \text{as} \quad x \to \infty, \end{aligned}\right\} t > t_c. \tag{3.7b, c, d}$$

We shall also require

$$s(t_c) = 0, \quad \lim_{t \to t_c^+} u(x,t) = \lim_{t \to t_c^-} u(x,t), \quad x > 0. \tag{3.8}$$

Here the interface C is given by $x = s(t)$ with D_+ being domain B and D_- being domain C.

We now make some observations concerning $s(t)$. Since $u(x,t)$ is piecewise-classical, we obtain from (3.6a, b)

$$R(\tilde{u}_c) + \dot{s} u_x(s^-(t),t) = 0, \quad t > t_c. \tag{3.9}$$

However, $R(\tilde{u}_c) > 0$ and $u_x(s^-(t),t) \leqslant 0$, which leads to

$$\dot{s}(t) > 0, \quad t > t_c, \tag{3.10}$$

via (3.9). Following part I we may also arrive at the upper bound

$$s(t) \leqslant \tilde{u}_c^{-1} A(t_c)\, \mathrm{e}^{t-t_c}, \quad t > t_c, \tag{3.11}$$

where

$$A(t_c) = \int_0^\infty u(x,t_c)\,\mathrm{d}x.$$

Thus, $s(t)$ is a monotone increasing function in $t > t_c$, and remains bounded for finite $t > t_c$. We next consider domains A, B, C separately.

4. Domain A

Here we examine the initial-boundary value problem (3.5a–d) in domain A, which we shall refer to as IBVPA. We first examine (3.5a–d) on D_T. It is readily established via the comparison theorem for scalar parabolic operators (see, for example, Fife 1979) that

$$0 < u(x,t) < 1 \quad \text{on} \quad D_T, \tag{4.1}$$

for any $T > 0$. The *a priori* bounds (4.1) then imply the global existence and uniqueness of a solution to IBVPA (see, for example, Smoller 1983) with $u(x,t) \in C^{\infty}[D_T]$ for any $T > 0$. Moreover, a further application of the comparison theorem gives

$$u(x,t) < u_0\,\mathrm{e}^t \quad \text{on} \quad D_T, \tag{4.2}$$

for any $T > 0$. We can also apply theorem (3.1) of Aronson & Weinberger (1975), which establishes that

$$u(x,t) \to 1 \quad \text{as} \quad t \to \infty, \tag{4.3}$$

uniformly on compact intervals in x. In addition we have the following theorem.

Theorem 4.4. *Let $u(x,t)$ be the solution of* IBVPA *on D_T (any $T > 0$). Then*
(i) $u_x \leqslant 0$,
and when $g''(x) + u_0^{-1} R(u_0 g(x)) \geqslant 0 \;\forall\; 0 \leqslant x \leqslant \sigma$, with $g'(0) = 0$,
(ii) $u_t \geqslant 0$.

Proof.
(i) Since $u \in C^{\infty}[D_T]$, then $\omega \equiv u_x$ satisfies the following initial-boundary value problem,

$$\left.\begin{aligned} &\omega_t = \omega_{xx} + R'(u)\,\omega \quad \text{on} \quad D_T, \\ &\omega(x,0) = \begin{cases} u_0\, g'(x), & 0 \leqslant x \leqslant \sigma, \\ 0, & x > \sigma, \end{cases} \\ &\omega(0,t) = 0, \quad 0 < t \leqslant T, \\ &\omega(x,t) \to 0 \quad \text{as} \quad x \to \infty, \quad 0 < t \leqslant T. \end{aligned}\right\} \tag{4.4}$$

We can now apply the parabolic maximum principle to (4.4) (recalling that $g'(x) \leqslant 0$ on $0 \leqslant x \leqslant \sigma$) (see, for example, Friedman 1964) to establish $\omega \leqslant 0$ on D_T, as required.

(ii) We consider first $u(x,t)$ and $g(x)$ on the domain $D_T^{\sigma} = (0,\sigma) \times (0,T]$, and define the operator

$$N[V] \equiv V_t - V_{xx} - R(V) \quad \text{on} \quad D_T^{\sigma}, \tag{4.5}$$

for any suitably differentiable function $V(x,t)$. We observe immediately that

$$N[u] \geqslant N[u_0\, g] \quad \text{on} \quad D_T^{\sigma}, \tag{4.6}$$

while

$$\left.\begin{aligned} u(x,0) &\geqslant u_0\, g(x), \quad x \in [0,\sigma], \\ u(\sigma,t) &\geqslant u_0\, g(\sigma), \quad t \in [0,T], \\ u_x(0,t) &\leqslant u_0\, g_x(0), \quad t \in [0,T], \end{aligned}\right\} \tag{4.7}$$

via (3.5*b*, *c*) and (4.1). Conditions (4.6, 4.7) together with the comparison theorem then give

$$u(x,t) \geqslant u_0\, g(x) \quad \text{on} \quad D_T^{\sigma}. \tag{4.8}$$

Therefore, from (4.1) and (4.8), we have

$$u(x,t) \geqslant u(x,0) \quad \text{on} \quad D_T. \tag{4.9}$$

Now, for any $\delta > 0$, define $\omega(x,t) \equiv u(x,t+\delta)$, on D_T. Then

$$N[\omega] \geqslant N[u] \quad \text{on} \quad D_T, \quad \omega_x(0,t) \leqslant u_x(0,t), \quad t \in [0,T], \tag{4.10}$$

while $\omega(x,0) = u(x,\delta)$, and so

$$\omega(x,0) \geqslant u(x,0), \quad x \in [0,\infty), \tag{4.11}$$

via (4.9). The comparison theorem, together with (4.10, 4.11) then gives $\omega(x,t) \geqslant u(x,t)$ on D_T. That is, $u(x,t+\delta) \geqslant u(x,t)$ in D_T for any $\delta > 0$. Thus $u_t \geqslant 0$ on D_T as required. ■

Now, since $u_0 < \tilde{u}_c < 1$ there exists a unique maximal $t_c > 0$ such that

$$u(x,t) < \tilde{u}_c \quad \text{on} \quad D_{t_c} \backslash \{(x,t_c) : x \geqslant 0\}, \tag{4.12}$$

via (4.3). Moreover, at $t = t_c$, $u(x,t_c)$ is monotone decreasing in x (via theorem 4.4) and

$$u(0,t_c) = \tilde{u}_c, \tag{4.13}$$

which requires $s(t_c) = 0$, as anticipated in (3.8). From (4.2) we obtain the lower bound

$$t_c > \log(\tilde{u}_c/u_0). \tag{4.14}$$

We may also follow part I and obtain the structure of $u(x,t)$ for $x \gg 1$ with $t = O(1)$ as,

$$u(x,t) \sim \frac{d_\infty t^{m+\frac{1}{2}}}{x^{m+1}} \, \mathrm{e}^{-(x^2/4t-t)}, \tag{4.15}$$

where d_∞ is a constant related to $g(x)$, and $m \in \mathbb{N}$ such that $g(x) = O([x-\sigma]^m)$ as $x \to \sigma^-$. In particular, with $u_c(x) = u(x,t_c)$, we have

$$u_c(x) \sim (C/x^{m+1}) \, \mathrm{e}^{-x^2/4t_c} \quad \text{as} \quad x \to \infty, \tag{4.16}$$

with C being constant.

The problem IBVPA thus has a unique solution on D_{t_c}, and we now consider domain B.

5. Domain B

It is convenient to define the inverse function of $s(t)$, which we denote by $\bar{s}(x), x \geqslant 0$ (so that $t \equiv \bar{s}(s(t)), \forall\, t \geqslant t_c$) with $\bar{s}(\cdot)$ being well defined via (3.10), (3.11). We have

$$\bar{s}'(x) = 1/\dot{s}(\bar{s}(x)) > 0 \quad \forall\, x > 0, \tag{5.1}$$

$$\bar{s}(0) = t_c. \tag{5.2}$$

The solution to (3.6a, b) can now be written implicity as

$$H(u) = t - \bar{s}(x), \quad x \geqslant 0, \quad t > \bar{s}(x), \tag{5.3}$$

where
$$H(y) = \int_{\lambda=\tilde{u}_c}^{\lambda=y} \frac{\mathrm{d}\lambda}{R(\lambda)}. \tag{5.4}$$

From (5.3, 5.4) we readily observe that $\tilde{u}_c \leqslant u < 1$ at each $x \geqslant 0$ for all $t > \bar{s}(x)$, with

$$u(x,t) \sim 1 - (1-\tilde{u}_c)\, \mathrm{e}^{R'(1)[t-\bar{s}(x)-\hat{c}]} \tag{5.5}$$

as $t \to \infty$, where

$$\hat{c} = \int_{\tilde{u}_c}^{1} \left\{ \frac{1}{R(\lambda)} + \frac{1}{R'(1)(1-\lambda)} \right\} \mathrm{d}\lambda.$$

Moreover, we have $u_t > 0$ for all $t \geqslant \bar{s}(x)$ while $u_x = -\bar{s}'(x) R(u) < 0$ for all $0 < x \leqslant s(t), t > t_c$, via (5.1), (5.3, 5.4). Therefore, for each $x \geqslant 0$ with $t \geqslant \bar{s}(x)$ we have that $u(x,t) \to 1^-$ as $t \to \infty$, monotonically in t, and the fully reacted state is reached in large time, with x fixed. However, when $x = s(t), u = \tilde{u}_c$ for all $t > t_c$ while $u \to 0$ for $x \gg s(t)$ for all t. This indicates the formation of a travelling wave structure as $t \to \infty$, which we shall investigate at a later stage in the paper.

6. The solution as $t \to t_c^+$, breakthrough

It has been established in §4 that for all initial data t_c is finite, and at $t = t_c, u(x, t_c)$ is monotone decreasing in x with $u(0, t_c) = \tilde{u}_c$. Moreover, either

$$u_t(0, t_c^-) > 0 \tag{6.1}$$

or there is $N \in \mathbb{Z}$ such that

$$\partial^n u/\partial t^n \,(0, t_c^-) = 0 \quad \forall\, n \leqslant 2N, \tag{6.2}$$

while

$$\partial^{2N+1} u/\partial t^{2N+1} \,(0, t_c^-) > 0. \tag{6.3}$$

We examine here the structure of $u(x,t)$ as $t \to t_c^+$ and $x \to 0$, that is as breakthrough occurs into $u > \tilde{u}_c$. Thus we must examine the structure of $u(x,t)$ in domains B and C. At $t = t_c$, we have, from §4, that

$$u(x, t_c) \sim u_c - a_2 x^2 + \sum_{n=3}^{\infty} a_n x^n, \tag{6.4}$$

as $x \to 0$, with $a_2 \geqslant 0$. When condition (6.1) holds, then equation (3.5a) establishes that

$$0 \leqslant a_2 < \tfrac{1}{2} R_c, \tag{6.5}$$

where $R_c = R(\tilde{u}_c)$. However, when conditions (6.2, 6.3) hold we have

$$a_2 = \tfrac{1}{2} R_c. \tag{6.6}$$

We expect the generic case to be $0 < a_2 < \frac{1}{2} R_c$, and we consider this case first. In this case $u_t(0, t_c) = R_c - 2a_2$, which, together with (6.4), suggests that $s(t) \sim O[(t-t_c)^{\frac{1}{2}}]$ as $t \to t_c^+$, and we expand

$$s(t) \sim \sum_{n=1}^{\infty} s_n (t-t_c)^{\frac{1}{2}n}, \tag{6.7}$$

with

$$u(\eta, t) \sim \begin{cases} \tilde{u}_c + \sum_{n=2}^{\infty} F_n(\eta)\,(t-t_c)^{\frac{1}{2}n} & \text{in domain C}, \\ \tilde{u}_c + \sum_{n=2}^{\infty} G_n(\eta)\,(t-t_c)^{\frac{1}{2}n} & \text{in domain B}, \end{cases} \tag{6.8}$$

as $t \to t_c^+$ with $\eta = x(t-t_c)^{-\frac{1}{2}} = O(1)$. We observe that the interface $x = s(t)$ corresponds to $\eta = s(t)\,(t-t_c)^{-\frac{1}{2}} \sim s_1 + o(1)$ as $t \to t_c^+$. We begin in domain C. On substitution from (6.8), (6.7) into (3.7a–c) and (3.8), (6.4) we obtain the leading order problem for $F_2(\eta), s_1$ as

$$\left.\begin{aligned} &F_2'' + \tfrac{1}{2}\eta F_2' - F_2 = -R_c, \quad \eta > s_1, \\ &F_2(s_1) = 0, \quad F_2'(s_1) = 0, \\ &F_2(\eta) \sim -a_2 \eta^2 \quad \text{as} \quad \eta \to \infty, \end{aligned}\right\} \tag{6.9a–d}$$

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which is an eigenvalue problem for s_1. The general solution of (6.9a) is

$$F_2(\eta) = C(1+\tfrac{1}{2}\eta^2)+E(1+\tfrac{1}{2}\eta^2)\int_\eta^\infty \frac{e^{-s^2/4}}{(1+\frac{1}{2}s^2)^2}\,ds+R_c, \quad \eta > s_1, \tag{6.10}$$

with C, E as yet undetermined constants. Condition (6.9d) readily gives $C = -2a_2$, after which conditions (6.9b, c) require

$$E = [2a_2(1+\tfrac{1}{2}s_1^2)-R_c]/(1+\tfrac{1}{2}s_1^2)\int_{s_1}^\infty F(s)\,ds, \tag{6.11}$$

with $F(s) = (1+\frac{1}{2}s^2)^{-2}\,e^{-s^2/4}$, and

$$\frac{2a_2}{R_c} = \frac{1}{(1+\frac{1}{2}s_1^2)} - s_1\,e^{s_1^2/4}\int_{s_1}^\infty F(s)\,ds \equiv Q(s_1), \tag{6.12}$$

which is to be solved for s_1. We observe from (6.12) that s_1 depends only upon the parameter a_2/R_c, while an examination of $Q(s_1)$ shows that

$$Q(s_1) \to \begin{cases} 1, & s_1 \to 0, \\ 0, & s_1 \to \infty, \end{cases}$$
$$Q'(s_1) < 0, \qquad s_1 \geqslant 0. \tag{6.13}$$

Therefore, in this case, equation (6.12) has a unique, positive, solution s_1, which is monotone decreasing with $0 < a_2/R_c < \frac{1}{2}$, and

$$s_1 \to \begin{cases} 0, & a_2/R_c \to \frac{1}{2}, \\ \infty, & a_2/R_c \to 0. \end{cases} \tag{6.14}$$

This completes the solution in domain C. To obtain the solution in domain B we substitute from (6.8), (6.7) into (3.6a, b). At leading order we obtain

$$\tfrac{1}{2}\eta G_2' - G_2 = -R_c, \quad 0 < \eta < s_1,$$
$$G_2(s_1) = 0,$$

which has solution,

$$G_2(\eta) = R_c\{1-(1/s_1^2)\,\eta^2\}, \quad 0 < \eta < s_1. \tag{6.15}$$

We conclude that an interface develops at t_c^+, and propagates away from $x = 0$ with a singular velocity $\dot{s} = O([t-t_c]^{-\frac{1}{2}})$. The jump in gradient at the interface is given with use of (6.15), (6.7),

$$J(t) \equiv u_x(s(t)^+, t) - u_x(s(t)^-, t) \sim (2R_c/s_1)\,(t-t_c)^{\frac{1}{2}}, \tag{6.16}$$

as $t \to t_c^+$.

The degenerate cases $a_2 = \frac{1}{2}R_c$ or 0 can be considered in a similar way. When $a_2 = 0$, then $u(x, t_c) \sim \tilde{u}_c - a_{2M}\,x^{2M}$ as $x \to 0$ for some $M = 2, 3, \ldots$, and $a_{2M} > 0$. It is then readily established that

$$\dot{s}(t) \sim O([t-t_c]^{1/2M-1}), \quad J(t) \sim O([t-t_c]^{1-1/2M}), \tag{6.17}$$

as $t \to t_c^+$. The final case has $a_2 = \frac{1}{2}R_c$, when (6.2), (6.3) hold for some $N = 1, 2, \ldots$. We establish that

$$\dot{s}(t) \sim O([t-t_c]^{N-\frac{1}{2}}), \quad J(t) \sim O([t-t_c]^{\frac{1}{2}-N}), \tag{6.18}$$

as $t - t_c^+$.

Thus, in the generic case, the interface has an unbounded velocity as $t \to t_c^+$, as it also does in the case $a_2 = 0$. However, in the case $a_2 = \frac{1}{2}R_c$ the interface initiates its motion with zero velocity. It should be noted that 'slow' fronts of the type (6.18) do not occur in the continuous diffusivity case (part I) and that in all present cases the gradient jumps at the interface are an order of magnitude larger than those generated in the continuous diffusivity case. In addition we observe that in all cases $0 \leqslant a_2 \leqslant R_c, \dot{s}(t)\, J(t) = O(1)$ as $t \to t_c^+$, representing continuity of concentration flux across the evolving interface.

7. Permanent form travelling waves

We expect that the long time development of the full initial-boundary value problem (2.1)–(2.6) may involve the propagation of a travelling wave of permanent form in $x > 0$, separating the unreacted state $u \equiv 0$ ahead from the fully reacted state $u \equiv 1$ to the rear. Thus, before examining the problem in domain C, we examine the possible class of piecewise-classical permanent form travelling waves that can be sustained by the integral conservation law (2.1). We make the following definition.

Definition 7.1. A permanent form travelling wave solution (PTW) of the integral conservation law (2.1) is a non-negative solution that depends only upon the single variable $z \equiv x - \gamma(t)$ (where $\gamma(t)$ is the wave-front position) and satisfies the conditions $u \to 0$ as $z \to \infty$ and $u \to 1$ as $z \to -\infty$. In addition, the solution should be continuous and piecewise-classical for $-\infty < z < \infty$.

We readily establish that a PTW has $0 \leqslant u(z) \leqslant 1$ and is monotone decreasing in z. Therefore $u(z)$ is a solution of the boundary value problem

$$u_{zz} + v u_z + R(u) = 0, \quad z > 0, \tag{7.2}$$

$$v u_z + R(u) = 0, \quad z < 0, \tag{7.3}$$

$$0 \leqslant u < \tilde{u}_c, \quad z > 0, \quad u_c < u \leqslant 1, \quad z < 0, \tag{7.4}$$

$$u \to 0 \quad \text{as} \quad z \to \infty, \tag{7.5}$$

$$u \to 1 \quad \text{as} \quad z \to -\infty, \tag{7.6}$$

$$u(0^+) = u(0^-) = \tilde{u}_c, \tag{7.7}$$

$$u_z(0^+) = 0. \tag{7.8}$$

In the above $v = \dot{\gamma}(t)$. However, u is a function of z alone, which determines that v must be constant, and without loss of generality we consider only $v > 0$. The problem (7.2–7.8) is a nonlinear eigenvalue problem with the positive propagation speed v being the eigenvalue. We study (7.2–7.8) in the phase plane.

(*a*) *The phase plane*

We consider first equation (7.2) for $z > 0$ in the (u, w) phase plane, where $w = u_z$. Equation (7.2) becomes the equivalent system

$$u_z = w, \quad w_z = -vw - R(u). \tag{7.9}$$

This system has equilibrium points at $\boldsymbol{e}_1 = (0, 0)$ and $\boldsymbol{e}_2 = (1, 0)$. A solution of (7.2) that satisfies conditions (7.4), (7.5), (7.7), (7.8) requires a directed integral path of the system (7.9) connecting the point $(\tilde{u}_c, 0)$ to the equilibrium point $\boldsymbol{e}_1$, lying entirely in the strip $0 \leqslant u \leqslant \tilde{u}_c$.

We observe first that the equilibrium point $\boldsymbol{e}_1$ is a spiral for $0 < v < 2$, becoming a node for $v \geqslant 2$. Therefore a necessary condition for the existence of a solution to (7.4, 7.5), (7.7, 7.8) is

$$v \geqslant 2. \tag{7.10}$$

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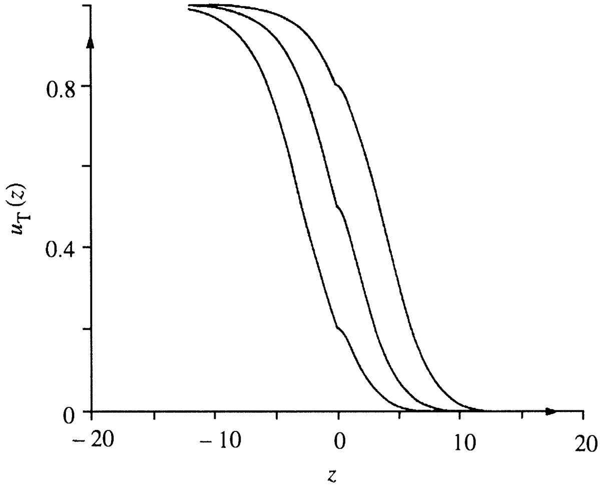

Figure 1. The minimum speed travelling wave $u_T(Z)$, when $R(u) = u(1-u)$ and $\tilde{u}_c = 0.2, 0.5, 0.8$.

However, it is also readily established that,

$$I = \{(u, w): 0 \leqslant u \leqslant 1, \quad -\tfrac{1}{2}vu \leqslant w \leqslant 0\} \tag{7.11}$$

in a positively invariant set for (7.9) for each $v \geqslant 2$, and so (via the Poincare–Bendixson theorem) we conclude that condition (7.10) is also a sufficient condition for the existence of a solution to (7.4, 7.5), (7.7, 7.8). We denote this solution by $u = u_+(z), z > 0$, and observe via (7.11) that $u_+(z)$ is monotone decreasing.

It remains to consider (7.3), (7.4), (7.6), (7.7) in $z < 0$. This problem has the solution $u = u_-(z)$, where $u_-(z)$ is given implicitly by

$$z = -\frac{1}{v}\int_{u_c}^{u_-} \frac{d\lambda}{R(\lambda)}, \quad z < 0. \tag{7.12}$$

We observe that $u_-(z)$ is also monotone decreasing.

We have established the following.

Theorem 7.13. *For each $v \geqslant 2$ there exists a unique* PTW*, given by*

$$u_T(z) = \begin{cases} u_+(z), & z \geqslant 0, \\ u_-(z), & z < 0; \end{cases}$$

$u_T(z)$ is monotone decreasing in z and has a single jump in gradient at $z = 0$, with

$$u'_T(0^+) - u'_T(0^-) = R_c/v.$$

For $0 < v < 2$, no PTW *exists.* ■

In the case when $R(u) = u(1-u)$ and $\tilde{u}_c = 0.2, 0.5, 0.8, u_T(z)$ when $v = 2$ (the minimum speed PTW) has been computed numerically and is illustrated in figure 1.

We remark finally that for $\tilde{u}_c \ll 1$ we have

$$u_+(z) \sim \begin{cases} 1/(\lambda_+ - \lambda_-)\{\lambda_+ e^{\lambda_- z} - \lambda_- e^{\lambda_+ z}\}, & v > 2, \\ (1+z)\,e^{-z}, & v = 2, \end{cases}$$

as $\tilde{u}_c \to 0$, where $\lambda_\pm = \tfrac{1}{2}\{-v \pm \sqrt{(v^2-4)}\}$. We next consider the problem in domain C.

8. The problem in domain C

In §4 we have discussed the development in domain A, while the problem in domain B has been completed in §5. Having established the details of breakthrough in §6, we can now consider the problem in domain C in more detail.

We introduce the travelling coordinates $y = x - s(t)$ and $\tau = t - t_c$, after which the problem in domain C becomes

$$u_\tau = u_{yy} + \dot{s}(\tau)\, u_y + R(u), \quad y, \tau > 0, \tag{8.1}$$

$$u(y, 0) = u_c(y), \quad y \geqslant 0, \tag{8.2}$$

$$u(0, \tau) = \tilde{u}_c, \quad u_y(0, \tau) = 0, \quad \tau \geqslant 0, \tag{8.3}$$

$$u(y, \tau) \to 0 \quad \text{as} \quad y \to \infty, \quad \tau \geqslant 0, \tag{8.4}$$

$$s(0) = 0, \tag{8.5}$$

where $u_c(y) > 0$ in a C^∞ function, with asymptotic form (4.16) as $y \to \infty$ and (6.4) as $y \to 0$. The problem (8.1)–(8.5) is an eigenvalue problem for $s(\tau)$.

Following arguments similar to the proof of theorem (4.4), we can readily establish that the solution to (8.1)–(8.5) has

$$0 \leqslant u(y, \tau) \leqslant \tilde{u}_c, \quad u_y(y, \tau) \leqslant 0, \tag{8.6}$$

with

$$0 \leqslant s(\tau) \leqslant \tilde{u}_c A(t_c)\, \mathrm{e}^\tau, \tag{8.7}$$

via (3.11). In examining (8.1)–(8.5) further, we shall restrict attention to the generic case (detailed in §6), for which

$$0 < -u_c''(0) < R_c. \tag{8.8}$$

We begin by constructing the small time asymptotic solution to (8.1)–(8.5), which has been partly established in §6. We now adopt a more formal approach.

Small time solution, $\tau \to 0$

With $u(y, \tau)$ being the solution to (8.1)–(8.5) then boundary condition (8.3) with (8.1) gives $\lim_{\tau\to 0} \lim_{y \to 0} u_{yy}(y, \tau) = -R_c$, while initial condition (8.2) with (8.8) gives $\lim_{y\to 0} \lim_{\tau\to 0} u_{yy}(y, \tau) = u_c''(0) > -R_c$. Thus $u(y, \tau)$ is not C^2 in a neighbourhood of $y = \tau = 0$ and we do not expect a regular expansion as $\tau \to 0$. This lack of smoothness indicates the present of an inner region where $y = o(1)$ and $u = \tilde{u}_c + o(1)$ as $\tau \to 0$. We denote this as region I and write

$$\left.\begin{aligned} y &= \bar{\eta}\psi(\tau), \\ u &= \tilde{u}_c + \chi(\tau)\, u_1(\bar{\eta}) + o(\chi(\tau)), \\ \dot{s}(\tau) &= \tfrac{1}{2}\ell\phi(\tau) + o(\phi(\tau)), \end{aligned}\right\} \tag{8.9}$$

with $\bar{\eta}, \ell, u = O(1), \psi(\tau), \chi(\tau) = o(1)$ as $\tau \to 0$, and the order of $\phi(\tau)$ to be determined. In region I, initial condition (8.2) becomes $u \sim \tilde{u}_c + \frac{1}{2} u_c''(0)\, \bar{\eta}^2 \psi^2(\tau) + \ldots$ for $\bar{\eta} \gg 1$ as $\tau \to 0$, which, on comparison with (8.9), requires $\chi(\tau) = O(\psi^2(\tau))$; so without loss of generality we put

$$\chi(\tau) = \psi^2(\tau). \tag{8.10}$$

In addition, after rewriting equation (8.1) in region I variables, via (8.9), a leading order balance requires $\psi\psi' = O(1)$ and $\phi = O(\psi')$ as $\tau \to 0$. This leads to

$$\psi(\tau) = \tau^{\frac{1}{2}}, \quad \phi(\tau) = \tau^{-\frac{1}{2}}, \quad \chi(\tau) = \tau \tag{8.11}$$

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as $\tau \to 0$. The problem at leading order in region I then becomes

$$\left.\begin{aligned} &u_1'' + \tfrac{1}{2}(l+\bar{\eta})\,u_1' - u_1 = -R_c, \quad \bar{\eta} > 0,\\ &u_1(0) = u_1'(0) = 0,\\ &u_1(\bar{\eta}) \sim \tfrac{1}{2}u_c''(0)\,\bar{\eta}^2 \quad \text{as} \quad \bar{\eta} \to \infty, \end{aligned}\right\} \tag{8.12}$$

where condition (8.4) has been dropped, and will be replaced by returning to the expansion for u when $y = O(1)$ as $\tau \to 0$. As expected, (8.12) is an eigenvalue problem for ℓ, and is equivalent to the eigenvalue problem (6.9) under a shift of origin in $\bar{\eta}$. Thus (8.12) has a unique solution, given by

$$u_1(\bar{\eta}) = F_2(\bar{\eta} + \ell), \quad \ell = s_1, \tag{8.13}$$

where $F_2(\cdot)$ and s_1 are given by (6.10–6.14), with a_2 replaced by $-\frac{1}{2}u_c''(0)$. Thus, (8.9)–(8.12) give the leading order development of u and $\dot{s}$ as $\tau \to 0$ with $y = O(\tau^{\frac{1}{2}})$.

We next introduce region II in which $y = O(1)$ and $u = O(1)$ as $\tau \to 0$. We write

$$u = u_c(y) + \nu(\tau)\,\bar{u}_1(y) + o(\nu(\tau)) \quad \text{as} \quad \tau \to 0, \tag{8.14}$$

with $\nu(\tau) = o(1)$ as $\tau \to 0$. On substitution from (8.14) into (8.1), a leading order balance requires $\nu(\tau) = \tau^{\frac{1}{2}}$, after which we obtain

$$\bar{u}_1(y) = l u_c'(y). \tag{8.15}$$

It is readily confirmed that expansion (8.14) with (8.15), as $y \to 0$, matches with expansion (8.9) as $\bar{\eta} \to \infty$. Finally we examine the expansion in region II for $y \gg 1$. After use of (4.16) we have

$$u \sim \frac{c\,\mathrm{e}^{-y^2/4t_c}}{y^{m+1}}\{1 - \tfrac{1}{2}\tau^{\frac{1}{2}}y + \dots\}, \tag{8.16}$$

as $\tau \to 0$ for $y \gg 1$. Clearly this expansion develops a non-uniformity for $y \gg 1$, in particular when $y = O(\tau^{-\frac{1}{2}})$ as $\tau \to 0$. We therefore introduce region III, in which $\hat{\eta} = \tau^{\frac{1}{2}}y = O(1)$ as $\tau \to 0$, and expand

$$u = \tau^{(m+1)/2}\,\mathrm{e}^{-\hat{\eta}^2/4t_c\tau}\{\hat{F}_0(\hat{\eta}) + \tau\hat{F}_1(\hat{\eta}) + \dots\} \tag{8.17}$$

as $\tau \to 0$, as suggested by (8.16). On substituting from (8.17) into (8.1) we obtain the leading order problem as

$$\hat{F}'_0 + (m + 1/\hat{\eta} - t_c^{-1})\hat{F}_0 = 0, \quad \hat{\eta} > 0, \tag{8.18}$$

$$\hat{F}_0 = o(e^{\hat{\eta}^2}) \quad \text{as} \quad \hat{\eta} \to \infty, \tag{8.19}$$

$$\hat{F}_0 \sim c\eta^{-(m+1)} \quad \text{as} \quad \hat{\eta} \to 0, \tag{8.20}$$

where (8.19) follows from (8.4) while (8.20) follows from (8.2) and matching to (8.16). The solution of (8.18)–(8.20) is readily obtained as

$$\hat{F}_0(\hat{\eta}) = c\hat{\eta}^{-(m+1)}\,\mathrm{e}^{\hat{\eta}/t_c}, \tag{8.21}$$

and so the expansion in region III becomes

$$u = \frac{c\tau^{(m+1)/2}}{\hat{\eta}^{(m+1)}}\exp\left\{-\frac{\hat{\eta}^2}{4t_c\,\tau} + \frac{\hat{\eta}}{t_c}\right\}\{1 + O(\tau)\}, \tag{8.22}$$

as $\tau \to 0$. An examination of higher order terms shows that (8.22) remains uniform as $\hat{\eta} \to \infty$, and no further regions are required.

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The asymptotic structure is now complete. In particular, we observe from (8.9), (8.13), (8.14), (8.15), (8.22) that $u_\tau(y,\tau)$ becomes unbounded as $\tau \to 0, y > 0$.

Asymptotic solution as $y \to \infty$

We next consider the asymptotic structure of the solution to (8.1)–(8.5) as $y \to \infty$ with $\tau = O(1)$. The form of expansion (8.22) for $\hat{\eta} \gg 1$ leads us to write

$$u = \exp(H(y,\tau)), \tag{8.23}$$

where

$$H(y,\tau) = h_0(\tau)\, y^2 + h_1(\tau)\, y + h_2(\tau) \log y + h_3(\tau) + o(1) \quad \text{as} \quad y \to \infty, \tag{8.24}$$

with $\tau = O(1)$. On substituting into (8.1) and solving at each order in turn, subject to matching with expansion (8.17) (for $\hat{\eta} \gg 1$) as $\tau \to 0$, we obtain

$$\left.\begin{aligned} h_0(\tau) &= -\frac{1}{4(\tau+t_c)}, \quad h_1(\tau) = \frac{1-\frac{1}{2}s(\tau)}{(\tau+t_c)}, \quad h_2(\tau) = -(m+1), \\ h_3(\tau) &= (m+\tfrac{1}{2}) \log\left(\frac{\tau}{t_c}+1\right) + \tau + \int_0^\tau \frac{\dot{s}(\lambda)(1-\frac{1}{2}s(\lambda))\, d\lambda}{(\lambda+t_c)} + \log C. \end{aligned}\right\} \tag{8.25}$$

From (8.25) we observe that

$$h_0(\tau) \sim O(\tau^{-1}), \quad h_1(\tau) \sim O(s(\tau)\,\tau^{-1}), \ldots, \quad \text{as} \quad \tau \to \infty, \tag{8.26}$$

since we expect $s(\tau) \to \infty$ as $\tau \to \infty$. Therefore, expansion (8.23)–(8.24) remains uniform for $\tau \gg 1$ *provided* $y \gg s(\tau)$. We now consider the long time development of the solution to (8.1)–(8.5).

Asymptotic solution as $\tau \to \infty$

For $y \gg s(\tau)$, the long time development of $u(y,\tau)$ is given by (8.23) and (8.24). However, a further region is required when $y = O(s(\tau))$ as $\tau \to \infty$. In this region we introduce the scaled variable $\hat{y} = y/s(\tau) = O(1)$ as $\tau \to \infty$. The form of expansion (8.23–8.24) then leads us to write

$$u(\hat{y},\tau) = \exp\{[s^2(\tau)/\tau]\, W(\hat{y},\tau)\}, \tag{8.27}$$

where

$$W(\hat{y},\tau) = W_0(\hat{y}) + o(1) \quad \text{as} \quad \tau \to \infty \tag{8.28}$$

with $\hat{y} = O(1)$. On substituting from (8.27), (8.28) into equation (8.1), a balancing of terms leads to the order relation

$$s\dot{s}/\tau = O(s^2/\tau^2) \quad \text{as} \quad \tau \to \infty,$$

which determines that

$$s(\tau) \sim v_0 \tau + o(\tau) \quad \text{as} \quad \tau \to \infty, \tag{8.29}$$

for some constant $v_0 > 0$ to be determined. The leading order problem for $W_0(\hat{y})$ is then

$$(W_0')^2 + (1+\hat{y})\, W_0' + (1/v_0^2 - W_0) = 0, \quad \hat{y} > 0, \tag{8.30}$$

$$W_0(\hat{y}) \sim -\tfrac{1}{4}\hat{y}^2 \quad \text{as} \quad \hat{y} \to \infty, \tag{8.31}$$

which matches (8.27), (8.28) to (8.23), (8.24). The solution to (8.30), (8.31) is readily obtained as

$$W_0(\hat{y}) = -\tfrac{1}{4}(\hat{y}+1)^2 + 1/v_0^2, \tag{8.32}$$

after which we have

$$u \sim \exp\{-v_0^2 \tau[\tfrac{1}{4}(\hat{y}+1)^2 - 1/v_0^2 + o(1)]\} \tag{8.33}$$

as $\tau \to \infty$ with $\hat{y} = O(1)$. The expansion (8.33) does not remain uniform as $\hat{y} \to 0$; it does not satisfy the boundary condition (8.3) at $y = 0$. We therefore require a further region in which $y = O(1)$ as $\tau \to \infty$ and we expand

$$u = u_0(y) + o(1) \quad \text{as} \quad \tau \to \infty, \quad y = O(1). (8.34)$$

At leading order we obtain

$$\left.\begin{aligned} &u_0'' + v_0 u_0' + R(u_0) = 0, \quad y > 0, \\ &u_0(0) = \tilde{u}_c, \quad u_0'(0) = 0, \\ &u_0(y) \to 0 \quad \text{as} \quad y \to \infty. \end{aligned}\right\} \tag{8.35}$$

This boundary value problem has been discussed in §7 ((7.2)–(7.8) with change of notation $u_0 \leftrightarrow u, y \leftrightarrow z, v_0 \leftrightarrow v$). In §7 it was established that (8.35) has a unique solution, denoted by $u_+(y; v_0)$ if and only if $v_0 \geqslant 2$. Thus we have

$$u \sim u_+(y; v_0) + o(1) \quad \text{as} \quad \tau \to \infty, \quad y = O(1). \tag{8.36}$$

It remains to match expansion (8.36) (as $y \to \infty$), with expansion (8.33) (as $\hat{y} \to 0$). We match the expansion of $l \equiv \log u$, which are

$$L(\hat{y}; \tau) = -v_0^2 \tau [\tfrac{1}{4}(\hat{y}+1)^2 - 1/v_0^2] + o(\tau); \quad \tau \to \infty, \quad \hat{y} = O(1), \tag{8.37}$$

$$L(y; \tau) = \log u_+(y; v_0) + o(1); \quad \tau \to \infty, \quad y = O(1). \tag{8.38}$$

To match expansion (8.37) (to $O(\tau)$) with expansion (8.38) (to $O(1)$) requires

$$\tfrac{1}{4}v_0^2 - 1 = 0, \quad \lambda_+(v_0) = -\tfrac{1}{2}v_0. \tag{8.39a, b}$$

Equation (8.39a) gives $v_0 = 2$, after which (8.39b) is satisfied automatically. This completes the long time asymptotic structure of (8.1)–(8.5).

We have seen that in the long time a permanent form travelling wave develops in domain C, and this has the minimum possible propagation speed $v_0 = 2$. This has been determined by the form of the initial data $u_c(y)$ for $y \gg 1$, via matching from the small τ solution to the large y solution, to the large t, y solution, to the large τ, $y = O(1)$ solution.

We now confirm the asymptotic solution of this section by considering numerical solutions of the full initial value problem.

9. Numerical method and results

As in part one of this work, the numerical solution of the reaction–diffusion problem in $x \geqslant s(t)$ can be considered in isolation to the pure reaction problem. Once the position of the interface is known it is simple to find the reaction zone solution via numerical integration of $u_t = R(u)$. We use the same method of solving the reaction–diffusion problem as in part I, and accordingly, only a brief description of this is now given. If the position of the interface is fixed by using the transformation $\xi = x - s(t)$ we need to solve the moving boundary problem in the domain of $0 \leqslant \xi \leqslant \infty$, $0 \leqslant t < \infty$,

$$\left.\begin{aligned} &u_t = u_{\xi\xi} + \dot{s} u_\xi + R(u), \\ &u(\xi, 0) = g(\xi), \quad u(0,t) = u_c \quad \text{and} \quad u_\xi(0,t) = 0, \\ \text{with} \quad &u \to 0 \quad \text{as} \quad \xi \to +\infty \quad \text{and} \quad s(0) = 0. \end{aligned}\right\} \tag{9.1}$$

Our analysis of the initial development of the interface indicates that $\dot{s} = 0(t^{-\frac{1}{2}})$ as

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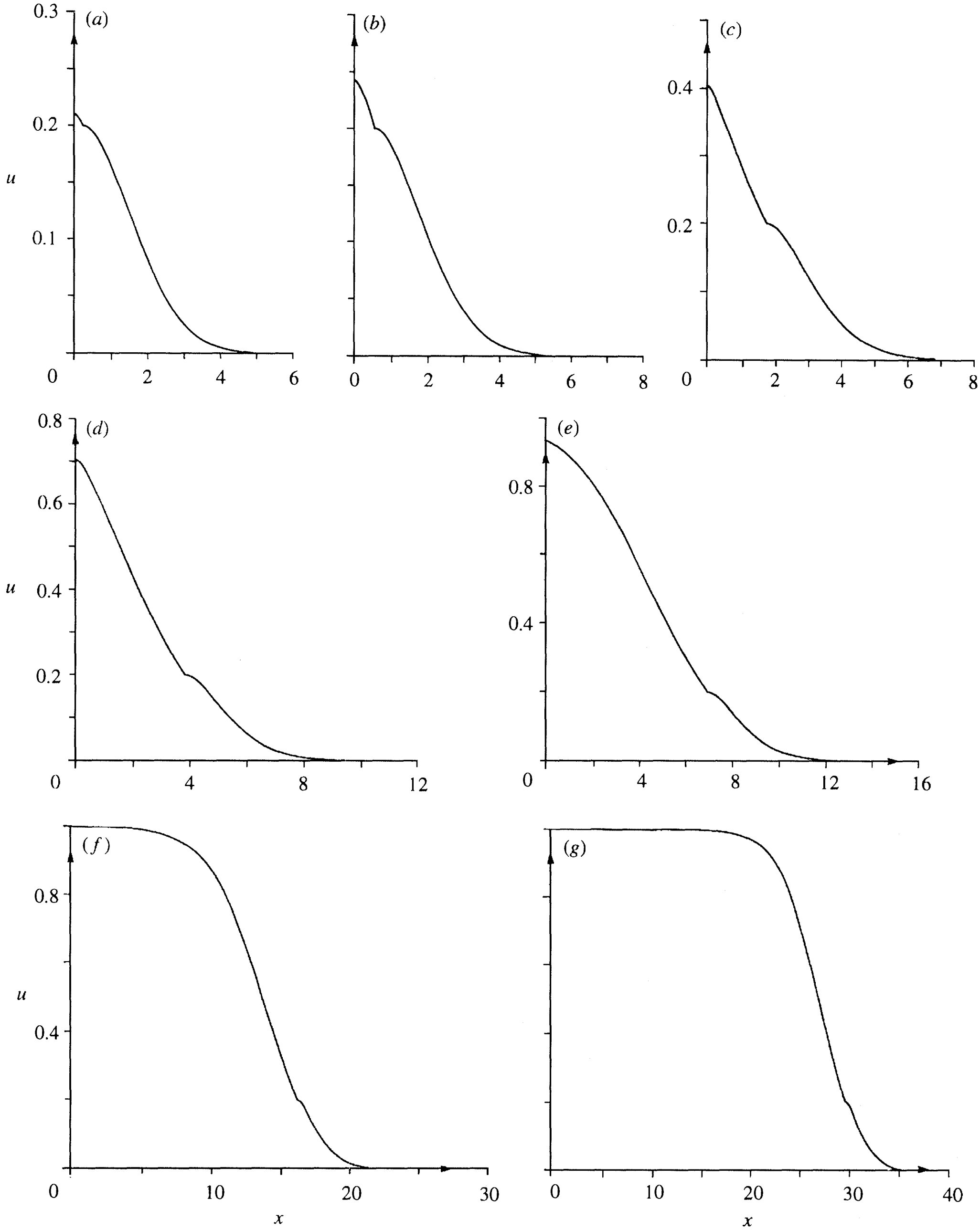

Figure 2. The solution of the initial-boundary value problem with $R(u) = u(1-u)$, $\tilde{u}_c = 0.2$, $t_c = 0.85$, at the following values of $t - t_c$: (*a*) 0.0625; (*b*) 0.25; (*c*) 1.0; (*d*) 2.25; (*e*) 4.0; (*f*) 9.0; (*g*) 16.0.

$t \to 0^+$. On introducing the time-like variable $\tau = t^{\frac{1}{2}}$ we force the initial velocity to be $O(1)$ and arrive at the modified system

$$\left.\begin{aligned} &u_\tau = 2\tau u_{\xi\xi} + s_\tau u_\xi + 2\tau R(u), \\ &u(\xi, 0) = g(\xi), \quad u(0, \tau) = u_c \quad \text{and} \quad u_\xi(0, \tau) = 0, \end{aligned}\right\} \tag{9.2}$$

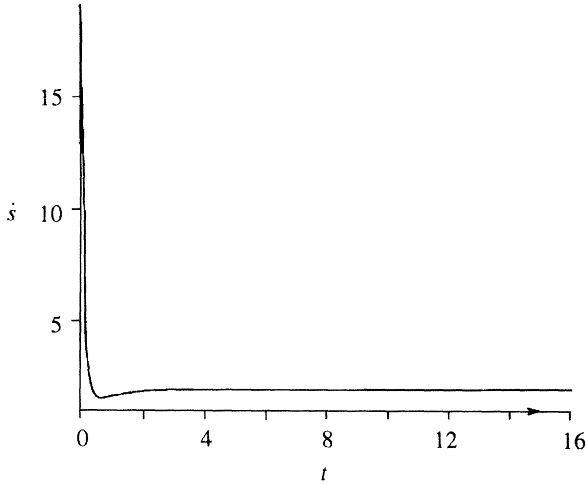

Figure 3. A plot of $\dot{s}(t)$ versus $(t-t_c)$ for the initial-boundary value problem, with details as in figure 2.

with $u \to 0$ as $\xi \to \infty$ and $s(0) = 0$ in the domain $0 \leqslant \xi \leqslant \infty, 0 \leqslant \tau < \infty$. By using finite difference approximations to the derivatives at the points $\xi_i, 1 \leqslant i \leqslant N$ and $t_{j+\frac{1}{2}}, j \geqslant 0$ we discretize equations (9.2) as a system of $N+1$ nonlinear algebraic equations in the $N+1$ unknowns $u_1^{j+1}, \ldots, u_N^{j+1}$ and s^{j+1}. These equations are solved iteratively at each time step by using a Newton method which, in general, was able to converge to a solution in three iterations with use of only one initial jacobian evaluation and produce a solution with an L_2 error norm of $O(10^{-8})$. In the solutions presented below our spatial step was taken to be 0.1, the time step was 0.05 and the extent of the mesh was $0 \leqslant \xi \leqslant 10$. With this choice of parameters the solutions are mesh independent, to within graphical accuracy, and the minimum speed travelling wave is captured, in terms of its known speed of 2, to within less than 3% error. This error arises principally from the truncation of an infinite domain and can be improved, as discussed in part I, by the use of a larger computational domain.

Numerical results, for Fisher reaction kinetics in the form $R(u) = u(1-u)$ and initial data in the form of a top hat of horizontal extent one unit and vertical extent 0.16 units when the diffusivity cuts off at 0.2 units, are shown in figures 2 and 3. Critical conditions are reached at the origin when $t_c = 0.850$. Figures 2(*a*–*c*) shows the initial development of the reaction and reaction–diffusion zones around the moving interface. Figure 2(*d*–*g*) shows the approach to the long time travelling wave structure predicted in earlier sections of this paper with the reaction zone pushing out a constant speed interface at large times. The speed of the interface is shown in this case in figure 3 and is seen to possess a (typical) minimum which separates the initial singular interface speed from the more gradual approach to a constant speed travelling wave.

10. Discussion

In part I and the present paper we have considered a scalar reaction–diffusion process, with autocatalytic kinetics and nonlinear variable diffusivity, as a simple model for a polymerization process. Here we have considered the case where, at low concentration, the diffusivity of the polymer solution is non-zero and approximately

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Table 1

((*a*) $u(x,t_c) \sim \tilde{u}_c - a_2 x^2 + \ldots; 0 < a_2 < \frac{1}{2}R_c$. (*b*) $u(x,t_c) \sim \tilde{u}_c - a_2 x^2 + \ldots; a_2 \geqslant \frac{1}{2}R_c(I), a_2 = \frac{1}{2}R_c\ (II)$. N defined in (6.2, 3). (*c*) $u(x,t_c) \sim \tilde{u}_c - a_{2p} x^{2p} + \ldots; a_{2p} > 0, p = 2, 3, 4 \ldots$.)

	part I		part II	
	$\dot{s}(t)$	$J(t)$	$\dot{s}(t)$	$J(t)$
(*a*)	$O([t-t_c]^{-\frac{1}{2}})$	$O([t-t_c]^{\frac{3}{2}})$	$O([t-t_c]^{-\frac{1}{2}})$	$O([t-t_c]^{\frac{1}{2}})$
(*b*)	$O([t-t_c]^{-\frac{1}{2}})$	$O([t-t_c]^{\frac{3}{2}})$	$O([t-t_c]^{N-\frac{1}{2}})$	$O([t-t_c]^{\frac{1}{2}-N})$
(*c*)	$O([t-t_c]^{1/2p-1})$	$O([t-t_c]^{3-3/2p})$	$O([t-t_c]^{1/2p-1})$	$O([t-t_c]^{1-1/2p})$

constant, on $[0, \tilde{u}_c]$, but suffers a rapid reduction at the critical concentration $\tilde{u}_c$, and is thereafter, $(\tilde{u}_c, \infty)$, zero, with the polymer being immobile. The fully reacted state is reached at $u = 1$, when the polymer is fully immobile. We have again considered the situation that arises when a localized quantity of polymer is used to initiate the reaction. This leads to an initial-boundary value problem for $u(x,t)$ in $x, t > 0$, and we examine piecewise-classical solutions to this problem. The initial data for $u(x,t)$ is continuous, monotone, with compact support. We have found that

(i) $u(x,t)$ is classical for $0 < t \leqslant t_c$, and monotone decreasing in u. The support of $u(x,t)$ becomes unbounded at $t = 0^+$.

(ii) an interface develops from $x = 0$ at $t = t_c^+$ and propagates into $x > 0$ in $t > t_c$. This interface at $x = s(t)$ separates $u > u_c$ (in $0 \leqslant x \leqslant s(t)$) from $0 < u < u_c$ (in $x > s(t)$) and represents a 'freezing' front for the polymer, i.e. the polymer is immobile for $0 \leqslant x \leqslant s(t)$ while it is in solution for $x > s(t)$.

(iii) as $t \to \infty$, the system approaches a permanent form travelling wave structure, selecting the travelling wave of minimum propagation speed. In line with this $\dot{s}(t) \to 2$ as $t \to \infty$ and a quasi-steady polymerization interface is established.

(iv) numerical evidence suggests that $\dot{s}(t)$ has a single minimum in (t_c, ∞).

All of the above qualitative features were also present in part I, when the diffusivity was reduced to zero at $u = \tilde{u}_c$ in a continuous rather than abrupt manner. However, a number of significant quantitative differences appear, which are associated with the interface between 'frozen' and mobile polymer. In both cases, the interface develops from $x = 0$ at $t = t_c^+$ and propagates into $x > 0$ in $t > t_c$. The quantitative differences that occur as $t \to t_c^+$ are summarized in table 1. From this table we observe that in all cases the gradient jump in $u(x,t)$ is an order of magnitude stronger for discontinuous diffusivity than for continuous diffusivity, as $t \to t_c^+$. For continuous diffusivity $J(t) \to 0$ as $t \to t_c^+$ in all cases. However, for discontinuous diffusivity $J(t)$ is unbounded as $t \to t_c^+$ in (*b*). Similarly, for continuous diffusivity $\dot{s}(t)$ is unbounded as $t \to t_c^+$ in all cases, while $\dot{s}(t) \to 0$ as $t \to t_c^+$ in (*b*) where the diffusivity is discontinuous. It may be expected that these order of magnitude differences should be observable experimentally.

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