PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A
MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

The Evolution of Travelling Waves in Reaction-Diffusion Equations with Monotone Decreasing Diffusivity. I. Continuous Diffusivity

D. J. Needham and A. C. King

Phil. Trans. R. Soc. Lond. A 1995 **350**, 335-360
doi: 10.1098/rsta.1995.0019

The evolution of travelling waves in reaction–diffusion equations with monotone decreasing diffusivity. I. Continuous diffusivity

By D. J. Needham[1] and A. C. King[2]†
[1] Department of Mathematics, University of Reading, White Knights, Reading RG6 2AX
[2] Department of Mathematics, University of Keele, Keele, Staffordshire ST5 5NU, U.K.

We examine the effects of a concentration dependent diffusivity on a reaction–diffusion process which has applications in chemical kinetics. The diffusivity is taken as a continuous monotone, a decreasing function of concentration that has compact support, of the form that arises in polymerization processes. We consider piecewise-classical solutions to an initial-boundary value problem. The existence of a family of permanent form travelling wave solutions is established, and the development of the solution of the initial-boundary value problem to the travelling wave of minimum propagation speed is considered. It is shown that an interface will always form in finite time, with its initial propagation speed being unbounded. The interface represents the surface of the expanding polymer matrix.

1. Introduction

There is a variety of chemical, biological and physical processes that can be modelled as simple closed systems in which the competing effects of reaction and diffusion predominate. One feature of the interplay between reaction and diffusion, which is often visible in laboratory experiments, is the formation of travelling chemical wave fronts. Well known examples of this are the spread of an advantageous gene through a population (Fisher 1937) and autocatalytic chemical systems such as the iodate–arsenous acid reaction (Hanna *et al.* 1982). Surveys of reaction–diffusion models in chemistry and biology can be found in Winfree (1980), Jones & Sleeman (1983), Murray (1989) and Gray & Scott (1990). In these works attention is generally focused upon systems in which the diffusivity between the reacting elements is constant. Some mention of the effects of variable diffusivity can be found in Murray, but discussion is limited to power law type behaviour in which the diffusivity vanishes as the concentration vanishes. A recent study of the evolution of initial data onto a travelling wave for this case can be found in King & Needham (1992).

In this paper we study the reaction–diffusion process in the case where the diffusivity vanishes at a finite and non-zero concentration. To motivate physically the study of such systems it is worth remarking on some basic facts concerned with the chemical process of polymerization in which the diffusivity may take on this form. A polymer is a large molecule formed by the linking together of a number of smaller molecules called monomers. Our attention here is restricted to radical chain polymerization (Odian 1970), which consists of initiation, propagation and

† Present address: Department of Theoretical Mechanics, University of Nottingham NG7 2RD.

Phil. Trans. R. Soc. Lond. A (1995) **350**, 335–360

Printed in Great Britain

termination stages. Initiation involves the production of a free radical and its reaction with a monomer molecule to produce a chain initiating species. Propagation consists of the addition of a large number of monomer molecules to this species to form a chain. The termination stage is representative of the slowing down of the polymerization process due to physical limitations on the chain length. After the propagation stage the nascent polymer structure may be linear, branched or cross-linked. The increasing molecule size, and its subsequent entanglement with other large molecules, restricts the diffusivity of the polymer and the termination stage can be considered diffusion limited. A general account of the statistical mechanics of polymer solutions is given in Doi & Edwards (1986), which establishes a theoretical basis (from microscopic considerations) for the observation of diffusivity reduction with increasing concentration in polymer solutions. Particular studies of the diffusion rate in the polymerization of methyl methacrylate by Regen (1975, 1976) show a rapid decrease in diffusivity with increasing polymer concentration. At 10% polymer concentration, the diffusivity, in appropriate units, is $O(10^2)$; at 80% concentration this value drops to $O(10^{-3})$. For both macroscopic theoretical studies and practical purposes we can regard this diffusivity as vanishing at a finite concentration. The behaviour of the diffusivity at values between these low and high concentrations can be complex and depends on the particular polymerization under consideration.

The aim of this paper is to study a reaction–diffusion equation with a general diffusivity and reaction function. The diffusivity function has the property of decreasing with increasing concentration and attaining zero at some critical concentration. This zero is approached continuously rather than abruptly. The reaction function is also chosen to be as general as reasonably possible. It is assumed that the reaction rate varies with concentration only and has two zeros. These represent the vanishing of any chemical reaction at zero concentration and at a finite saturation level. In §2 we provide a natural foundation for the study of such equations by considering integral conservation laws associated with the reaction–diffusion process, with some uniqueness and boundedness results also being established. Section 3 demonstrates the existence of a class of piecewise-classical permanent form travelling wave solutions in systems of this type. The evolution of the various types of initial data in the small time (t) limit is considered in §4, while the asymptotic structure of the solution for large distance (x) is considered in §5. A non-uniformity in this asymptotic expansion, when t is large, is revealed. This non-uniformity, which is associated with the selection of a minimum speed travelling wave, is resolved in §8. A detailed discussion of the behaviour of the solution and the genesis of a moving boundary as the critical concentration is approached is given in §6. A numerical method for solving the moving boundary problem is described in some detail in §7. Numerical results which confirm the mathematical analysis are also presented.

2. Conservation laws and differential equations

As a simple 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 a concentration of the autocatalytic chemical species (polymer). Under reaction u reproduces itself at a rate $R_0 R(u/u_r)$ and diffuses (in an unstirred environment) at a rate equal to the gradient of the flux function

$F_0\hat{F}(u/u_c)$. Here $R(\cdot)$ and $\hat{F}(\cdot)$ are dimensionless functions, with $\hat{F}\in C^\infty[0,1]$, $R\in C^\infty[0,\infty)]$, and R_0, F_0, u_r, u_c are appropriately dimensional constants. We restrict attention to the case when $\hat{D}(u)\equiv\{F_0\hat{F}(u/u_c)\}_u$ has

$$\hat{D}(0)>0 \tag{2.1}$$

and is monotone decreasing in $0<u<u_c$, with

$$\hat{D}(u_c)=0 \tag{2.2}$$

and

$$\hat{D}(u)\equiv 0,\quad u>u_c. \tag{2.3}$$

Moreover, we choose F_0 so that $\hat{D}_u(u_c^-)=-F_0u_c^{-2}$, which fixes

$$\hat{F}''(1^-)=-1. \tag{2.4}$$

The reaction function $R_0R(u/u_r)$ is taken to have two zeros in $u\geqslant 0$ at $u=0$ (the unreacted state) and $u=u_r$ (the fully reacted state) with $R(u/u_r)>0$ for $0<u<u_r$. The equilibrium states $u=0, u_r$ are non-degenerate, so that $R'(0)>0$ and $R'(1)<0$. In particular, we set R_0 so that

$$R'(0)=1. \tag{2.5}$$

In dimensional form, the integral conservation law governing the one-dimensional reaction and diffusion of u is

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{x_1}^{x_2}u\,\mathrm{d}x=[F_0\hat{F}(u/u_c)_x]_{x_1}^{x_2}+\int_{x_1}^{x_2}R_0R(u/u_r)\,\mathrm{d}x, \tag{2.6}$$

for any $x_2>x_1\geqslant 0$, $t>0$. Here $x\geqslant 0$ is the spatial coordinate and $t\geqslant 0$ is time. We next introduce dimensionless quantities

$$u=u_r u',\quad x=(F_0/R_0)^{\frac{1}{2}}\tilde{u}_c^{-1}x',\quad t=(u_r/R_0)t'. \tag{2.7}$$

After substitution from (2.7) into (2.6) and dropping primes for convenience, we arrive at the dimensionless conservation law

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{x_1}^{x_2}u\,\mathrm{d}x=[F_x(u)]_{x_1}^{x_2}+\int_{x_1}^{x_2}R(u)\,\mathrm{d}x, \tag{2.8}$$

where now

$$F(X)\equiv\tilde{u}_c^2\hat{F}(X/\tilde{u}_c), \tag{2.9}$$

with $\tilde{u}_c$ being the dimensionless parameter

$$\tilde{u}_c=u_c/u_r. \tag{2.10}$$

It is convenient to introduce

$$D(u)\equiv F'(u),\quad u\geqslant 0, \tag{2.11}$$

after which we have the following conditions on $D(u)$:

$$\left.\begin{array}{ll}\text{(i)} & D(u)\text{ is continuous in }u\geqslant 0,\\ \text{(ii)} & D(0)=\tilde{u}_c\hat{F}'(0)>0,\quad D(\tilde{u}_c)=0,\quad D'(\tilde{u}_c^-)=-1,\\ \text{(iii)} & D(u)\equiv 0\text{ in }u>\tilde{u}_c,\\ \text{(iv)} & D(u)\text{ is }C^\infty\text{ and monotone in }0\leqslant u\leqslant\tilde{u}_c;\\ & D'(u)<0\text{ for }0<u<\tilde{u}_c,\end{array}\right\} \tag{2.12}$$

via (2.1)–(2.9). In dimensionless form the conditions on $R(u)$ become

$$\left.\begin{array}{ll}\text{(i)} & R(u)\text{ is }C^\infty\text{ in }u\geqslant 0,\\ \text{(ii)} & R(0)=R(1)=0,\quad R'(0)=1,\\ \text{(iii)} & R(u)\leqslant u,\quad u\in[0,1].\end{array}\right\} \tag{2.13}$$

The condition (iii) limits the curvature of $R(u)$ in $[0,1]$ and arises through a technical requirement that will be discussed at a later stage. In terms of polymer reactions, we also make the restriction

$$0 < \tilde{u}_c < 1, \tag{2.14}$$

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

In the remainder of the paper we examine the initial-boundary value problem which arises when a localized quantity of u is introduced initially into the otherwise unreacting state $u \equiv 0$. Under these circumstances equation (2.8) must be solved in $x, t > 0$ subject to the following initial and boundary conditions,

$$u(x,0) = \begin{cases} u_0 g(x), & 0 \leqslant x \leqslant \sigma, \\ 0, & x > 0, \end{cases} \tag{2.15}$$

$$u_x(0,t) = 0, \quad t > 0, \tag{2.16}$$

$$u(x,t) \to 0 \quad \text{as} \quad x \to \infty, \quad t > 0. \tag{2.17}$$

The function $g(x)$ is positive, monotone decreasing, and analytic in $0 \leqslant x \leqslant \sigma$, with $\max_{0 \leqslant x \leqslant \sigma}\{g(x)\} = 1$ and

$$g(x) \sim g_m (x-\sigma)^m \quad \text{as} \quad x \to \sigma^-, \tag{2.18}$$

for some non-zero constant g_m and $m \in \mathbb{N}$. The dimensionless parameter σ defines the support of the initial data $g(x)$, while u_0 is a measure of the maximum input concentration in u, which, for the polymer problem has

$$0 < u_0 < \tilde{u}_c. \tag{2.19}$$

Following King & Needham (1992), we consider solutions $u(x,t)$ to the initial-boundary value problem (2.8), (2.15–2.17) 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 throughout D_T *except* along piecewise differentiable curves $x = s(t)$, say, upon which $u(s(t),t) = \tilde{u}_c$. However, we require that the limits of u_t, u_x, u_{xx} 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 (2.8), (2.15–2.17) on D_T. Clearly, all operations in (2.8) are well defined for $u \in C_p[D_T]$.

(a) *Piecewise-classical solutions*

Let $u(x,t)$ be a piecewise-classical solution of (2.8), (2.15–2.17) 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 $D_\pm$ (note that D_+, D_-, C are disjoint, and $D_+ \cup D_- \cup C = D_T$). It is then clear that $u(x,t)$ satisfies the partial differential equations

$$u_t = D(u)\, u_{XX} + D'(u)\, u_X^2 + R(u), \quad (x,t) \in D_-, \tag{2.20a}$$

$$u_t = R(u), \quad (x,t) \in D_+, \tag{2.20b}$$

while across C (2.8) requires

$$u|_{C^+} = u|_{C^-} = \tilde{u}_c, \tag{2.21}$$

where $u|_{C^\pm}$ denotes the limit of u on approaching C from $D_\pm$ respectively. With the curve C described by $x = s(t)$, conditions (2.21) and equation (2.20a, b) lead to

$$[\dot{s} u_x + R(\tilde{u}_c)]_{C^+} = [\dot{s} u_x - u_x^2 + R(\tilde{u}_c)]_{C^-} = 0, \tag{2.22}$$

which express the regularity conditions, on $u(x,t)$ as C is approached from $D_{\pm}$ respectively.

(b) *Reformulation of the initial-boundary value problem*

For simplicity we restrict attention to the case when $g(x)$ is monotone decreasing in $0 \leqslant x \leqslant \sigma$. To examine the initial-boundary value problem (2.8), (2.15)–(2.17), we first consider the modified initial-boundary value problem

$$\omega_t = [D_\epsilon(\omega)\,\omega_x]_x + R(\omega), \quad (x,t)\in D_T, \tag{2.23a}$$

$$\omega(x,0) = \omega_0(x) = \begin{cases} u_0\, g(x), & 0 \leqslant x \leqslant \sigma, \\ 0, & x > \sigma, \end{cases} \tag{2.23b}$$

$$\omega_x(0,t) = 0, \quad t > 0, \tag{2.23c}$$

$$\omega(x,0) \to 0 \quad \text{as} \quad x\to\infty, \quad t>0, \tag{2.23d}$$

where

$$D_\epsilon(\omega) = \begin{cases} D(\omega), & 0 \leqslant \omega \leqslant \tilde{u}_c - \epsilon, \\ \chi(\omega), & \omega > \tilde{u}_c - \epsilon, \end{cases} \tag{2.24}$$

with

$$\chi(\omega) = D_c + \{a(\omega-\tilde{u}_c+\epsilon) + b(\omega-\tilde{u}_c+\epsilon)^2 + c(\omega-\tilde{u}_c+\epsilon)^3\}\{1+\lambda(\omega-\tilde{u}_c+\epsilon)^4\}^{-1} \tag{2.25}$$

and
$$D_c = D(\tilde{u}_c-\epsilon), \quad a = D'(\tilde{u}_c-\epsilon), \quad 2b = D''(\tilde{u}_c-\epsilon), \quad 6c = D'''(\tilde{u}_c-\epsilon). \tag{2.26}$$

Here, $\epsilon, \lambda > 0$ are real parameters with $0 < \epsilon < \epsilon_c$ where $\epsilon_c < \tilde{u}_c - u_0$. A solution to (2.23) will be a solution in the classical sense.

We first observe that, with λ taken sufficiently large, the modified diffusivity $D_\epsilon(\omega)$ satisfies the following conditions for each $0 < \epsilon < \epsilon_c$,

$$\left.\begin{aligned} &D_\epsilon(\omega)\in C^3[\mathbb{R}^+], \\ &D_\epsilon(\omega) > 0 \quad \text{for} \quad \omega \geqslant 0, \\ &D_\epsilon(\omega) \to D_c(>0) \quad \text{as} \quad \omega\to\infty. \end{aligned}\right\} \tag{2.27a–c}$$

Also, with a suitable extension of the definitions of $D_\epsilon(\omega)$ and $R(\omega)$ into $\omega < 0$, we can readily establish (following King & Needham 1992) that a solution of (2.23) (henceforth referred to as $I_\epsilon[D_T]$) has

$$\omega(x,t) \geqslant 0 \quad \text{for all} \quad (x,t)\in D_T. \tag{2.28}$$

Finally we note that

$$R'(\omega) \text{ is bounded above, } \omega\in[0,\infty), \tag{2.29a}$$

$$D_\epsilon(\omega) \text{ is bounded above and below (above zero), } \omega\in[0,\infty), \tag{2.29b}$$

$$R(\omega)\in C^\infty[\mathbb{R}^+]. \tag{2.29c}$$

We also require some notation. With $V(x,t)$ being a suitably smooth function on D_T, we define (following Oleinik & Kruzhkov 1961)

$$\left.\begin{aligned} &|V|_0 = \sup_{D_T}|V|, \quad |V|_\alpha = |V|_0 + \sup_{P_1,P_2\in D_T} \frac{|V(P_1)-V(P_2)|}{d(P_1,P_2)^\alpha}, \\ &|V|_{1+\alpha} = |V|_\alpha + |V_x|_\alpha, \quad |V|_{2+\alpha} = |V|_{1+\alpha} + |V_x|_{1+\alpha} + |V_t|_\alpha \end{aligned}\right\} \tag{2.30}$$

with $0<\alpha<1$ and $d(P_1,P_2) = [(x_1-x_2)^2+(t_1-t_2)^2]^{\frac{1}{2}}$ where $(x_1,t_1), (x_2,t_2)$ are the coordinates of P_1, P_2 respectively. Corresponding to (2.30) we write $V(x,t)\in C_q[D_T]$

($q = 0, \alpha, 1+\alpha, 2+\alpha$), if $|V|_q$ is finite. We note that $V(x,t) \in C_{2+\alpha}[D_T]$ implies that V, V_X, V_t, V_{XX} are well defined, bounded and continuous, together with satisfying a uniform Hölder condition of degree α throughout D_T.

We can now state the following.

Theorem 2.31. *When $\omega_0(x) \in C_{2+\nu}[D_T]$, there exists a unique classical solution $\omega_\epsilon(x,t)$ to $I_\epsilon[D_T]$, for any $T > 0$ and $0 < \epsilon < \epsilon_c$. Moreover, $\omega_\epsilon(x,t) \in C_{2+\nu}[D_T]$.*

Proof. First note that $\omega_0(x) \in C_{2+\nu}[D_T]$ implies that ω_0', ω_0'' exist, are bounded and continuous, and satisfy a uniform Hölder condition of degree, ν, on $\mathbb{R}^+$. The proof then follows from Oleinik & Kruzhkov (1961, theorem 14, p. 132). We are required to check that $D_\epsilon(\omega) \in C^{2+\nu}[\mathbb{R}^+]$, $D_\epsilon(\omega)$ is bounded above and below (above zero) on $\mathbb{R}^+$, and that $R'(\omega)$ is bounded above on $\mathbb{R}^+$ (note that we need only consider $\omega \in \mathbb{R}^+$ because of (2.28)). All of these conditions are satisfied via (2.27)–(2.29). ■

In addition, we have that

$$|\omega_\epsilon|_{2+\nu} \leqslant M, \quad \text{on} \quad D_T, \tag{2.32}$$

where M depends only on $\omega_0(x)$, which follows from Oleinik & Kruzhkov (1961, theorem 12, p. 130).

Now, since $u_0 < \tilde{u}_c - \epsilon$ for $0 < \epsilon < \epsilon_c$, then $\omega_0 < \tilde{u}_c - \epsilon$ for all $x \geqslant 0$, and so there exists a unique, maximal $t_\epsilon > 0$, such that

$$\omega_\epsilon(x,t) < \tilde{u}_c - \epsilon \quad \text{on} \quad D_{t_\epsilon}/\{(x, t_\epsilon) : x > 0\} \tag{2.33}$$

where we set $t_\epsilon = \infty$ if $\omega_\epsilon(x,t) < \tilde{u}_c - \epsilon$ for all $t \geqslant 0$, $x > 0$. We also recall that

$$D_\epsilon(X), R(X) \in C^\infty[0, \tilde{u}_c - \epsilon] \tag{2.34}$$

for any $0 < \epsilon < \epsilon_c$, which enables us to establish the following lemma.

Lemma 2.35. *With $\omega_\epsilon(x,t)$ being the solution of $I_\epsilon[D_{t_\epsilon}]$ for any $0 < \epsilon < \epsilon_c$, then $\omega_\epsilon(x,t) \in C^\infty[D_{t_\epsilon}]$ (under the conditions of theorem* (2.31)).

Proof. We denote by $H_{p+\alpha}[D_{t_\epsilon}]$, $p \in \mathbb{N}$, $0 < \alpha < 1$, the set of functions $V : D_{t_\epsilon} \to \mathbb{R}$ which are p times continuously differentiable in x, with each derivative satisfying a Hölder condition of degree α. We first show that $\omega_\epsilon(x,t) \in H_{2p+\nu}[D_{t_\epsilon}]$ for any $p \in \mathbb{N}$ and with ν as defined in theorem (2.31).

(i) From theorem (2.31) we know that

$$\omega_\epsilon(x,t) \in H_{2+\nu}[D_{t_\epsilon}], \tag{2.36}$$

as $C_{2+\nu}[D_{t_\epsilon}] \subset H_{2+\nu}[D_{t_\epsilon}]$. Now suppose that, as an induction hypothesis,

$$\omega_\epsilon(x,t) \in H_{2m+\nu}[D_{t_\epsilon}], \tag{2.37}$$

for some $m \in \mathbb{N}$. Then since $0 < \omega_\epsilon \leqslant \tilde{u}_c - \epsilon$ (via (2.33)) on D_{t_ϵ} we have via (2.34) and (2.37)

$$D_\epsilon(\omega_\epsilon(x,t)), \quad R(\omega_\epsilon(x,t)) \in H_{2m+\nu}[D_{t_\epsilon}]. \tag{2.38}$$

An application of Oleinik & Kruzhkov (1961, theorem 9, p. 121) with (2.38) then establishes that

$$\omega_\epsilon(x,t)) \in H_{2(m+1)+\nu}[D_{t_\epsilon}].$$

Therefore, with (2.36), we have via induction that

$$\omega_\epsilon(x,t) \in H_{2n+\nu}[D_{t_\epsilon}], \tag{2.39}$$

for any $n \in \mathbb{N}$, as required.

(ii) As $\omega_\epsilon(x,t)$ is a solution to $I_\epsilon[D_{t_\epsilon}]$, then for ω_ϵ we have the operator relation

$$\frac{\partial}{\partial t} \equiv D_\epsilon(\cdot)\frac{\partial^2}{\partial x^2} + D'_\epsilon(\cdot)\left[\frac{\partial}{\partial x}\right]^2 + R(\cdot). \tag{2.40}$$

On D_{t_ϵ}, $\omega_\epsilon(x,t)$ satisfies (2.33), (2.39), with $D_\epsilon(\cdot)$ and $R(\cdot)$ satisfying (2.34). Therefore, from (2.40), all t and mixed x,t derivatives of $\omega_\epsilon(x,t)$ exist and are continuous in D_{t_ϵ}, which with (2.39) establishes that

$$\omega_\epsilon(x,t) \in C^\infty[D_{t_\epsilon}],$$

as required. ∎

We now have the following theorem.

Theorem 2.41. *With $\omega_\epsilon(x,t)$ being the solution of $I_\epsilon[D_{t_\epsilon}]$ (for any $0<\epsilon<\epsilon_c$), then $\omega_{\epsilon_x}(x,t) \leqslant 0$ throughout D_{t_ϵ}. In addition, with $\omega_0(x) \in C^2[0,\infty]$ and such that $[D(\omega_0)\,\omega_{0_x}]_x + R(\omega_0) \geqslant 0$, then $\omega_{\epsilon_t}(x,t) \geqslant 0$ throughout D_{t_ϵ}.*

Proof. Recall first that $\omega_0(x)$ is monotone decreasing for $x \geqslant 0$. Now via lemma (2.35) $\omega_{\epsilon_x} \in C^\infty[D_{t_\epsilon}]$ and hence from equation (2.23*a*) we have

$$\phi_t = [D_\epsilon(\omega_\epsilon)\,\phi]_{xx} + R'(\omega_\epsilon)\,\phi, \quad (x,t)\in D_{t_\epsilon}, \tag{2.42}$$

with
$$\phi(x,0) = \phi_0(x)\,(=w'_0(x)) \leqslant 0, \quad x \geqslant 0, \tag{2.43}$$

$$\phi(0,t) = 0, \quad 0<t\leqslant t_\epsilon, \tag{2.44}$$

$$\phi(x,t) \to 0 \quad \text{as} \quad x\to\infty, \quad 0<t\leqslant t_\epsilon, \tag{2.45}$$

where
$$\phi(x,t) \equiv \omega_{\epsilon_x}(x,t), \quad (x,t)\in D_{t_\epsilon}, \tag{2.46}$$

and we recall that $\phi(x,t)$, $\omega_\epsilon(x,t) \in C^\infty[D_{t_\epsilon}]$, with $0 \leqslant \omega_\epsilon \leqslant \tilde{u}_c - \epsilon$ and $D_\epsilon(X)$, $R(X) \in C^\infty[0, \tilde{u}_c - \epsilon]$.

We can re-write equation (2.42) as

$$a(x,t)\,\phi_{xx} + b(x,t)\,\phi_x + h(x,t)\,\phi - \phi_t = 0, \quad (x,t)\in D_{t_\epsilon}, \tag{2.47}$$

where

$$\left.\begin{aligned} a(x,t) &= D_\epsilon(\omega_\epsilon), \quad b(x,t) = 2D_\epsilon(\omega_\epsilon)_x, \\ h(x,t) &= R'(\omega_\epsilon) + D_\epsilon(\omega_\epsilon)_{xx}. \end{aligned}\right\} \tag{2.48}$$

We note that $a(x,t)$, $b(x,t)$ and $h(x,t)$ are bounded C^∞ functions in D_{t_ϵ} (via above and theorem (2.31)) and $a(x,t)$ is bounded above zero ($a(x,t) \geqslant D_\epsilon(\tilde{u}_c - \epsilon) > 0$) in D_{t_ϵ}.

We next introduce $\psi = \phi\,\mathrm{e}^{-\lambda t}(\lambda \in \mathbb{R})$, and rewrite (2.47) in terms of ψ as,

$$a(x,t)\,\psi_{xx} + b(x,t)\,\psi_x + (h(x,t) - \lambda)\,\psi - \psi_t = 0, \quad (x,t)\in D_{t_\epsilon}, \tag{2.49}$$

with conditions (2.43)–(2.45) becoming

$$\left.\begin{aligned} &\psi(0,t) = 0, \quad 0<t\leqslant t_\epsilon, \\ &\psi(x,t) \to 0 \quad \text{as} \quad x\to\infty, \quad 0<t\leqslant t_\epsilon, \\ &\psi(x,0) = \phi_0(x) \leqslant 0, \quad x \geqslant 0. \end{aligned}\right\} \tag{2.50}$$

With $h(x,t)$ bounded on D_{t_ϵ}, we can choose λ sufficiently large so that $(h(x,t)-\lambda) \leqslant 0$ on D_{t_ϵ}. We now suppose that there exists a point $(x_0,t_0)\in D_{t_\epsilon}$ such that $\psi(x_0,t_0) > 0$. Conditions (2.50) then imply that $\psi(x,t)$ achieves its maximum $M>0$ on $\bar{D}_{t_\epsilon}$ *within* D_{t_ϵ}. That is, there exists a point $(x_1,t_1)\in D_{t_\epsilon}$, such that $\psi(x_1,t_1) = M$. An application of the maximum principle of Protter & Weinberger (1967, ch. 3, §2, theorem 4) then establishes that $\psi(x,t) \equiv M > 0$ for all $(x,t) \leqslant \bar{D}_{t_\epsilon}$. In particular this leads to $\phi_0(x) \equiv M > 0$, which contradicts (2.50). We conclude that $\psi(x,t) \leqslant 0$ throughout $\bar{D}_{t_\epsilon}$, and hence that $\phi(x,t) \leqslant 0$ throughout $\bar{D}_{t_\epsilon}$, as required.

The proof of the second part follows similarly, on noting that the condition $[D(\omega_0)\,\omega_0']' + R(\omega_0) \geqslant 0$ ensures that $\omega_{\epsilon_t}(x,t) \geqslant 0$ as $t \to 0^+$ for all $x > 0$. ■

We can further establish the following.

Lemma 2.52. *For each* $0 < \epsilon < \epsilon_c$, t_ϵ *is finite, under the conditions of theorem* (2.41).

Proof. For a given $0 < \epsilon < \epsilon_c$, suppose that t_ϵ is unbounded. Then by definition of t_ϵ we have

$$0 \leqslant \omega_\epsilon(x,t) \leqslant \tilde{u}_c - \epsilon \quad \text{on} \quad D_T, \tag{2.53}$$

for any $T > 0$. Thus (via theorem (2.41)), for each $x \geqslant 0$, $\omega_\epsilon(x,t)$ is monotone increasing in t and bounded above, and so

$$\omega_\epsilon(x,t) \to u_\infty(x) \quad \text{as} \quad t \to \infty, \quad x \geqslant 0, \tag{2.54a}$$

with

$$0 \leqslant u_\infty(x) \leqslant \tilde{u}_c - \epsilon, \quad x \geqslant 0, \tag{2.54b}$$

and $u_\infty(x)$ satisfying

$$(D(u_\infty)\,u_\infty')' + R(u_\infty) = 0, \quad x > 0. \tag{2.54c}$$

However, it is readily established that (2.54*b*, *c*) has no solution and we conclude that t_ϵ must be finite, as required. ■

By construction of $D_\epsilon(\cdot)$ it is also clear that for $0 < \epsilon_2 < \epsilon_1 < \epsilon_c$

$$t_{\epsilon_2} > t_{\epsilon_1} \tag{2.55}$$

and via theorem (2.31) that

$$\omega_{\epsilon_2}(x,t) \equiv \omega_{\epsilon_1}(x,t) \tag{2.56}$$

on $D_{t_{\epsilon_1}}$. We can now state the following.

Theorem 2.57. *For each* $0 < \epsilon < \epsilon_c$ *the initial-boundary value problem* (2.8), (2.15–2.17) *has a unique solution on* D_{t_ϵ} *in* $C_p[D_{t_\epsilon}]$. *This solution is given by* $u = \omega_\epsilon(x,t)$.

Proof. By construction $\omega_\epsilon(x,t)$ is a solution to (2.8), (2.15)–(2.17) in $C_p[D_{t_\epsilon}]$ on D_{t_ϵ}. We now consider uniqueness. Let $u(x,t) \in C_p[D_{t_\epsilon}]$ be a solution to (2.8), (2.15)–(2.17) on D_{t_ϵ}.

(i) Suppose that $u(x,t) \leqslant \tilde{u}_c - \epsilon$ on D_{t_ϵ}. Then $u(x,t)$ satisfies $I_\epsilon[D_{t_\epsilon}]$. However, the solution to $I_\epsilon[D_{t_\epsilon}]$ is unique (theorem (2.31)) and so $u(x,t) \equiv \omega_\epsilon(x,t)$ on D_{t_ϵ}.

(ii) Suppose that $u(x,t) \nleqslant \tilde{u}_c - \epsilon$ on D_{t_ϵ}. Then, as $\epsilon_c < \tilde{u}_c - u_0$, $\exists t^*(< t_\epsilon)$, $x^*(> 0)$ such that

$$u(x^*, t^*) = \tilde{u}_c - \epsilon, \tag{2.58}$$

while

$$u(x,t) \leqslant \tilde{u}_c - \epsilon,$$

on D_{t^*}. Thus, following (i), we conclude that $u(x,t) \equiv \omega_\epsilon(x,t)$ on D_{t^*}, which gives, via (2.58), $\omega_\epsilon(x^*, t^*) = \tilde{u}_c - \epsilon$, contradicting the definition of t_ϵ. Thus $u(x,t) \leqslant \tilde{u}_c - \epsilon$ on D_{t_ϵ}, and uniqueness again follows via (i). ■

Finally we show that t_ϵ remains bounded as $\epsilon \to 0$. Now, via (2.55), t_ϵ is increasing as $\epsilon \to 0$ and we suppose that $t_\epsilon \to \infty$ as $\epsilon \to 0$. We next consider $\omega_\epsilon(x, t_\epsilon)$. Via theorem (2.41) and (2.56), we deduce that $\omega_\epsilon(x, t_\epsilon)$ is monotone increasing as $t_\epsilon \to \infty$ for fixed

$x \geqslant 0$, with $0 \leqslant \omega_\epsilon(x, t_\epsilon) \leqslant \tilde{u}_c$, by definition of t_ϵ. Therefore, as $\epsilon \to 0$, $\omega_\epsilon(x, t_\epsilon)$ is monotone increasing and bounded above, for each $x \geqslant 0$, and so

$$\omega_\epsilon(x, t_\epsilon) \to \omega_\infty(x) \quad \text{as} \quad \epsilon \to 0,$$

where, by construction,

$$(D(\omega_\infty)\,\omega_\infty')' + R(\omega_\infty) = 0, \quad x \geqslant 0,$$
$$0 \leqslant \omega_\infty(x) \leqslant \tilde{u}_c.$$

However, it is readily established that this problem has no solution, and we conclude that t_ϵ is bounded as $\epsilon \to 0$, which (since t_ϵ is increasing as $\epsilon \to 0$) ensures that $t_c = \lim_{\epsilon\to 0} t_\epsilon$ exists and we define

$$\omega_c(x,t) = \omega_\epsilon(x,t); \quad x \geqslant 0, \quad 0 \leqslant t \leqslant t_\epsilon < t_c. \tag{2.59}$$

We then have the following theorem.

Theorem 2.60. *With the condition of theorem* (2.41) *satisfied, the initial-boundary value problem* (2.8), (2.15)–(2.17) *has a unique solution on* $x \geqslant 0$, $0 \leqslant t < t_c$ *given by* $u = \omega_c(x,t)$. *Moreover,*

(i) $0 \leqslant \omega_c(x,t) < \tilde{u}_c$,
(ii) $\omega_c(x,t) \in C^\infty$,
(iii) $\omega_{c_x}(x,t) \leqslant 0$,
(iv) $\lim_{t\to t_c} \omega_c(0,t) = \tilde{u}_c$,
(v) $\omega_{c_t}(x,t) \geqslant 0$ on $x > 0$, $0 < t < t_c$.

Proof. This follows from theorem (2.41), (2.54), theorem (2.57) and construction of $\omega_c(x,t)$. ■

The results of this subsection direct us to look for a solution to the initial-boundary value problem (2.8), (2.15)–(2.17) in three distinct domains.

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

$$u_t = D(u)\,u_{xx} + D'(u)\,u_x^2 + R(u), \quad 0 \leqslant u < \tilde{u}_c, \tag{2.60a}$$

$$u(x,0) = \begin{cases} u_0\,g(x), & 0 \leqslant x \leqslant \sigma, \\ 0, & x > \sigma, \end{cases} \tag{2.60b}$$

$$u_x(0,t) = 0, \quad t > 0, \tag{2.60c}$$

$$u(x,t) \to 0 \quad \text{as} \quad x \to \infty, \quad t \geqslant 0. \tag{2.60d}$$

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

$$u_t = R(u), \quad u > \tilde{u}_c, \tag{2.61a}$$

$$u(x,t) \to \tilde{u}_c \quad \text{as} \quad x \to s^-(t). \tag{2.61b}$$

Domain III, $s(t) \leqslant x < \infty$, $t \geqslant t_c$

$$u_t = D(u)\,u_{xx} + D'(u)\,u_x^2 + R(u), \quad 0 \leqslant u \leqslant \tilde{u}_c, \tag{2.62a}$$

$$u(x,t) \to \begin{cases} \tilde{u}_c, & x \to s^+(t), \\ 0, & x \to \infty. \end{cases} \tag{2.62b}$$

We also require,

$$s(t_c) = 0, \quad \lim_{t\to t_c^+} u(x,t) = \lim_{t\to t_c^-} u(x,t). \tag{2.63}$$

Here the interface C is given by $x = s(t)$ with D_+ being domain II and D_- being domain III. The problem in domain I has a unique solution, $u = \omega_c(x,t)$, via theorem (2.60). Also, since $u(x,t) > u_c$ in domain II, condition (2.22) requires that

$$\dot{s}(t) > 0, \quad t \geqslant t_c, \tag{2.64}$$

as u_x must remain bounded as $x \to s(t)^-$ ($u \in C_p[D_T]$). To obtain an upper bound on $s(t)$ we consider the problem in domain III. We define the quantity

$$A(t) = \int_{s(t)}^{\infty} u(x,t)\,\mathrm{d}t, \quad t \geqslant t_c,$$

and apply the operation $\int_{s(t)}^{\infty} \ldots \mathrm{d}x$ to expression (2.62 a), which leads to

$$A_t = -\dot{s}\tilde{u}_c + \int_{s(t)}^{\infty} R(u)\,\mathrm{d}x, \quad t \geqslant t_c. \tag{2.65}$$

After use of condition (2.13) (iii), we obtain

$$A_t - A \leqslant -\dot{s}\tilde{u}_c, \quad t \geqslant t_c. \tag{2.66}$$

An integration of the differential inequality (2.66) gives

$$A(t) \leqslant A(t_c)\,\mathrm{e}^{t-t_c} - \tilde{u}_c\left\{s(t) + \mathrm{e}^t \int_{t_c}^{t} s(\tau)\,\mathrm{e}^{-\tau}\,\mathrm{d}\tau\right\}$$

in $t \geqslant t_c$, after use of (2.63). However, $A(t)$, $s(t) \geqslant 0$ in $t \geqslant t_c$, which leads to

$$s(t) \leqslant \tilde{u}_c^{-1} A(t_c)\,\mathrm{e}^{t-t_c}, \quad t \geqslant t_c. \tag{2.67}$$

Thus $s(t)$ is monotone increasing in $t \geqslant t_c$ and remains bounded for all finite t.

We next consider the development of $u(x,t)$ in domain II. It is convenient to define the inverse function of $s(t)$, which we denote by $\bar{s}(x)$, $x \geqslant 0$ (so that $t = \bar{s}(s(t))\ \forall\, t \geqslant t_c$, with $\bar{s}(\cdot)$ being well defined via (2.64) and (2.67)). We have

$$\bar{s}'(x) = 1/\dot{s}(\bar{s}(x)) > 0, \quad \forall\, x > 0, \tag{2.68}$$

$$\bar{s}(0) = t_c. \tag{2.69}$$

The solution to (2.61 a, b) can now be written implicitly as

$$H(u) = t - \bar{s}(x), \quad x \geqslant 0, \quad t > \bar{s}(x), \tag{2.70}$$

where

$$H(y) = \int_{\lambda=\tilde{u}_c}^{\lambda=y} \frac{\mathrm{d}\lambda}{R(\lambda)}. \tag{2.71}$$

From (2.70), (2.71) we readily observe that $\tilde{u}_c \leqslant u < 1$ at each $x \geqslant 0$ for all $t > \bar{s}(x)$, with,

$$u(x,t) \sim 1 - (1-\tilde{u}_c)\,\mathrm{e}^{R'(1)[t-\bar{s}(x)-c]} \tag{2.72}$$

as $t \to \infty$, where

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

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 (2.68) and (2.70). Thus 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 reacted in large time, with x fixed. However, when $x = s(t)$, $u = \tilde{u}_c$ for all t, while $u \to 0$ for $x \gg s(t)$ for all t. This indicates the formation of a travelling wave structure as $t \to \infty$.

Before studying the problems in domains (I)–(III) further, we first examine the possible class of piecewise-classical permanent form travelling wave solutions of the integral conservation law (2.8), which could develop from the initial-boundary value problem in the long time.

3. Permanent form travelling waves

We expect that the long time development of the initial-boundary value problem (IBVP) 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. Therefore, before developing IBVP further, we examine the possible class of piecewise-classical permanent form travelling waves that can be sustained by the integral conservation law (2.8).

We make the following definition:

Definition 3.1. A permanent form travelling wave solution (PTW) of the integral conservation law (2.8) is a non-negative solution that depends on the single variable $z \equiv x - \gamma(t)$ (where $\gamma(t)$ is the position of the wave-front), 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 $-\infty < z < \infty$.

It is readily deduced that a PTW has $0 \leqslant u(z) \leqslant 1$ and is monotone decreasing in z. Thus, $u(z)$ is a solution of the boundary value problem

$$D(u)\,u_{zz} + D'(u)\,u_z^2 + vu_z + R(u) = 0, \quad z > 0, \tag{3.2}$$

$$vu_z + R(u) = 0, \quad z < 0, \tag{3.3}$$

with conditions

$$0 \leqslant u < \tilde{u}_c, \quad z > 0; \quad \tilde{u}_c < u \leqslant 1, \quad z < 0, \tag{3.4a}$$

$$u \to 0 \quad \text{as} \quad z \to \infty, \tag{3.4b}$$

$$u \to 1 \quad \text{as} \quad z \to -\infty, \tag{3.5}$$

$$u(0^+) = u(0^-) = \tilde{u}_c. \tag{3.6}$$

In the above $v = \dot{\gamma}(t)$. However, since u is a function of z alone, equations (3.2), (3.3) determine that the wave-front propagation speed v must be constant. Moreover, the symmetry of (3.2)–(3.6) implies that we need only consider $v > 0$. The problem (3.2)–(3.6) can be thought of as a nonlinear eigenvalue problem, with the positive propagation speed v being the eigenvalue. We study (3.2)–(3.6) in the phase plane.

(a) *The phase plane*

We consider equation (3.2) for $z > 0$ in the (u, w) phase plane, where $w = u_z$. In terms of u, w equation (3.2) can be written as the equivalent system

$$u_z = w, \quad w_z = \{-D'(u)\,w^2 - vw - R(u)\}/D(u). \tag{3.7}$$

The trajectories of system (3.7) in the (u, w) phase plane satisfy the first order ordinary differential equation

$$\frac{\mathrm{d}w}{\mathrm{d}u} = -\frac{D'(u)\,w^2 - vw - R(u)}{wD(u)}, \tag{3.8}$$

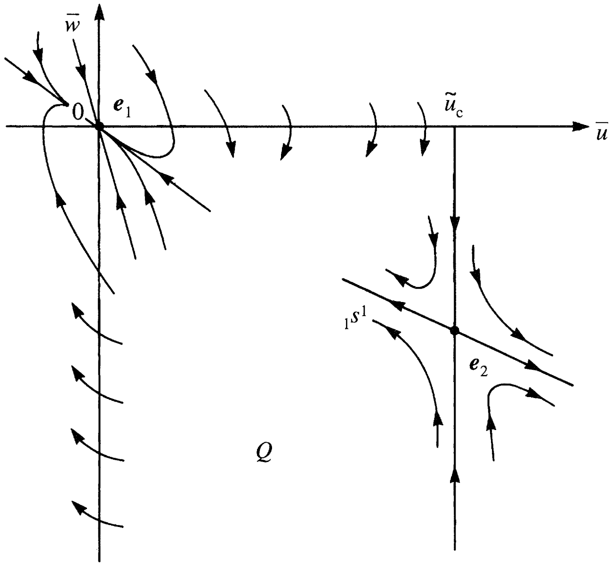

Figure 1. Local behaviour in the $(\bar{u}, \bar{w})$ phase plane, with $v_0 \geqslant \sqrt{D_0}$.

from which it is clear that the singular system (3.7) has the same phase portrait as the regular system

$$\bar{u}_z = \bar{w}D(\bar{u}), \quad \bar{w}_z = -D'(\bar{u})\,\bar{w}^2 - v\bar{w} - R(\bar{u}). \tag{3.9a, b}$$

We are thus able to characterize the phase portrait of the singular system (3.7) via that of the regular system (3.9). The phase portrait of (3.9a, b) need only be investigated in the domain $\bar{w} \leqslant 0$, $0 \leqslant \bar{u} \leqslant \tilde{u}_c$, which we denote by Q. The system (3.9) has two equilibrium points in Q at $\boldsymbol{e}_1 = (0, 0)$ and $\boldsymbol{e}_2 = (\tilde{u}_c, \Omega)$, where

$$\Omega = \tfrac{1}{2}\{v - (v^2 + 4R_c)^{\frac{1}{2}}\}, \tag{3.10}$$

with $R_c = R(\tilde{u}_c)$. We also observe that the line $\bar{u} \equiv \tilde{u}_c$ is an integral path of the system in Q. Thus a solution to equation (3.2) in $z > 0$ that satisfies conditions (3.4) and (3.6) requires a directed integral path of the system (3.9a, b) connecting the equilibrium point $\boldsymbol{e}_1$ to the equilibrium point $\boldsymbol{e}_2$ and lying entirely in Q.

We begin by examining the equilibrium point $\boldsymbol{e}_2$. Linearization of equations (3.9) at $\boldsymbol{e}_2$ shows that it is a simple saddle point for all $v > 0$, with eigenvalues given by

$$\lambda_1 = \tfrac{1}{2}\{-v + (v^2 + 4R_c)^{\frac{1}{2}}\}, \quad \lambda_2 = -(v^2 + 4R_c)^{\frac{1}{2}}.$$

The stable manifold at $\boldsymbol{e}_2$ coincides with the line $\bar{u} \equiv \tilde{u}_c$, while the unstable manifold cuts the line $\bar{u} \equiv \tilde{u}_c$. Thus, there is just one possible integral path that will satisfy condition (3.6) and remain in Q, this being the part of the unstable manifold at $\boldsymbol{e}_2$ that points into Q. We label this as S, and the local behaviour in the neighbourhood of $\boldsymbol{e}_2$ is shown in figure 1.

Linearization of equation (3.9) about the equilibrium point $\boldsymbol{e}_1$ shows that it is a stable spiral for $0 < v < 2\sqrt{D_0}$, while it is a stable node for $v \geqslant 2\sqrt{D_0}$, with

$$D_0 = D(0) = \tilde{u}_c \hat{F}'(0). \tag{3.11}$$

The eigenvalues are given by

$$\mu_1 = \tfrac{1}{2}\{-v + (v^2 - 4D_0)^{\frac{1}{2}}\}, \quad \mu_2 = \tfrac{1}{2}\{-v - (v^2 - 4D_0)^{\frac{1}{2}}\}$$

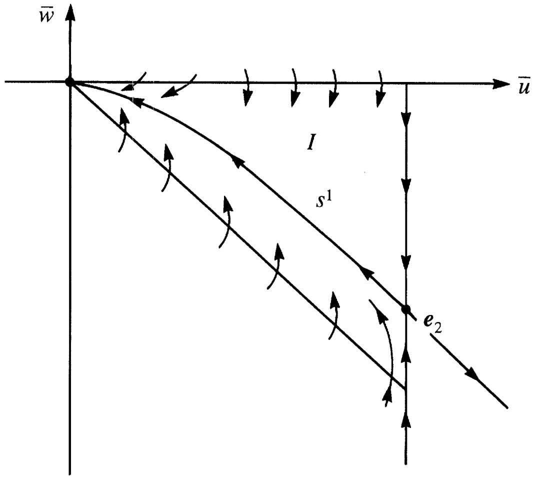

Figure 2. The integral path S in the $(\bar{u}, \bar{w})$ phase plane, with $v_0 \geqslant \sqrt{D_0}$.

with the two straight line paths having slopes

$$c_{\pm} = (2D_0)^{-1}[-v \pm (v^2 - 4D_0)^{\frac{1}{2}}], \tag{3.12}$$

when $v \geqslant 2\sqrt{D_0}$. Note that both $c_{\pm} < 0$. Therefore, a necessary condition for a solution to (3.2), (3.4*a*), (3.4*b*) and (3.6) is that

$$v \geqslant 2\sqrt{D_0}. \tag{3.13}$$

The condition (3.13) will also be sufficient if we can show that the integral path S, which leaves $\boldsymbol{e}_2$ as the unstable manifold in Q, remains in Q and connects to the node at $\boldsymbol{e}_1$. The local behaviour in the neighbourhood of $\boldsymbol{e}_1$ (for $v \geqslant 2\sqrt{D_0}$) is illustrated in figure 1.

To proceed we require the following lemma.

Lemma 3.14. *For each* $v \geqslant 2\sqrt{D_0}$ *the region*

$$I = \{(\bar{u}, \bar{w}) \in \mathbb{R}^2 : 0 \leqslant \bar{u} \leqslant \tilde{u}_c, \quad -\alpha(v)\,\bar{u} \leqslant \bar{w} \leqslant 0\}$$

is a positively invariant region for the system (3.9), *with*

$$\alpha(v) = (2D_0)^{-1}[v + (v^2 - 4D_0)^{\frac{1}{2}}].$$

Proof. We define the vector field $H(\bar{u}, \bar{w})$ as

$$H(\bar{u}, \bar{w}) = (\bar{w}D(\bar{u}), -D'(\bar{u})\,\bar{w}^2 - v\bar{w} - R(\bar{u}))^{\mathrm{T}}. \tag{3.15}$$

An inspection of H readily shows that any integral path starting within I cannot subsequently leave I via the edges that have $\bar{u} \equiv \tilde{u}_c$ or $\bar{w} \equiv 0$. It remains to consider the third edge of I, $\bar{w} = -\alpha(v)\,\bar{u}$, $0 < \bar{u} < \tilde{u}_c$, which we denote by ζ. We must show that the vector field $\boldsymbol{H}$ is directed strictly into I on ζ. This requires that

$$F(\bar{u}, v) \equiv \boldsymbol{H}|_{\zeta} \cdot (\alpha, 1)^{\mathrm{T}} > 0 \;\forall\; 0 < \bar{u} < \tilde{u}_c, \tag{3.16}$$

where, with use of (3.15),

$$F(\bar{u}, v) = -\alpha^2 \bar{u} D(\bar{u}) - D'(\bar{u})\,\alpha^2 \bar{u}^2 + v\alpha\bar{u} - R(\bar{u}), \quad 0 < \bar{u} < \tilde{u}_c. \tag{3.17}$$

Now via (2.12) (iv)

$$F(\bar{u}, v) > -\alpha^2 \bar{u} D(\bar{u}) + v\alpha\bar{u} - R(\bar{u}), \quad 0 < \bar{u} < \tilde{u}_c.$$

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

Furthermore, using (2.12) (iv) and (2.13) (iii) we have

$$F(\bar{u}, v) > \bar{u}(-D_0\alpha^2 + v\alpha - 1) = 0, \quad 0 < \bar{u} < \tilde{u}_c,$$

on using the expression for $\alpha(v)$, and the result is established. ∎

We now show that the equilibrium point $\boldsymbol{e}_2 \in I$ for all $v \geqslant 2\surd D_0$. For $\boldsymbol{e}_2 \in I$ we require

$$\tilde{u}_c\,\alpha(v) + \Omega > 0, \quad v \geqslant 2\surd D_0. \tag{3.18}$$

First we consider the case with $v = 2\surd D_0$, when

$$\tilde{u}_c\,\alpha(v) + \Omega \equiv D_0^{-\frac{1}{2}}\{(\tilde{u}_c + D_0) - \surd D_0 (R_c + D_0)^{\frac{1}{2}}\}. \tag{3.19}$$

However, via (2.13) (iii), $R_c \leqslant \tilde{u}_c$; so (3.19) leads to

$$\tilde{u}_c\,\alpha(v) + \Omega \geqslant D_0^{-\frac{1}{2}}(\tilde{u}_c + D_0)^{\frac{1}{2}}\{(\tilde{u}_c + D_0)^{\frac{1}{2}} - \surd D_0\} > 0 \tag{3.20}$$

and $\boldsymbol{e}_2 \in I$ for $v = 2\surd D_0$. We now consider the case when $v > 2\surd D_0$, and observe that $\alpha(v)$ is a monotone increasing function of $v \geqslant 2\surd D_0$. Furthermore, it is readily checked that Ω is a monotone increasing function of $v \geqslant 2\surd D_0$. Hence $\tilde{u}_c\,\alpha(v) + \Omega$ is a monotone increasing function of $v \geqslant 2\surd D_0$, and, since (3.18) holds for $v = 2\surd D_0$, then it must hold for $v \geqslant 2\surd D_0$. Therefore,

$$\boldsymbol{e}_2 \in I \;\forall\, v \geqslant 2\surd D_0, \tag{3.21}$$

as required. The integral path S therefore enters I as it leaves $\boldsymbol{e}_2$. However, it cannot leave I, and must connect with the equilibrium point $\boldsymbol{e}_1$ at the origin (via the Poincaré–Bendixson theorem). Moreover, $I \subset Q$ and so S remains within Q. A sketch of the integral path S with $v \geqslant 2\surd D_0$ is shown in figure 2. We have established the following proposition.

Proposition 3.22. *The equation* (3.2), *subject to conditions* (3.4*a*, *b*) *and* (3.6) *has a unique solution* $u_+(z)$ *for each* $v \geqslant 2\surd D_0$. ∎

We note that, for each $v \geqslant 2\surd D_0$, the integral path S lies in $w < 0$ in the (u, w) phase plane, and so $u_+(z)$ is monotone decreasing in $z > 0$. In particular,

$$u_+(z) \sim \begin{cases} A\exp(c_+ z), & v > 2\surd D_0, \\ Bz\exp(-z/\surd D_0), & v = 2\surd D_0, \end{cases} \tag{3.23}$$

as $z \to \infty$, while

$$u_+(z) \sim \tilde{u}_c + \Omega(v)\,z \quad \text{as} \quad z \to 0^+. \tag{3.24}$$

Here A, B are positive constants.

To continue $u_+(z)$ into a PTW, we must now consider equation (3.3) in $z < 0$ subject to the conditions (3.4*a*), (3.5), (3.6). This problem has a unique solution for each $v \geqslant 2\surd D_0$, given by $\boldsymbol{u} = \boldsymbol{u}_-(z)$, which is given implicitly by

$$z = v\int_{u_-(z)}^{\tilde{u}_c} \frac{\mathrm{d}\phi}{R(\phi)}, \quad z < 0. \tag{3.25}$$

An examination of (3.25) shows that $u_-(z)$ is monotone decreasing in $z < 0$, with

$$u_-(z) \sim 1 - c\exp(-R'(1)\,z/v) \quad \text{as} \quad z \to -\infty \tag{3.26}$$

and $c > 0$ constant, while

$$u_-(z) \sim \tilde{u}_c - (R_c/v)\,z \quad \text{as} \quad z \to 0^-. \tag{3.27}$$

Therefore we have established the following theorem.

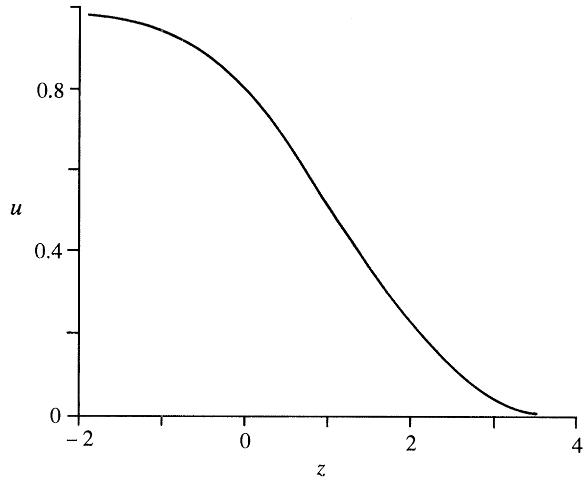

Figure 3. The minimum speed PTW when $D(u) \equiv \frac{3}{2}(\frac{1}{2}-u)(\frac{1}{6}+u)$ and $R(u) \equiv u(1-u)$ with $\tilde{u}_c = 0.5$.

Theorem 3.28. *For each* $v \geqslant 2\surd D_0$ *there exists a unique, piecewise-classical, permanent form travelling wave solution to the integral conservation law* (2.8), *say* $u_T(z)$. *Moreover,* $u_T(z)$ *is classical in* $z>0$ *and* $z<0$ *with*

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

For $0<v<2\surd D_0$, *no such solution exists.* ■

Finally, we consider the jump in derivative of $u_T(z)$ at $z=0$. From (3.27) and (3.24) we find that

$$[u_{T_z}(0^+)-u_{T_z}(0^-)] = \tfrac{1}{2}\{v-(v^2+4R_c)^{\frac{1}{2}}\}+R_c/v>0, \tag{3.29}$$

for all $v \geqslant 2\surd D_0$.

For the case where $D(u) \equiv \frac{3}{2}(\frac{1}{2}-u)(\frac{1}{6}+u)$, $\tilde{u}_c = \frac{1}{2}$, $D_0 = \frac{1}{8}$ and $R(u) \equiv u(1-u)$ the minimum speed PTW has been computed numerically and is shown in figure 3.

4. Small time development, $t \to 0$

The existence of a solution to the initial-boundary value problem in domain I, (2.60*a–d*), has been established in §2, where it was further established that the solution is C^∞ on D_{t_ϵ}. Here we examine the structure of this solution as $t \to 0$. There are two cases to consider depending upon the behaviour (2.18) of $g(x)$ as $x \to \sigma^-$.

(*a*) *Case* (i), $m=0$

In this case $g(x) \to g_0 > 0$ as $x \to \sigma^-$. Since $g(x)$ has compact support, we anticipate that the structure of the solution to (2.60*a–d*) as $t \to 0$ has primarily three asymptotically defined regions in x. We thus proceed to construct the asymptotic solution via the method of matched asymptotic expansions. The three regions are labelled as follows:

$$\left.\begin{array}{lll} \text{region A} & 0 \leqslant x \leqslant \sigma - O(\delta(t)), & u = O(1), \\ \text{region B} & x = \sigma + O(\delta(t)), & u = O(1), \\ \text{region C} & x \geqslant \sigma + O(\delta(t)), & u = o(1), \end{array}\right\} \quad \text{as} \quad t \to 0, \tag{4.1}$$

where $\delta(t) = o(1)$ as $t \to 0$. This structure follows immediately from the initial

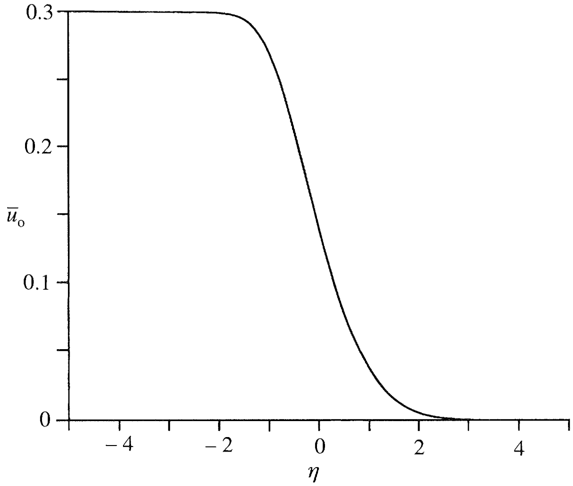

Figure 4. A graph of $\bar{u}_0(\eta)$ versus η in the case where $D(u) \equiv (\tilde{u}_c - u)$ and $\tilde{u}_c = 0.5$.

condition (2.15) when $m = 0$. The function $\delta(t)$ is to be chosen to retain, at leading order in region B, the term $(D(u)\,u_x)_x$ in equation (2.60*a*). It readily follows that $\delta(t) = O(t^{\frac{1}{2}})$ as $t \to 0$, and without loss of generality we put $\delta(t) = t^{\frac{1}{2}}$.

We begin in region A. Since $u(x,0) > 0$ and analytic in A, with $u = O(1)$ as $t \to 0$, we expand $u(x,t)$ as a regular power series in t. After substitution into equation (2.60*a*) and applying initial condition (2.60*b*) we obtain

$$u(x,t) = u_0\,g(x) + t[D(u_0\,g(x))\,u_0\,g''(x) + D'(u_0\,g(x))\,u_0^2(g'(x))^2 + R(u_0\,g(x))] + O(t^2) \quad \text{as} \quad t \to 0, \tag{4.2}$$

with $0 < x \leqslant \sigma - O(t^{\frac{1}{2}})$. Now, with $(\sigma - x) \ll 1$, (4.2) becomes

$$u(x,t) \sim u_0\,g_0 + t\{D(u_0\,g_0)\,u_0\,g''(\sigma) + D'(u_0\,g_0)\,u_0^2(g'(\sigma))^2 + R(u_0\,g_0)\} + \cdots \quad \text{as} \quad t \to 0.$$

This suggests that in region B we have

$$u(\eta,t) \sim \sum_{r=0}^{\infty} t^r \bar{u}_r(\eta) \quad \text{as} \quad t \to 0. \tag{4.3}$$

With $\eta = O(1)$, where $\eta = (x-\sigma)/t^{\frac{1}{2}}$. On substituting from (4.3) into (2.60*a*) (when written in terms of η and t) we obtain, at leading order,

$$D(\bar{u}_0)\,\bar{u}_{0\eta\eta} + D'(\bar{u}_0)\,(\bar{u}_{0\eta})^2 + \tfrac{1}{2}\eta\bar{u}_{0\eta} = 0, \quad -\infty < \eta < \infty, \tag{4.4}$$

to be solved subject to matching with regions A and C as $\eta \to \pm\infty$ respectively. Via (4.1) and (4.2) these matching conditions are

$$\left.\begin{aligned} \bar{u}_0(\eta) &\to u_0\,g_0 \quad \text{as} \quad \eta \to -\infty \\ \bar{u}_0(\eta) &\to 0 \quad\quad\ \ \text{as} \quad \eta \to +\infty \end{aligned}\right\}. \tag{4.5}$$

The solution to the boundary value problem (4.4), (4.5) has not been found for general $D(\cdot)$. However, it has been solved numerically in the case $D(u) = (\tilde{u}_c - u)$, $\tilde{u}_c = 0.5$, $u_0\,g_0 = 0.3$ and a graph of the solution is shown in figure 4.

However, the form of $\bar{u}_0(\eta)$ as $\eta \to \pm\infty$ can be obtained directly from (4.4), (4.5) as

$$\bar{u}_0(\eta) \sim \begin{cases} c_\infty\,\eta^{-1}\exp[-\eta^2/4D_0] & \text{as} \quad \eta \to +\infty \\ u_0\,g_0 + c_{-\infty}\,\eta^{-1}\exp[-\eta^2/4D(u_0\,g_0)] & \text{as} \quad \eta \to -\infty \end{cases} \tag{4.6}$$

for some constants $c_\infty > 0$ and $c_{-\infty} < 0$.

Finally we move to region C, in which (4.4) and (4.6) suggest that we write

$$u(x,t) = \exp[-\psi(x,t)\,t^{-1}], \tag{4.7}$$

with $\psi(x,t) = O(1)$ as $t \to 0$ in C, and $\psi(x,t) > 0$. We expand

$$\psi(x,t) = \psi_0(x) + t[\psi_2(x)\log t + \psi_1(x)] + o(t) \tag{4.8a}$$

as $t \to 0$ in C as suggested by (4.3) and (4.6). After substitution from (4.7), (4.8a) into (2.60a) and solving at each order in turn, together with matching to expansion (4.3) as $x \to \sigma^+$, we obtain

$$\psi(x,t) = (x-\sigma)^2/4D_0 - t[\tfrac{1}{2}\log t + \log c_\infty - \log(x-\sigma)] + o(t) \tag{4.8b}$$

as $t \to 0$ in region C. This gives, via (4.7),

$$u(x,t) = \frac{c_\infty t^{\frac{1}{2}}}{(x-\sigma)} \exp[-(x-\sigma)^2/4D_0 t]\{1+o(1)\} \quad \text{as} \quad t \to 0, \tag{4.9}$$

with $x = \sigma + O(1)$. We note that expansion (4.8) remains uniform as $t \to 0$ for $x \gg 1$, and no further regions are required to complete the asymptotic structure of $u(x,t)$ as $t \to 0$.

(b) *Case* (ii), $m \geqslant 1$

As in case (i) we again require three asymptotic regions A, B, C, with $\delta(t) = t^{\frac{1}{2}}$ as $t \to 0$. The difference in this case is that now $u = o(1)$ as $t \to 0$ in region B, and the leading order problem in this region is then solved exactly. In region A the development of u is as in (a), given by (4.2). In region B we have that

$$u(\eta,t) = t^{m/2}\hat{u}_0(\eta) + o(t^{m/2}) \quad \text{as} \quad t \to 0 \tag{4.10}$$

with $\eta = O(1)$, where

$$\left.\begin{aligned} &\hat{u}_{0_{\lambda\lambda}} + \tfrac{1}{2}\lambda \hat{u}_{0_\lambda} - \tfrac{1}{2}m\hat{u}_0 = 0, \quad -\infty < \lambda < \infty, \\ &\hat{u}_0 \to 0 \quad \text{as} \quad \lambda \to +\infty, \\ &\hat{u}_0 \sim u_0 \hat{g}_m(-\lambda)^m \quad \text{as} \quad \lambda \to -\infty, \end{aligned}\right\} \tag{4.11}$$

with $\lambda = D_0^{-\frac{1}{2}}\eta$ and $\hat{g}_m = (-1)^m g_m D_0^{m/2}$. The solution to (4.11) is readily obtained as

$$\hat{u}(\lambda) = \begin{cases} \dfrac{2^{m-1}(\frac{1}{2}m)!\,u_0\hat{g}_m}{\pi^{\frac{1}{2}}} A_m(\lambda) \displaystyle\int_\lambda^\infty \frac{e^{-s^2/4}}{A_m^2(s)}\,ds, & m \text{ even}, \\[2ex] \dfrac{m!\,u_0\hat{g}_m}{K_m[\frac{1}{2}(m-1)]!} A_m(\lambda) \displaystyle\int_\lambda^\infty \frac{e^{-s^2/4}}{A_m^2(s)}\,ds, & m \text{ odd}, \end{cases} \tag{4.12}$$

where

$$A_m(\lambda) = \begin{cases} \displaystyle\sum_{i=0}^{\frac{1}{2}m} \frac{(\frac{1}{2}m)!\,\lambda^{2i}}{(2i)!\,(\frac{1}{2}m-i)!}, & m \text{ even}, \\[2ex] \displaystyle\sum_{i=0}^{\frac{1}{2}(m-1)} \frac{(\frac{1}{2}[m-1])!\,\lambda^{2i+1}}{(2i+1)!\,[\frac{1}{2}(m-i)-i]!}, & m \text{ odd}, \end{cases}$$

and

$$K_m = \int_{-\infty}^\infty \left(\frac{e^{-s^2/4}}{A_m^2(s)} - \frac{1}{s^2}\right) ds, \quad m \text{ odd}.$$

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

We note from (4.12) that $\hat{u}_0(\eta)$ is positive and monotone decreasing for all $-\infty < \eta < \infty$. From (4.10) and (4.12) we also have, for $\eta \gg 1$,

$$\hat{u}_0(\eta) \sim \hat{c}_\infty \exp[-\eta^2/4D_0]/\eta^{m+1}, \tag{4.13}$$

with
$$\hat{c}_\infty = D_0^{(\frac{1}{2}m+1)} \begin{cases} 2^m m!\, u_0 \hat{g}_m/\pi^{\frac{1}{2}}, & m \text{ even} \\ 2(m!)^2 u_0 \hat{g}_m/(\frac{1}{2}m)!\,[\frac{1}{2}(m-1)]!\,K_m, & m \text{ odd}. \end{cases}$$

The expansion in region C follows (4.7) and (4.8), with now

$$\psi(x,t) = ((x-\sigma)^2/4D_0) - t[(m+\tfrac{1}{2})\log t + \log \hat{c}_\infty - (m+1)\log(x-\sigma)] + o(t) \tag{4.14}$$

as $t \to 0$ with $x = \sigma + O(1)$. This leads to, via (4.7),

$$u(x,t) = \frac{\hat{c}_\infty t^{m+\frac{1}{2}}}{(x-\sigma)^{m+1}} \exp[-(x-\sigma)^2/4D_0 t]\{1+o(1)\} \quad \text{as} \quad t \to 0 \tag{4.15}$$

with $x = \sigma + O(1)$. The expansion (4.14) remains uniform for $x \gg 1$ as $t \to 0$, and the asymptotic structure of $u(x,t)$ as $t \to 0$ is complete.

In both cases (i) and (ii) there are two points to note in the small t development of $u(x,t)$. First, the support of $u(x,t)$ extends to $x = \infty$ immediately and, secondly, reaction is only significant within the original support domain, region A, with diffusion dominating in regions B and C. We next consider the asymptotic behaviour of $u(x,t)$ as $x \to \infty$ with $t = O(1)$.

5. Asymptotic solution as $x \to \infty$

We examine the structure of the solution $u(x,t)$ in domains I and II as $x \to \infty$ with $t = O(1)$. The boundary conditions (2.60d) and (2.62b) imply that $u = o(1)$ as $x \to \infty$, $t = O(1)$. Moreover, the structure of $u(x,t)$ in region I as $t \to 0$ with $x \gg 1$, as given in (4.7), (4.8b), (4.14), indicates that we write

$$u(x,t) = \exp\{-\theta(x,t)\} \quad \text{as} \quad x \to \infty, \tag{5.1}$$

with $t = O(1)$, and

$$\theta(x,t) = \theta_0(t)(x-\sigma)^2 + \theta_1(t)(x-\sigma) + \theta_2(t)\log(x-\sigma) + \theta_3(t) + o(1), \tag{5.2}$$

as $x \to \infty$ with $t = O(1)$. After substitution into equations (2.60), (2.61a) and solving at each order in turn, we obtain

$$\theta_0(t) = (4D_0 t)^{-1}, \quad \theta_1(t) \equiv 0, \quad \theta_2(t) \equiv (m+1), \quad \theta_3(t) = -(m+\tfrac{1}{2})\log t - t - \log d_\infty. \tag{5.3}$$

Here $d_\infty = c_\infty$ or $\hat{c}_\infty$ for $m = 0$ or $m \geq 1$ respectively, and arbitrary constants have been chosen to satisfy boundary conditions (2.60d), (2.62b) and to match with expansion (4.7), (4.8) ($m = 0$) or expansion (4.7), (4.14) ($m \geq 1$) in the overlapping domain $x \gg 1$, $t \ll 1$. Therefore we have

$$\theta(x,t) = (x-\sigma)^2/4D_0 t + (m+1)\log(x-\sigma) - \{(m+\tfrac{1}{2})\log t + t + \log d_\infty\} + o(1) \tag{5.4}$$

as $x \to \infty$ with $t = O(1)$. After substitution into (5.1) we arrive at

$$u(x,t) = \frac{d_\infty t^{m+\frac{1}{2}}}{(x-\sigma)^{m+1}} \exp(-\{x^2/4D_0 t - t\})[1+o(1)] \tag{5.5}$$

as $x \to \infty$ with $t = O(1)$. An important point to note is that $u(x,t)$ is exponentially small as $x \to \infty$, and the expansion (5.5) remains uniformly valid for t large *provided* $x \gg O(t)$. However, expression (5.5) fails for $t \gg 1$ when $x = O(t)$ and $u(x,t)$ is then only algebraically small in t. We discuss this long-time non-uniformity in (5.5) in §8, where it is shown to play a significant role in determining the propagation speed of a travelling wave that develops in the initial-boundary value problem when $t \gg 1$. However, before examining the long-time structure of $u(x,t)$, we first consider the asymptotic structure of $u(x,t)$ when $t \sim t_c$ and $u \sim \tilde{u}_c$.

6. Development at breakthrough $t \to t_c^+$

Here we examine 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 II and III. At $t = t_c$, $u(x,t_c)$ is monotone decreasing in x, with a local maximum at $x = 0$, where $u = \tilde{u}_c$ (via theorem (2.60)). Therefore, as $x \to 0^+$, we have

$$u(x,t_c) \sim \tilde{u}_c - a_2 x^2 + \sum_{n=3}^{\infty} a_n x^n, \tag{6.1}$$

with $a_2 \geqslant 0$. We expect the generic condition to be $a_2 \neq 0$, and we begin with this case. We say that breakthrough occurs at $t = t_c$ if $u(0,t) > \tilde{u}_c$ for $0 < t - t_c \ll 1$. Now, in $t < t_c$ equation (2.60*a*) gives, as $x \to 0^+$,

$$u_t(0,t) = D(u(0,t))\, u_{xx}(0,t) + R(u(0,t)), \tag{6.2}$$

which gives, on using (6.1) and allowing $t \to t_c^-$ in (6.2),

$$u_t(0,t_c) = R(\tilde{u}_c) > 0. \tag{6.3}$$

Therefore breakthrough always occurs at $t = t_c$. Furthermore (6.3) and (6.1) (with $a_2 \neq 0$) suggest that $s(t) = O[(t-t_c)^{\frac{1}{2}}]$ as $t \to t_c^+$, and we expand

$$s(t) \sim \sum_{n=1}^{\infty} s_n (t-t_c)^{n/2}, \tag{6.4}$$

with

$$u(\hat{\eta},t) \sim \begin{cases} \tilde{u}_c + \sum_{n=2}^{\infty} F_n(\hat{\eta})\,(t-t_c)^{n/2} & \text{in domain III} \\ \tilde{u}_c + \sum_{n=2}^{\infty} G_n(\hat{\eta})\,(t-t_c)^{n/2} & \text{in domain II} \end{cases} \tag{6.5}$$

at $t \to t_c^+$. Here $\hat{\eta} = x/(t-t_c)^{\frac{1}{2}} = O(1)$ as $t \to t_c^+$, with $x = s(t)$ corresponding to $\hat{\eta} = s_1 + o(1)$ as $t \to t_c^+$. After substitution from (6.5) into (2.61*a*), (2.62*a*) and solving at each order in turn, we obtain

$$u(\hat{\eta},t) = \begin{cases} \tilde{u}_c + (t-t_c)\{R(\tilde{u}_c) - a_2\hat{\eta}^2\} + a_3(t-t_c)^{\frac{3}{2}}\hat{\eta}^3 \\ \quad + (t-t_c)^2[\tfrac{1}{2}R(\tilde{u}_c)\{R'(\tilde{u}_c)+2a_2\} - a_2\{R'(\tilde{u}_c)+6a_2\}\hat{\eta}^2 \\ \quad + a_4\hat{\eta}^4] + O([t-t_c]^{\frac{5}{2}}) \quad \text{in III} \\ \tilde{u}_c + (t-t_c)[R(\tilde{u}_c) + \hat{A}\hat{\eta}^2] + \hat{B}(t-t_c)^{\frac{3}{2}}\hat{\eta}^3 \\ \quad + (t-t_c)^2[\tfrac{1}{2}R(\tilde{u}_c)R'(\tilde{u}_c) + \hat{A}R'(\tilde{u}_c)\hat{\eta}^2 + \hat{C}\hat{\eta}^4] \\ \quad + O([t-t_c]^{\frac{5}{2}}) \quad \text{in II} \end{cases} \tag{6.6}$$

MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES
THE ROYAL SOCIETY A
PHILOSOPHICAL TRANSACTIONS OF

where the initial condition (6.1) has been satisfied by the expansion in domain III as $\hat{\eta} \to \infty$. Here $\hat{A}, \hat{B}, \hat{C}$ are as yet undetermined constants. It remains to apply the interface condition that $u \to \tilde{u}_c$ as $x \to s(t)^{\pm}$. This determines (via (6.6) and (6.4)) the remaining unknowns as

$$\left.\begin{aligned} s_1 &= (R_c/a_2)^{\frac{1}{2}}, \quad s_2 = R_c a_3/2a_2^2, \\ s_3 &= \frac{5a_3^2 R_c^{\frac{3}{2}}}{8a_2^{\frac{7}{2}}} + \frac{a_4 R_c^{\frac{3}{2}}}{2a_2^{\frac{5}{2}}} - \frac{R_c^{\frac{1}{2}} R_c'}{4a_2^{\frac{1}{2}}} - \frac{5a_2^{\frac{1}{2}} R_c^{\frac{1}{2}}}{2}, \\ \hat{A} &= -a_2, \quad \hat{B} = a_3, \quad \hat{C} = a_4 - 5a_2^3/R_c, \end{aligned}\right\} \tag{6.7}$$

where $R_c = R(\tilde{u}_c)$, $R_c' = R'(\tilde{u}_c)$. We can now determine the jump in gradient across $x = s(t)$. On using (2.22) we find that

$$J(t) \equiv u_x(s(t)^+, t) - u_x(s(t)^-, t) = \dot{s}^{-1} u_x^2(s(t)^+, t)), \tag{6.8}$$

which, after substitution from (6.4), (6.6), (6.7), leads to

$$J(t) \sim 8a_2^{\frac{3}{2}} R_c^{\frac{1}{2}} (t - t_c)^{\frac{3}{2}} \quad \text{as} \quad t \to t_c^+. \tag{6.9}$$

We next examine the general case in which $a_2 = \ldots = a_{2p-1} = 0$, $a_{2p} \neq 0$, $p \in \mathbb{N}$ and $a_{2p} < 0$, in (6.1). Again (6.2) and (6.3) establish that breakthrough occurs at $t = t_c$. However, (6.3) and (6.1) now suggest that $s(t) = O[(t-t_c)^{1/2p}]$ as $t \to t_c^+$, and we expand

$$s(t) \sim s_1 (t - t_c)^{1/2p} + \cdots \tag{6.10}$$

with

$$u(\tilde{\eta}, t) \sim \begin{cases} \tilde{u}_c + \sum\limits_{n=2}^{\infty} \tilde{F}_n(\tilde{\eta})\,(t-t_c)^{n/2} & \text{in domain III} \\ \tilde{u}_c + \sum\limits_{n=2}^{\infty} \tilde{G}_n(\tilde{\eta})\,(t-t_c)^{n/2} & \text{in domain II} \end{cases} \tag{6.11}$$

at $t \to t_c^+$. Here $\tilde{\eta} = x/(t-t_c)^{1/2p} = O(1)$ as $t \to t_c^+$. After substitution from (6.10), (6.11) into (2.61a), (2.62a), we obtain the leading order development as

$$u(\tilde{\eta}, t) \sim \begin{cases} \tilde{u}_c + (t-t_c)\,[R_c + a_{2p}\,\tilde{\eta}^{2p}] & \text{in domain III} \\ \tilde{u}_c + (t-t_c)\,[R_c + \tilde{A}\tilde{\eta}^{2p}] & \text{in domain II} \end{cases} \tag{6.12}$$

and $\tilde{A}$ is an as yet undetermined constant. It remains to apply the interface condition ($u \to \tilde{u}_c$ as $x \to s(t)^{\pm}$) which fixes the remaining unknowns as

$$\tilde{A} = a_{2p}, \quad s_1 = (-R_c/a_{2p})^{1/2p}. \tag{6.13}$$

Finally we determine from (6.8), (6.10), (6.12) and (6.13) that the gradient jump is given by

$$J(t) \sim 8p^3 a_{2p}^2 (-R_c/a_{2p})^{4p-3/2p}\,(t-t_c)^{3(2p-1)/2p} \tag{6.14}$$

as $t \to t_c^+$.

In both cases we see that breakthrough occurs at $t = t_c$, and the front initiates its motion with a singular velocity, given by $\dot{s}(t) = O([t-t_c]^{1/2p-1})$ as $t \to t_c^+$.

7. Numerical solutions

In this section we consider numerical solutions of the initial-boundary value problem (2.60)–(2.63). For initial data whose maximum value is below the critical level ($\tilde{u}_c$) the numerical problem is classical, at least until the effects of reaction increase u up to the critical level. To avoid unnecessary computation we only consider initial data whose maximum is at the critical level, this maximum occurring at the origin. The functional form of initial data is chosen so that a moving boundary is immediately formed. As noted earlier the moving boundary problem splits into a purely reactive equation for $x < s(t)$ and a reaction–diffusion equation for $x \geqslant s(t)$. If the solution of the reaction–diffusion problem can be found, in isolation from the reaction problem, it is then possible to return to the reaction problem with knowledge of $s(t)$ and compute this separately and very easily.

The reaction–diffusion problem, to be solved on the domain $s(t) < x < \infty$, is written in the form

$$\left.\begin{aligned} u_t &= D(u)\,u_{xx} + D'(u)\,u_x^2 + R(u), \\ u(x,0) &= g(x), \quad u(s(t),t) = \tilde{u}_c, \\ s(0) &= 0, \quad u \to 0 \quad \text{as} \quad x \to \infty. \end{aligned}\right\} \tag{7.1}$$

A further boundary condition, which is useful in the numerical solution of this problem, can be found by considering the form of $u(x,t)$ close to the moving boundary. If we pose an expansion

$$u(x,t) = u_c + a(t)\,(x - s(t)) + 0((x - s(t))^2) \tag{7.2}$$

then a simple calculation reveals

$$a(t) = -\tfrac{1}{2}\{-\dot{s}(t) + \surd([s(t)]^2 + 4R(\tilde{u}_c))\}. \tag{7.3}$$

This asymptotic development can be used exactly at the moving boundary $x = s(t)$ to give the condition

$$u_x(s,(t),t) = -\tfrac{1}{2}\{-\dot{s}(t) + \surd([\dot{s}(t)]^2 + 4R(\tilde{u}_c))\}. \tag{7.4}$$

For numerical purposes it is desirable to compute the evolving solution over a fixed domain. This is effected by the introduction of a new independent variable $\xi = x - s(t)$ and leads to the modified system, to be solved over the domain $0 \leqslant \xi < \infty$,

$$\left.\begin{aligned} u_t &= D(u)\,u_{\xi\xi} + D'(u)\,u_\xi^2 + \dot{s}u_\xi + R(u), \\ u(\xi,0) &= g(\xi), \quad u(0,t) = \tilde{u}_c, \\ u_\xi(0,t) &= -\tfrac{1}{2}\{-\dot{s}(t) + \surd([s(t)]^2 + 4R(\tilde{u}_c))\}, \\ s(0) &= 0, \quad u \to 0 \quad \text{as} \quad \xi \to \infty \end{aligned}\right\} \tag{7.5}$$

In earlier analysis we have shown that the moving boundary has an initial velocity $\dot{s} = O(t^{-\frac{1}{2}})$. To keep an accurate representation of the boundary position it is necessary to account for this singular velocity. This is done by introducing a new variable $\tau = t^{\frac{1}{2}}$ (in this variable the initial velocity of the boundary is $O(1)$) and leads to the system

$$\left.\begin{aligned} u_\tau &= 2\tau D(u)\,u_{\xi\xi} + 2\tau D'(u)\,u_\xi^2 + \dot{s}u_\xi + 2\tau R(u), \\ u(\xi,0) &= g(\xi), \quad u(0,\tau) = \tilde{u}_c, \\ 2\tau u_\xi(0,\tau) &= -\tfrac{1}{2}\{-\dot{s}(\tau) + \surd([s(\tau)]^2 + 4\tau^2 R(\tilde{u}_c))\}, \\ s(0) &= 0, \quad u \to 0 \quad \text{as} \quad \xi \to \infty, \end{aligned}\right\} \tag{7.6}$$

where dotted quantities now represent $\mathrm{d}/\mathrm{d}\tau$.

A finite-difference approximation of equations (7.6), of implicit form so as to ensure reasonable accuracy and stability, is constructed by defining a mesh of ξ and

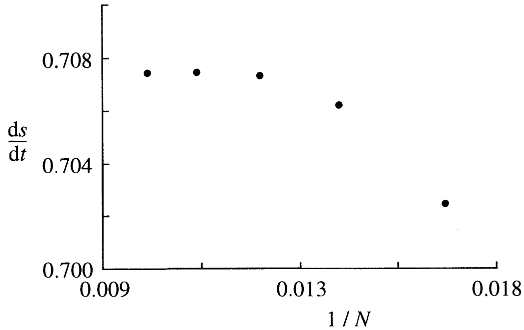

Figure 5. The dependence of $\dot{s}(t)$ at $t = 16$ with $1/N$.

t points by $\zeta_i = ih$, $1 \leqslant i \leqslant M$, and $t_j = jk$, $j \geqslant 0$, and leads to the discrete system of the form

$$\left.\begin{aligned} u_i^{j+1} - u_i^j = {} & k\tau_{j+\frac{1}{2}} D(\tfrac{1}{2}(u_i^{j+1}+u_i^j))((u_{\xi\xi})_i^{j+1} + (u_{\xi\xi})_i^j) \\ & + \tfrac{1}{2}k\tau_{j+\frac{1}{2}} D'(\tfrac{1}{2}(u_i^{j+1}+u_i^j))((u_\xi)_i^{j+1} + (u_\xi)_i^j) \\ & + \tfrac{1}{2}(s^{j+1}-s^j)((u_\xi)_i^{j+1} + (u_\xi)_i^j) + 2k\tau_{j+\frac{1}{2}} R(\tfrac{1}{2}(u_i^{j+1}+u_i^j)), \\ u_i^0 = g_i, \quad u_0^j = \tilde{u}_c, & \quad s^0 = 0, \quad u_{n+1}^j = 0, \\ -2k\tau_{j+\frac{1}{2}}((u_\xi)_0^{j+1} + (u_\xi)_0^j) = {} & -(s^{j+1}-s^j) + \surd\{(s^{j+1}-s^j)^2 + 4k^2\tau_{j+\frac{1}{2}}^2 R(\tilde{u}_c)\}, \end{aligned}\right\} \tag{7.7}$$

where $u_i^j = u(ih, jk)$ in the usual notation. The above system may be written in a fully discretized form by replacing all spatial derivatives that occur by quadratically accurate finite difference representations. As a result of this equations (7.7) are recognized as a system of $N+1$ nonlinear algebraic equations in the $N+1$ unknowns $u_1^{j+1}, \ldots u_N^{j+1}, s^{j+1}$. These equations were solved using the NAG routine CO5NBF which uses a combination of Newtonian and steepest descent iterations. This method generally only required three iterations per time step to produce a solution whose error, in L^2 norm, was $O(10^{-8})$. The choice of mesh parameters h, k and N is a matter of trial and error in a nonlinear problem. It was found that the choice $h = 0.1$, $k = 0.05$ produced a stable solution for times up to $O(25)$. The effect of truncation of the infinite domain is well known to have a serious effect on eigenvalue problems for differential equations. We investigated truncation error as a numerical experiment in this problem by considering the approach of the velocity of the moving boundary to the minimum speed travelling wave. Figure 5 shows the value of $\mathrm{d}s/\mathrm{d}t$ at $t = 16$ with the above mesh parameters and N varying. With increasing N, $\mathrm{d}s/\mathrm{d}t$ rapidly approaches a value of 0.7046, whereas the exact minimum speed travelling wave for this example has a speed of $1/\surd 2$. These results give some confidence that our numerical scheme is quadratically accurate.

To study the evolution of any initial data it is necessary to assign a functional form to $D(u)$ and $R(u)$; these choices must fall within the classes of functions discussed earlier in the paper. We chose $D(u) = \frac{3}{2}(\frac{1}{2}-u)(\frac{1}{6}+u)$, $\tilde{u}_c = \frac{1}{2}$, $D_0 = \frac{1}{8}$ and $R(u) = u(1-u)$. This choice of $R(u)$ enables us to integrate the reaction equation for u in the form

$$u = \frac{\tilde{u}_c \exp\{-s^{-1}(x)+t\}}{1-\tilde{u}_c+\tilde{u}_c \exp\{-s^{-1}(x)+t\}} \tag{7.8}$$

in the domain $0 \leqslant x \leqslant s(t)$, $t > 0$.

The evolution of the initial data $u(x, 0) = \frac{1}{2}\,\mathrm{e}^{-\frac{1}{2}x^2}$ is shown for $t = 0.25$, 1.0, 4.0, 9.0 and 16.0 in figure 6 (*a*–*e*), with the gradient jump shown on an inset. The variation

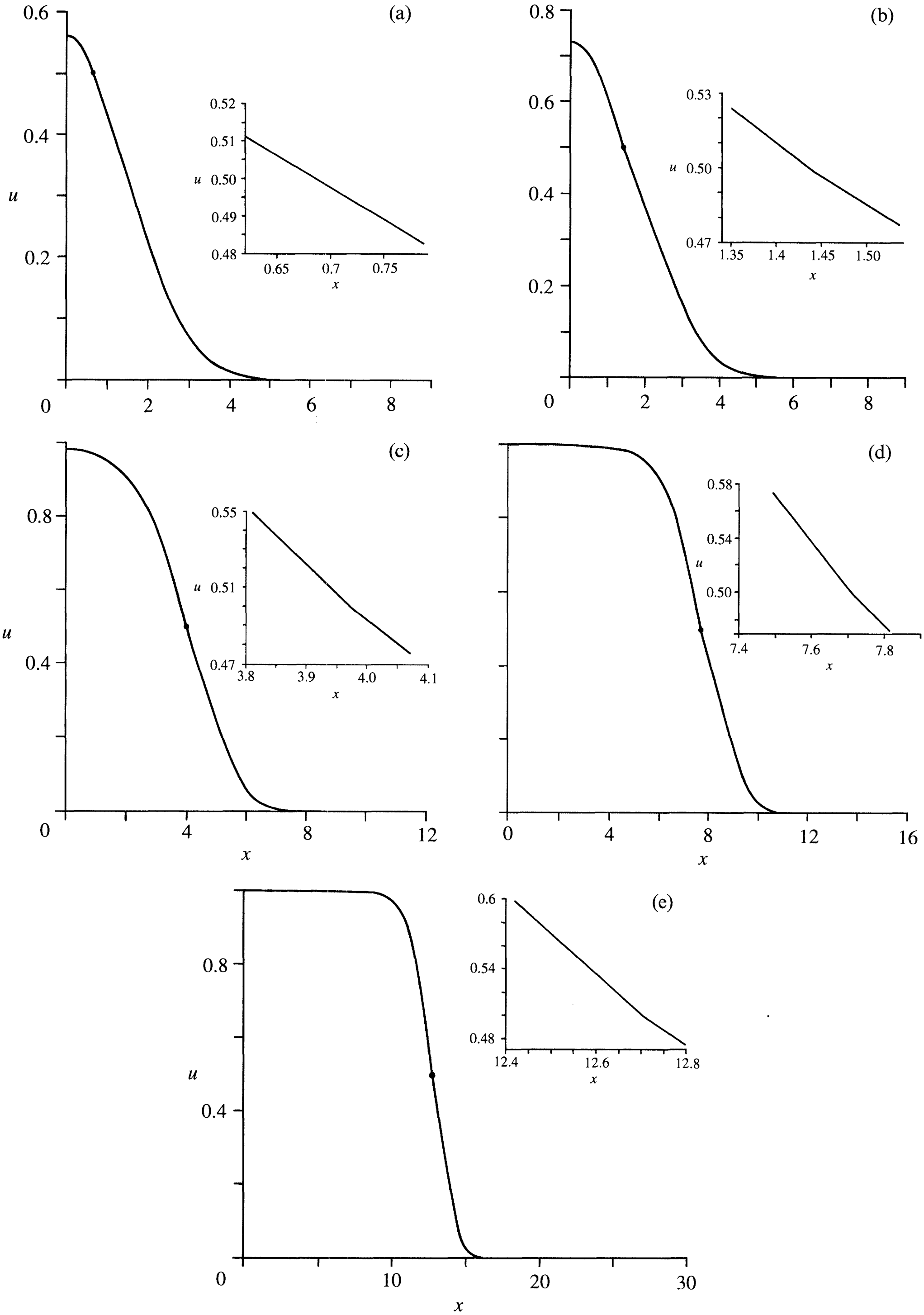

Figure 6. The numerical solution of (7.1) with $D(u) \equiv \frac{3}{2}(\frac{1}{2}-u)(\frac{1}{6}+u), R(u) = u(1-u), \tilde{u}_c = 0.5$, $g(x) = \frac{1}{2}e^{-\frac{1}{2}x^2}$ at $t =$ (*a*) 0.25, (*b*) 1.0, (*c*) 4.0, (*d*) 9.0, (*e*) 16.0.

MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES
THE ROYAL SOCIETY
PHILOSOPHICAL TRANSACTIONS OF

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

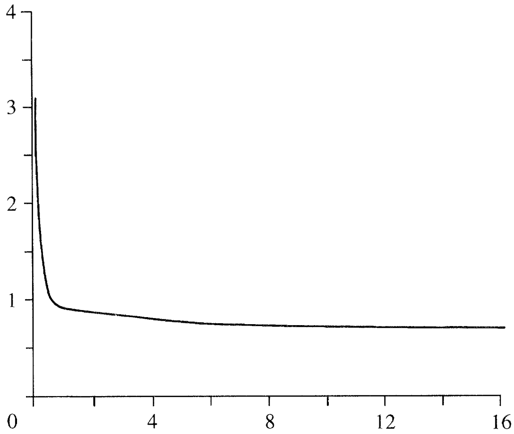

Figure 7. A graph of $\dot{s}(t)$ versus t for use in figure 6.

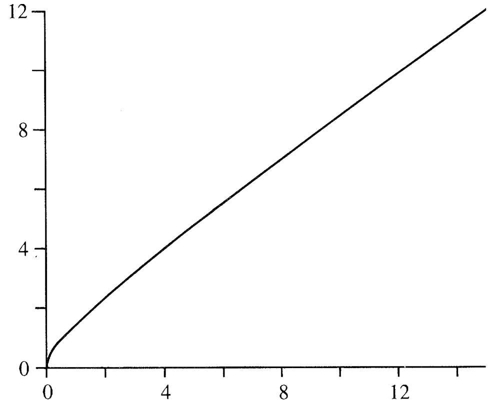

Figure 8. A graph of $s(t)$ versus t for use in figure 6.

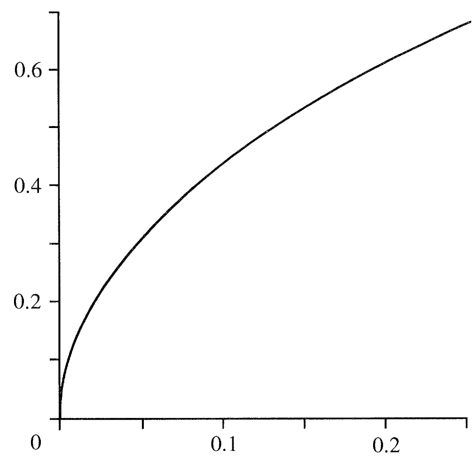

Figure 9. A graph of the small time behaviour of $s(t)$ for use in figure 6.

of $\mathrm{d}s/\mathrm{d}t$ with t is shown in figure 7. The evolution of a fully reacted state behind an (asymptotically) constant speed moving boundary is clearly illustrated. A graph of $s(t)$ versus t is shown in figure 8. It can be noted from this graph that there is an initial rapid acceleration of the moving boundary which slows down over an $O(1)$ timescale into a constant speed wave form. The speed and form of this constant speed wave form are in agreement with those of the minimum speed permanent form travelling wave available to the system (§3). The initial behaviour of the moving boundary is shown rather more clearly in figure 9, where the predicted $O(t^{\frac{1}{2}})$ behaviour is obvious. Similar behaviour to this was found for a wide variety of initial data.

8. Large time behaviour

This section is concerned with examining the asymptotic structure of the solution to IBVP as $t \to \infty$. The numerical solutions of §7 have shown that a permanent form travelling wave develops in IBVP as $t \to \infty$, and it is indicated that the PTW that develops is that which has the minimum propagation speed $2\sqrt{D_0}$. Here we formally establish this result, on the assumption that a PTW develops as $t \to \infty$, via the method of matched asymptotic expansions.

For $t \gg 1$, we have from §5 ((5.1), (5.4)) that,

$$u(x,t) \sim \exp\{-(x-\sigma)^2/4D_0 t - (m+1)\log(x-\sigma) + \{(m+\tfrac{1}{2})\log t + t + \log d_\infty\} + \cdots\} \quad (8.1)$$

for $x \gg O(t)$ as $t \to \infty$. However, this asymptotic expansions fails when $x = O(t)$, when the travelling wave structure appears. Thus when $x = O(t)$ we introduce the independent variable $y = x - s(t)$ and expand as follows,

$$\left.\begin{aligned} u(y,t) &\sim u_0(y) + t^{-1}u_1(y) + \cdots \\ \dot{s}(t) &\sim v_0 + v_1 t^{-1} + \cdots \end{aligned}\right\} \quad \text{as} \quad t \to \infty, \quad y = O(1), \quad \begin{aligned}(8.2)\\(8.3)\end{aligned}$$

where the algebraic correction terms are suggested by the form of (8.1) when $x = O(t)$.

After substitution from (8.2, 8.3) into (2.61), (2.62) we obtain at leading order as $t \to \infty$ the eigenvalue problem (3.2), (3.3) for $u_0(y)$ (with y replacing z and v_0 replacing v), together with conditions (3.4)–(3.6), which are required to match with expansion (8.1) as $y \to \infty$ and with the asymptotic form (2.72) as $y \to -\infty$. This problem has a solution $u_T(y, v_0)$ for each $v_0 \geqslant 2\sqrt{D_0}$ (see §3). Thus we may write

$$u(y,t) \sim \exp[\log u_T(y, v_0) + O(t^{-1})] \quad \text{as} \quad t \to \infty \quad (8.4)$$

with $y = O(1)$. We now determine v_0 by matching (8.1) to (8.4) up to terms of $O(t)$. We first write the exponent of (8.4), up to $O(t)$, when $x \gg O(t)$. This gives

$$E \sim xc_+(v_0) - v_0 c_+(v_0)\,t + o(t), \quad (8.5)$$

where E represents the exponent of u and $u_T(y, v_0)$ is expanded as in §3. Next we write the exponent of (8.1) in terms of y, and expand up to $O(t)$. After rewriting in terms of x we arrive at

$$E \sim -\tfrac{1}{2}v_0/D_0\,x + (1 + \tfrac{1}{4}v_0^2/D_0)\,t + o(t). \quad (8.6)$$

The matching principle (see, for example, Van Dyke 1975) requires that (8.5) and (8.6) agree up to $o(t)$, which requires

$$c_+(v_0) + \tfrac{1}{2}v_0/D_0 = 0, \quad v_0 c_+(v_0) + \tfrac{1}{4}v_0^2/D_0 + 1 = 0. \quad (8.7, 8.8)$$

We eliminate $c_+(v_0)$ between (8.7, 8.8) which leaves $-\tfrac{1}{4}v_0^2/D_0 + 1 = 0$, resulting in

$$v_0 = 2\sqrt{D_0}, \quad (8.9)$$

which is the minimum speed of propagation for a PTW (see §3). It remains to show that (8.7) is satisfied, and this follows automatically on using (8.9) with (3.12). We have thus established that, when a PTW develops in IBVP as $t \to \infty$, it is the PTW with minimum propagation speed that occurs.

9. Discussion

We have considered a scalar reaction–diffusion process with autocatalytic kinetics and a nonlinear variable diffusivity as a simple model for a polymerization process. In particular the diffusivity is taken to be monotone decreasing in concentration with finite support $[0, \tilde{u}_c]$. For concentrations $u > \tilde{u}_c$ (< 1) the polymer is assumed to be immobile, while remaining mobile at the lower concentrations $0 < u < \tilde{u}_c$. The fully reacted state is reached at $u = 1$, when the polymer is fully immobile. We have considered the situation that arises when a localized quantity of polymer is used to initiate the reaction. This leads to a 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 monotone, with compact support, and we have found that

(i) $u(x,t)$ is classical for $0 < t \leqslant t_c$, and monotone decreasing in x. 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 $x > x(t)$) and represents a 'freezing' front for the polymer, i.e. the polymer is immobile for $0 < x < s(t)$, while it is in solution for $x > s(t)$. As $t \to t_c^+$, $\dot{s}(t) = O([t-t_c]^{-\frac{1}{2}})$, with $\dot{s}(t) > 0$ in $t > t_c$. The 'freezing' front initiates its motion with singular velocity.

(iii) as $t \to \infty$, the system approaches a PTW structure, selecting the PTW of minimum speed. In line with this $\dot{s}(t) \to 2\sqrt{D_0}$ as $t \to \infty$ and a quasi-steady polymerization interface is established. The fully reacted state $u \equiv 1$ is achieved to the rear of this interface as $t \to \infty$.

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

References

Doi, M. & Edwards, S. F. 1986 *The theory of polymer dynamics*. Oxford: Clarendon Press.

Fisher, R. A. 1937 *Ann. Eug.* **7**, 355.

Friedman, A. 1964 *Partial differential equations of parabolic type*. New Jersey: Prentice-Hall.

Gray, P. & Scott, S. K. 1990 *Chemical oscillations and instabilities*. Oxford: Clarendon Press.

Hanna, A., Saul, A. & Showalter, K. 1982 *J. Am. chem. Soc.* **104**, 3838.

Jones, D. S. & Sleeman, B. D. 1983 *Differential equations and mathematical biology*. London: Allen and Unwin.

King, A. C. & Needham, D. J. 1992 *Proc. R. Soc. Lond.* A **437**, 657.

Murray, J. D. 1989 *Mathematical biology*. Berlin: Springer.

Odion, G. 1970 *Principles of polmerization*. New York: Wiley.

Oleinik, O. A. & Kruzhkov, S. N. 1961 *Translations of contents of Usp. mat. Nauk*. vol. XVI, no. 5, p. 105.

Regen, S. L. 1975 *J. Am. chem. Soc.* **97**, 5956.

Regen, S. L. 1976 *J. Am. chem. Soc.* **98**, 6270.

Van Dyke, M. 1975 *Perturbation methods in fluid mechanics*. Stamford: Parabolic Press.

Winfree, A. T. 1980 The geometry of biological time. Berlin: Springer.

Received 24 May 1993; accepted 22 October 1993

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES