

## Parabolic Free Boundary Problems Arising in Porous Medium Combustion

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[Received 1 May 1987]

A parabolic partial differential equation approximating the evolution of temperature in highly exothermic porous-medium combustion at low driving velocities is examined. The equation is of reaction-diffusion type with a reaction term which is discontinuous as a function of the dependent variable.

Firstly the variation of the steady solution set with the scaled heat of the reaction is described and the related time-dependent behaviour analysed. The stability results follow from characterizing the ends of the solution branch and fold points explicitly and deducing global stability results about the whole of the continuous solution branch. The results are used to indicate the parameter regimes and temporal scales on which the small driving velocity approximation ceases to be valid.

Secondly the behaviour of the discontinuous partial differential equation is compared with that of a continuous equation which it approximates. This provides justification for the approximation of reaction terms possessing steep gradients by discontinuous functions; the large activation energy limit in porous-medium combustion involves such a process.

### 1. Introduction

IN NATURE there are a number of biological and chemical processes which, when viewed on an appropriate time-scale, exhibit switch-like behaviour. Thus it is natural to model such phenomena by introducing functions which are discontinuous in the appropriate variable.

In particular we are motivated by the study of combustion of solid porous media (see (Norbury & Stuart, 1987a)) where, in the limit of large activation energy, the reaction rate is discontinuous as a function of the temperature in the combustible solid. The discontinuity represents the switch between a state of near-frozen chemistry, in which the temperatures are too low to allow combustion to occur, and a state in which the combustion reaction has significant effect, but is limited by the ability of the gaseous reactants to diffuse into the reaction sites in the solid. Mathematically the switch arises because the two-stage chemical reaction in this form of heterogeneous combustion is a *rational function* of the Arrhenius reaction rate. This contrasts with the theory of homogeneous combustion, where the reaction rate is *proportional* to the Arrhenius term.

In (Stuart, 1987) the model derived in (Norbury & Stuart, 1987a) is simplified in

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the case of highly exothermic chemical reactions when  $\mu$ , the inlet velocity of the gas flow through the porous medium, is small. It is shown that the initial evolution of the solid temperature  $T \sim u + O(\mu^{\frac{1}{2}})$  is governed by an equation of the form (P1), below, where  $t$  represents time and  $x$  is a spatial coordinate parallel to the direction of the driving gas flow. A model such as (P1), however, has applications to a variety of biological and chemical phenomena.

Thus

$$\left. \begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial}{\partial x} \left( K(u) \frac{\partial u}{\partial x} \right) + \lambda H(u-1)f(u) \quad \text{for } x \in (-1, 1), \\ \text{with } u(\pm 1, t) &= 0 \quad \text{and initial conditions.} \end{aligned} \right\} \quad (\text{P1})$$

Here  $H(\cdot)$  is the function which is defined to be zero when its argument is negative, one-half when its argument is zero and unity otherwise. The continuous problem which (P1) approximates is (P2), defined by

$$\left. \begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial}{\partial x} \left( K(u) \frac{\partial u}{\partial x} \right) + \frac{\lambda f(u)}{1 + \exp((1-u)/\varepsilon)} \quad \text{for } x \in (-1, 1), \\ \text{with } u(\pm 1, t) &= 0 \quad \text{and initial conditions.} \end{aligned} \right\} \quad (\text{P2})$$

For both (P1) and (P2) we take initial data with support on  $(-1, 1)$  satisfying  $u(\pm 1) = 0$ . The particular form of the continuous reaction rate chosen in (P2) is motivated by the original form of the reaction rate in porous-medium combustion (see (Norbury & Stuart, 1987a)) before the limit of large activation energy is taken. Note that, for fixed  $\lambda$ , equation (P1) approximates (P2) in the limit  $\varepsilon \rightarrow 0$ .

We assume that  $K(u) \in C^1$  and satisfies  $K(u) \geq \bar{K} > 0$  so that the equations are uniformly parabolic. We also assume that  $f(u) \in C^2$  and that  $f(u) > 0$  for all  $u \geq 1$  and  $\lambda > 0$  so that the forcing term is positive. We seek solutions which are  $C^1(0, T)$  in  $t$  and piecewise  $C^2(-1, 1)$  in  $x$  (in fact  $C^2(-1, 1)$  except where  $u(x, t) = 1$ ). In other words we assume that the discontinuity induced by the forcing term is taken up entirely in the second  $x$ -derivative of  $u$ , rather than in the first  $t$ -derivative of  $u$  or a combination of these. Implicit in problem (P1) is the presence of moving boundaries at  $x = s_i(t)$  defined by  $u(s_i(t), t) = 1$  for  $i = 0, \dots, n$  for some integer  $n$  (which may vary with  $t$  as internal boundaries coalesce or are formed).

Our objective in this paper is twofold. First to understand the large-time behaviour of problem (P1) in order that we may deduce the validity of the approximation of the temperature  $T$  by  $T \sim u + O(\mu^{\frac{1}{2}})$  for small driving velocities  $\mu$ . Secondly to validate the approximation of the continuous problem (P2) by its discontinuous counterpart (P1).

In Section 2 we describe the bifurcation surface for the steady solutions  $U(x)$  of problem (P1) as  $\lambda$  varies, by considering the projection of  $U$  onto  $\|U\|_\infty$ , the maximum norm of  $U$ . The structure of the bifurcation diagram for the steady solutions is discussed by Nistri (1979), who demonstrated that a generic form of bifurcation from  $\lambda \sim \infty$  occurs (see Fig. 1). In Section 3 we show that the temporal growth rates of the linearized version of (P1) are real (Theorem 3.1). We use this result to facilitate a linear stability analysis of the steady solutions for the singularly perturbed version of problem (P1) when  $\lambda \gg 1$  and demonstrate that

the solutions are unstable. In Section 4 we examine the particular case of  $K(u)$  constant and  $f(u)$  linear. We demonstrate the existence of either one, two or three steady solutions, depending on  $\lambda$ , and examine the linear stability of these solutions by characterizing the fold point explicitly (Theorem 4.1). These results are summarized in Fig. 1 for the case considered in Section 4. In Section 5 we describe numerical results from the solution of problem (P1) to illustrate the analytic results on the stability and domains of attraction of the steady states. Finally, in Section 6 we compare the qualitative structure of the steady solution set and the time-dependent behaviour of problems (P1) and (P2).

Previous work on time-dependent problems with discontinuous nonlinearities is limited; see for example (Lacey, 1981; Terman 1983). Lacey considers a semilinear parabolic equation with a piecewise constant forcing term and examines the spatial dependence of the time-evolving system. Terman analyses a problem related to (P1) arising from the study of nerve conduction in which the piecewise linear forcing term is of indeterminate sign.

## 2. Steady solutions

The steady solutions of problem (P1) satisfy

$$(K(U)U_x)_x + \lambda H(U - 1)f(U) = 0 \tag{2.1}$$

and

$$U(\pm 1) = 0. \tag{2.2}$$

Clearly  $U \equiv 0$  is a solution to this problem. Since  $K(U) \geq \bar{K} > 0$  we know that in any region where  $U(x) < 1$ ,  $U_x(x)$  is of one sign. Hence any non-trivial solution must satisfy  $U(x) > 1$  somewhere and this can only happen over one interval. This demonstrates that there is no bifurcation from the trivial solution  $U \equiv 0$ .

If we define the two points  $s_1$  and  $s_2$  ( $s_1 < s_2$ ) by  $U(s_i) = 1$ ,  $i = 1, 2$  then it can be shown that  $s_1 = -s_2$ . Thus, without loss of generality we consider the solution of (2.1) subject to the symmetry boundary conditions

$$U_x(0) = U(1) = 0, \tag{2.3}$$

and define the unique point  $s$  by  $U(s) = 1$ .

An analytic expression for the bifurcation surface defining this steady problem is most easily derived by noting that the function  $\lambda(U(0))$  is uniquely defined. This approach was introduced by Laetsch (1970) for general two-point boundary-value problems and is valuable in both analytic and numerical studies (see (Budd & Norbury 1987; Nistri 1979; Smoller & Wasserman 1981)). Under the transformation  $y = x/\lambda$  the equation (2.1) is independent of  $\lambda$ . The bifurcation surface may then be determined by solving the rescaled equation as an initial-value problem. For each initial value  $U(0)$  ( $= \|U\|_\infty$ , by the maximum principle (Protter & Weinberger, 1976)) greater than one this determines a unique point  $y = \bar{y}(\|U\|_\infty)$  at which  $U(\bar{y}) = 0$ . Since  $\lambda = \bar{y}^2$  at such a point, this defines the bifurcation surface.

This approach to the semilinear version ( $K(u) \equiv 1$ ) of (2.1) and (2.3) is described by Nistri (1979). Under the transformation  $S' = K$  and  $w(x) = S(u(x))$ ,

equation (2.1) may be converted into a semilinear equation for  $w(x)$  so that the results of Nistri are directly applicable. However, since we are ultimately interested in the time-dependent problem (P1), we chose to work directly with the quasilinear equation (2.1).

Non-trivial steady solutions satisfy  $U(x) > 1$  in  $(0, s)$  and  $U(x) < 1$  in  $(s, 1)$ . Multiplying equation (2.1) by  $K(U)U_x$ , integrating in the two separate regions  $0 < x < s$  and  $s < x < 1$  and using the condition that  $U_x(s)$  is continuous to eliminate  $s$ , we obtain the following expression for the variation of  $\lambda$  with  $U(0)$ :

$$\sqrt{2\lambda} = \frac{\int_0^1 K(U) dU}{[h(1, U(0))]^{\frac{1}{2}}} + \int_1^{U(0)} \left( \frac{K(U) dU}{[h(U, U(0))]^{\frac{1}{2}}} \right). \tag{2.4}$$

where

$$h(U, U(0)) = \int_U^{U(0)} f(\xi)K(\xi) d\xi; \tag{2.5}$$

$s$  is determined by

$$s = \int_1^{U(0)} \left( \frac{K(U)}{[2\lambda h(U, U(0))]^{\frac{1}{2}}} \right) dU. \tag{2.6}$$

Elimination of  $\sqrt{2\lambda}$  between (2.4) and (2.6) shows that

$$\int_0^1 K(U) dU \left( \frac{s}{1-s} \right) = \int_1^{U(0)} K(U) \left( \frac{h(1, U(0))}{h(U, U(0))} \right)^{\frac{1}{2}} dU. \tag{2.7}$$

Because  $h(X, X) = 0$  equations (2.4), (2.6), and (2.7) suffer from a weakly singular kernel, and are thus unsuitable for differentiation or for direct numerical integration. However this singularity may be removed by integrating by parts and using the fact that  $h_U(U, U(0)) = -f(U)K(U)$ .

After doing this, taking the limit  $U(0) \rightarrow 1$  in equations (2.4) and (2.6) we obtain

$$\lambda \rightarrow \infty \quad \text{and} \quad s \rightarrow 0 \quad \text{as} \quad U(0) \rightarrow 1. \tag{2.8}$$

Thus the existence of a branch of solutions bifurcating from  $\lambda = \infty$  is established. This result is derived by Nistri (1979) and may also be proved by employing a local bifurcation theory to a suitably transformed problem; see (Stuart, 1987).

### 3. Eigenvalues of the linearized evolutionary operator

In this section we prove that the eigenvalues of the linearized version of equation (2.1) are real. We then employ this result to perform a linear-stability analysis of the steady solutions of (P1) which bifurcate from infinity.

**THEOREM 3.1** *The eigenvalues of the formal linearized version of (2.1) subject to boundary conditions (2.3) are real.*

*Proof.* The linearized version of (2.1) has eigenvalues  $\omega$  and corresponding eigenfunctions  $G(x)$  determined, for  $U(x)$  the solution of (2.1) and (2.3), by

$$\omega G = (K(U)G)_{xx} + \lambda H(U - 1)f'(U)G, \tag{3.1}$$

with

$$G_x(0) = G(1) = 0 \tag{3.2}$$

and the jump condition

$$\int_{s_-}^{s_+} (K(U)G)_{xx} dx + \lambda \int_{s_-}^{s_+} \delta(U - 1)f(U)G dx = 0. \tag{3.3}$$

Here we have interpreted the derivative of the Heaviside step function as a Dirac delta function in the sense of generalized functions (see (Lighthill, 1970)). Integrating (3.3) gives the jump condition

$$K(1)[G']_{x=s} = \frac{\lambda f(1)G(s)}{U_x(s)}, \tag{3.4}$$

which represents the effect of perturbing the free boundary.

Using the standard technique employed in the analysis of the stability of inviscid fluid flows (Drazin & Reid, 1981) we multiply (3.1) by  $(K(U)G)^*$  (where  $*$  denotes complex conjugation), integrate by parts, and take the imaginary part. This gives

$$K(1)^2 \operatorname{Im} [G'(s_-)G^*(s_-)] - \operatorname{Im}(\omega) \int_0^{s_-} K(U) |G|^2 dx = 0$$

and

$$-K(1)^2 \operatorname{Im} [G'(s_+)G^*(s_+)] - \operatorname{Im}(\omega) \int_{s_+}^1 K(U) |G|^2 dx = 0.$$

Adding these and using the jump condition (3.4) gives us

$$K(1)^2 \operatorname{Im} \left[ \frac{-\lambda f(1)}{U_x(s)} |G|^2 \right] - \operatorname{Im}(\omega) \int_0^1 K(U) |G|^2 dx = 0.$$

Since  $f(U)$  and  $K(U)$  are real-valued functions, this gives

$$\operatorname{Im}(\omega) \int_0^1 K(U) |G|^2 dx = 0.$$

As we are considering eigenvalues  $\omega$ ,  $G \neq 0$  and in addition  $K(U) > 0$ ; thus the result follows.

**COROLLARY** *No Hopf bifurcation can occur in problem (P1).*

(This result may also be proved by constructing a Liapunov function.)

### 3.1 The Semilinear Equation $\lambda \gg 1$

We construct a power-series expansion for the solution of the symmetric steady problem defined by (2.1) and (2.3), for  $\lambda \gg 1$  and  $\|U\|_\infty \sim 1$ . We then show that this solution is linearly unstable.

We anticipate from (2.8) that for  $\lambda \gg 1$ ,  $s$  will be small. Thus we rescale the independent variable  $x = sy$ , for  $0 < x < s$ , to obtain from (2.1) and (2.3)

$$(K(U)U_y)_y + \lambda s^2 f(U) = 0, \tag{3.5}$$

and

$$U_y(0) = 0 \quad \text{and} \quad U(1) = 1. \tag{3.6}$$

We seek expansions of the form

$$U = 1 + U_1/\lambda^\delta \quad \text{and} \quad s = s_1/\lambda^{\frac{1}{2}(\delta+1)}$$

giving, for  $0 < x < s$ ,

$$U(x) \sim 1 + \frac{s_1^2 f(1)}{2K(1)} \left[ 1 - \frac{x^2 \lambda^{\delta+1}}{s_1^2} \right] \frac{1}{\lambda^\delta} \tag{3.7}$$

and

$$U_x(s) \sim -\frac{f(1)}{K(1)} \lambda x. \tag{3.8}$$

Solving equations (2.1) and (2.3) in  $s < x < 1$  yields

$$U_x(s) = -\frac{\int_0^1 K(\xi) d\xi}{(1-s)K(1)} \sim -\frac{\int_0^1 K(\xi) d\xi}{K(1)}. \tag{3.9}$$

Imposing continuity of  $U_x(s)$  at  $x = s$  we obtain

$$\frac{\int_0^1 K(\xi) d\xi}{K(1)} = \frac{f(1)s_1}{K(1)\lambda^{\frac{1}{2}(\delta-1)}}, \tag{3.10}$$

and so we deduce that  $\delta = 1$  and  $s_1 = \int_0^1 K(\xi) d\xi / f(1)$ .

**THEOREM 3.2** *The power-series expansion for  $U(x)$  as  $\lambda \rightarrow \infty$  derived above is convergent.*

*Proof.* The proof employs local bifurcation theory and may be found in (Stuart, 1987).

We now perform a linear stability analysis for the steady solutions corresponding to  $U(0) \sim 1$ ,  $\lambda \gg 1$  in the case of linear diffusion ( $K(U) \equiv 1$ ). The results may also be proved for non-constant  $K$  but we do not detail this case in order to clarify the exposition. Seeking perturbations to the steady solutions of the form  $e^{\omega t} G(x)$  yields the eigenvalue problem

$$\omega G = G_{xx} + \lambda H(U - 1) f'(U) G, \tag{3.11}$$

with

$$G_x(0) = G(1) = 0 \tag{3.12}$$

and the jump condition

$$[G']_{x=s} = \frac{\lambda f(1)G(s)}{U_x(s)}. \tag{3.13}$$

(This is taken from equations (3.1), (3.2) and (3.4) with  $K \equiv 1$ .) Again, since  $s \ll 1$  for  $\lambda \gg 1$  we rescale the equation for  $0 < x < s$  by setting  $y = x/s$ . We obtain

$$G_{yy} + s^2(\lambda f'(U) - \omega)G = 0, \tag{3.14}$$

subject to  $G_y(0) = 0$ .

We seek expansions such that  $s^2\omega \sim \omega_0 + \omega_1/\lambda + \dots$  and  $G \sim G_0 + O(\lambda^{-1})$ . Then  $G_0$  satisfies

$$G_{0yy} - \omega_0 G_0 = 0 \quad \text{and} \quad G_{0y}(0) = 0.$$

This gives, in  $0 < x < s$ ,

$$G_0(x) = A \cosh(\omega_0^{1/2} x/s)$$

and

$$G_{0x}(x) = \frac{A\omega_0^{1/2}}{s} \sinh(\omega_0^{1/2} x/s).$$

In  $s < x < 1$   $G$  satisfies  $G_{xx} - \omega G = 0$  and  $G(1) = 0$  and hence

$$G_0 \sim G = B \sinh(\omega_0^{1/2}(1-x)/s).$$

Imposing continuity of  $G_0(s)$  at  $x = s$  implies that

$$A \cosh \omega_0^{1/2} = B \sinh(\omega_0^{1/2}(1-s)/s),$$

and using this in the jump condition (3.13) gives the following expression for  $\omega_0$ :

$$-\frac{\omega_0^{1/2}}{s} \cosh \omega_0^{1/2} \coth\left(\omega_0^{1/2} \frac{1-s}{s}\right) - \frac{\omega_0^{1/2}}{s} \sinh \omega_0^{1/2} = \frac{\lambda f(1)}{U_x(s)} \cosh \omega_0^{1/2}. \tag{3.15}$$

However, from equations (3.9) and (3.10) we know that  $U_x(s) \sim -s_1 f(1)$  and, as  $s \sim s_1/\lambda \ll 1$ , (3.15) reduces to

$$\omega_0^{1/2}(1 + \tanh \omega_0^{1/2}) = 1. \tag{3.16}$$

The only solution of this equation is  $\omega_0 \sim 0.4086$  and hence we have demonstrated the existence of a positive eigenvalue  $\omega \sim 0.4086\lambda^2/s_1^2$ . This result shows that the branch of solutions bifurcating from infinity is linearly unstable as a solution of problem (P1).

*Note.* In the case where  $K(u)$  is constant and  $f(u) = 1 + au$  a similar analysis demonstrates that in the neighbourhood of  $\|U\| = \infty$  (where  $\lambda = \pi^2/4a$ ; see Section 4) the branch of solutions is stable.

**4. Local stability of the fold point for  $K(u) \equiv 1$  and  $f(u)$  linear**

In the following section we consider problem (P1) in the case where  $K(u) = 1$  and  $f(u) = 1 + au$ . (By virtue of the transformation described in Section 2 the

results on the steady problem also apply to functions  $K(u)$  and  $f(u)$  related by  $f^{-1}(1 + aw) = S^{-1}(w)$ , where  $S'(w) = K(w)$ ). In this case the non-trivial solution of the steady problem may be found explicitly, and is given by

$$U(x) = \begin{cases} -\frac{1}{a} + \left(\frac{a+1}{a}\right) \frac{\cos(\lambda a)^{\frac{1}{2}} x}{\cos(\lambda a)^{\frac{1}{2}} s} & \text{for } 0 < x < s, \\ \left(\frac{1-x}{1-s}\right) & \text{for } s < x < 1. \end{cases} \tag{4.1}$$

The continuity condition on  $U_x(s)$ , which determines  $s$ , is

$$\left(\frac{a+1}{a}\right)(\lambda a)^{\frac{1}{2}} \tan(\lambda a)^{\frac{1}{2}} s = \frac{1}{1-s}. \tag{4.3}$$

Using equations (2.4) to (2.6), the equation for the bifurcation curve is

$$(\lambda a)^{\frac{1}{2}} = [(1 + aU(0))^2 - (1 + a)^2]^{-\frac{1}{2}} + \frac{\pi}{2a} - \frac{1}{a} \sin^{-1}\left(\frac{1+a}{1+aU(0)}\right), \tag{4.4}$$

with  $s$  determined by

$$(1-s) = \left(\frac{s}{\lambda}\right)^{\frac{1}{2}} [(1 + aU(0))^2 - (1 + a)^2]^{-\frac{1}{2}}. \tag{4.5}$$

The curve (4.4) is plotted in Fig. 1. Note the presence of a fold point at  $\lambda = \lambda_c$ ,  $U(0) = U_c$ . The number of solutions of the steady problem may be summarized as follows:

- (i) one solution ( $U \equiv 0$ ) for  $0 \leq \lambda < \lambda_c$ ,
- (ii) two solutions for  $\lambda = \lambda_c$ ,
- (iii) three solutions for  $\lambda_c < \lambda < \pi^2/4a$ ,
- (iv) two solutions for  $\lambda \geq \pi^2/4a$ .

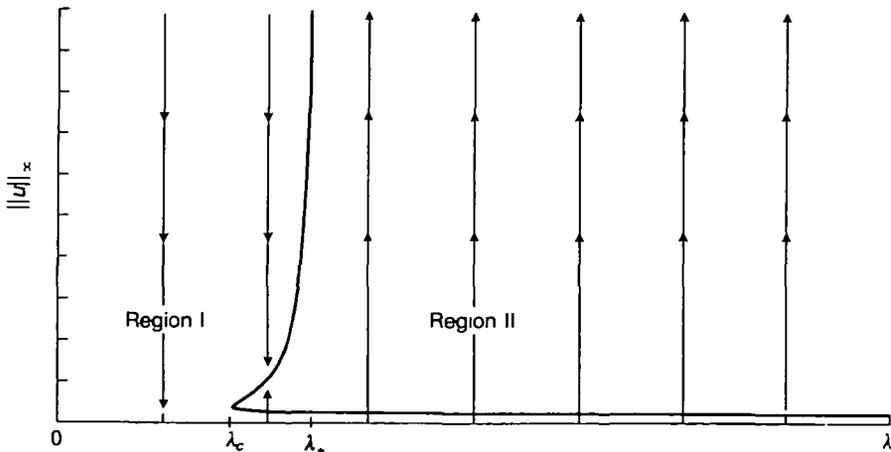


FIG. 1. The bifurcation curve (4.4);  $\lambda_* = \pi^2/4a$

By differentiating expression (4.4) with respect to  $U(0)$  we can determine  $U_c$ . Substituting this back into (4.4) and (4.5) gives  $\lambda_c$  and  $s_c$ . These values at the fold point are

$$\left(\frac{\lambda_c}{a}\right)^{\frac{1}{2}} = \frac{1}{(1+a)a^{\frac{1}{2}}} + \frac{\pi}{2a} - \frac{1}{a} \sin^{-1}[(1+a)^{\frac{1}{2}}]. \tag{4.6}$$

$$U_c = -\frac{1}{a} + \frac{(1+a)^{\frac{1}{2}}}{a} \tag{4.7}$$

and

$$1 - s_c = \frac{1}{(1+a)(\lambda_c)^{\frac{1}{2}}}. \tag{4.8}$$

**THEOREM 4.1** *The point  $(U_c, \lambda_c)$  is a point of neutral stability, according to linear theory. In its neighbourhood the upper branch of solutions (see Fig. 1) corresponds to locally stable solutions and the lower branch to locally unstable solutions.*

*Proof.* Seeking perturbations to the steady problem  $U(x)$  of the form  $e^{\omega t}G(x)$  leads us to the following eigenvalue problem for  $\omega$ :

$$G_{xx} - \omega G + \lambda H(U - 1)aG = 0, \tag{4.9}$$

with

$$G_x(0) = G(1) = 0 \tag{4.10}$$

and jump condition

$$[G']_{x=s} = \lambda(1+a)G(s)/U_x(s). \tag{4.11}$$

(This eigenvalue problem derives from equations (3.1), (3.2), and (3.4) with  $K(u) \equiv 1$  and  $f(u) = 1 + au$ .) Solving the two ordinary differential equations and applying the jump condition gives an expression  $E(\omega) = 0$  to determine  $\omega$ , where, for  $0 < \omega < a\lambda$ ,

$$E(\omega) = (\lambda a - \omega)^{\frac{1}{2}} \tan(\lambda a - \omega)^{\frac{1}{2}} s - \omega^{\frac{1}{2}} \coth \omega^{\frac{1}{2}}(1-s) + \lambda(1+a)(1-s)$$

and, for  $a\lambda \leq \omega$ ,

$$E(\omega) = -(\omega - \lambda a)^{\frac{1}{2}} \tanh(\omega - \lambda a)^{\frac{1}{2}} s - \omega^{\frac{1}{2}} \coth \omega^{\frac{1}{2}}(1-s) + \lambda(1+a)(1-s).$$

By Theorem 3.1 we know that all solutions of this equation lie on the real axis. Also,  $E(\omega)$  is a continuous function of  $\omega$  for  $\omega > 0$ ,  $E'(\omega) < 0$  for all  $\omega > 0$  whenever  $\lambda < \pi^2/4a$  and  $\lim_{\omega \rightarrow \infty} E(\omega) = -\infty$ . Thus the linear-stability properties of the steady solutions with  $\lambda < \pi^2/4a$  are determined entirely by  $E(0)$ . If  $E(0) > 0$  there exists a positive eigenvalue  $\omega = 0$ , indicating instability. If  $E(0) = 0$  we have an eigenvalue  $\omega = 0$  and thus we have neutral stability. If  $E(0) < 0$  then there are no non-negative eigenvalues and hence we expect stability. Consequently we examine  $E(0)$ .

Now

$$\lim_{\omega \rightarrow 0} E(\omega) = (\lambda a) \tan(\lambda a) s - \frac{1}{(1-s)} + \lambda(1+a)(1-s).$$

Using the matching condition (4.3) this expression may be rewritten as

$$E(0) = \lambda(1+a)(1-s) - \left(\frac{1}{1-s}\right)\left(\frac{1}{1+a}\right).$$

We now examine  $E(0)$  in the neighbourhood of the fold point. Perturbing (4.7) to give

$$U(0) = -\frac{1}{a} + \frac{(1+a)^{\frac{1}{2}}}{a} + \varepsilon = U_c + \varepsilon,$$

we find from equations (4.4) and (4.5) that

$$\left(\frac{\lambda}{a}\right) = \left(\frac{\lambda_c}{a}\right) + O(\varepsilon^2) \quad (4.12)$$

and

$$(1-s) = \frac{1}{(1+a)\lambda_c^{\frac{1}{2}}} - \frac{\varepsilon}{(1+a)^{\frac{3}{2}}\lambda_c^{\frac{1}{2}}} + O(\varepsilon^2). \quad (4.13)$$

Substituting these expressions into  $E(0)$  shows that in the neighbourhood of the fold point we have

$$E(0) \sim -\frac{2\lambda_c^{\frac{1}{2}}\varepsilon}{(1+a)^{\frac{1}{2}}}.$$

Since the upper branch corresponds to  $\varepsilon > 0$ , the fold point to  $\varepsilon = 0$  and the lower branch to  $\varepsilon < 0$ , the result follows.

The work of Section 3 indicates that the end points of the global steady solution branch shown in Fig. 1 have the corresponding stabilities in the neighbourhood of the fold point. Since there are no secondary bifurcations on the solution branch we deduce that the entire upper branch is locally stable and that the entire lower branch is locally unstable. Furthermore, we expect that the global time-dependent behaviour of (P1) will be as indicated by the arrows in Fig. 1.

In Norbury and Stuart (1987b) the maximum principle is employed to prove rigorously that all ordered data (that is data lying strictly above or below a steady solution) evolve according to the arrows shown in Fig. 1. An energy method is also employed to prove that for  $\lambda < \lambda_c$ ,  $u \rightarrow 0$  as  $t \rightarrow \infty$ , for all initial data.

We may employ the results summarized in Fig. 1 to discuss the validity of the approximation of temperature by the equation (P1) for small driving velocities  $\mu$ . This approximation can become invalid after a sufficient length of time as the effect of solid reactant consumption becomes significant. Specifically, when the product of time  $t$  and reaction rate  $f(u)$  becomes of  $O(\mu^{-1})$ , in addition to the temperature remaining bounded above unity on a finite interval, the effect of solid reactant consumption must be included in (P1).

The results in this section indicate that for  $\lambda < \lambda_c$  equation (P1) remains a valid approximation to the temperature for small driving velocities for all time, since  $u \rightarrow 0$  as  $t \rightarrow \infty$  for all initial data. For  $\lambda_c \leq \lambda$  the results show that again the

approximation is valid for all time provided that the initial temperature profile lies strictly below the lower (unstable) solution branch shown in Fig. 1, since then  $u \rightarrow 0$  as  $t \rightarrow \infty$ . Thus combustion is not sustained, nor are appreciable quantities of reactant consumed, for these ranges of parameter and initial data.

For  $\lambda_c \leq \lambda < \pi^2/4a$  with initial data lying above the lower solution branch,  $u$  remains bounded above unity on an interval of finite length for all time; also  $u(x, t)$  evolves to a solution on the upper branch in Fig. 1 as  $t \rightarrow \infty$ . In this case the effect of reactant consumption becomes important and the approximation breaks down for times of  $O(\mu^{-1/2})$ . Finally, if  $\lambda \geq \pi^2/4a$  and the initial data lies above the lower solution branch then  $u$  grows without bound. In (Norbury and Stuart, 1987b) it is shown that the rate of growth is exponential in time and thus the small driving velocity approximation breaks down on a time-scale of  $O(\ln \mu)$ .

In this section we have considered only the specific case of  $K(u) = 1$  and  $f(u) = 1 + au$ . However, by employing the global results in (Norbury and Stuart, 1987b) more general classes of nonlinearity may be treated in a similar fashion.

**5. Numerical results**

A description and evaluation of various numerical methods for parabolic problems of the form (P1) is given in (Stuart, 1985). In this section we describe numerical results obtained by implementing the most effective of these methods on problem (P1), with  $K(u) = 1$  and  $f(u) = 1 + au$ . The method employs a coordinate transformation (see (Landau, 1950)) to fix the position of the moving boundary  $s(t)$ ; the continuity of the spatial derivative is imposed to determine  $s(t)$ . It is worth noting that the same transformation of coordinates is of analytic value in deriving comparison principles. See (Norbury & Stuart, 1987b).

The results are shown in Figs 2, 3, and 4. Figure 2 shows how data lying

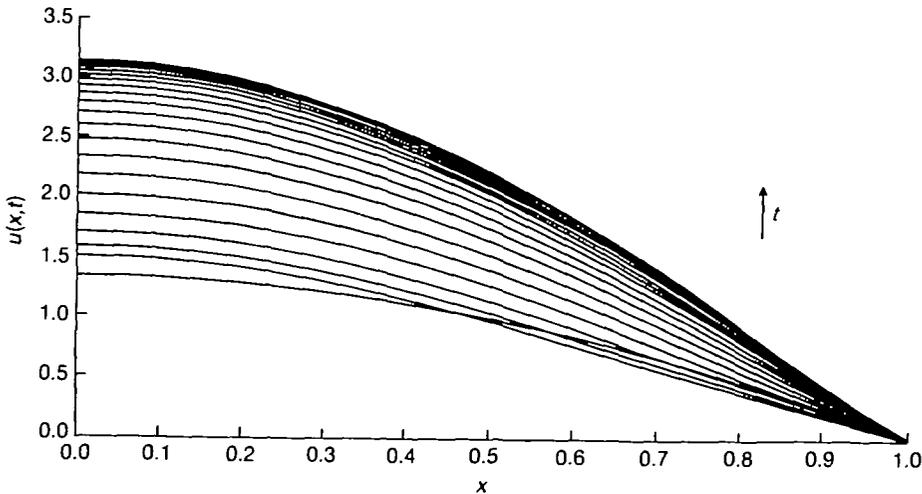


FIG. 2. The solution of equation (P1);  $f(u) = 1 + au$ ,  $K(u) = 1$

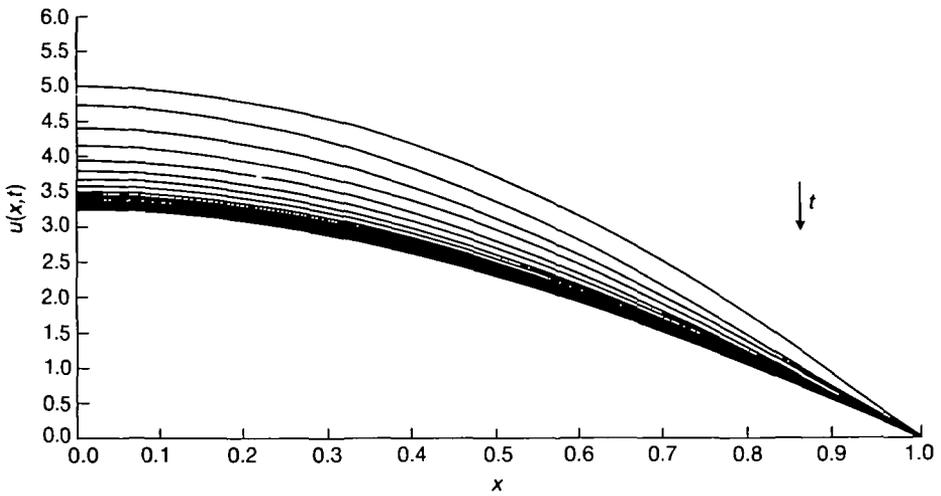


FIG. 3. The solution of equation (P1);  $f(u) = 1 + au$ ,  $K(u) = 1$

between the unstable and non-trivial stable branches in Fig. 1 evolve towards the upper stable branch as  $t$  increases. In Fig. 3 we see the evolution of data lying above the stable branch towards the stable branch. Finally, in Fig. 4, we show the evolution of data lying above the unstable branch in the parameter regime  $\lambda > \pi^2/4a$ . In this case there is no upper limiting steady state and we see how the solution grows without bound.

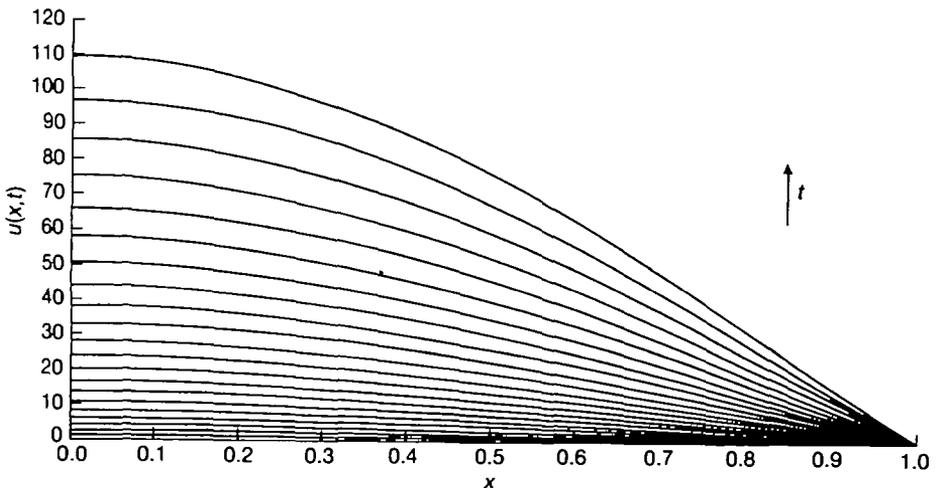


FIG. 4. The solution of equation (P1);  $f(u) = 1 + au$ ,  $K(u) = 1$

**6. The validity of the discontinuous approximation**

We now consider the semilinear parabolic equation

$$\left. \begin{aligned} u_t &= \Delta u + \lambda g(u; \varepsilon) \quad \text{in } \Omega \times (0, T), \\ \text{with } u &= 0 \text{ on } \delta\Omega \times (0, T) \text{ and some initial conditions.} \end{aligned} \right\} \quad (6.1)$$

Here  $\delta\Omega$  is the (smooth) boundary of  $\Omega$ ,  $\lambda \geq 0$  and the function  $g(u; \varepsilon)$  is defined by

$$g(u; \varepsilon) = \frac{f(u)}{1 + \exp((1 - u)/\varepsilon)}, \quad (6.2)$$

where  $f(u) \geq 0$  and  $f(u) \in C^2(0, \infty)$ . We examine the case of  $\varepsilon \ll 1$ . It is clear that

$$\lim_{\varepsilon \rightarrow 0} g(u) = H(u - 1)f(u). \quad (6.3)$$

Hence a natural approximation to equation (6.1) for small  $\varepsilon$  is

$$\left. \begin{aligned} u_t &= \Delta u + \lambda H(u - 1)f(u) \quad \text{in } \Omega \times (0, T), \\ \text{with } u &= 0 \text{ on } \delta\Omega \times (0, T). \end{aligned} \right\} \quad (6.4)$$

This approximation is not uniformly valid in  $\lambda$  — more specifically it breaks down for values of  $\lambda$  of order  $\exp(1/\varepsilon)$ . Thus we might expect that the qualitative behaviour of equation (6.4) and equation (6.1) (subject to the same initial and boundary conditions) will be the same for moderate values of  $\lambda$ . However, for large values of  $\lambda$  we expect the behaviour to be different.

Consider the time-independent solutions of (6.1) and (6.4). Note that equation (6.4) possesses the trivial solution  $U \equiv 0$  whereas, in general, equation (6.1) does not. Furthermore, when considered as a steady solution of the evolution equation (6.4), the trivial solution is stable. Thus we expect that, for moderate values of  $\lambda$ , there will be a corresponding small-norm solution to equation (6.1) which is stable.

**THEOREM 6.1** *There exists a positive steady solution of equation (6.1) whenever there exists a positive solution  $V$  of the equation*

$$\Delta V + \lambda f(V) = 0 \quad \text{in } \Omega \quad \text{and} \quad V = 0 \quad \text{on } \delta\Omega. \quad (6.5)$$

*Furthermore, this solution is a stable solution when viewed as a steady state of equation (6.1).*

*Proof.* The proof is by the method of upper and lower solutions (described in (Smoller, 1982: Theorem 10.3)). Since any solution constructed by this method is a stable solution of the corresponding parabolic equation, we need only demonstrate the existence of a positive solution.

We take zero as our lower solution, since

$$\Delta 0 + \lambda g(0; \varepsilon) = \lambda f(0)/[1 + \exp(1/\varepsilon)] \geq 0.$$

As our upper solution we take  $V$ , since

$$\Delta V + \lambda g(V; \varepsilon) \leq \Delta V + \lambda f(V) = 0$$

and  $V = 0$  on  $\delta\Omega$ . As the upper solution is assumed to be positive and the lower solution is zero the proof is complete.

Now we return to the specific piecewise linear problem that we considered in Section 4. Thus  $\Omega = (-1, 1)$  and  $f(u) = 1 + au$ . In this case equation (6.5) is a linear ordinary differential equation and the solution is

$$V = \frac{1}{a} \left( \frac{\cos\{(\lambda a)^{\frac{1}{2}}x\}}{\cos\{(\lambda a)^{\frac{1}{2}}\}} - 1 \right).$$

Hence  $V$  is a positive solution provided that  $\lambda < \pi^2/4a$ . We now have the following theorem.

**THEOREM 6.2** *In the case  $\Omega = (-1, 1) \in \mathbb{R}^1$  and  $f(u) = 1 + au$ , there exists a positive stable steady solution of equations (6.1), (6.2) for all  $\varepsilon$ , whenever  $\lambda < \pi^2/4a$ .*

*Proof.* The proof is a direct application of Theorem 6.1.

### 6.1 Bifurcation Diagram

Using Theorem 6.2 we compare the solutions of problems (P1) and (P2). We construct the bifurcation diagram for the steady solution of equation (6.1), in the case  $\Omega = (-1, 1)$  and  $f(u) = 1 + au$ .

As described in Section 2 it is advantageous to rescale the independent variable. Again we set  $y = \sqrt{\lambda} x$  and obtain

$$U_{yy} + g(U; \varepsilon) = 0 \quad \text{in } (-\sqrt{\lambda}, \sqrt{\lambda}) \quad \text{with } U(\pm\sqrt{\lambda}) = 0. \quad (6.6)$$

If we seek symmetric solutions we have

$$U_y(0) = 0 \quad (6.7)$$

and so for each value of  $U(0) \equiv \|U\|_\infty$  we may determine the appropriate value of  $\lambda$  by integrating (6.6) numerically, subject to (6.7), until we reach  $\bar{y} : U(\bar{y}) = 0$ . (Since  $U_{yy} < 0$  we are assured that this point exists.) We then have  $\lambda = \bar{y}^2$ . By plotting the locus of  $\lambda$  against  $\|U\|_\infty$  the bifurcation diagram may be constructed. Since  $\lambda$  is uniquely determined by  $\|U\|_\infty$  we automatically capture all the folds present in the bifurcation surface and avoid the numerical difficulties inherent in solving boundary-value problems with multiple solutions.

The results are shown in Fig. 5. Notice the three branches of solutions. This structure is characteristic of the solution to many elliptic equations arising in combustion theory (Aris, 1975). Since the lowest branch is unique for  $\lambda$  sufficiently small we deduce from Theorem 6.2 that it is stable, as a solution of the associated parabolic equation (6.1), for  $\lambda < \pi^2/4a$ . Furthermore, since equation (6.1) is in gradient form, we know that no Hopf bifurcation is possible (Berger, 1977) and thus that the whole lower branch is stable. However, at the

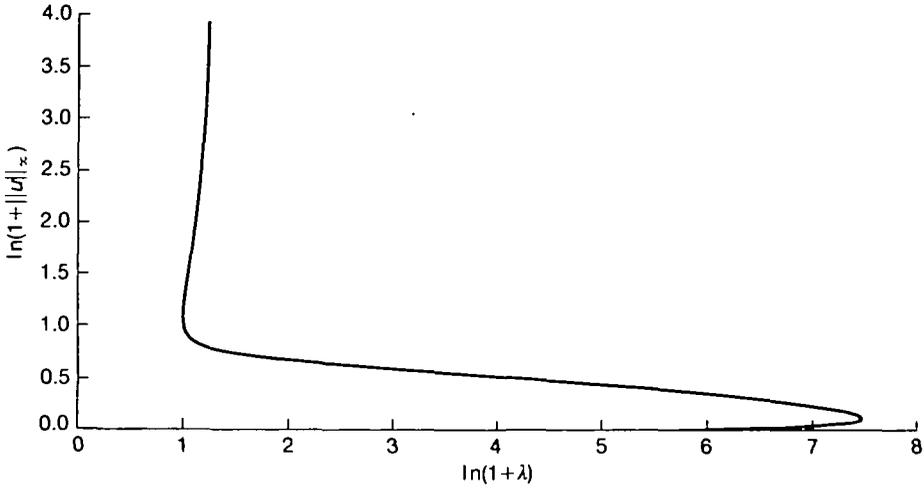


FIG. 5. The bifurcation diagram for equation (6.1);  $f(u) = 1 + au$ ,  $\varepsilon = 0.1$

two fold points, we expect a change in stability and thus we deduce that the middle branch is unstable and the upper branch stable.

If we now compare these results with those for the piecewise linear approximation of equation (6.6) summarized in Fig. 6, we see that the essential structure of the two bifurcation diagrams is the same for moderate values of  $\lambda$ , although the stable trivial state in Fig. 6 has been replaced by a stable solution of very small norm in Fig. 5. However, as conjectured earlier, the approximation breaks down for large values of  $\lambda$ .

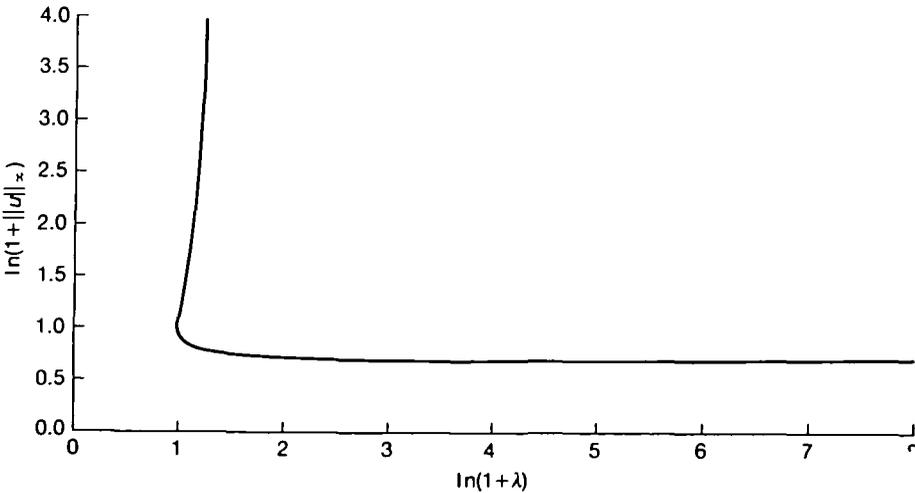


FIG. 6. The bifurcation diagram for equation (6.4);  $f(u) = 1 + au$

## 7. Conclusion

We have studied problem (P1) in detail. We have investigated the local stability properties of the steady solutions (Sections 3 and 4) and related these results to the global time-dependent behaviour of (P1). We have also described numerical calculations which complement the analytic study.

These results have enabled us to examine the validity of equation (P1) as an approximation for the evolution of temperature in highly exothermic chemical reactions with small driving velocities. In particular we can predict the parameter regimes in which, and the temporal scales on which, the effect of reactant consumption becomes important. This information is detailed at the end of Section 4.

We have also compared problems (P1) and (P2) and demonstrated that the approximation of (P2) by (P1) as  $\varepsilon \rightarrow 0$  (which corresponds to the large activation energy limit) is valid for moderate values of  $\lambda$  ( $\ll O(\exp(1/\varepsilon))$ ). In addition, the analysis of (P1) conducted in the limit  $\lambda \rightarrow \infty$  is of value since it may be employed to infer stability results for the whole (unstable) solution branch which exists for  $\lambda_c < \lambda < \infty$ ; see Fig. 1. These results are of importance because the approximating problem (P1) is frequently easier to analyse than (P2) and, in certain circumstances may be more suitable for numerical study. In addition, the limiting process linking problems (P1) and (P2) may be applied to the eight partial differential equations governing full porous-medium combustion—see (Norbury and Stuart, 1987a).

## Acknowledgement

The second author is grateful to the Science and Engineering Research Council for financial support.

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