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Similarity Solutions of a Heat Equation with Nonlinearly Varying Heat Capacity

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A reaction-diffusion equation, coupled through variable heat capacity and source term to a temporally evolving ordinary differential equation, is examined. The model is a prototype for the study of combustion processes where the heat capacity of a composite solid medium changes significantly as the reactant within the medium is consumed.

Similarity solutions are sought by analysing the invariance of the equations to various stretching groups. The resulting two-point boundary-value problem is singular at the origin and posed on the semi-infinite domain. By employing series expansion techniques we derive a *regular* problem posed on a *finite* domain. This problem is amenable to standard numerical solution by means of Newton–Kantorovich iteration. Results of the computations are presented and interpreted in terms of the governing partial differential equation.

1. Introduction

IN THIS paper we analyse the time-dependent problem

$$\sigma u_t = u_{xx} + \sigma^p u^q \quad \text{and} \quad \sigma_t = -\lambda \sigma^p u^q,$$

together with the boundary conditions

$$u(0, t) = A > 0 \quad \text{and} \quad \lim_{x \to \infty} u(x, t) = 0,$$

and initial conditions

$$u(x, 0) = 0 \quad \text{and} \quad \sigma(x, 0) = \sigma_0(x) > 0.$$

We call this the problem (P).

The variable u represents a (non-dimensional) temperature, governed by a reaction-diffusion equation, and σ is a (non-dimensional) heat capacity, governed by an ordinary differential equation. Our motivation is the study of chemically reacting systems in which the solid (non-diffusing) reactant forms a significant proportion of the composite solid comprising the one reactant and various inerts. In such cases the variation of physical properties associated with the composite solid, such as the overall heat capacity, must be allowed for—as reactant is consumed these properties can change significantly. We assume that $\lambda > 0$ so that the heat capacity decreases as the reaction progresses. In the theory of homogeneous combustion it is frequently assumed that the concentration of inerts is large relative to that of the reactant, and significant progress can be made upon the assumption of constant heat capacities [3, 9]. However, in the theory of

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heterogeneous combustion it is necessary to allow for the variation of heat capacity with reactant concentration in order that sustained combustion can occur (see [10: Theorem 4.1]).

Problem (P) defines the canonical problem for chemically reacting systems in which the variation of heat capacity is significant. Typically the heat capacity is linearly related to the reactant concentration so that (P) defines the simplest system governing evolution of solid temperature and concentration. The form of reaction term ($\propto \sigma^p u^q$) is chosen to have algebraic dependence since this is the usual form arising in heterogeneous combustion; a more complete description of the relevance of (P) in porous-medium combustion is given in section 2. However, we believe that (P) is important in its own right as a prototype problem including the effect of a nonlinearly varying heat capacity in a reaction-diffusion equation.

In particular we are interested in the limiting behaviour of (P) as $t \to \infty$. We note that, for $\lambda > 0$, σ is a monotone decreasing function and that $\sigma(x, t) \to 0$ as $t \to \infty$. Thus a singularity develops in the equation for u and we examine this effect. Physically, the effect of a vanishing heat capacity can be interpreted as modelling a combustion process in a porous solid in which the residue (ash) has a negligible heat capacity. Thus, as all the reactant is consumed, the composite solid tends to a limiting state with negligible heat capacity.

In section 2 we derive problem (P) as a distinguished limit of the equations governing porous-medium combustion. The group invariance of (P) under stretching transformations is discussed in section 3 and appropriate similarity variables deduced; thus (P) may be reduced to the study of a third-order boundary-value problem on $\mathbb{R}^+$ with a singularity at the origin. This singularity forces a constraint on two components of the solution at the origin if the necessary regularity (for the partial differential equation) is imposed.

In section 4 we prove local existence of a one-parameter family of solutions to the initial-value problem satisfying the constraint at the origin. The proof employs the contraction mapping theorem to prove the existence of a solution lying close to an appropriate series expansion. In section 5 we deduce the asymptotic behaviour of the ordinary differential equations at infinity.

By employing the series expansion constructed and validated in section 4 we may define a regular shooting problem for the numerical solution of the boundary-value problem on $\mathbb{R}^+$, avoiding numerical difficulties associated with the singularity at the origin; furthermore, by utilizing the analysis at infinity from section 5, we derive a shooting problem posed on a finite domain. This regularization is described in section 6. We use Newton–Kantorovich iteration to solve the regularized problem, and a global a priori bound is derived and employed to simplify the initial guess for the iteration. In section 7 numerical results are presented and interpreted in the context of problem (P).

2. Derivation and discussion of the model

In [11] a simplified model for porous medium combustion is derived with the form

$$\sigma_t = -\lambda r, \tag{2.1}$$

$$\sigma u_t = u_{xx} + (w - u) + r, \tag{2.2}$$

$$\mu w_x = (u - w), \tag{2.3}$$

$$g_x = -ar/\mu, \tag{2.4}$$

where the reaction rate r is given by

$$r = \mu^{\frac{1}{2}} H(u - u_c) H(\sigma - \sigma_c) g f(w). \tag{2.5}$$

Here $H(\cdot)$ is the Heaviside unit step function defined by $H(X) = 0$ if $X \leq 0$ and $H(X) = 1$ if $X > 0$. Typically $f(w) \propto w^q$ (see [2, 11]). In [6] it is proved that this model has a solution globally defined in time (for arbitrary positive $f(w)$).

The variables σ, u, w and g represent respectively, the (scaled) solid heat capacity, solid and gas temperatures and the flux of oxygen, respectively. The heat capacity σ is related to the solid concentration γ by

$$\sigma = \sigma_c + \lambda\gamma,$$

where λ is proportional to the specific heat of the combustion solid.

The assumptions made in deriving (2.1) to (2.5) are as follows.

(i) The non-dimensional activation energy is large—this results in the discontinuous form (2.5) for the reaction rate.

(ii) The ratio of gas heat storage to solid heat storage is small—this means that the time-derivative of the gas temperature may be neglected, resulting in equation (2.3).

(iii) The rate of consumption of oxygen and the rate of production of carbon dioxide are nearly equal and the specific heats of these two gases are nearly equal—this allows the effect of the gas velocity field to be reduced to a parameter-dependence of equations (2.1) to (2.5) on μ, proportional to the inlet gas velocity.

We emphasize that the limit process described below does not invalidate any of the assumptions (i) to (iii) made in deriving (2.1) to (2.5).

The reaction rate (2.5) shows that if *either* the solid temperature falls below a certain temperature, *or* the solid reactant is exhausted, then the reaction terminates. Otherwise the reaction proceeds at a rate proportional to $gf(w)$; this term represents the product of oxygen concentration and the rate of oxygen diffusion into the reaction sites in the solid. In [11] an expression for this rate of oxygen diffusion is employed following the experimental work of Baker [2]. This expression is independent of the concentration of solid reactant. It is possible, however, that the effect of reactant concentration *can* affect the rate of oxygen diffusion since the surface area of reactant changes significantly as it is consumed and since the shrinking reactant is surrounded by an increasing quantity of ash. This effect can be allowed for by letting the expression for oxygen diffusion be proportional to γ^p ($p > 0$). If this is done, then an analysis similar to that in [11] shows that, in the limit of large activation energy, r takes the form

$$r = \mu^{\frac{1}{2}} H(u - u_c) g f(w) (\sigma - \sigma_c)^p / \lambda^p, \qquad p \geq 1.$$

By considering only the case when $p \geq 1$ we prevent the possibility of finite-time exhaustion of the solid $\gamma = (\sigma - \sigma_c)/\lambda$, so that the $H(\sigma - \sigma_c)$ term no longer appears. We assume that $p \geq 1$ henceforth. With $f(w)$ in the form prescribed above we obtain

$$r = \mu^{\frac{1}{2}} d H(u - u_c) g w^q (\sigma - \sigma_c)^p / \lambda^p. \tag{2.6}$$

We now examine (2.1) to (2.4) and (2.6) in the distinguished limit

$$\mu \to 0, \quad \mu^{\frac{1}{2}} d \to \text{const.}, \quad a\mu^{-\frac{1}{2}} \to \text{const.}, \quad \sigma_c \mu^{-\frac{1}{2}} \to \text{const.},$$

where the constants are of $O(1)$ with respect to μ. Expanding in powers of $\mu^{\frac{1}{2}}$ and substituting into (2.1) to (2.5) yields

$$\sigma_{0t} = -\lambda r_0, \qquad \sigma_0 u_{0t} = u_{0xx} + r_0,$$
$$w_0 = u_0, \qquad g_0 = \text{const.},$$
$$r_0 \propto H(u_0 - u_c)\sigma_0^p w_0^q.$$

Here a subscript zero denotes an $O(1)$ quantity. We have assumed that the initial conditions are compatible with the assumption that $w_0 = u_0$; that is, we assume that initially the gas and solid phases are at the same temperature to within variations of $O(\mu^{\frac{1}{2}})$. We have also assumed that the oxygen flux at the boundary is constant so that g_0 is constant in both space and time.

If we scale the independent variables appropriately (posing the problem on $x > 0$) and neglect the $H(u_0 - u_c)$ contribution to r_0 then we obtain (P) (dropping the subscripts zero). Ignoring the switch term, $H(u_0 - u_c)$ may be formally justified provided that u_c is small; we make this assumption.

We do not claim that the limiting process described above to derive (P) from (2.1) to (2.5) corresponds very closely to any naturally occurring combustion phenomena: the parameter μ represents the inlet gas velocity through the porous medium, d is a scaled heat of reaction and a determines the rate of oxygen consumption relative to that of the solid reactant. Thus the limit process above describes the highly exothermic combustion of a porous solid fuel in a slowly driven gas flow with negligible oxygen depletion. None the less, by considering the limit, we have extracted a problem (P) which describes the coupling between the equations for solid temperature and solid heat capacity. This coupling is of paramount importance in the analysis of the full model defined by (2.1) to (2.5)—in particular in determining parameter regimes of existence and non-existence for sustained combustion; see [10, 12]—and the limiting process may be justified purely as a means of elucidating this coupling further.

3. The group invariance of (P); Similarity solutions

We examine the group invariance of (P) under the scalings

$$\sigma' = \lambda^\alpha \sigma, \quad u' = \lambda^\beta u, \quad t' = \lambda^\gamma t, \quad x' = \lambda x.$$

By determining the values of α, β and γ for which (P) is invariant under these transformations we can determine appropriate similarity variables [4]. Substitution demonstrates that (P) is invariant for $\alpha = -2/p$, $\beta = 0$ and $\gamma = 2(p-1)/p$.

Following Dresner [4] we deduce that (P) admits solutions of the form

$$u(x,t)=f(\eta) \quad \text{and} \quad \sigma(x,t)=t^{-1/(p-1)}g(\eta),$$

where $\eta=xt^{-p/2(p-1)}$.

Substituting these similarity forms into (P) we obtain the following boundary-value problem: find a pair $(f,g)\in C^2(0,\infty)\times C(0,\infty)$ satisfying

$$f''+\frac{p\eta g f'}{2(p-1)}+g^p f^q=0, \tag{3.1}$$

$$p\eta g'+2g-2\lambda(p-1)g^p f^q=0, \tag{3.2}$$

where the prime means differentiate with respect to η. Here, and throughout the following, $C^n(a,b)$ denotes the space of functions whose first n derivatives are continuous on the *closed* interval $[a,b]$ (unless $b=\infty$ in which case the interval is open at the right-hand end.)

The initial and boundary conditions on $u(x,t)$ transform to

$$f(0)=A \quad \text{and} \quad \lim_{\eta\to\infty} f(\eta)=0. \tag{3.3}$$

If we assume that $\sigma(x,0)$ is bounded for all $x>0$ then we require that

$$\lim_{\eta\to\infty} \eta^{2/p}g(\eta)=1/C \quad (\text{of } O(1)). \tag{3.4}$$

Thus (3.3), (3.4) provide three boundary conditions for the third order system (3.1), (3.2).

Note that we only require continuity of $g(\eta)$. In fact $g(\eta)$ will be a C^1 function everywhere except at the origin. Since $g(\eta)$ is assumed to be uniformly continuous $g'(\eta)$ cannot grow as strongly as $1/\eta$ at the origin. This forces us to the conclusion that $g(0)=\lambda(p-1)g^p(0)f^q(0)$. For non-trivial solutions $g(\eta)$ this implies that

$$\lambda(p-1)g^{(p-1)}(0)f^q(0)=1. \tag{3.5}$$

Thus all uniformly continuous solutions of (3.1) to (3.4) must satisfy the constraint (3.5).

If we consider (3.1) to (3.4) as a shooting problem for fixed A and C then we require two shooting parameters at $\eta=0$ in order that we may satisfy both (3.3) and (3.4). In a regular shooting problem it would be natural to choose $f'(0)$ and $g(0)$ to be the two shooting parameters. However, the constraint (3.5) means that we are not free to choose $g(0)$. In the following section we prove that there exists a one-parameter family of solutions to the initial-value problem defined by (3.1), (3.2) and the constrained initial conditions

$$f(0)=A, \quad f'(0)=D, \quad \lambda(p-1)g^{(p-1)}(0)A^q=1. \tag{3.6}$$

Thus, by varying D, we have the two parameters required for a properly posed shooting problem.

Henceforth we specialize to the case in which $p=2$ and $q=1$ in order to simplify the algebra. However, the analysis may be extended to general p and q

in a fairly straightforward fashion. The case when $p=2$ and $q\neq 1$ is very similar and differs only in the algebra. The case when $p\neq 2$ requires more care as the nature of the singularity at $\eta=0$ is changed and a form other than (4.4) must be sought for $g(\eta)$.

4. Similarity solutions; $\eta \ll 1$

In the case when $p=2$ and $q=1$ equations (3.1), (3.2) reduce to

$$f''+\eta g f'+g^2 f=0, \tag{4.1}$$

$$\eta g'+g-\lambda g^2 f=0. \tag{4.2}$$

For fixed A, D and λ we prove the local existence of a *one-parameter family* of solutions satisfying (4.1), (4.2) and the initial conditions

$$f(0)=A, \quad f'(0)=D, \quad \lambda g(0)A=1. \tag{4.3}$$

Thus, although the singularity at $\eta=0$ in (4.2) forces a constraint on the initial conditions for (4.1), (4.2), this is compensated for by the fact that a one-parameter family of solutions satisfies the constrained initial-value problem (4.1) to (4.3). This result is important since the existence of this family of solutions is necessary to define a shooting problem which solves (3.1) to (3.4).

The proof proceeds by constructing power-series solutions to (4.1) to (4.3) and employing the contraction mapping theorem [7] to prove the existence of a solution lying close to the power-series construction. The key to the analysis is to find an appropriate integral-equation formulation for (4.2) subject to the (constrained) initial condition. Once this has been done, the proof follows by fairly standard use of the contraction mapping theorem, and we shall omit the tedious algebraic details.

We seek a solution of (4.2) satisfying

$$g(\eta)=[\lambda f(\eta)-\lambda\eta\,\mathrm{Ln}\,(\eta)f'(\eta)+B\eta+\lambda\eta k(\eta)]^{-1} \tag{4.4}$$

for *arbitrary* $B\in\mathbb{R}$, with $k(\eta)$ (a continuous function) to be found. Since B is arbitrary we set $k(0)=0$. Note that (4.4) implies that $g(0)=[\lambda f(0)]^{-1}$ as required by (4.3).

Substituting (4.4) into (4.2) yields $k'(\eta)=\mathrm{Ln}\,(\eta)f''(\eta)$. Thus we deduce from (4.4) that $g(\eta)$ satisfies the integral equation

$$g(\eta)=\left[\lambda f(\eta)-\lambda\eta\,\mathrm{Ln}\,(\eta)f'(\eta)+B\eta+\lambda\eta\int_0^\eta \mathrm{Ln}\,(\xi)f''(\xi)\,\mathrm{d}\xi\right]^{-1}. \tag{4.5}$$

Equivalently, by (4.1),

$$g(\eta)=\left[\lambda f(\eta)-\lambda\eta\,\mathrm{Ln}\,(\eta)f'(\eta)+B\eta \right.$$
$$\left. -\lambda\eta\int_0^\eta \mathrm{Ln}\,(\xi)(\xi g(\xi)f'(\xi)+g^2(\xi)f(\xi))\,\mathrm{d}\xi\right]^{-1}. \tag{4.6}$$

Note that (4.5), (4.6) are parametrized by $B \in \mathbb{R}$ and this is the key to establishing the existence of a one-parameter family of solutions of (4.1) to (4.3).

We now construct power series solutions of (4.1) to (4.3) and (4.5), seeking expansions for $f(\eta)$ and $g(\eta)$ of the form

$$f(\eta) \approx f_0 + f_1\eta + f_2\eta^2 + f_3\eta^3 \operatorname{Ln}(\eta) + O(\eta^3), \tag{4.7}$$

$$g \approx g_0 + g_1\eta \operatorname{Ln} \eta + g_2\eta + O(\eta^2 \operatorname{Ln}(\eta)). \tag{4.8}$$

Substituting (4.7), (4.8) into (4.5) yields the following expressions for the g_i:

$$g_0 = 1/\lambda f_0, \quad g_1 = f_1/\lambda f_0^2, \quad g_2 = -\frac{\lambda f_1 + B}{\lambda^2 f_0^2}. \tag{4.9}$$

Multiplying (4.1) through by g^{-2} and substituting (4.7) for $f(\eta)$ and (4.8), (4.9) for $g(\eta)$ we obtain the following expressions for the f_i:

$$f_2 = -1/2\lambda^2 f_0 \quad \text{and} \quad f_3 = -f_1/3\lambda^2 f_0^2. \tag{4.10}$$

Since, by (4.3) $f_0 = A$ and $f_1 = D$, equations (4.9), (4.10) determine series expansions for $f(\eta)$ and $g(\eta)$ respectively. We may now prove the following theorem.

THEOREM 4.1 *There exists $\bar{\eta} > 0$ such that equations* (4.1) *to* (4.3) *possess a one-parameter family of solutions $(f, g) \in C^2(0, \bar{\eta}) \times C(0, \bar{\eta})$, satisfying*

$$\left.\begin{aligned} &\|f(\eta) - \bar{f}(\eta)\| \leq C_1\bar{\eta}^3, \qquad \|h(\eta) - \bar{h}(\eta)\| \leq C_2\bar{\eta}^2, \\ &\|g(\eta) - \bar{g}(\eta)\| \leq C_3\bar{\eta}^2 \operatorname{Ln}(\bar{\eta}), \end{aligned}\right\} \tag{4.11}$$

where

$$h(\eta) \equiv f'(\eta), \qquad \|\cdot\| = \sup_{0 \leq \eta \leq \bar{\eta}} |\cdot|, \qquad \bar{f}(\eta) = f_0 + f_1\eta + f_2\eta^2 + f_3\eta^3 \operatorname{Ln}(\eta),$$

$$\bar{h}(\eta) = f_1 + 2f_2\eta + 3f_3\eta^2 \operatorname{Ln}(\eta), \qquad \bar{g}(\eta) = g_0 + g_1\eta \operatorname{Ln}(\eta) + g_2\eta.$$

Here f_i, $i = 0, \ldots, 3$ and g_i, $i = 0, \ldots, 2$ are as defined preceding the theorem, for arbitrary $B \in \mathbb{R}$.

Proof. The proof is a fairly standard application of the contraction mapping theorem and the details are omitted. Using equation (4.6), we may write (4.1) to (4.3) as the equivalent nonlinear integral equations:

$$f(\eta) = A + \int_0^\eta h(\xi)\, d\xi,$$

$$h(\eta) = D - \int_0^\eta [\xi g(\xi)h(\xi) + g^2(\xi)f(\xi)]\, d\xi,$$

$$g(\eta) = \left[\lambda f(\eta) - \lambda\eta \operatorname{Ln}(\eta)h(\eta) + B\eta - \lambda\eta \int_0^\eta \operatorname{Ln}(\xi)[\xi g(\xi)h(\xi) + g^2(\xi)f(\xi)]\, d\xi\right]^{-1}.$$

We now define the associated fixed point mappings

$$\left.\begin{aligned} f_{n+1}(\eta) &= A + \int_0^\eta h_n(\xi)\,\mathrm{d}\xi, \\ h_{n+1}(\eta) &= D - \int_0^\eta [\xi g_n(\xi) h_n(\xi) + g_n^2(\xi) f_{n+1}(\xi)]\,\mathrm{d}\xi, \\ g_{n+1}(\eta) &= [\lambda f_{n+1}(\eta) - \lambda\eta\,\mathrm{Ln}\,(\eta) h_{n+1}(\eta) + B\eta - \lambda\eta \\ &\quad \times \int_0^\eta \mathrm{Ln}\,(\xi)[\xi g_n(\xi) h_{n+1}(\xi) + g_n^2(\xi) f_{n+1}(\xi)\,\mathrm{d}\xi]^{-1}. \end{aligned}\right\} \tag{4.12}$$

We denote by X the set of functions $(f, h, g) \in C(0, \bar{\eta}) \times C(0, \bar{\eta}) \times C(0, \bar{\eta})$, and by X_s the closed subset of X such that (4.11) holds. Clearly a fixed point of (4.12) is a solution of the integral equations above, and hence of (4.1) to (4.3); functions $(f, g, h) \in X$ satisfying (4.1) automatically yield $f \in C^2(0, \bar{\eta})$ and so a fixed point of (4.12) has the desired regularity properties for f and g.

We prove that (4.12) maps X_s into itself and is contractive in the (supremum) norm of the product Banach space X. By the contraction mapping theorem this proves the existence of a unique solution lying in X_s. Since X_s is parametrized by $B \in \mathbb{R}$ (through g_2) this yields the required result.

We note first that if $(f_n, h_n, g_n) \in X$ then $(f_{n+1}, h_{n+1}, g_{n+1}) \in X$ for η sufficiently small. The requirement that η be sufficiently small is necessary only to ensure that $g_{n+1}(0)$ remains bounded; this is achieved for $\eta \ll 1$ since $g_{n+1} = [\lambda A + O(\eta\,\mathrm{Ln}\,(\eta))]^{-1}$. This last fact is verified below, since $f_{n+1}(\eta)$ satisfies (4.13).

Standard manipulations show that, if $(f_n, h_n, g_n) \in X$, then

$$\|f_{n+1}(\eta) - \bar{f}(\eta)\| \leq \left(\frac{|D|}{9\mu^2 A^2} + \frac{|C_2|}{3}\right)\bar{\eta}^3, \tag{4.13}$$

$$\|h_{n+1}(\eta) - \bar{h}(\eta)\| \leq (C_4)\bar{\eta}^2, \qquad \|g_{n+1}(\eta) - \bar{g}(\eta)\| \leq (C_5)\bar{\eta}^2\,\mathrm{Ln}\,(\bar{\eta}).$$

The constants C_4 and C_5 are independent of C_1, C_2 and C_3 and depend only upon the f_i and g_i. Thus, by setting

$$C_1 \geq \frac{|D|}{9\mu^2 A^2} + \frac{|C_2|}{3},$$

$C_2 = 2C_4$ and $C_3 = 2C_5$ then we deduce that (4.13) maps X_s into itself. The proof that (4.13) is contractive for η sufficiently small is standard and not of sufficient interest to warrant presentation. This completes the proof of the theorem.

5. Similarity solutions; $\eta \gg 1$

We now examine the asymptotic behaviour of (4.1), (4.2) subject to (3.3) and (3.4). In the case when $p = 2$ equation (3.4) implies that $g(\eta)$ has the asymptotic form

$$g(\eta) \approx 1/\eta C \tag{5.1}$$

as $\eta \to \infty$. With the ansatz (5.1), equation (4.1) becomes

$$\eta^2(f'' + f'/C) + f/C^2 \approx 0. \tag{5.2}$$

We seek solutions of (5.2) with the form

$$f(\eta) = \exp(-\eta/2C)u(\eta/C) \tag{5.3}$$

which symmetrizes the leading-order part (in powers of η^{-2}) of the differential operator in (5.2). For $z = \eta/C$ this yields Whittakers' equation [1: equation 13.1.31], namely

$$z^2 u_{zz} + \left(\frac{1}{C^2} - \frac{z^2}{4}\right)u = 0. \tag{5.4}$$

From [5] we deduce that (5.4) has linearly independent solutions with the asymptotic behaviour

$$u(z) = \begin{cases} e^{z/2}[1 + O(|z|^{-1})], \\ e^{-z/2}[1 + O(|z|^{-1})] \end{cases} \tag{5.5}$$

as $z \to \infty$. Thus, as $\eta \to \infty$, $f(\eta)$ has solutions of the form

$$f(\eta) = \begin{cases} 1 + O(|\eta|^{-1}), \\ e^{(-\eta/C)}[1 + O(|\eta|^{-1})], \end{cases} \tag{5.6}$$

Since we are interested in solutions of (4.1) satisfying $f \to 0$ as $\eta \to \infty$ we deduce that

$$f(\eta) \approx E e^{(-\eta/C)} \quad \text{as } \eta \to \infty. \tag{5.7}$$

Thus, in solving the boundary-value problem defined by (4.1), (4.2), (3.3), (5.1) we wish to choose values of the shooting parameters B and D (see the end of section 3) such that (5.1) and (5.7) are satisfied. A numerical procedure for achieving this is described in the following section.

6. Numerical approximation of similarity solutions

We wish to find solutions $(f, g) \in C^2(0, \infty) \times C(0, \infty)$ of (4.1), (4.2) satisfying

$$f(0) = A, \quad \lim_{\eta \to \infty} f(\eta) = 0, \quad \lim_{\eta \to \infty} \eta g(\eta) = 1/C.$$

To solve this problem directly by a numerical method is inpractical for two reasons: first equation (4.2) is singular at $\eta = 0$ and secondly the problem is posed on the semi-infinite domain. We overcome these problems by taking account of the asymptotic form of the solutions for $\eta \ll 1$ and $\eta \gg 1$ derived in the two preceding sections. By so doing we obtain a *regular* two-parameter shooting problem on a *finite domain*. This problem may be solved directly by means of Newton–Kantorovich iteration.

The expansions in section 4 show that for $\eta = \eta_l \ll 1$ solutions of (4.1), (4.2) with the required regularity, subject to $f(0) = A$, are approximated by the two-parameter ($(B, D) \in \mathbb{R}^2$) family

$$f(\eta_l) = A + D\eta_l - \frac{\eta_l^2}{2\lambda^2 A} - \frac{D\eta_l^3 \operatorname{Ln}(\eta_l)}{3\lambda^2 A^2}, \tag{6.1}$$

$$f'(\eta_l) = D - \frac{\eta_l}{\lambda^2 A} - \frac{D\eta_l^2 \operatorname{Ln}(\eta_l)}{\lambda^2 A^2}, \tag{6.2}$$

$$g(\eta_l) = \frac{1}{\lambda A} + \frac{D\eta_l \operatorname{Ln}(\eta_l)}{\lambda A^2} - \frac{\lambda D + B}{\lambda^2 A^2}\eta_l. \tag{6.3}$$

For $\eta \gg 1$ we want the pair (f, g) to have asymptotic behaviour defined by (5.1) and (5.7). From the two linearly independent solutions in (5.6) we deduce that satisfying (5.7) is equivalent to choosing initial conditions (6.1) to (6.3) so that the (approximately constant) solution $f(\eta) \propto 1 + O(\eta^{-1})$ is not picked up for $\eta \gg 1$. This unwanted solution may be difficult to eradicate if equations (4.1), (4.2) are solved directly. However, by using the approximate symmetrization of the differential equation governing $f(\eta)$ described in section 5, we convert the unwanted constant solution into an exponentially growing solution (see equation (5.5)). As such it is far more easily identified and eradicated by a numerical procedure.

Thus we apply the transformation (5.3) to equation (4.1) and change the independent variable to $z = \eta/C$. Under this transformation, equations (4.1), (4.2) become

$$u_{zz} + (gzC^2 - 1)u_z + (C^2g^2 - \tfrac{1}{2}gzC^2 + \tfrac{1}{4})u = 0, \tag{6.4}$$

$$zg_z + g = \lambda g^2 u \exp(-\tfrac{1}{2}z). \tag{6.5}$$

Note that setting $g(z) \approx 1/zC^2$ reduces (6.4) to (5.4) as expected.

From the asymptotic relations (5.1) and (5.5) we deduce that appropriate end conditions for (6.4) and (6.5) are, for $z_u \gg 1$,

$$u_z(z_u) + \tfrac{1}{2}u(z_u) = 0, \tag{6.6}$$

$$z_u g(z_u) = 1/C^2. \tag{6.7}$$

Thus, numerically, we solve the two-parameter shooting problem for $(B, D) \in \mathbb{R}^2$ so that solutions of (6.4), (6.5) subject to appropriately transformed initial conditions (6.1) to (6.3) satisfy (6.6), (6.7). This is now a regular two-point boundary-value problem readily solvable by standard numerical techniques. We employ Newton–Kantorovich iteration for the solution (see, for example, [8]). This requires tripling the dimensionality of the ordinary differential equation system to be solved; we solve the resulting ninth-order system by means of a Runge–Kutta method, as implemented in the NAG library. We use different values of η_l and η_u ($= z_u C$) to verify the robustness of the solutions obtained.

We now derive an important bound on D which is useful as a guide to making initial approximations to D for the Newton iteration. In the following we assume that $\lambda > 0$ as discussed in the introduction.

LEMMA 6.1 *The shooting parameter D satisfies*

$$D \leqslant 1/\lambda C. \tag{6.8}$$

Proof. Integrate equation (4.1) from $\eta = 0$ to $\eta = \infty$, employing parts on the second term. This yields

$$f'(0) = D = \int_0^\infty [g^2 f - (\eta g)' f] \, d\eta.$$

Noting, from (4.2), that $(\eta g)' = \lambda g^2 f$, we obtain

$$D = \int_0^\infty \left[\frac{(\eta g)'}{\lambda} - \lambda (gf)^2 \right] d\eta,$$

so that

$$D = \frac{1}{\lambda C} - \int_0^\infty \lambda (gf)^2 \, d\eta \leqslant \frac{1}{\lambda C}.$$

This completes the proof.

7. Results and conclusions

In this section we present some numerical results obtained by employing the method described in section 6. We also interpret these results in the context of the partial differential equation problem (P).

Extensive computations indicate the existence of only a single solution pair (f, g) satisfying (3.1) to (3.4) (in the case when $p = 2$ and $q = 1$) for each value of the parameters λ, A, C. This is not surprising since solutions of (3.1) to (3.4) are solutions of the initial-value problem (P) with the (singular) initial condition

$$\sigma(x, 0) = 1/Cx^{2/p}. \tag{7.1}$$

Although this singular initial condition is clearly unrealistic, the similarity solutions are still important since they may describe the limiting behaviour of the system (P) for large time. The stability of the similarity solutions will be analysed in a subsequent paper.

To fix ideas, we set $A = C = 1$ for all the graphical output discussed in this section. First we examine the variation of solution pairs (f, g) with λ. Figures 1 and 2 show the graphs of the values of the shooting parameters B and D, which solve (3.1) to (3.4), against λ. The variation of D with λ is consistent with equation (6.8). From Fig. 2 we deduce the existence of a critical value of λ, λ_c, for which $D = 0$.

Figures 3 and 4 show profiles of f, f', ηg and g against η for two different values of λ, one greater than and the other less than λ_c. In Fig. 3a, f contains a single maximum; this is consistent with equation (4.1) which implies (by the maximum principle) that f has no positive minimum. In Fig. 4a, however, f is

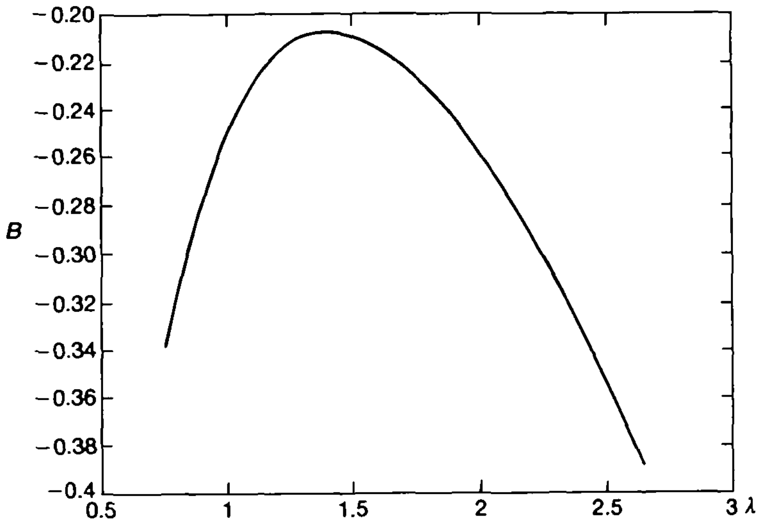

FIG 1. B versus λ

monotonic decreasing since $\lambda > \lambda_c$. Figures 3c and 4c show clearly that $\eta g(\eta)$ tends to a limiting constant value of C (= 1 in this case) as required by (5.1).

By employing the similarity variables described at the beginning of section 3 we can determine solutions $u(x, t)$ and $\sigma(x, t)$ of (P). Figures 5 and 6 show profiles of u and σ against x at successive time intervals. We note that the temperature profile u behaves like a progressive wave with ignition initiated at the boundary, and the temperature raised to the value A (the boundary value). In

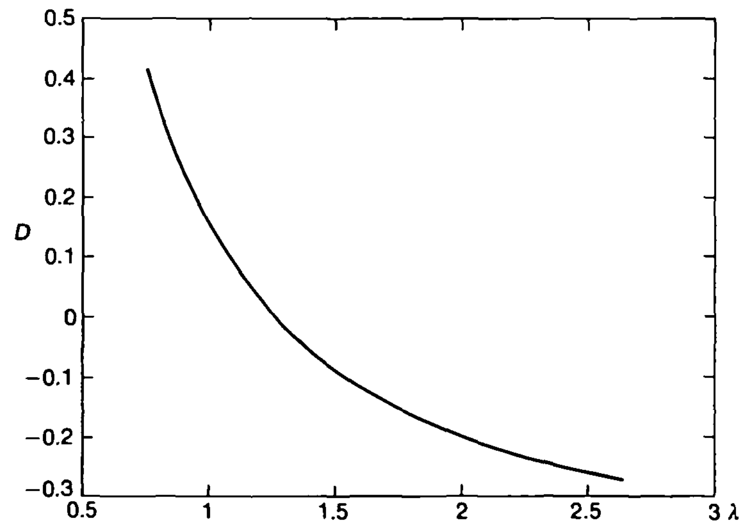

Fig. 2. D versus λ

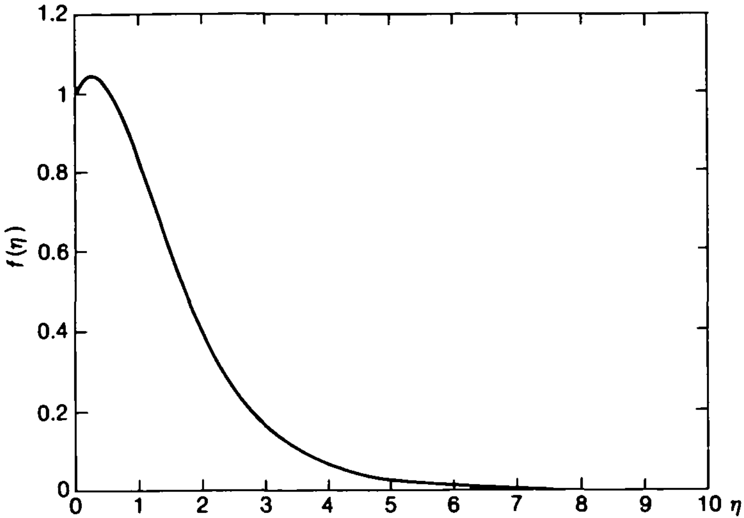

FIG 3a. $f(\eta)$ versus η. $\lambda=0.8$

the case shown ($\lambda<\lambda_c$) D is positive and the wave has a peak temperature greater than A; for $\lambda>\lambda_c$ this is not the case. The heat capacity profile, shown in Fig. 6, behaves as a progressive, damped wave with a limiting value of zero as $t\to\infty$.

The limiting behaviour of $u(x, t)$ and $\sigma(x, t)$ as $t\to\infty$ can be verified directly from the form of the similarity solutions. From the discussion at the beginning of

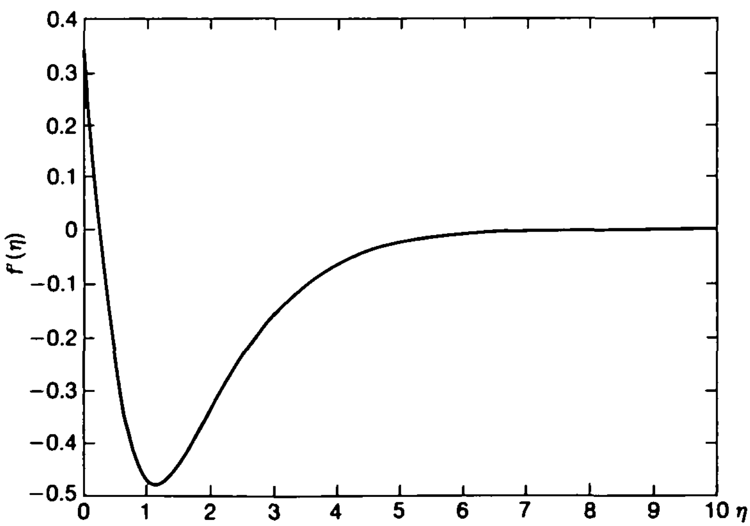

FIG 3b. $f'(\eta)$ versus η. $\lambda=0.8$

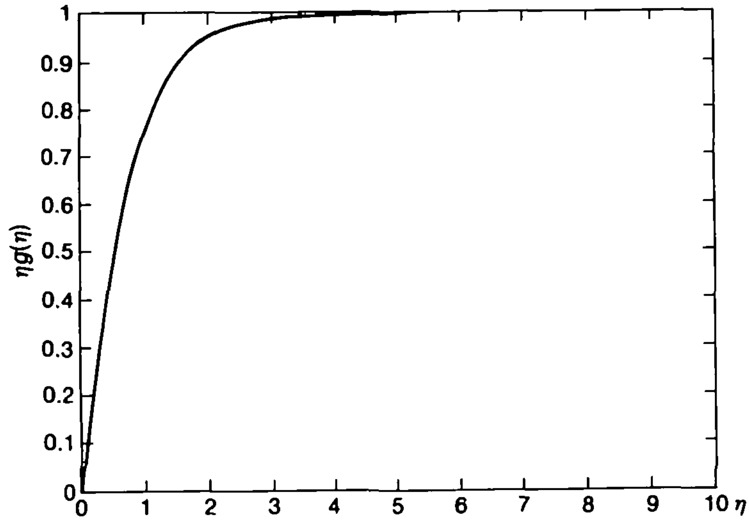

FIG 3c. $\eta g(\eta)$ versus η. $\lambda=0.8$

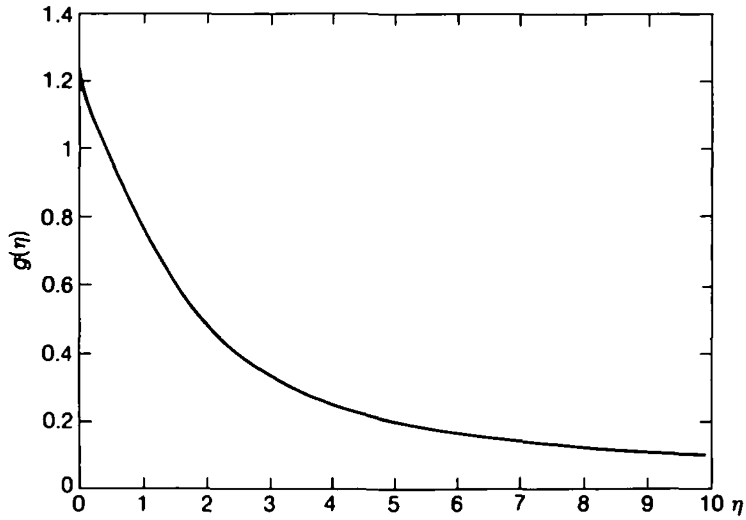

FIG 3d. $g(\eta)$ versus η. $\lambda=0.8$

section 3 we deduce that, for $p=2$,

$$u(x,t)=f(x/t) \quad \text{and} \quad \sigma(x,t)=t^{-1}g(x/t).$$

Thus, as $t\to\infty$, with x fixed, we obtain

$$u(x,t)\to f(0)=A, \qquad t\sigma(x,t)\to g(0)=1/\lambda A.$$

This demonstrates an important balance between the limiting profiles of $u(x,t)$

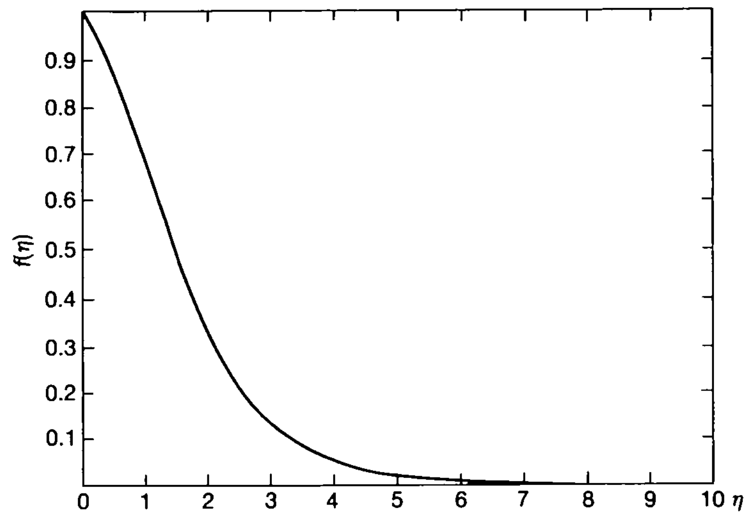

FIG 4a. $f(\eta)$ versus η. $\lambda=2.0$

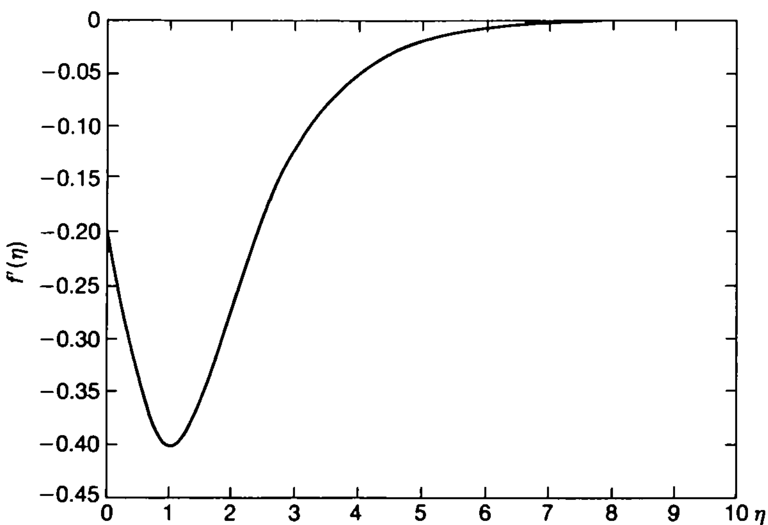

FIG 4b. $f'(\eta)$ versus η. $\lambda=2.0$

and $\sigma(x, t)$, namely that

$$\lim_{t\to\infty} t\sigma(x, t)u(x, t) = 1/\lambda. \tag{7.2}$$

This result is independent of the prescribed boundary and initial conditions, that is, the dependence of (P) and (7.1) on A and C. Equation (7.2) reflects the delicate balance between heat produced and solid consumed (since the heat

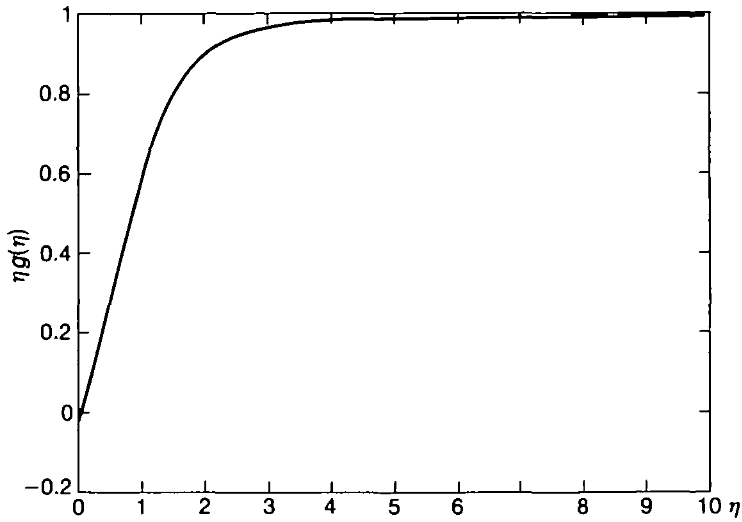

FIG 4c. $\eta g(\eta)$ versus η. $\lambda=2.0$

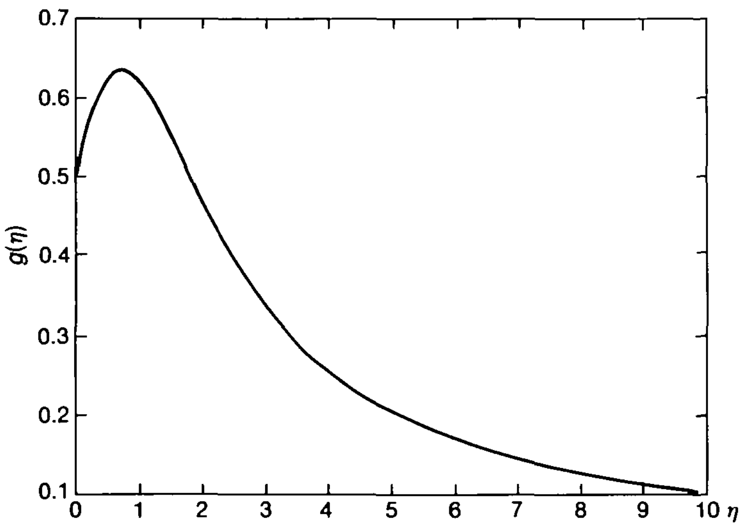

FIG 4d. $g(\eta)$ versus η. $\lambda=2.0$

capacity σ is linearly related to solid concentration). As mentioned before, this balance is crucial in determining regions of existence and non-existence for sustained combustion in the full model for porous-medium combustion described in section 2 [10, 12]. Equation (7.2) provides another interpretation of this balance in the context of the limiting behaviour of the simplified problem (P).

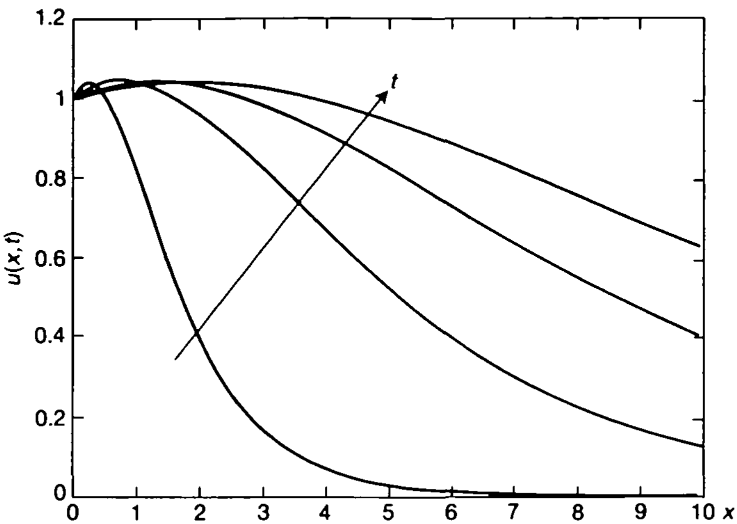

FIG 5. $u(x, t)$ versus x at t-intervals of 2 units from $t=1$ to $t=7$. $\lambda=0.8$

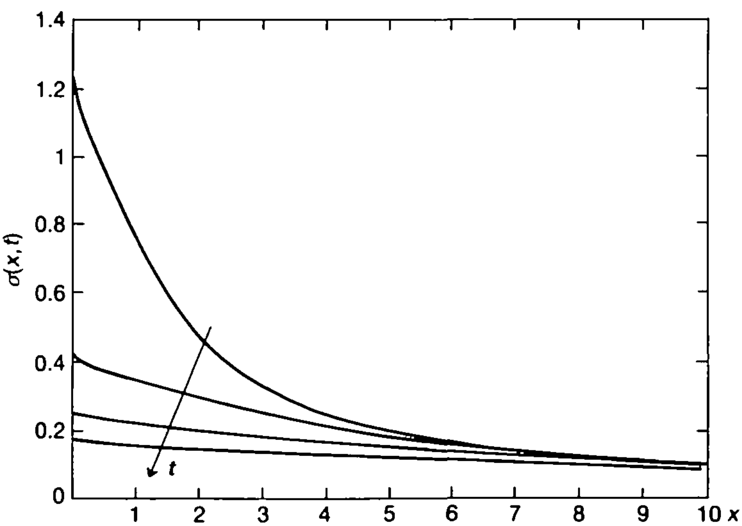

FIG 6. $\sigma(x, t)$ versus x at t-intervals of 2 units from $t=1$ to $t=7$. $\lambda=0.8$

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