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Diffusion Controlled Smoulder Propagation in a Thin Slab

J. ADLER
Department of Mathematics, Imperial College of Science, Technology & Medicine, London SW7 2BZ, U.K.

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Abstract. Complex variable techniques are used to determine the shape of the smouldering reaction front and the concentration of the oxidizer behind the front for steady smoulder propagation in a solid slab of exothermically reacting material. It extends an earlier free boundary problem of Adler and Herbert which considered diffusion controlled smoulder propagation in a half-space. The region behind the reaction front is assumed to be porous, the oxidizer diffusing from both planar surfaces to the front, where its concentration vanishes. Suitable scaling allows the oxidizer concentration to be expanded in powers of a small parameter. The resulting coupled differential equations for the coefficients are solved in terms of functional equations. Some consideration is given to the regions where the front meets the planar surfaces. It is shown that, close to the leading edge, the surface concentration varies monotonically with distance from the edge.

1. Introduction

Smouldering is a combustion phenomenon that lies between the extremes of negligible exothermic reaction and flame-like burning. It is known that smouldering only takes place in char forming materials [1], that is, a porous solid remains after the combustion process has passed through the material. The reaction is sustained and controlled by the rate at which oxidizer is able to reach the reaction zone, which lies between the char and unburnt solid.

The initiation of smouldering can be defined theoretically in terms of turning-point bifurcations in a suitable parameter space [2,3]. These lie intermediate to those defining the quiescent state and flame-like burning.

An asymptotic theory of steady smouldering in a half-space has been considered by Adler and Herbert [4]. It is based on earlier work of Ohlemiller [5], in which a thin reaction zone propagates parallel to a planar surface on which a constant oxidizer concentration is maintained. It is found that, to first order, the shape of the reaction front is parabolic, a consequence of the conditions at the reaction front where the concentration of oxidizer vanishes and where the rate of oxygen supply balances the rate at which fuel is consumed. The asymptotic theory of Adler and Herbert is not valid in the region where the reaction front meets the planar surface. Using Alt's method, Kerr [6] has computed the shape of the front and the oxidizer concentration in this region for various surface conditions.

In the work presented below, the reacting material is confined between parallel planes with a thin reaction front moving with constant speed parallel to the surfaces. Constant oxidizer concentration is initially assumed on the planar surfaces behind the reaction front with the concentration vanishing on the reaction front. It is shown, however, that at the leading edge the planar surface concentration varies monotonically with distance from the edge. In the analysis of Adler and Herbert, the reduction of the equations to dimensionless form produced a single small parameter s. For the slab geometry considered here, a similar but not identical reduction introduces an additional mass transfer Peclét number p. The problem has symmetry about

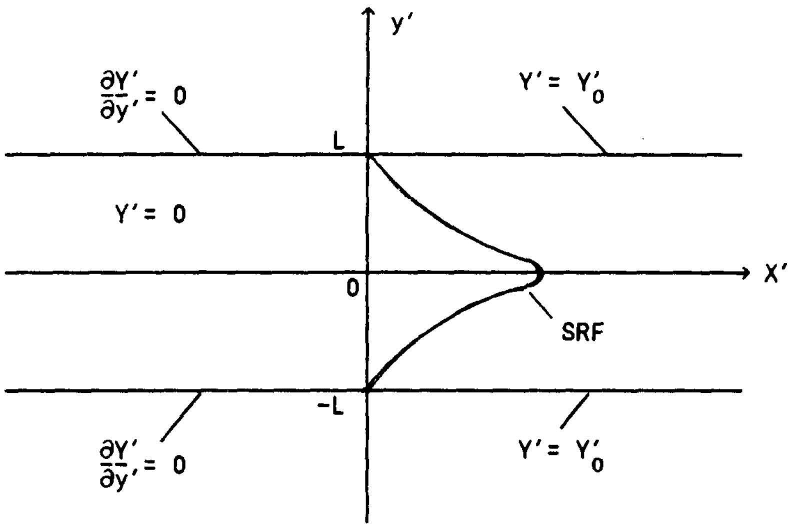

Figure 1. Smouldering reaction front (SRF) and boundary conditions for a thin slab.

the midplane; as $s/p \to 0$ the asymptotic solution derived by Adler and Herbert becomes relevant for the half-slab. For thin slabs, $p = O(s)$, as demonstrated in the discussion below. The analysis which we give assumes this relationship between s and p.

2. Conservation Equations

Let the solid occupy the region $-L \leq y' \leq L$ and take x' in a direction parallel to the surfaces. The fractional concentration of oxidizer $Y'(x', y')$ satisfies the 2D diffusion equation

$$\frac{\partial Y'}{\partial t'} = D\left(\frac{\partial^2 Y'}{\partial x'^2} + \frac{\partial^2 Y'}{\partial y'^2}\right), \tag{2.1}$$

where t' is the time and D a constant diffusion coefficient. We assume that a thin smouldering reaction front (SRF) moves with constant speed u' parallel to the slab surfaces. Introducing a coordinate relative to the moving front, $X' = x' + u't'$, Equation (2.1) becomes

$$\frac{u'}{D}\frac{\partial Y'}{\partial X'} = \frac{\partial^2 Y'}{\partial X'^2} + \frac{\partial^2 Y'}{\partial y'^2}. \tag{2.2}$$

A schematic diagram of the smouldering process is shown in Figure 1. To the left of the SRF is a compacted region of unburnt fuel in which there is no oxidizer. In the porous region to the right of the front, oxidizer diffuses from the planar surfaces, where its concentration is specified, to the SRF where it vanishes. The rate of oxidizer diffusion to the front balances the rate at which fuel is consumed at the front [4]. The condition at the SRF may be written:

$$n_0 \rho_{\mathrm{F}} u' \frac{\mathrm{d}y'}{\mathrm{d}X'} = \rho_0 D\left(-\frac{\partial Y'}{\partial y'} + \frac{\partial Y'}{\partial X'}\frac{\mathrm{d}y'}{\mathrm{d}X'}\right), \tag{2.3}$$

and

$$Y' = 0$$

where ρ_0 is the surface gas density, ρ_F is the fuel density and n_0 is the stoichiometric coefficient of the reaction. If the SRF meets the plane of symmetry $y = 0$ at $X' = X'_0$, then

$$\frac{\partial Y'}{\partial y'}(X', 0) = 0, \qquad X' \geq X'_0 > 0. \tag{2.4}$$

Suitable plane surface conditions are

$$\begin{aligned} \frac{\partial Y'}{\partial y'}(X', \pm L) &= 0, \qquad X' < X'_1, \\ Y'(X', \pm L) &= Y'_0, \qquad X' > X'_1, \end{aligned} \tag{2.5}$$

where Y'_0 is the fractional surface concentration and X'_0, X'_1 are to be determined such that $0 < X'_1 < X'_0$.

3. Dimensionless Equations

Put

$$X = X'/L, \quad y = y'/L, \quad Y = Y'/Y'_0, \tag{3.1}$$

$$p = Lu'/D, \quad \text{Péclet number for mass transfer}$$

$$s = \left(\frac{\rho_0}{\rho_F}\right)\frac{Y'_0}{n_0}. \tag{3.2}$$

Equation (2.2) becomes

$$p\frac{\partial Y}{\partial y} = \frac{\partial^2 Y}{\partial X^2} + \frac{\partial^2 Y}{\partial y^2}, \tag{3.3}$$

where

$$\left.\begin{aligned} \frac{\partial Y}{\partial y}(X, \pm 1) &= 0, \qquad X < X_1, \\ Y(X, \pm 1) &= 1, \qquad X > X_1, \\ \frac{\partial Y}{\partial y}(X, 0) &= 0, \qquad X > X_0. \end{aligned}\right\} \tag{3.4}$$

The conditions at the SRF are:

$$p\frac{\mathrm{d}y}{\mathrm{d}X} = s\left(-\frac{\partial Y}{\partial y} + \frac{\partial Y}{\partial X}\frac{\mathrm{d}y}{\mathrm{d}X}\right), \tag{3.5}$$

and

$$Y = 0.$$

The parameter s involves the ratio of gas to solid density and is small, typically $s \sim 10^{-2}$. With a thin slab assumption, we put $p = \lambda s$, where λ is an $O(1)$ constant. Equations (3.3) and (3.5) now become

$$\lambda s\frac{\partial Y}{\partial X} = \frac{\partial^2 Y}{\partial X^2} + \frac{\partial^2 Y}{\partial y^2}, \tag{3.6}$$

and at SRF:

$$\lambda \frac{dy}{dX} = -\frac{\partial Y}{\partial y} + \frac{\partial Y}{\partial X}\frac{dy}{dX}, \tag{3.7}$$

$$Y = 0.$$

4. The First Order Problem

If $y = \pm f(X)$ is the equation of the SRF we now restrict attention to the region $0 \le X \le X_0$, $f(X) \le y \le 1$.

With

$$Y(X,y) = Y_0(X,y) + \lambda s Y_1(X,y) + \cdots, \tag{4.1}$$

substitution in (3.6), (3.7) gives

$$\frac{\partial^2 Y_0}{\partial X^2} + \frac{\partial^2 Y_0}{\partial y^2} = 0 \tag{4.2}$$

at SRF:

$$\lambda \frac{dy}{dX} = -\frac{\partial Y_0}{\partial y} + \frac{\partial Y_0}{\partial X}\frac{dy}{dX}, \tag{4.3}$$

and

$$Y_0 = 0,$$

with appropriate boundary conditions (3.4).

From the second of Equations (4.3),

$$\frac{\partial Y_0}{\partial X} + \frac{\partial Y_0}{\partial y}\frac{dy}{dX} = 0, \tag{4.4}$$

which, together with the first equation, gives

$$-\frac{dy}{dX} = \left(\frac{\partial Y_0}{\partial X}\right) \Big/ \left(\frac{\partial Y_0}{\partial y}\right) = \left(\frac{\partial Y_0}{\partial y}\right) \Big/ \left(\lambda - \frac{\partial Y_0}{\partial X}\right). \tag{4.5}$$

From (4.5) it follows that on the SRF,

$$0 \le \frac{\partial Y_0}{\partial X} \le \lambda, \qquad -\frac{1}{2}\lambda \le \frac{\partial Y_0}{\partial y} \le \frac{1}{2}\lambda. \tag{4.6}$$

It is convenient to treat the above problem in terms of complex variables. The technique which we shall use is related to the Schwarz function method [7]. Complex variable methods have been shown by Howison [8] to be useful in solving moving boundary problems in fluid mechanics.

Put

$$Y_0(X,y) = 1 + i[\phi(z) - \phi(\bar{z})], \tag{4.7}$$

where

$$z = X + i(1 - y),$$
$$\bar{z} = X - i(1 - y),$$

and $\phi(z)$ is a real function of the complex variable z. Expression (4.7) satisfies (4.2) and $Y_0(X, 1) = 1(z = \bar{z})$. Treating z and $\bar{z}$ as new independent variables, Equations (4.5) can be written

$$\frac{1}{i}\frac{\mathrm{d}z - \mathrm{d}\bar{z}}{\mathrm{d}z + \mathrm{d}\bar{z}} = \frac{i[\phi'(z) - \phi'(\bar{z})]}{\phi'(z) + \phi'(\bar{z})} = \frac{\phi'(z) + \phi'(\bar{z})}{\lambda - i[\phi'(z) - \phi'(\bar{z})]}, \tag{4.8}$$

from which it follows that

$$4\phi'(z) = i\lambda\left(\frac{\phi'(z)}{\phi'(\bar{z})} - 1\right). \tag{4.9}$$

On the SRF the concentration vanishes, hence

$$Y_0 = 1 + i(\phi(z) - \phi(\bar{z})) = 0, \tag{4.10}$$

so that

$$\phi'(z)\,\mathrm{d}z - \phi'(\bar{z})\,\mathrm{d}\bar{z} = 0.$$

Substitution in (4.9) gives

$$4\phi'(z) = i\lambda\left(\frac{\mathrm{d}\bar{z}}{\mathrm{d}z} - 1\right). \tag{4.11}$$

Equation (4.11) expresses the fact that on the SRF, $\bar{z}$ is a function of z. Integration gives

$$\phi(z) = \frac{i\lambda}{4}(\bar{z} - z) + \tfrac{1}{2}i,$$

hence

$$\bar{z} = z - i\frac{4}{\lambda}\phi(z) - \frac{2}{\lambda}. \tag{4.12}$$

On substituting for $\bar{z}$ in (4.10)

$$\phi(z) - \phi\left(z - i\frac{4}{\lambda}\phi(z) - \frac{2}{\lambda}\right) = i, \tag{4.13}$$

which is a functional equation for $\phi(z)$. A solution may be written

$$\phi(z) = \left(\frac{\lambda z}{2} + b\right)^{1/2}, \tag{4.14}$$

where b is a real constant. Although other solutions exist, the above form is appropriate since it leads to a parabolic shape for the SRF. From (4.10)

$$\left(\frac{\lambda z}{2} + b\right)^{1/2} - \left(\frac{\lambda \bar{z}}{2} + b\right)^{1/2} = i,$$

hence

$$2\lambda X + 4b + 1 = \lambda^2(1-y)^2.$$

Here b is a constant which shifts the profile parallel to the x-axis. Choose $b = -\frac{1}{4}$, then

$$\frac{2}{\lambda}X = (1-y)^2 \tag{4.15}$$

is the equation of the SRF, and this meets the plane of symmetry, $y = 0$ where $X = X_0 = \frac{1}{2}\lambda$.

With (4.14) and $b = -\frac{1}{4}$, the solution to the 1st order problem becomes

$$\begin{aligned} Y_0(X,y) &= 1 + i\left[\left(\frac{\lambda z}{2} - \frac{1}{4}\right)^{1/2} - \left(\frac{\lambda \bar{z}}{2} - \frac{1}{4}\right)^{1/2}\right] \\ &= 1 - \lambda^{1/2}\left[\left\{\left(X - \frac{1}{2\lambda}\right)^2 + (1-y)^2\right\}^{1/2} - X + \frac{1}{2\lambda}\right]^{1/2}, \end{aligned} \tag{4.16}$$

which has a branch-point at $X = X_1 = 1/2\lambda, y = 1$.

Put

$$\frac{\lambda z}{2} - \frac{1}{4} = \frac{\lambda}{2}\,\mathrm{r}e^{i\theta}, \tag{4.17}$$

where (r, θ) are plane polar coordinates. Then

$$Y_0(X,y) = 1 - (2\lambda r)^{1/2}\sin\tfrac{1}{2}\theta. \tag{4.18}$$

In this form the 'upstream influence' on the solution is clearly demonstrated. Without this effect a solution does not appear possible [9].

From (4.18),

$$|\nabla Y_0| = (\lambda/2r)^{1/2}, \tag{4.19}$$

hence on the SRF, where $r = X + 1/2\lambda$,

$$|\nabla Y_0| = \left(\frac{\lambda}{2}\right)^{1/2}\frac{1}{(X+\frac{1}{2}\lambda)^{1/2}}. \tag{4.20}$$

The oxidizer flux through the SRF, from (0, 1) to $(\frac{1}{2}\lambda, 0)$, is

$$\begin{aligned} &\int_0^{1/2\lambda} |\nabla Y_0|\left[1 + \left(\frac{\mathrm{d}y}{\mathrm{d}X}\right)^2\right]^{1/2}\mathrm{d}X \\ &= \left(\frac{\lambda}{2}\right)^{1/2}\int_0^{1/2\lambda}\frac{1}{(X+\frac{1}{2}\lambda)^{1/2}}\left(1 + \frac{1}{2\lambda X}\right)^{1/2}\mathrm{d}X = \lambda, \end{aligned} \tag{4.21}$$

giving a physical interpretation to the parameter λ.

Since the problem has symmetry about the midplane, $y = 0$, the equation of the SRF and solution for $y < 0$ may be obtained by reflection. Thus

$$Y_0(X,y) = 1 - \lambda^{1/2}\left[\left\{\left(X - \frac{1}{2\lambda}\right)^2 + (1+y)^2\right\}^{1/2} - X + \frac{1}{2\lambda}\right]^{1/2}, \tag{4.22}$$

at the SRF:

$$\frac{2}{\lambda}X = (1+y)^2, \tag{4.23}$$

where

$$0 \le X \le \tfrac{1}{2}\lambda, \qquad -1 \le y \le 0.$$

To first order, the equation of the SRF in $-1 \le y \le 1$ thus has a cusp at $(\frac{1}{2}\lambda, 0)$. The appearance of a cusp on the plane of symmetry is clearly undesirable from a physical point of view. Some attempt to remedy this has been made in Section 6, below. Nearly cusp-like solutions have, however, been obtained by numerical integration of the equations for $s \ll p$ [6a]

The above problem, for a somewhat different physical situation and with $\lambda = 1$, has been solved by Siegel [10] using conformal mapping. His solution is obtained in terms of elliptic functions and would not be useful for a development of our solution in powers of s. Unlike the 'simple' solution derived above it does not have a cusp-like behaviour on the plane of symmetry. Away from this plane the solution for the 'front' is nearly parabolic, as shown in Figure 5 of his paper.

5. The Second Order Problem

With (4.1) substituted in (3.6), the $O(s)$ terms are

$$\frac{\partial^2 Y_1'}{\partial X^2} + \frac{\partial^2 Y_1'}{\partial y^2} = \frac{\partial Y_0}{\partial X}. \tag{5.1}$$

In terms of variables $z, \bar{z}$, as in (4.7), this can be written as

$$\begin{aligned} 4\frac{\partial^2 Y_1'}{\partial z\,\partial \bar{z}} &= \frac{\partial Y_0}{\partial z} + \frac{\partial Y_0}{\partial \bar{z}}, \\ &= \frac{i\lambda}{4}\left[\left(\frac{\lambda z}{2} - \frac{1}{4}\right)^{-1/2} - \left(\frac{\lambda \bar{z}}{2} - \frac{1}{4}\right)^{-1/2}\right] \end{aligned} \tag{5.2}$$

on using Equation (4.16). A solution of (5.2), which satisfies $Y_1 = 0$ when $z = \bar{z}(y = 1)$, is

$$Y_1 = \frac{i}{4}\left[\bar{z}\left(\frac{\lambda z}{2} - \frac{1}{4}\right)^{1/2} - z\left(\frac{\lambda \bar{z}}{2} - \frac{1}{4}\right)^{1/2}\right] + \frac{i}{4}[\psi(z) - \psi(\bar{z})], \tag{5.3}$$

where $\psi(z)$ is a real function of the complex variable z.

Consider conditions on the SRF. From Equation (3.7) we obtain

$$\frac{\mathrm{d}X}{\mathrm{d}y} = \left(\frac{\partial Y}{\partial X} - \lambda\right) \Big/ \left(\frac{\partial Y}{\partial y}\right), \tag{5.4}$$

hence

$$\frac{\mathrm{d}X + i\,\mathrm{d}y}{\mathrm{d}X - i\,\mathrm{d}y} = \left(\frac{\partial Y}{\partial X} + i\frac{\partial Y}{\partial y} - \lambda\right) \Big/ \left(\frac{\partial Y}{\partial X} - i\frac{\partial Y}{\partial y} - \lambda\right),$$

so that

$$\frac{d\bar{z}}{dz} = \left(\frac{\partial Y}{\partial z} - \frac{\lambda}{2}\right) \Big/ \left(\frac{\partial Y}{\partial \bar{z}} - \frac{\lambda}{2}\right). \tag{5.5}$$

On the SRF, $\bar{z}$ is a function of z. Since $Y(z, \bar{z}) = 0$,

$$\frac{\partial Y}{\partial z}\, dz + \frac{\partial Y}{\partial \bar{z}}\, d\bar{z} = 0, \tag{5.6}$$

which, combined with (5.5), gives

$$\frac{d\bar{z}}{dz} - 1 + \frac{4}{\lambda}\frac{\partial Y}{\partial z}(z, \bar{z}(z)) = 0. \tag{5.7}$$

Put

$$\bar{z}(z) = \bar{z}_0(z) + s\bar{z}_1(z) + \cdots, \tag{5.8}$$

where

$$\bar{z}_0(z) = z - \frac{2}{\lambda} - i\frac{4}{\lambda}\left(\frac{\lambda z}{2} - \frac{1}{4}\right)^{1/2}.$$

Here $\bar{z}_0$ is the 1st order solution to the shape of the SRF. Substituting in (5.7) and equating terms of $O(s)$, we obtain

$$\frac{d\bar{z}_1}{dz} + i\left[\frac{\lambda \bar{z}_0}{4}\left(\frac{\lambda z}{2} - \frac{1}{4}\right)^{-1/2} - \left(\frac{\lambda \bar{z}_0}{2} - \frac{1}{4}\right)^{1/2} + \psi'(z)\right] = 0, \tag{5.9}$$

which simplifies to

$$\frac{d\bar{z}_1}{dz} + i\left[-\frac{1}{2}\left(\frac{\lambda z}{2} - \frac{1}{4}\right)^{1/2} - \frac{3}{8}\left(\frac{\lambda z}{2} - \frac{1}{4}\right)^{-1/2} + \psi'(z)\right] = 0. \tag{5.10}$$

Integration gives

$$\bar{z}_1(z) = i\frac{2}{3\lambda}\left(\frac{\lambda z}{2} - \frac{1}{4}\right)^{3/2} + i\frac{3}{2\lambda}\left(\frac{\lambda z}{2} - \frac{1}{4}\right)^{1/2} - i\psi(z) + \text{constant}. \tag{5.11}$$

A further equation involving $\bar{z}_1$ and ψ can be found from the condition $Y(z, \bar{z}) = 0$. Substituting (5.8) and noting that $Y = Y_0 + \lambda s Y_1 + \ldots$, the terms of $O(s)$ give

$$z_1 \frac{\partial Y_0}{\partial \bar{z}}(z, \bar{z}_0) + \lambda Y_1(z, \bar{z}_0) = 0. \tag{5.12}$$

Hence

$$\bar{z}_1 = \left(\lambda\frac{\bar{z}_0}{2} - \frac{1}{4}\right)^{1/2}\left[\bar{z}_0\left(\frac{\lambda z}{2} - \frac{1}{4}\right)^{1/2} - z\left(\lambda\frac{\bar{z}_0}{2} - \frac{1}{4}\right)^{1/2} + \psi(z) - \psi(\bar{z}_0)\right]. \tag{5.13}$$

From the 1st order problem

$$Y_0(z, \bar{z}_0) = 1 + i\left[\left(\frac{\lambda z}{2} - \frac{1}{4}\right)^{1/2} - \left(\frac{\lambda \bar{z}_0}{2} - \frac{1}{4}\right)^{1/2}\right] = 0,$$

hence

$$\left(\frac{\lambda z}{2}-\frac{1}{4}\right)^{1/2}-\left(\frac{\lambda \bar{z}_0}{2}-\frac{1}{4}\right)^{1/2}=i.$$

Put

$$Z=\left(\frac{\lambda z}{2}-\frac{1}{4}\right)^{1/2}-\frac{i}{2}=\left(\frac{\lambda \bar{z}_0}{2}-\frac{1}{4}\right)^{1/2}+\frac{i}{2}. \tag{5.14}$$

Then

$$\begin{aligned} z &= \frac{2}{\lambda}(Z^2+iZ), \\ \bar{z}_0 &= \frac{2}{\lambda}(Z^2-iZ), \end{aligned} \tag{5.15}$$

and (5.15) is the 1st order parametric form of the SRF equation with Z a real parameter such that $0 \leq Z \leq \frac{1}{2}\lambda$. In terms of Z, Equation (5.13) becomes

$$\bar{z}_1=\left(Z-\frac{i}{2}\right)\left[-i\frac{2}{\lambda}Z^2+\psi\left(\frac{2}{\lambda}(Z^2+iZ)\right)-\psi\left(\frac{2}{\lambda}(Z^2-iZ)\right)\right], \tag{5.16}$$

and Equation (5.11) can be written

$$\bar{z}_1=\frac{i}{\lambda}\left(\frac{2}{3}Z^3+iZ^2+Z\right)-i\psi\left(\frac{2}{\lambda}(Z^2+iZ)\right)+iK, \tag{5.17}$$

where K is a real constant.

From (5.16) and (5.17) we obtain

$$\begin{aligned} &\left(Z+\frac{i}{2}\right)\psi\left(\frac{2}{\lambda}(Z^2+iZ)\right)-\left(Z-\frac{i}{2}\right)\psi\left(\frac{2}{\lambda}(Z^2-iZ)\right) \\ &=\frac{i}{\lambda}\left(\frac{8}{3}Z^3+Z\right)+iK, \end{aligned} \tag{5.18}$$

a functional equation for ψ. Equation (5.18) can be simplified by setting

$$\chi(z)=z\psi\left(\frac{2}{\lambda}\left(z^2+\frac{1}{4}\right)\right), \tag{5.19}$$

in which case

$$\chi\left(Z+\frac{i}{2}\right)-\chi\left(Z-\frac{i}{2}\right)=\frac{i}{\lambda}\left(\frac{8}{3}Z^3+Z\right)+iK. \tag{5.20}$$

The required solution of (5.20) is

$$\chi(z)=\frac{2}{3\lambda}z^4+\frac{5}{6\lambda}z^2+Kz, \tag{5.21}$$

hence

$$\psi(z)=\frac{2}{3\lambda}\left(\frac{\lambda z}{2}-\frac{1}{4}\right)^{3/2}+\frac{5}{6\lambda}\left(\frac{\lambda z}{2}-\frac{1}{4}\right)^{1/2}+K. \tag{5.22}$$

Substitution of (5.22) in (5.3) determines Y_1, and in (5.13) $\bar{z}_1$, the constant K cancelling in both cases. Thus

$$\bar{z}_1 = \frac{1}{3\lambda}(1 + i2Z), \tag{5.23}$$

and

$$\bar{z}_0 = \frac{2}{\lambda}\left(Z^2 - iZ\right).$$

The equation of the SRF becomes

$$\begin{aligned} \bar{z} &= \bar{z}_0 + s\bar{z}_1 + \cdots \\ &= \frac{2}{\lambda}Z^2 + \frac{s}{3\lambda} - i\left(\frac{2Z}{\lambda} - 2\frac{sZ}{3\lambda}\right) + \cdots \\ &= X - i(1-y). \end{aligned}$$

Hence

$$\begin{aligned} X &= \frac{2}{\lambda}Z^2 + \frac{s}{3\lambda} + O(s^2), \\ 1 - y &= \frac{2Z}{\lambda} - 2\frac{sZ}{3\lambda} + O(s^2). \end{aligned} \tag{5.24}$$

The SRF meets the plane of symmetry $y = 0$, where

$$X = \frac{\lambda}{2} + \frac{s}{3}\left(\lambda + \frac{1}{\lambda}\right) + O(s^2),$$

and the upper surface $y = 1$, where

$$X = \frac{s}{3\lambda} + O(s^2).$$

The effect of the perturbation is to shift the profile in the direction of the surface branch-point.

Substituting (4.17) and (5.22) in (5.3) we find

$$Y_1 = -r^{1/2}\left[\frac{2}{3(2\lambda)^{1/2}} - \frac{1}{4}(2\lambda)^{1/2}r\right]\sin\frac{\theta}{2} - \frac{1}{12}(2\lambda)^{1/2}r^{3/2}\sin\frac{3\theta}{2}. \tag{5.25}$$

Finally

$$\begin{aligned} Y(X,y) = {} & 1 - (2\lambda)^{1/2}r^{1/2}\sin\frac{\theta}{2} - \\ & -\lambda s\left\{r^{1/2}\left[\frac{2}{3(2\lambda)^{1/2}} - \frac{1}{4}(2\lambda)^{1/2}r\right]\sin\frac{\theta}{2} + \right. \\ & \left. + \frac{1}{12}(2\lambda)^{1/2}r^{3/2}\sin\frac{3\theta}{2}\right\} + O(s^2), \end{aligned} \tag{5.26}$$

where

$$X - \frac{1}{2\lambda} = r\cos\theta,$$

$$1 - y = r\sin\theta,$$

which gives the concentration of oxidizer between the surface $y = 1$ and the reaction front. Equations (5.24) show that this may be written

$$\frac{2}{\lambda}\left(X - \frac{s}{3\lambda}\right) = \frac{(1-y)^2}{(1-\frac{s}{3})^2} + O(s^2). \tag{5.27}$$

6. The SRF Turning-Point Region

In solving the above free-boundary problem, no consideration has been given to the region where the SRF meets the midplane other than that the behaviour there is cusp-like. We seek here the oxidizer concentration and shape of the SRF under more realistic boundary conditions. The solution, which will be derived by methods similar to those above, is only valid in the neighbourhood of the SRF turning-point.

Put

$$Y(X,y) = \tilde{Y}_0(X,y) + \lambda s \tilde{Y}_1(X,y) + \cdots \tag{6.1}$$

in Equation (3.6) and equate terms of like order. Then

$$\frac{\partial^2 \tilde{Y}_0}{\partial X} + \frac{\partial^2 \tilde{Y}_0}{\partial y^2} = 0, \tag{6.2}$$

$$\frac{\partial^2 \tilde{Y}_1}{\partial X} + \frac{\partial^2 \tilde{Y}_1}{\partial y^2} = \frac{\partial \tilde{Y}_0}{\partial X}. \tag{6.3}$$

The conditions on the SRF are

$$\lambda\frac{\mathrm{d}y}{\mathrm{d}X} = -\frac{\partial Y}{\partial y} + \frac{\partial Y}{\partial X}\frac{\mathrm{d}y}{\mathrm{d}X}, \quad Y = 0. \tag{6.4}$$

If the SRF meets the midplane at $X = X_0$, then

$$\frac{\partial \tilde{Y}_i}{\partial y}(X,0) = 0, \quad X \geq X_0, \quad i = 0,1,2,\ldots. \tag{6.5}$$

7. The First Order Turning-Point Problem

Put $\zeta = X + iy$, $\bar{\zeta} = X - iy$ and consider $\tilde{Y}_0$ as a function of ζ and $\bar{\zeta}$. A solution of (6.2) which satisfies (6.5) is

$$\tilde{Y}_0 = \Phi(\zeta) + \Phi(\bar{\zeta}), \tag{7.1}$$

where $\Phi(\zeta)$ is a real function of the complex variable ζ. Consider the conditions on the SRF. From (6.4)

$$-\frac{\mathrm{d}y}{\mathrm{d}X} = \frac{\left(\dfrac{\partial \tilde{Y}_0}{\partial X}\right)}{\left(\dfrac{\partial \tilde{Y}_0}{\partial y}\right)} = \frac{\left(\dfrac{\partial \tilde{Y}_0}{\partial y}\right)}{\lambda - \left(\dfrac{\partial \tilde{Y}_0}{\partial X}\right)}, \tag{7.2}$$

hence

$$-\frac{(\mathrm{d}\zeta - \mathrm{d}\bar{\zeta})}{\mathrm{d}\zeta + \mathrm{d}\bar{\zeta}} = \frac{\Phi'(\zeta) + \Phi'(\bar{\zeta})}{\Phi'(\zeta) - \Phi'(\bar{\zeta})} = \frac{\Phi'(\zeta) - \Phi'(\bar{\zeta})}{\Phi'(\zeta) + \Phi'(\bar{\zeta}) - \lambda}. \tag{7.3}$$

From the last two expressions of (7.3) we obtain

$$\lambda\left[\frac{\Phi'(\zeta)}{\Phi'(\bar{\zeta})} + 1\right] - 4\Phi'(\zeta) = 0. \tag{7.4}$$

On the SRF,

$$\tilde{Y}_0 = \Phi(\zeta) + \Phi(\bar{\zeta}) = 0, \tag{7.5}$$

hence

$$\Phi'(\zeta)\,\mathrm{d}\zeta + \Phi'(\bar{\zeta})\,\mathrm{d}\bar{\zeta} = 0.$$

Substitution in (7.4) gives

$$\Phi'(\zeta) = \frac{\lambda}{4}\left(1 - \frac{\mathrm{d}\bar{\zeta}}{\mathrm{d}\zeta}\right), \tag{7.6}$$

which implies that here $\bar{\zeta}$ is a function of ζ. Integration gives

$$\Phi(\zeta) = \frac{\lambda}{4}(\zeta - \bar{\zeta}), \tag{7.7}$$

where we ignore the possible additive constant iM, M real, since this only modifies Φ. Substituting

$$\bar{\zeta} = \zeta - \frac{4}{\lambda}\Phi(\zeta)$$

in (7.5), gives

$$\Phi(\zeta) + \Phi\left(\zeta - \frac{4}{\lambda}\Phi(\zeta)\right) = 0, \tag{7.8}$$

a functional equation for $\Phi(\zeta)$. The solution of (7.8) is

$$\Phi(\zeta) = \frac{\lambda}{2}\zeta + b, \tag{7.9}$$

where b is a real constant. It is easily shown that this form is unique, the equation being reducible to a particular case of 'Babbage's equation' [11]. From (7.5), the equation of the SRF is given by

$$\frac{\lambda}{2}(\zeta + \bar{\zeta}) + 2b = 0,$$

hence

$$\tilde{Y}_0(X, y) = \frac{\lambda}{2}(\zeta + \bar{\zeta}) + 2b = \lambda(X - X_0), \quad X \geq X_0. \tag{7.10}$$

8. The Second Order Turning-Point Problem

The equation for the component $\tilde{Y}_1$ becomes

$$\frac{\partial^2 \tilde{Y}_1}{\partial X^2} + \frac{\partial^2 \tilde{Y}_1}{\partial y^2} = \lambda. \tag{8.1}$$

Let the equation of the SRF be

$$X(y) = X_0 + \lambda s X_1(y) + \cdots . \tag{8.2}$$

From Equations (6.4) we obtain

$$\frac{\partial Y_1}{\partial X}(X_0, y) = 0 \tag{8.3}$$

and

$$X_1(y) = -\frac{1}{\lambda} Y_1(X_0, y). \tag{8.4}$$

A solution of Equation (8.1) can be written

$$\tilde{Y}_1 = \frac{\lambda}{4}\zeta\bar{\zeta} + \Psi(\zeta) + \Psi(\bar{\zeta}), \tag{8.5}$$

where $\Psi(\zeta)$ is a real function of ζ, and this satisfies condition (6.5).

From (8.3), we obtain

$$\left(\frac{\partial}{\partial\zeta} + \frac{\partial}{\partial\bar{\zeta}}\right)\tilde{Y}_1 = \frac{\lambda}{4}(\zeta + \bar{\zeta}) + \Psi'(\zeta) + \Psi'(\bar{\zeta}) = 0,$$

when $X = \frac{1}{2}(\zeta - \bar{\zeta}) = X_0$. Thus

$$\frac{\lambda}{2} X_0 + \Psi'(\zeta) + \Psi'(2X_0 - \zeta) = 0. \tag{8.6}$$

Integration gives

$$\frac{\lambda}{2} X_0\zeta + \Psi(\zeta) - \Psi(2X_0 - \zeta) = \frac{\lambda}{2} X_0^2,$$

hence

$$\Psi(\zeta) - \Psi(2X_0 - \zeta) = \frac{\lambda}{2} X_0(X_0 - \zeta), \tag{8.7}$$

a functional equation for $\Psi(\zeta)$. The required solution of (8.7), such that $\tilde{Y}_1 = 0$ when $\zeta = \bar{\zeta} = X_0$, is

$$\Psi(\zeta) = -\frac{\lambda}{8}[A(\zeta - X_0)^2 + X_0(2\zeta - X_0)], \tag{8.8}$$

where A is a real constant. Substitution in (8.5) gives

$$\tilde{Y}_1(X, y) = \frac{\lambda}{4}[(1 - A)(X - X_0)^2 + (1 + A)y^2], \tag{8.9}$$

and from (8.4)

$$X_1(y) = -\frac{1}{4}(1+A)y^2. \tag{8.10}$$

Finally, the oxidizer concentration near the turning-point is

$$Y(X,y) = \lambda(X - X_0) + \frac{s\lambda^2}{4}[(1-A)(X-X_0)^2 + (1+A)y^2] + O(s^2), \tag{8.11}$$

and the equation of the SRF is

$$X(y) = X_0 - \frac{s\lambda}{4}(1+A)y^2 + O(s^2). \tag{8.12}$$

Equation (8.12) shows that on the SRF near the turning-point, $X = X_0 + O(s)$ when $y = O(1)$. On substituting this in (5.27) and matching like powers of s, we obtain $X_0 = 1/2\lambda$ and $y = O(s)$. This leads to a contradiction unless $A = -1$ in (8.12). The oxidizer concentration near the turning-point thus becomes

$$Y(X,y) = \lambda(X - \tfrac{1}{2}\lambda) + s\tfrac{1}{2}\lambda^2(X - \tfrac{1}{2}\lambda)^2 + O(s^2), \tag{8.13}$$

where

$$0 \le X - \tfrac{1}{2}\lambda \le O(s).$$

9. The SRF–Plane Surface Corner Problem

In considering smoulder propagation in a half-space, Adler and Herbert [4] failed to obtain an analytic solution near to where the SRF meets the plane surface. The numerical solutions of Kerr [6] appear to indicate that the shape of the SRF is parabolic in this region. In view of the solution to the 1st order problem obtained in Section 4, it is of some interest to examine the complete equations in the corner regions.

The parameters s and p may be scaled out of the equations by the substitutions

$$\begin{aligned} \xi &= \frac{p}{s^2 L}(sx' + u't'), \\ \eta &= \frac{p}{s}\left(1 - \frac{y'}{L}\right). \end{aligned} \tag{9.1}$$

Equation (2.1) becomes

$$\frac{\partial Y}{\partial \xi} = \frac{\partial^2 Y}{\partial \xi^2} + \frac{\partial^2 Y}{\partial \eta^2}, \tag{9.2}$$

and the conditions on the SRF become

$$\frac{\mathrm{d}\eta}{\mathrm{d}\xi} = -\frac{\partial Y}{\partial \eta} + \frac{\partial Y}{\partial \xi}\cdot\frac{\mathrm{d}\eta}{\mathrm{d}\xi}, \tag{9.3}$$

and

$$Y = 0.$$

Introduce complex variables

$$\rho = \xi + i\eta, \qquad \bar{\rho} = \xi - i\eta, \tag{9.4}$$

and consider Y as a function of ρ and $\bar{\rho}$. Equation (9.2) becomes

$$\frac{\partial^2 Y}{\partial\rho\,\partial\bar{\rho}} - \frac{1}{4}\frac{\partial Y}{\partial\rho} - \frac{1}{4}\frac{\partial Y}{\partial\bar{\rho}} = 0. \tag{9.5}$$

Rearrangement of (9.3) gives

$$\frac{\mathrm{d}\xi}{\mathrm{d}\eta} = \left(\frac{\partial Y}{\partial\xi} - 1\right) \Big/ \frac{\partial Y}{\partial\eta},$$

hence

$$\frac{\mathrm{d}\zeta - i\,\mathrm{d}\eta}{\mathrm{d}\xi + i\,\mathrm{d}\eta} = \left(\frac{\partial Y}{\partial\xi} - i\frac{\partial Y}{\partial\eta} - 1\right) \Big/ \left(\frac{\partial Y}{\partial\xi} + i\frac{\partial Y}{\partial\eta} - 1\right),$$

which in terms of $\rho, \bar{\rho}$ is

$$\frac{\mathrm{d}\bar{\rho}}{\partial\rho} = \left(\frac{\partial Y}{\partial\rho} - \frac{1}{2}\right) \Big/ \left(\frac{\partial Y}{\partial\bar{\rho}} - \frac{1}{2}\right). \tag{9.6}$$

Since on the SRF, $Y(\rho, \bar{\rho}) = 0$, we also have

$$\frac{\partial Y}{\partial\rho} + \frac{\partial Y}{\partial\bar{\rho}}\frac{\mathrm{d}\bar{\rho}}{\mathrm{d}\rho} = 0, \tag{9.7}$$

which combined with (9.6) gives

$$\frac{\mathrm{d}\bar{\rho}}{\mathrm{d}\rho} - 1 + 4\frac{\partial Y}{\partial\rho}(\rho, \bar{\rho}) = 0. \tag{9.8}$$

Equation (9.8) implies that on the SRF, $\bar{\rho}(\rho)$ is a function of ρ. In general, let

$$Y(\rho, \bar{\rho}) = e^{\frac{1}{4}(\rho+\bar{\rho})}\tilde{\tilde{Y}}(\rho, \bar{\rho}). \tag{9.9}$$

Equation (9.5) becomes

$$\frac{\partial^2 \tilde{\tilde{Y}}}{\partial\rho\,\partial\bar{\rho}} - \frac{1}{16}\tilde{\tilde{Y}} = 0, \tag{9.10}$$

and the conditions on the SRF are

$$\begin{aligned} &\bar{\rho} = \bar{\rho}(\rho) \\ &\frac{\partial\tilde{\tilde{Y}}}{\partial\rho}(\rho, \bar{\rho}) = \frac{1}{4}\left(1 - \frac{\mathrm{d}\bar{\rho}}{\mathrm{d}\rho}\right) e^{-\frac{1}{4}(\rho+\bar{\rho})}, \\ &\tilde{\tilde{Y}}(\rho, \bar{\rho}) = 0. \end{aligned} \tag{9.11}$$

A solution of (9.10) may be written in terms of the Riemann–Green function $I_0(\frac{1}{2}\sqrt{(\rho - \omega)(\bar{\rho} - \bar{\omega}}$, where $I_0(t)$ is the modified Bessel function of order zero [12]. Taking the SRF as the datum curve, with A and B on the curve,

$$\tilde{\tilde{Y}}(\omega, \bar{\omega}) = \int_{AB} I_0(\tfrac{1}{2}\sqrt{(\rho - \omega)(\bar{\rho} - \bar{\omega})}\,\frac{\partial\tilde{\tilde{Y}}}{\partial\rho}\,\mathrm{d}\rho. \tag{9.12}$$

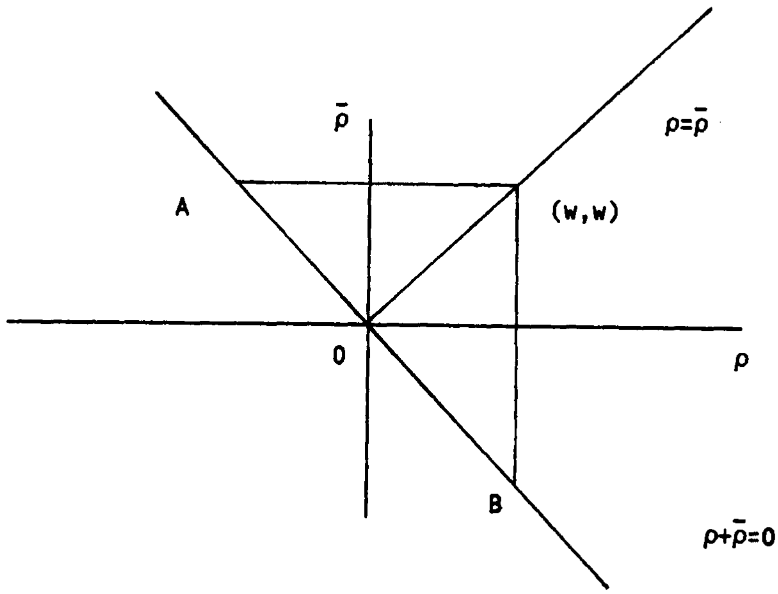

Figure 2. Path of integration in the $(\rho, \bar{\rho})$ plane for determining the oxidizer concentration at the leading edge of the SRF.

Hence for points on the plane surface $\omega = \bar{\omega}$, $(y' = L)$, and using (9.11)

$$\tilde{\bar{Y}}(\omega, \bar{\omega}) = \frac{1}{4}\int_{AB} I_0\big(\tfrac{1}{2}\sqrt{(\rho-\omega)(\bar{\rho}-\omega)}\big)\left(1 - \frac{\mathrm{d}\bar{\rho}}{\mathrm{d}\rho}\right) e^{-\frac{1}{4}(\rho+\bar{\rho})}\,\mathrm{d}\rho. \tag{9.13}$$

Let the equation of the SRF near where it meets the plane surface be $\rho + \bar{\rho} = 0$. The plane surface oxidizer concentration becomes (see Figure 2)

$$\begin{aligned} Y(\omega,\omega) &= \frac{1}{2}e^{1/2\omega}\int_{-\omega}^{\omega} I_0\big(\tfrac{1}{2}\sqrt{\omega^2-\rho^2}\big)\,\mathrm{d}\rho \\ &= e^{1/2\omega}\int_{0}^{\omega} I_0\big(\tfrac{1}{2}\sqrt{\omega^2-\rho^2}\big)\,\mathrm{d}\rho, \end{aligned} \tag{9.14}$$

where ω is now a real parameter $(\xi = \omega)$. The integral in (9.14) may be evaluated for small ω by use of the series expansion for $I_0(t)$. The result is

$$Y(\omega,\omega) = \omega + \frac{1}{2}\omega^2 + \frac{1}{6}\omega^3 + \cdots. \tag{9.15}$$

The dependence on ω as $\omega \to 0$ may be compared with the result of Section 4 by setting $\omega = \lambda X$.

A different approach to the corner problem is possible using an analysis similar to that of Blackwell and Ockendon [13] for the continuous casting of a metal bar from a mold.

Equations (9.3) can be combined to give the SRF condition

$$\frac{\partial Y}{\partial \xi} = \left[1 + \left(\frac{\mathrm{d}\xi}{\mathrm{d}\eta}\right)^2\right]^{-1}. \tag{9.16}$$

Introduce new independent variables, u, v, given by

$$\begin{aligned} \xi + \xi_0 &= u^2 - v^2, \\ \eta &= 2uv, \end{aligned} \tag{9.17}$$

where ξ_0 is a constant to be determined.

The coordinate transformation (9.17) permits a solution of (9.2) which depends only on v. The function $Y(v)$ satisfies

$$Y'' + 2vY' = 0, \tag{9.18}$$

with solution

$$Y(v) = 1 - \mathrm{erf}(v)/\mathrm{erf}(v_0), \tag{9.19}$$

where $v = v_0$ is the equation of the SRF.

Condition (9.16) on the SRF becomes

$$Y'(v_0) = -2v_0. \tag{9.20}$$

Substitution of (9.19) then shows that v_0 must be the solution of

$$\pi^{1/2} v_0 e^{v_0^2}\, \mathrm{erf}(v_0) = 1. \tag{9.21}$$

The substitution $v_0 = z_0/2^{1/2}$ shows that this is identical to the equation for z_0 derived by Adler and Herbert [4].

With $\xi_0 = -v_0^2$, the equation for the SRF becomes

$$\xi = \eta^2/4v_0^2. \tag{9.22}$$

From (9.17) and (9.19), the oxidizer concentration in the corner region becomes

$$Y(\xi, \eta) = 1 - \int_0^v e^{-t^2}\,\mathrm{d}t \Big/ \int_0^{v_0} e^{-t^2}\,\mathrm{d}t, \tag{9.23}$$

where

$$v = 2^{-1/2}[\{(\xi - v_0^2)^2 + \eta^2\}^{1/2} - \xi + v_0^2]^{1/2}.$$

The result (9.23) shows that there is a branch point at $(v_0^2, 0)$ and that the concentration is continuous on $\eta = 0$. Near the origin, the surface concentration is found to be

$$Y(\xi, 0) = \xi + 1/2(1 + 1/2v_0^2)\xi^2 + \cdots. \tag{9.24}$$

In comparing (9.24) with (9.15) we note that the latter was only derived with the assumption that the SRF meets the planar surface at right angles.

Discussion

The close analogy between smoulder propagation in a slab and the continuous casting of a metal bar from a liquid pool has already been mentioned above. Numerical solutions for the latter problem, using a boundary integral method and more general surface boundary conditions, have been obtained by Dewynne, Howison and Ockendon [14].

For smoulder propagation in a half-space, Adler and Herbert [4] assumed a constant oxidizer concentration on the planar surface and a vanishing concentration on the SRF, producing a singularity at $X = 0, y = 1$. [9] has recently shown that this problem is not well-posed but may be made regular by assuming that in the corner region the surface concentration varies linearly with distance. Referring to the 1st order problem of Section 4, we see that the singular points $(0, \pm 1)$ are replaced by branch points at $(1/2\lambda, \pm 1)$ and that the oxidizer concentration is now continuous on the planar surfaces and SRF.

To first order, the parameter λ was found to represent the oxidizer flux through one-half of the SRF and by continuity this must also be the flux through one of the planar surfaces. By definition, $\lambda = p/s$, where $p = Lu'/D$, hence for constant s, λ increases or decreases with p. The total 'length' ℓ of the SRF, obtainable from Section 4, is

$$\begin{aligned}\ell &= 2\int_0^{1/2\lambda}\left[1+\left(\frac{\mathrm{d}y}{\mathrm{d}X}\right)^2\right]^{1/2}\mathrm{d}X\\ &= (1+\lambda^2)^{1/2}+\frac{1}{\lambda}\log[\lambda+(1+\lambda^2)^{1/2}].\end{aligned}$$

The SRF is thus stretched or shortened by an increase or decrease in p, provided $\lambda > 1$.

The above analysis is based on a thin slab assumption, namely, that the Peclét number, p, for mass transfer is of the order of the small parameter s as defined by Equation (3.2). The definition of p involves the propagation speed, u', which is assumed known. This must be determined by considering the thermodynamics, chemical kinetics and material properties in a finite reaction zone. Some typical smouldering reactions are discussed in the paper by Drysdale [1]. Physically, it is seen that the oxidizer flux through the planar boundaries increases with u' and slab thickness L. The dominant term for the shape of the front is given by Equation (4.15), which shows that the front moves closer to the plane boundaries as the Peclét number increases.

Smouldering velocities are typically, $u' \sim 10^{-3}$ cm sec^{-1} [1], so that for a 2-cm-thick slab and reasonable values for $D, p \sim 10^{-1}$. Values of s depend on the material, but typically $s \sim 10^{-2}$, giving $\lambda \sim 10$.

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