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Self-similar reacting flows in variable density media

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Abstract. A theoretical study of self-similar detonations is undertaken in the case that the shock is propagating into a medium whose density varies by an algebraic power law. The non-constant density case permits the inclusion of Arrhenius and depletion factors in the reaction rate function. Special solutions are obtained that illustrate the nature of the singular locus, found even in the constant density case, and a necessary condition for the solution to intersect the singular locus is given in terms of the action of the piston. We are able to identify the appearance of the singular locus with an underdriven detonation that goes to failure in one of the special solutions, and in general with a reaction that does not go to completion.

1. Introduction

We consider the motion of a strong, planar shock wave moving into a one-dimensional reactive medium and initiating a chemical reaction that takes place behind the shock. The gas-dynamic flow of the chemical mixture behind the shock is described by the ZND (Zel'dovich–von Neumann–Doering) model that consists of the adiabatic, inviscid, one-dimensional fluid equations, plus constitutive relations for the equation of state and a rate equation governing the evolution of the chemical species. Self-similar solutions to the problem of describing this time-dependent reactive flow have been studied by several authors in the case that the density ahead of the shock is *constant*. See, for example, Sternberg (1970), Cowperthwaite (1979), Logan and Pérez (1980), Holm and Logan (1983) and Logan and Woerner (1989). One difficulty with all these studies is that the class of self-similar solutions does not include the case when the reaction rate contains either simple depletion or Arrehnius factors. In fact, it is shown in Logan and Pérez (1980) (also see Rogers and Ames 1989) that a necessary condition for self-similar motions to exist is that the reaction rate function governing the irreversible, exothermic chemical reaction $A \to B$ must have the form $r = p^{\beta} F(\rho, \lambda/p)$, where p is pressure, ρ is the density, λ is the mass fraction of the product species B, β is a constant and F is an arbitrary function. The case examined most often is the case that $r = \alpha p/\rho$ ($\beta = 1$ and $F \equiv \alpha/\rho$, α a constant), where the rate is proportional to the internal energy.

If one considers a shock propagating into a medium with *non-constant* density, however, one does not have to abandon Arrhenius kinetics and depletion factors to obtain self-similar motions of the reactive flow. The study of some these solutions is the content of this work. We classify all reaction rates and density distributions under which the governing equations and strong shock conditions admit self-similar solutions in the variable density case. In non-reactive media, self-similar solutions in the variable density case have been investigated by Sedov (1959) and Korobeinikov (1973).

In one special case an exact, analytic solution is found when the density is increasing ahead of a constant velocity shock. In a decreasing density case, under a special assumption, the problem is reduced to a single integration. These special solutions provide insights into the nature of the singular locus that is present in some self-similar detonations, a behaviour noticed by earlier authors in the constant density case. Bounds are obtained on the reaction progress variable and a necessary condition for the reaction not to go to completion is given. In the last section some numerical results are presented to illustrate the various cases. For one of the special solutions we are able to identify the presence of the singular locus with an underdriven detonation that leads to failure.

2. Self-similar solutions

At time $\bar{t}=0$ a piston located at $\bar{x}=0$ moves forward with initial velocity u_i into a one-dimensional reactive medium occupying $\bar{x}>0$ and having density $\bar{\rho}_0(\bar{x})$, $\bar{x}\geqslant 0$. The motion of the piston generates a strong shock with speed $\bar{D}(\bar{t})>0$, which in turn initiates an irreversible, exothermic chemical reaction $A\to B$ which then supplies energy to the flow behind the shock; no reaction is assumed to occur in the shock itself. Behind the shock the flow is governed by the scaled Eulerian equations (see Fickett and Davis 1979):

$$\dot{\rho}+\rho u_x=0 \tag{2.1}$$

$$\dot{u}+\rho^{-1}p_x=f/(u_i\tau_0^{-1}) \tag{2.2}$$

$$\dot{p}-\frac{\gamma p}{\rho}\dot{\rho}=k(\gamma-1)\rho\dot{\lambda} \tag{2.3}$$

$$\dot{\lambda}=r(\rho, p, \lambda) \tag{2.4}$$

where the overdot denotes the material derivative $\partial/\partial t+u\partial/\partial x$. These equations represent conservation of mass, momentum, energy, and the species equation, respectively. Here, ρ, u, p and λ represent the scaled density, particle velocity, pressure and mass fraction of B. The parameters γ and k represent the polytropic index and a dimensionless modelling number ($k\equiv u_i^2/q$, where q is the specific heat of reaction), respectively; f is the body force and r is the chemical reaction rate. To obtain (2.1)–(2.4) we have used the scalings

$$t=\tau_0^{-1}\bar{t} \qquad x=\bar{x}/(u_i\tau_0) \qquad u=\bar{u}/u_i$$

$$\rho=\bar{\rho}/\rho_0(0) \qquad p=\bar{p}/(\bar{\rho}_0(0)u_i^2) \qquad f=\bar{f}/(u_i\tau_0^{-1})$$

where the barred quantities are the original dimensioned quantities and τ_0 is a given chemical time scale; λ is already dimensionless. The presence of the body force f in the governing equations is required since a non-constant density distribution requires an external force to maintain equilibrium ahead of the shock. However, for detonations, where particle velocities and accelerations are large, we assume $|f|\ll u_i\tau_0^{-1}$, and therefore we neglect the body force in (2.2) in the subsequent analysis of the flow behind the shock. Alternatively, we could regard the reactive medium as a solidly packed condensed explosive with density variations caused by the packing; the small forces holding the components together are negligible compared with the pressure generated in a detonation.

Across the shock the Rankine–Hugoniot strong shock conditions are assumed to hold. In dimensionless form these conditions are

$$p_1(x)=\frac{2\rho_0(x)}{\gamma+1}D^2 \qquad \rho_1(x)=\frac{\gamma+1}{\gamma-1}\rho_0(x) \qquad u_1(x)=\frac{2}{\gamma+1}D \qquad \lambda_1=0 \tag{2.5}$$

where the subscript unity denotes the value of the quantity immediately behind the shock; $\bar{D}$ has been scaled by u_i and $\bar{\rho}_0(x)$ has been scaled by $\bar{\rho}_0(0)$. The shock velocity D is another unknown in the problem.

In the above formulation of the equations we have assumed that the equation of state of the reacting mixture behind the shock is $e=p/((\gamma-1)\rho)-q\lambda$, where e is the specific internal energy. This polytropic gas equation of state is assumed to hold even though the material ahead of the shock may be a solid combustible material. Typical values of γ for the gaseous products of a solid explosive are $\gamma\geqslant 6$ (see Fickett and Davis 1979).

Our goal is to find transformations under which (2.1)–(2.5) are invariant and determine the resulting self-similar solutions. We begin with the following general result regarding the invariance group of the governing partial differential equations (2.1)–(2.4).

Proposition 2.1 (Holm and Logan 1983). The one-parameter local lie group Γ_ε under which (2.1)–(2.4) with $f\equiv 0$ are constant conformally invariant is given by

$$\bar{t}=\varepsilon^{b}(t+1)-1 \qquad \bar{x}=\varepsilon^{a+b}(x+1)-1$$

$$\bar{\rho}=\varepsilon^{c}\rho \qquad \bar{u}=\varepsilon^{a}u \qquad \bar{p}=\varepsilon^{2a+c}p \qquad \bar{\lambda}=\varepsilon^{2a}\lambda$$

and r must have the form

$$r=\frac{p^{\beta+1}}{\rho}H\left(\frac{p^{\alpha}}{\rho},\frac{\lambda}{p^{1-\alpha}}\right) \tag{2.6}$$

where a, b and c are constants and

$$\alpha\equiv\frac{c}{2a+c} \qquad \beta\equiv\frac{-b}{2a+c}$$

and ε is the group parameter.

Remark. The similarity method is well catalogued in Bluman and Kumei (1989) or Rogers and Ames (1989). See also Logan (1987) for a brief introduction.

The infinitesimal generators for the x and t transformations above are $X=(a+b)(x+1)$ and $T=b(t+1)$. The similarity variable s may be taken as a first integral of $\mathrm{d}x/X=\mathrm{d}t/T$, or

$$s=\frac{x+1}{(t+1)^{\xi+1}} \qquad \xi=a/b. \tag{2.7}$$

Thus the shock path is the similarity curve $s=1$ passing through $x=t=0$. So the shock locus is

$$x=(t+1)^{\xi+1}-1 \tag{2.8}$$

and the shock speed D is

$$D=(\xi+1)(t+1)^{\xi}. \tag{2.9}$$

First integrals of the characteristic system

$$\frac{\mathrm{d}t}{b(t+1)}=\frac{\mathrm{d}\rho}{c\rho}=\frac{\mathrm{d}u}{au}=\frac{\mathrm{d}p}{(2a+c)p}=\frac{\mathrm{d}\lambda}{2a\lambda}$$

where the denominators are the corresponding generators of the group, define the self-similar motion. The form of the motion is

$$\begin{aligned} \rho&=(t+1)^{\eta}R(s) \qquad & p&=(t+1)^{2\xi+\eta}P(s) \\ u&=(t+1)^{\xi}\tilde{U}(s) \qquad & \lambda&=(t+1)^{2\xi}\Lambda(s) \end{aligned} \tag{2.10}$$

where $\eta\equiv c/b$.

Now we depart from previous work and consider the variable density case. The jump conditions (2.10) should also be invariant under Γ_{ε}. Hence the density relationship should be

$$\bar{\rho}_1=\frac{\gamma+1}{\gamma-1}\rho_0(\bar{x}).$$

Taking $\partial/\partial\varepsilon$ at the identity $\varepsilon=1$ gives, after some manipulation,

$$c\rho_0(x)=(a+b)(x+1)\rho_0'(x).$$

This differential equation for $\rho_0(x)$ is easily solved to get

$$\rho_0(x)=\rho_0(0)(x+1)^{c/(a+b)}. \tag{2.11}$$

Consequently, if the jump conditions are invariant under Γ_{ε}, then $\rho_0(x)$ must necessarily have the form (2.11). Because of the scalings, we get $\rho_0(0)\equiv 1$.

To obtain a self-similar reaction rate with an Arrhenius factor and depletion we adjust the parameters *a, b, c*. From (2.6) we observe that $\alpha=1$ (forcing $a=\xi=0$) will permit the arbitrary function H to depend on p/ρ (proportional to temperature) and λ alone. Then

$$r=\frac{p^{\beta+1}}{\rho}H(\theta,\lambda) \tag{2.12}$$

where $\theta\equiv p/\rho$ is the temperature. Taking

$$H(\theta,\lambda)=(1-\lambda)\exp(-E^*/\theta)$$

will then allow more realistic chemical kinetics than previously examined with self-similar solution in the constant density case. In this case ($\alpha=1$), the shock locus (2.8) becomes $x=t$ and the scaled shock velocity is $D=1$. The similarity curves $s=(x+1)/(t+1)=\text{constant}$ are straight lines in xt space. The density distribution ahead of the shock is $\rho_0(x)=(x+1)^{\eta}$ and the jump conditions become

$$\tilde{U}(1)=P(1)=\frac{2}{\gamma+1} \qquad R(1)=\frac{\gamma+1}{\gamma-1} \qquad \Lambda(1)=0. \tag{2.13}$$

If we make the definition $U \equiv \tilde{U} - s$, then substitution of (2.10) into the governing equations (2.1)-(2.4) gives a system of ordinary differential equations for U, P, R and Λ:

$$\eta R + UR' + R(U'+1) = 0 \tag{2.14}$$

$$U(U'+1) + P'/R = 0 \tag{2.15}$$

$$\eta P + UP' - \gamma PR^{-1}(\eta R + UR') = (\gamma - 1)kP^{1-1/\eta}H(PR^{-1}, \Lambda) \tag{2.16}$$

$$U\Lambda' = P^{1-1/\eta}R^{-1}H(PR^{-1}, \Lambda) \tag{2.17}$$

where also

$$U(1) = \frac{1-\gamma}{1+\gamma} < 0 \tag{2.18}$$

and the prime denotes differentiation with respect to s, with $0 < s \leqslant 1$.

We remark that the translated particle velocity U is introduced to obtain an autonomous system. Also, we assume $\eta \neq 0$; if $\eta = 0$ then $c = 0$ and the initial density would be constant, forcing $H \equiv 0$. Finally, we note that the power law density also allows self-similar solutions in cylindrical and spherical geometries, cases we do not consider here since no elementary solutions have been found in these cases.

Equations (2.14)-(2.17) can be written in normal form as

$$R' = -\frac{\eta R}{U} - \frac{P[\eta - (\gamma-1)kP^{-1/\eta}H]}{U\Delta} \tag{2.19}$$

$$U' = -1 + \frac{PR^{-1}[\eta - (\gamma-1)kP^{-1/\eta}H]}{\Delta} \tag{2.20}$$

$$P' = \frac{UP[k(\gamma-1)P^{-1/\eta}H - \eta]}{\Delta} \tag{2.21}$$

$$\Lambda' = P^{1-1/\eta}U^{-1}R^{-1}H \tag{2.22}$$

where $\Delta \equiv U^2 - \gamma PR^{-1}$. Since $U(1) < 0$ and $\Delta(1) < 0$, solutions will exist only for those values of s where Δ and U are negative. We shall refer to the set of (U, P, R) where $\Delta \equiv 0$ as the singular surface. Note that $\Delta = 0$ is not the sonic surface since U is not the particle velocity, but rather the translated particle velocity.

Before proceeding further, we note the properties of the self-similar solution along the shock locus. We denote

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)_s \equiv \left(\frac{\partial}{\partial t} + D\frac{\partial}{\partial x}\right)_{s=1}.$$

The following proposition is straightforward to verify.

Proposition 2.2. For the similarity solution propagating into a medium with density $\rho_0(x) = (x+1)^\eta$, $\eta \neq 0$, we have

$$\left(\frac{\mathrm{d}u}{\mathrm{d}t}\right)_s = \left(\frac{\mathrm{d}\lambda}{\mathrm{d}t}\right)_s = \left(\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{p}{\rho}\right)\right)_s = 0$$

$$\left(\frac{\mathrm{d}p}{\mathrm{d}t}\right)_s = \frac{2(t+1)^{\eta-1}\eta}{\gamma+1} \qquad \left(\frac{\mathrm{d}\rho}{\mathrm{d}t}\right)_s = \frac{(\gamma+1)(t+1)^{\eta-1}\eta}{\gamma-1}.$$

Thus u, λ, and $\theta \equiv p/\rho$ are constant along the shock while p and ρ are increasing when $\eta > 0$ (increasing density ahead) and p and ρ are decreasing when $\eta < 0$ (decreasing density ahead).

For any $H = H(PR^{-1}, \Lambda)$ equations (2.19)–(2.22) can be solved numerically, subject to initial conditions (2.13) and (2.18) at the shock. Substitution of this result into (2.10) would then give a class of self-similar motions for the problem. In the following we examine some special cases.

3. The case H = constant

In the special case H = constant we can obtain a simple analytic solution; such solutions are rare in reactive flow problems, even in simplified cases. We take, for convenience, $H = (\gamma - 1)^{-1}$ so that the reaction rate r is given by

$$r = \frac{p^{1-1/\eta}}{(\gamma-1)\rho}. \tag{3.1}$$

This rate function resembles the 'internal energy' rate functions often studied in the constant density case (see the references in section 1). To simplify the problem still further, we choose k and η to lie on the locus $\eta = (2/(\gamma+1))^{-1/\eta}k$. Thus $\eta > 0$, and (2.13) and (2.21) permit us to choose $P = 2(\gamma+1)^{-1}$ for all s. Then from (2.15) we obtain $U' + 1 = 0$ which integrates to give $\tilde{U}(s) = 2(\gamma+1)^{-1}$. Then (2.14) becomes

$$\eta R + \left(\frac{2}{\gamma+1} - s\right) R' = 0$$

yielding

$$R = \left(\frac{\gamma+1}{\gamma-1}\right)^{\eta+1} \left(s - \frac{2}{\gamma+1}\right)^{\eta}. \tag{3.2}$$

As a consequence the species equation (2.22) may be integrated to obtain

$$\Lambda = L\left\{\left(s - \frac{2}{\gamma+1}\right)^{-\eta} - \left(\frac{\gamma+1}{\gamma-1}\right)^{\eta}\right\} \tag{3.3}$$

where

$$L \equiv \left(\frac{2}{\gamma+1}\right)^{1-1/\eta} \left[(\gamma-1)\eta \left(\frac{\gamma+1}{\gamma-1}\right)^{\eta+1}\right]^{-1}.$$

The energy equation (2.16) is now satisfied identically. We summarize this result as follows, where we have combined the above results with (2.10).

Proposition 3.1. If the reaction rate is given by (3.1) and η and k related by the nonlinear equation

$$\eta = \left(\frac{2}{\gamma+1}\right)^{-1/\eta} k \qquad (\eta > 0) \tag{3.4}$$

then a self-similar solution to (2.1)–(2.5) with $f \equiv 0$ is given by

$$p = \frac{2}{\gamma+1}(t+1)^{\eta} \qquad u = \frac{2}{\gamma+1}$$
$$\rho = \left(\frac{\gamma+1}{\gamma-1}\right)^{\eta+1}\left(\frac{x+1}{t+1} - \frac{2}{\gamma+1}\right)(t+1)^{\eta} \tag{3.5}$$
$$\lambda = L\left\{\left(\frac{x+1}{t+1} - \frac{2}{\gamma+1}\right)^{-\eta} - \left(\frac{\gamma+1}{\gamma-1}\right)^{\eta}\right\} \qquad D = 1$$

for $x < t$.

Remark 3.1. The solution in proposition 3.1 has the property that there always exists an $s = s^*$ such that $\Lambda(s^*) = 1$. That is, the reaction always goes to completion. This result follows immediately from (3.3).

Remark 3.2. The solution (3.5) has the property that each term in the momentum balance equation (2.2) is identically zero; consequently, the reactive flow represented by this solution does not transfer momentum. The density is also constant on particle paths, the latter being given by $x - x_0 = 2(t - x_0)(\gamma+1)^{-1}$, where x_0 is the time $t = 0$ location of the particle. The piston path is the particle path $x_0 = 0$. Figure 1 shows the spacetime diagram for this solution and in figures 2 and 3 graphs of the solution surfaces for $\rho(x, t)$ and $\lambda(x, t)$ are shown.

We conclude this section with some general comments about the behaviour of self-similar reacting flows in the nonconstant density case; these are governed by (2.19)–(2.22) with initial data (2.13). If the condition

$$k(\gamma-1)P^{-1/\eta}H - \eta > 0 \tag{3.6}$$

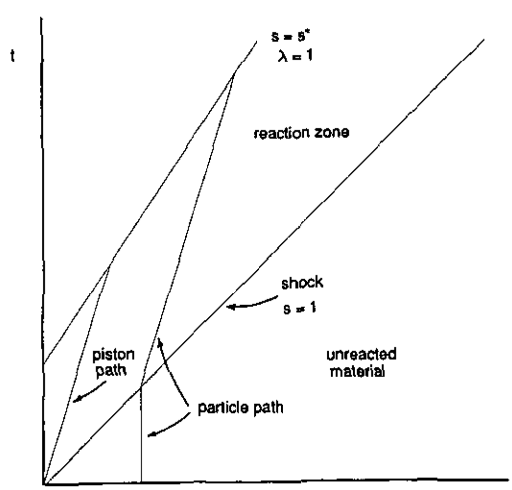

Figure 1. A spacetime representation of the solution (3.5) showing a typical particle path, the piston path and the shock. Each particle intersects the $\lambda = 1$ locus so that the reaction goes to completion.

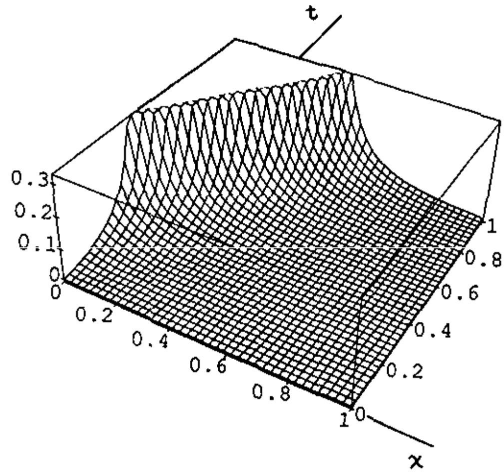

Figure 2. The density surface $\rho = \rho(x, t)$ for the solution (3.5) with $\eta = \gamma = 2$. The increase in density ahead of the shock is quadratic in t. The solution ends when the reaction is complete ($\lambda = 1$).

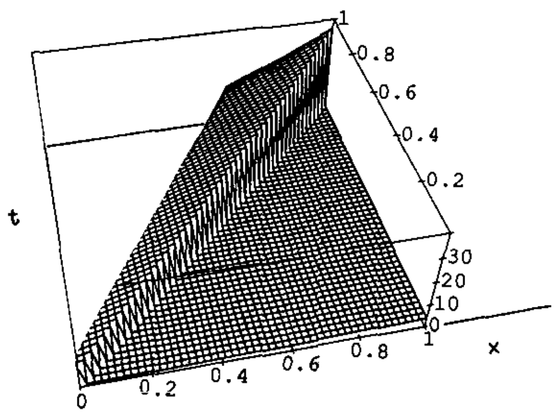

Figure 3. The progress variable surface $\lambda = \lambda(x, t)$ for the solution (3.5) with $\eta = \gamma = 2$.

holds, then (2.21) shows P is decreasing behind the shock. We always have $H > 0$, and therefore $\eta < 0$ guarantees (3.6). Further, (3.6) and (2.20) imply $\tilde{U}$ decreases behind the shock. Similarly, if (3.6) fails then P and $\tilde{U}$ increase behind the shock. Thus, for self-similar solutions with density variations $\rho_0(x) = (1+x)^\eta$, $\eta \neq 0$, ahead of the shock, along similarity curves $s =$ constant where (3.6) holds, fluid particles are decelerating; and, along those where (3.6) fails to hold, fluid particles are accelerating. As a consequence, if a rate function contains a depletion factor $1-\lambda$ and if the reaction goes to completion, then $H = 0$ when $\lambda = 1$. So, (3.6) is equivalent to $\eta < 0$. On the other hand, if $\eta > 0$, i.e. if a detonation is propagating into a medium of increasing density, and if the reaction rate has a depletion factor, then as $\lambda \to 1$ the flow must be accelerating. Finally, noting that

$$\dot{u} = u_t + uu_x = -\frac{x+1}{t+1}\tilde{U}' + \frac{\tilde{U}\tilde{U}'}{t+1} = \frac{\tilde{U}'U}{t+1}$$

we observe $\tilde{U}'<0$ implies $\dot{u}>0$ (since $U<0$); therefore the sign of $\tilde{U}'$ relates to the acceleration and deceleration of the fluid particles in a direct way.

4. The decreasing density case ($\eta<0$)

We now consider (2.14)–(2.17) in the case that $\eta=-1$, or $\rho_0(x)=(x+1)^{-1}$. Then (2.14) integrates to

$$UR=-1 \tag{4.1}$$

and (2.15) becomes

$$-\frac{1}{R}\left(\frac{R'}{R^2}+1\right)+\frac{P'}{R}=0$$

which integrates to $P+R^{-1}-s=$ constant. Again, from the initial conditions (2.13) and (2.18) we find the constant of integration to be zero, and therefore

$$P=s-R^{-1}. \tag{4.2}$$

Equations (2.16) and (2.17) can then be written

$$(\gamma-1)s-(\gamma+1)\frac{R'}{R^3}-\gamma\left(\frac{s}{R}\right)'=(1-\gamma)k\Lambda' \tag{4.3}$$

$$\Lambda'=-P^2H. \tag{4.4}$$

Next we integrate (4.3) to find

$$\frac{\gamma-1}{2}s^2+\left(\frac{\gamma+1}{2}\right)R^{-2}-\gamma sR^{-1}=(1-\gamma)k\Lambda$$

where the constant of integration is zero from the initial conditions. Therefore, in terms of $\Lambda(s)$,

$$R=(\gamma-1)[\gamma s-\sqrt{s^2-2(\gamma^2-1)k\Lambda}]^{-1} \tag{4.5}$$

$$U=(\gamma+1)^{-1}[-\gamma s+\sqrt{s^2-2(\gamma^2-1)k\Lambda}] \tag{4.6}$$

$$\tilde{U}=P=(\gamma+1)^{-1}[s+\sqrt{s^2-2(\gamma^2-1)k\Lambda}]. \tag{4.7}$$

Before (4.4) can be integrated to determine $\Lambda(s)$, a rate function H must be specified. It appears that there is no simple choice for H which would allow (4.4) to be integrated in closed form. (Note that the solution (4.5)–(4.7) coupled with (4.4) is reminiscent of the classical, steady ZND solution for the constant density case; however, there is no obvious transformation that relates the two.)

Even though (4.4) cannot be integrated in closed form, it is possible to deduce some conclusions on the size of Λ and hence upon the extent of completion of the reaction. From (4.4),

$$\Lambda(s)=-\int_1^s HP^2(\sigma)\,\mathrm{d}\sigma \qquad s<1.$$

Since $\eta<0$, the pressure P is decreasing (see the discussion at the end of section 3) and so its maximum value is attained on $[s,1]$ at $s=1$. Therefore

$$\Lambda(s)\leqslant-\left(\frac{2}{\gamma+1}\right)^2\int_1^s H\,\mathrm{d}\sigma\leqslant\left(\frac{2}{\gamma+1}\right)^2\|H\|_{\infty,s}(1-s) \tag{4.8}$$

where $\|H\|_{\infty,s}$ denotes the supremum norm on $[s, 1]$. When H has the form of the product of an Arrhenius factor with a depletion factor,

$$H \equiv (1-\lambda)\exp(-E^*/\theta) \qquad E^* > 0 \tag{4.9}$$

we see that $\|H\|_{\infty,s} < 1$ for $0 \leq s \leq 1$ and therefore $\Lambda(s) < 2(\gamma+1)^{-2}(1-s) < 2(\gamma+1)^{-2}$. Since $\gamma > 1$, we conclude that the reaction will *not* go to completion for the special case (4.9).

The mathematical reason that the reaction does not go to completion for some forms of H lies in the existence of a singular locus for the differential equations (2.19)–(2.22) governing the self-similar flow. We have, for the solution (4.5)–(4.7),

$$U^2 - \frac{\gamma p}{R} = R^{-1}[R^{-1} - \gamma s + \gamma R^{-1}] = -R^{-1}\sqrt{s^2 - 2(\gamma-1)k\Lambda}.$$

Since $U \equiv -R^{-1}$ is never zero, the singularity occurs in (2.19)–(2.22) when

$$s^2 - 2(\gamma-1)k\Lambda(s) = 0$$

which may have solutions $s_0 \in (0, 1)$, depending on H. Figure 4 shows a spacetime diagram for an H of the form (4.9). From (4.5)–(4.7) we observe that P, R and U (and hence $\tilde{U}$) are finite at s_0 even though their derivatives become infinite. In particular, we see from (4.7) that $\tilde{U}(s_0) > 0$; i.e. at the singularity the flow velocity is positive. We remark that this result is in contrast to the results for constant density in Logan and Woerner (1989); there it was found that a singularity in the flow developed only for decelerating pistons with negative velocity. In the next section we shall give a necessary condition for the existence of a singularity in terms of the piston motion and therefore pose a physical reason for some reactions going to completion, and others not.

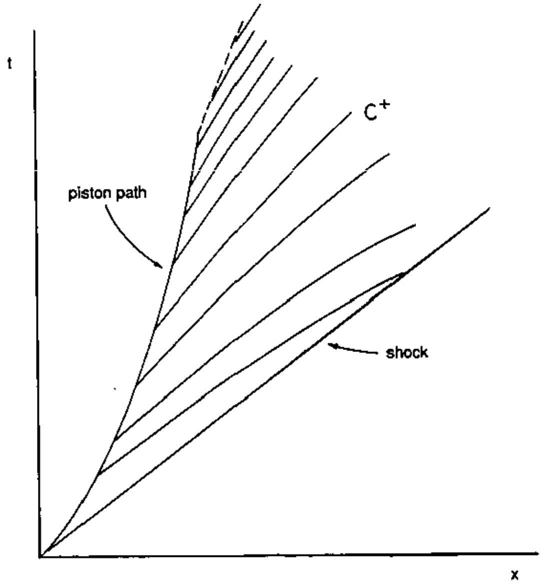

Figure 4. Spacetime diagram showing the shock $x = t$ and the decelerating piston in the case $r = p^2(1-\lambda)\exp(-E^*/\theta)$ where $E^* = 0.222$, $\gamma = 2$, $k = 1$, $\eta = -1$. The C^+ characteristics have envelope $s = 0.385$ (dashed line) and the reaction does not go to completion. This solution was computed numerically from (4.4)–(4.7).

5. Nature of the singular points

In this section we give some insight into the nature of the self-similar flow when the appearance of a singular point occurs in (2.14)–(2.17). Singular lines, also termed limit lines, are not uncommon in gas-dynamic theory (see von Mises 1958).

The governing equations (2.1)–(2.3) can be written in characteristic form in the usual way (see, for example, Whitham 1974):

$$\left(\frac{\mathrm{d}p}{\mathrm{d}t}\right) \pm \rho c\left(\frac{\mathrm{d}u}{\mathrm{d}t}\right) = (\gamma-1)k\rho r \qquad \text{on } \frac{\mathrm{d}x}{\mathrm{d}t} = u \pm c \tag{5.1}$$

$$\frac{\mathrm{d}p}{\mathrm{d}t} - c^2\frac{\mathrm{d}\rho}{\mathrm{d}t} = k(\gamma-1)\rho r \qquad \text{on } \frac{\mathrm{d}x}{\mathrm{d}t} = u \tag{5.2}$$

and

$$\frac{\mathrm{d}\lambda}{\mathrm{d}t} = r \qquad \text{on } \frac{\mathrm{d}x}{\mathrm{d}t} = u \tag{5.3}$$

where $c^2 \equiv \gamma p\rho^{-1}$. In terms of the similarity variables, (5.1) becomes

$$\eta P + P'(U \pm C) \pm RC(U'+1)(U \pm C) = k(\gamma-1)P^{1-1/\eta}H(\theta, \Lambda) \tag{5.4}$$

where $C^2 = \gamma PR^{-1}$. On the singular surface $\Delta \equiv U^2 - C^2 = 0$, equation (5.4) becomes

$$\eta = (\gamma-1)kP^{-1/\eta}H(\theta, \Lambda). \tag{5.5}$$

Therefore, if a trajectory of (2.19)–(2.22) approaches the singular surface $\Delta = 0$ for some $s = s_0 < 1$, then (5.5) must hold in the limit $s \to s_0^+$ in order to have a valid solution at that point. Otherwise, the trajectory cannot enter the singular surface and the solution would have to terminate at $s = s_0$, whether or not the reaction is complete. Condition (5.5) relates the density index η to the rate factor $H(\theta, \Lambda)$. If $\eta < 0$ then (5.5) can never hold; thus in media with decreasing density ahead of the shock, any trajectory entering the singular surface must terminate there.

If (5.5) fails to hold so that the solution must end on the singular surface, then it is the positive characteristic equation (with the plus sign in (5.4)) that produces the singularity since $U < 0$ and $C > 0$. In this case (5.1) shows that the C^+ characteristics have slope $\mathrm{d}x/\mathrm{d}t = \tilde{U} + C = U + C + s$, and so $\mathrm{d}x/\mathrm{d}t = s_0$ at the singular point. But this is precisely the slope of the similarity curve $s(x, t) = s_0$. Consequently, the similarity curve $s = s_0$ in xt space is an envelope of the positive characteristics. An example of this phenomenon is illustrated in figure 4.

The governing equations (2.19)–(2.22) also exhibit singular behaviour at $U = \tilde{U} - s = 0$. In this case we can show that it is the behaviour of the particle paths near a critical similarity curve that causes the singularity. If (5.2) is written in terms of the similarity solution we obtain

$$\eta P + UP' - C^2(\eta R + UR') = k(\gamma-1)P^{1-1/\eta}H. \tag{5.6}$$

When $U = 0$ we have

$$kP^{-\eta}H(\theta, \Lambda) = -\eta. \tag{5.7}$$

Therefore, if a trajectory of (2.19)–(2.22) approaches the surface $U = 0$ for some $s = s_0 < 1$, then (5.7) must hold as $s \to s_0^+$ in order to have a valid solution at that point; otherwise the solution must terminate at s_0. We note that if the solution becomes singular at $s = s_0$ and enters the surface $U = 0$, then the particle paths have slope $\mathrm{d}x/\mathrm{d}t = \tilde{U} = U + s = s_0$, which is the same as the slope of the similarity curve $s = s_0$. Thus the similarity curve $s = s_0$ in xt space forms an envelope of the particle paths. The evolution of the chemical progress variable Λ is determined by the species equation (2.22). An example of such a singular flow is shown in figure 5.

The question of whether the singular surface $\Delta = 0$ appears in a given self-similar flow can be partially answered in terms of the piston motion. We prove the following.

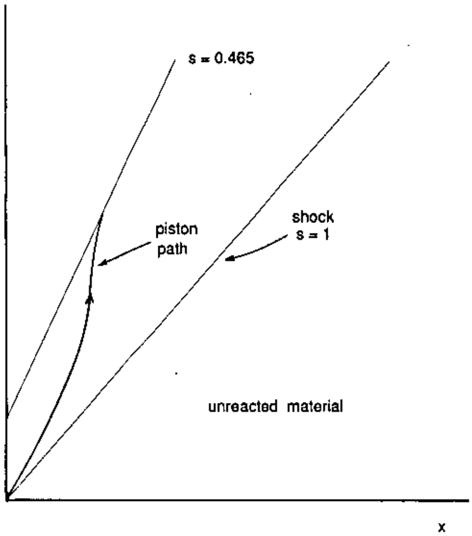

Figure 5. The piston path (not drawn to scale) in the case $k = 3$, $\eta = 1$, $\gamma = 2$ with the reaction rate H given by (4.9) with $E^* = 0.222$. The reaction goes to completion ($\lambda = 1$) as the particle paths approach the line $s = 0.465$, which is an envelope of the particle paths.

Proposition 5.1. A necessary condition that $\Delta(s_0) = 0$, $s_0 < 1$, for the self-similar solution (2.1)–(2.5) with $\rho_0(x) = (1 + x)^\eta$, $\eta \neq 0$, is that the piston decelerate on some interval of time.

Proof. First we note that by definition

$$\Delta' = 2UU' - \gamma P'/R + \gamma PR'/R^2.$$

Using the mass and momentum equations (2.14) and (2.15), we may eliminate R' to obtain

$$\Delta' = 2UU' - \frac{\gamma\eta P}{RU} - \frac{\gamma P'}{RU^2}\left(U^2 - \frac{P}{R}\right). \tag{5.8}$$

By way of contradiction, assume that the piston is everywhere accelerating, that is,

$$\dot{u}_{\text{piston}} > 0.$$

Since the solution is self-similar, every particle is likewise accelerating. Thus $\dot{u} > 0$ everywhere. Then by the remarks at the end of section 3, we have

$$\tilde{U}' < 0 \qquad U' > 0 \qquad P' < 0 \qquad P, R > 0 \qquad U < 0.$$

From (3.6) we also have $\eta > 0$ as a necessary condition for accelerating fluid particles. Therefore, the first two terms on the right-hand side of (5.8) are positive. Further, since $\gamma > 1$,

$$U^2 - \frac{P}{R} > \Delta.$$

Let s_0 be the first value of s smaller than one where $\Delta(s_0) = 0$; then $(U^2 - P/R)(s_0) > 0$ and from (5.8) we must have $\Delta'(s_0) > 0$. But this contradicts the fact that $\Delta(1) < 0$ and $\Delta(s) < 0$ for $s_0 < s < 1$, and the proof is complete. □

The detonation presented in proposition 3.1 always goes to completion because the piston is never decelerating. The converse of proposition 5.1 is false; sufficient conditions must involve k and form of H, as well as the action of the piston.

We may gain further physical insight into the existence of the singular line by transforming the solution (4.4)–(4.7) in the case $\eta = -1$ into quantities $\hat{\Lambda}$, $\hat{R}$, $\hat{U}$ and $\hat{P}$ defined by

$$\hat{R} = sR = \frac{\gamma + 1}{\gamma - \sqrt{1 - 2(\gamma^2 - 1)k\hat{\Lambda}}} \qquad \hat{\Lambda} = s^{-2}\Lambda \tag{5.7}$$

$$\hat{U} = \hat{P} = s^{-1}\tilde{U} = s^{-1}P = \frac{1 - \sqrt{1 - 2(\gamma^2 - 1)k\hat{\Lambda}}}{\gamma + 1}. \tag{5.8}$$

In these variables the solution resembles the classical ZND steady solution (see Fickett and Davis (1979)). The quantity $2(\gamma^2 - 1)k$ under the radical in (5.7)–(5.8) is analogous to the overdrive parameter $(D_j/D)^2$ in the ZND solution, where D_j is the Chapman–Jouget velocity and D is the detonation velocity. If $2(\gamma^2 - 1)k > 1$, which is analogous to $D < D_j$ (underdriven case), then the reaction will not go to completion since the quantity under the radical in (5.7) and (5.8) would become negative before $\Lambda = 1$. Thus, in the solution (4.4)–(4.7) there is a correspondence between being underdriven and having a trajectory reach the singular surface, the latter leading to an incomplete reaction.

This observation is consistent with the results obtained in Logan and Woerner (1989) in the constant density case. There, the appearance of a limit line was accompanied by a piston that was decelerating infinitely fast (essentially becoming a massless piston). Thus, the limit line appeared when the flow was strongly underdriven and the reaction did not go to completion. Physically, one could infer that the piston behind the flow is pulled backwards so rapidly that the resulting rarefaction causes the chemical reaction to end before it goes to completion.

6. Discussion and examples

The trajectories of the self-similar system (2.19)–(2.22) lie in a four-dimensional phase space; there are three adjustable parameters (γ, k and η) plus an arbitrary reaction rate function $H(\theta, \Lambda)$. With this high degree of generality it is difficult to make specific assertions regarding the behaviour of the phase trajectories. In special cases, however, some conclusions can be drawn. For example, in section 3 we examined an exact solution when H = constant and there was a nonlinear, simplifying relationship (equation (3.4)) between k and η. This solution had the property that the chemical reaction always goes to completion. On the other hand, the reaction for the special solution in section 4 with $\eta = -1$ and H given by (4.9) never goes to completion because of the appearance of the singularity in the flow.

One reason for examining self-similar detonations in a medium with variable density is that solutions can be obtained when the rate law contains Arrhenius and depletion factors. In the case studies for detonations in constant density media, the invariance hypothesis forced the rate law to be of the form $r = p^{\beta} f(\rho, \lambda/p)$, thus excluding the physically relevant Arrhenius and depletion factors; in these studies it was not clear if the mechanism producing singular lines in the flow was the rate law, often taken to be a simple power law $r = p/\rho = \theta$ (see Logan and Woerner 1989). Therefore, rather than undertake an exhaustive numerical study and examine large classes of rate laws and parameter ranges, we limit the discussion to rate laws of the form (4.9) with the shock propagating into a medium of increasing density ($\eta = 1$); we then examine the behaviour of the trajectories for different values of k, the ratio of the specific chemical energy release q to the initial piston velocity u_i^2.

Figure 6 illustrates trajectories in RUP-phase space when $\eta = 1$ and H is given by (4.9) with $E^* = 0.222$ and $\gamma = 2$. The singular surface $\Delta \equiv U^2 - \gamma P/R = 0$ is shown as a sheet varying parabolically in the U direction and linearly in the R direction. The shock is represented as a point $((\gamma+1)/(\gamma-1), (1-\gamma)/(1+\gamma), 2/(\gamma+1))$ which lies above the surface $\Delta = 0$. Numerical calculations indicate three possibilities. For $k < k^* \simeq 4.430\,316\,75$ the trajectory enters the singular surface $U = 0$ and the reaction goes to completion, as may be expected from (2.22) where U appears in the denominator on

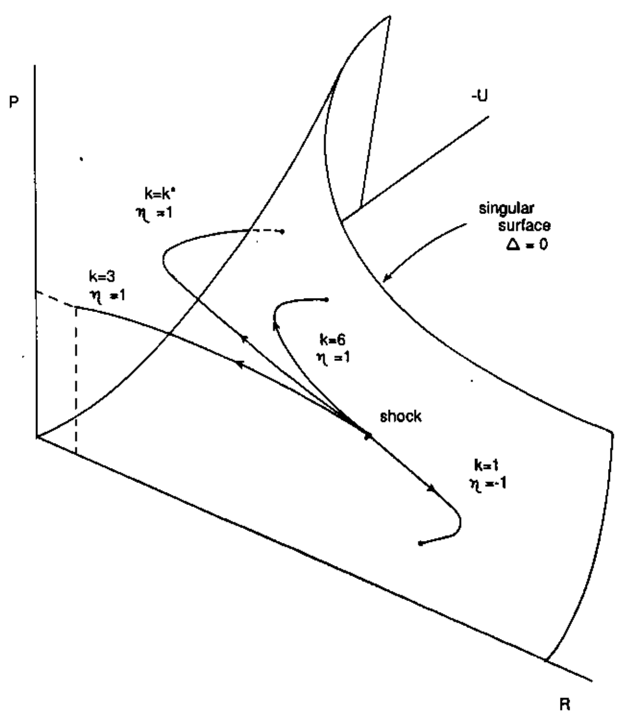

Figure 6. Trajectories of (2.19)–(2.22) in RUP-space when H is given by (4.9) with $E^* = 0.222$ for different values of η and k. The point representing the shock lies above the $\Delta = 0$ surface.

the right-hand side. For $k > k^*$ the trajectory enters the singular surface $\Delta = 0$ before the reaction is complete. For $k = k^*$ the reaction is complete just at the singular surface $\Delta = 0$. Three such trajectories (for $k = 3$, k^* and 6) are shown in figure 6. In this special case, one important conclusion can be drawn from proposition 5.1; namely, a necessary condition for the chemical reaction *not* to go to completion is that the piston decelerate on some interval of time. (Thus, the detonation given in proposition 3.1 always goes to completion because the piston is never decelerating.) Figure 7 shows the calculated values of the reaction progress variable λ as a function of $1-s$ for $k = 1$ and $k = 3$; we note the different shapes of the curves. The piston path for $k = 3$ is depicted in figure 5.

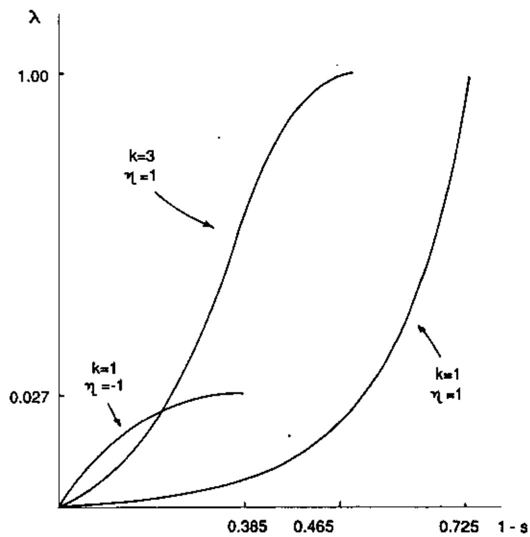

Figure 7. The reaction progress variable λ graphed against $1-s$ (making the shock at the origin) for different values of k and η with H given by (4.9) with $E^* = 0.222$. The graph for $\eta = -1$ is not drawn to correct vertical scale.

Figure 6 also shows a typical trajectory for a decreasing medium ($\eta = -1$). In this case the trajectory intersects the singular surface $\Delta = 0$ before the reaction is complete. The particle velocity is continuously decreasing along the trajectory (see figure 4); the reaction progress variable curve is shown in figure 7.

The numerical results in the case $\eta = 1$ and H given by (4.9) are consistent with the results of the constant density case discussed in Logan and Woerner (1989). For small values of the modelling parameter k there is a smooth solution behind the shock and the reaction goes to completion. As k increases, that is, as more chemical energy is released with respect to the mechanical energy u_i^2, there is a value ($k = k^*$) beyond which the flow is characterized by the presence of a singular surface and an incomplete chemical reaction. We have shown that if the reaction is incomplete, that is, if a trajectory intersects the singular surface, then necessarily the driving piston must decelerate on some interval of time. Again, this result is consistent with the constant density case where it was observed (but not proved) that the presence of a limit line in the flow was associated with a rapidly decelerating piston. Thus, there are not substantial changes in a medium of increasing density from the constant density case;

but in the non-constant case the kinetics are not restricted and it appears that the presence of limit lines is not an artifact of over-simplified rate laws, like the power laws used by the authors in the constant density case (Logan and Woerner 1989).

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