Self-similar detonation waves

Darryl D Holm† and J David Logan‡

† Los Alamos National Laboratory of the University of California, Los Alamos, New Mexico 87545.
‡ Department of Mathematics and Statistics, University of Nebraska, Lincoln, Nebraska 68588. Partially supported by Group M-3 of Los Alamos National Laboratory and the Air Force Office of Scientific Research.

Abstract. New results on similarity solutions to one-dimensional reactive flow problems with strong shocks are presented. Using dimensional methods, two modelling numbers for the flow are identified and the possible equations of state, including Mie–Grüneisen forms, which admit similarity solutions are characterised. In a special case the entire problem is reduced to a nonlinear eigenvalue problem in a sound speed–particle velocity phase plane. In this plane the critical points are analysed and the relationship between singular points in the self-similar solution and the characteristics of the Zel'dovich–von Neumann–Doering equations is found.

1. Introduction

The problem statement is as follows. We consider self-similar motion of a strong shock wave moving into a reactive medium and initiating a chemical reaction which takes place behind the shock. The self-similar flow of the chemical mixture behind the shock is described by the ZND (Zel'dovich–von Neumann–Doring) model (see Fickett and Davis 1979) which consists of the adiabatic, inviscid, one-dimensional fluid equations, plus constitutive relations for the equation of state and for the local chemical reaction rate(s).

The first part of the problem is to determine the general constitutive relations for which the ZND model possesses self-similar detonation waves as solutions. The main problem then is to characterise the resultant self-similar waves physically. This is done by interpreting the critical points and singular points of the self-similar equations in terms of physical quantities. Such interpretation is accomplished most directly by reducing the self-similar equations to motion in a 'phase plane' whose coordinates are the local sound speed and particle velocity.

In recent years several investigators have studied such problems of self-similar detonation waves in the ZND model. In these studies, the equation of state of the chemical mixture is that of a polytropic gas and the chemical kinetics are given by various interpolation functions for reaction rates; for example, a reaction rate proportional to the internal energy or the temperature is known to simplify the self-similar calculations. For such reaction rate functions, Sternberg (1970) has given a relatively complete description of self-similar ZND flows in Eulerian coordinates. Logan and Pérez (1980) have characterised the general form of reaction rates for ideal gas equations of state under which the ZND model admits self-similar solutions and have

also computed the local Lie group under which the one-dimensional problem in Lagrangian variables is invariant. In a special case Logan and Bdzil (1982) have reduced the problem of self-similar ZND waves in spherical geometry to phase-plane analysis in a 'Lie plane', whose coordinates, however, have no physical significance. Cowperthwaite (1978) has used self-similar solutions in conjunction with Lagrangian gauge data to determine energy release rates. Bisimov *et al* (1970), Lee *et al* (1969), and recently Kamel and Oppenheim (1979) have also studied self-similar solutions where energy is deposited continuously in the flow regime behind the shock. Further references on these types of problems as well as on problems where the energy is released either in the shock front or after an induction time period can be found in Korobeinikov (1976).

In the present paper we first answer the question of which equations of state $e = e(p, \rho, \lambda)$ admit self-similar solutions and we determine Mie–Grüneisen forms of the equation of state. Here, e is internal energy, p is pressure, ρ is density and λ is the degree of chemical reaction. Classical dimensional analysis of the governing ZND equations then leads us to identify two dimensionless modelling numbers whose values decisively affect the flow. Indeed, the product of these two modelling numbers acts as a nonlinear eigenvalue for the existence of regular solutions in the self-similar ZND problems for which the reaction rate is taken to be proportional to the internal energy. For that class of ZND problems, by choosing phase-plane variables to be particle velocity and local sound speed, we determine the physical nature of the critical and singular points encountered in spherical geometry by Logan and Bdzil. In addition, we determine in general the relationship between the singular points in the self-similar flow and the characteristics of the original ZND equations.

In §§ 2 and 3 the ZND equations are recalled and made dimensionless. In § 4, imposition of scale invariance upon the ZND system restricts the functional forms of the ZND constitutive relations to a class which includes state equations of Mie–Grüneisen type. Thereupon, scale invariance is used to reduce the ZND system to ordinary differential equations for the self-similar solutions. In § 5 we consider the particular class of constitutive functions for which solution of the similarity equations reduces to phase-plane analysis plus quadratures. Significantly, in § 6 the critical points of this phase-plane problem are seen to be determined by the characteristic equations of the original ZND system. Then in § 7 an example is studied for planar geometry and for a polytropic equation of state with $\gamma = 3$. In the example, most of the phase-plane analysis can be done without numerical aid, except to determine a nonlinear eigenvalue for which there exists a regular solution over the entire range of integration. From that example, in § 8 we supply the physical interpretation of the critical-point results obtained in spherical geometry by Logan and Bdzil.

2. The governing equations

In Eulerian form, the ZND equations governing the flow of a reacting fluid are given by (see Fickett and Davis 1979)

$$\mathrm{d}\rho/\mathrm{d}t + \rho(u_r + \nu u/r) = 0 \tag{2.1}$$

$$\mathrm{d}u/\mathrm{d}t + p_r/\rho = 0 \tag{2.2}$$

$$\mathrm{d}p/\mathrm{d}t - (B/\rho)\,\mathrm{d}\rho/\mathrm{d}t = q^2 l\Gamma\rho Q/\tau \tag{2.3}$$

$$\mathrm{d}\lambda/\mathrm{d}t = Q/\tau \tag{2.4}$$

where ρ, u, p are the density, particle velocity, and pressure, respectively, and λ is the dimensionless progress variable of a single, irreversible chemical reaction (λ represents the mass fraction of the product). Equations (2.1) and (2.2) are the usual conservation laws for mass and momentum with $\nu = 0, 1, 2$ the geometric factor for planar, cylindrical, spherical symmetry, respectively, and $\mathrm{d}/\mathrm{d}t = \partial/\partial t + u\,\partial/\partial r$ the convective derivative. Equation (2.3) is the expression for the conservation of energy, where $B = B(\rho, p, \lambda)$ is the bulk modulus, $l = l(\rho, p, \lambda)$ is the chemical potential, $\Gamma = \Gamma(\rho, p, \lambda)$ is the Grüneisen function and $Q = Q(\rho, p, \lambda)$ is the chemical reaction rate with $1/\tau$ being the rate constant. The functions B, l and Γ are related to the equation of state $e = e(\rho, p, \lambda)$, where e is the internal energy, via the equations

$$\left(\frac{\partial e}{\partial v}\right)_{\lambda, p} = \frac{B}{\Gamma} - p \qquad \left(\frac{\partial e}{\partial p}\right)_{\rho, \lambda} = \frac{1}{\rho \Gamma} \qquad \left(\frac{\partial e}{\partial \lambda}\right)_{p, \rho} = -q^2 l \tag{2.5}$$

where $v = 1/\rho$ is the specific volume and q^2 is the heat of reaction. Equation (2.3) follows easily from the adiabatic equation $\mathrm{d}e = -p\,\mathrm{d}v$ and the definitions (2.5). The reader may more readily recognise (4.3) as conservation of energy, from which (2.3) follows. Finally, (2.4) is the rate equation governing the evolution of the chemical reaction. The requirement of Galilean invariance precludes dependence upon u in the constitutive functions B, l, Γ and Q.

The equilibrium state just behind a shock with velocity D propagating into a quiescent material with initial states p_0, ρ_0, $u_0 = 0$, $\lambda_0 = 0$ is determined by the Rankine–Hugoniot jump conditions. These relations are

$$u_1/D = 1 - \rho_0/\rho_1 \tag{2.6}$$

$$p_1 - p_0 = \rho_0 u_1 D \tag{2.7}$$

$$e_1 - e_0 = (p_1 + p_0)(v_0 - v_1)/2 = u_1^2/2 + p_0(v_0 - v_1) \tag{2.8}$$

$$\lambda_1 - \lambda_0 = 0. \tag{2.9}$$

Equation (2.9) indicates that no reactions occur in the shock front. For strong shocks, the terms involving p_0 are to be neglected. We note that no viscous or heat conduction effects are present to disperse the shock.

3. Scaling

In order to write the equations in dimensionless form we introduce the following dimensionless variables:

$$\bar{t} = t/(r_0/D_0) \qquad \bar{r} = r/r_0 \qquad \bar{u} = u/D_0$$
$$\bar{\rho} = \rho/\rho_0 \qquad \bar{p} = p/\rho_0 D_0^2 \qquad \bar{\lambda} = \lambda \tag{3.1}$$

where r_0 is a length scale for the problem and D_0 is the initial (time $t = 0$) shock speed. The partial differential equations (2.1)–(2.4) become, upon dropping the bar notation,

$$\mathrm{d}\rho/\mathrm{d}t + \rho(u_r + \nu u/r) = 0 \tag{3.2}$$

$$\mathrm{d}u/\mathrm{d}t + p_r/\rho = 0 \tag{3.3}$$

$$dp/dt - (B/\rho)\, d\rho/dt = k_e k_t \rho \Gamma lQ \tag{3.4}$$

$$d\lambda/dt = k_t Q \tag{3.5}$$

where k_t and k_e are dimensionless modelling numbers given by

$$k_t = (r_0/D_0)/\tau \qquad k_e = q^2/D_0^2. \tag{3.6}$$

Hence k_t is the ratio of the hydrodynamic time scale to the time scale for the chemical reaction, and k_e is the ratio of the specific energies for the chemical reaction and the hydrodynamics. The competition between the chemistry and the hydromechanical flow shows up in equations (3.4) and (3.5). For $k_e = O(1)$, the reactive equations become those of inert flow in the limit that $k_t \ll 1$, i.e. when the chemistry takes place much more slowly than the mechanical processes. If $k_t \gg 1$, then the time scale for the chemistry is fast compared with that of the flow; in this limit the reaction zone length is small and approaches that of a Chapman–Jouget detonation where the reaction is instantaneous and takes place in the shock front. For $k_t = O(1)$ and $k_e \ll 1$ the chemical energy release is small and is coupled to the flow only through the bulk modulus B and the reaction rate Q.

In scaled variables, the Rankine–Hugoniot conditions (2.6)–(2.9) become

$$u_1/D = 1 - 1/\rho_1 \qquad p_1 - p_0 = u_1 D \qquad \lambda_1 - \lambda_0 = 0$$

$$e_1 - e_0 = u_1^2/2 + p_0(1 - 1/\rho_1). \tag{3.7}$$

Again, the terms containing p_0 are to be neglected in the strong shock case.

4. Self-similar solutions

The general group under which the governing partial differential equations and Rankine–Hugoniot conditions are invariant has been computed by Logan and Pérez (1980) under the assumption of polytropic equation of state and in the strong shock limit. Here we make no assumptions concerning the functional form of the equation of state, $e = e(\rho, p, \lambda)$. In fact, we wish to determine forms of the equation of state and reaction rate for which self-similar solutions can be found.

It is easy to see that the mass equation (3.2), the momentum equation (3.3) and the rate equation (3.5) admit the following transformation group[†]:

$$\bar{t} = e^b(t + t_0) - t_0 \qquad \bar{r} = e^{a+b} r$$

$$\bar{\rho} = e^c \rho \qquad \bar{u} = e^a u \tag{4.1}$$

$$\bar{p} = e^{2a+c}(p + p_0) - p_0 \qquad \bar{\lambda} = e^{2a}(\lambda + \lambda_0) - \lambda_0$$

where a, b, c, p_0, λ_0 are arbitrary group parameters, and provided that the reaction rate $Q = Q(\rho, p + p_0, \lambda + \lambda_0)$ is of the form

$$Q = \frac{(p + p_0)^{\beta+1}}{\rho} H\left(\frac{(p + p_0)^\alpha}{\rho}, \frac{\lambda + \lambda_0}{(p + p_0)^{1-\alpha}}\right) \tag{4.2}$$

with H an arbitrary function and $\alpha = c/(2a + c)$, $\beta = -b/(2a + c)$. We remark that the two arguments in H are each invariant under transformations (4.1).

[†] In the planar case, $\bar{r} = e^{a+b}(r + r_0) - r_0$, $\bar{u} = e^a(u + u_0) - u_0$.

To determine the equation of state $e = e(\rho, p + p_0, \lambda + \lambda_0)$ that will admit self-similar solutions, we work with the energy conservation law in the form

$$d(\rho e)/dt + (\rho e + p)\,\mathrm{div}\,u = 0 \tag{4.3}$$

rather than (3.4). By observation, ρe must scale like p; in fact,

$$\frac{\mathrm{d}}{\mathrm{d}\bar{t}}(\overline{\rho e}) + (\overline{\rho e} + \bar{p})\,\overline{\mathrm{div}}\,\bar{u} = \frac{\mathrm{d}}{\mathrm{d}t}(\overline{\rho e}) + (\overline{\rho e} + \mathrm{e}^{2a+c}(p + p_0) - p_0)\,\mathrm{div}\,u.$$

Therefore we will have invariance if

$$\overline{\rho e} - p_0 = \mathrm{e}^{2a+c}(\rho e - p_0).$$

Writing out this condition to first-order terms in the parameters a, b and c forces $g \equiv \rho e$ to satisfy the first-order quasi-linear equation

$$(p + p_0)g_p + \alpha\rho g_\rho + (1 - \alpha)(\lambda + \lambda_0)g_\lambda = g - p_0.$$

Solving the resulting characteristic equations gives

$$e - e_0 = \frac{p_0}{\rho} + \frac{p + p_0}{\rho}E\left(\frac{(p + p_0)^\alpha}{\rho}, \frac{\lambda + \lambda_0}{(p + p_0)^{1-\alpha}}\right) \tag{4.4}$$

which is the general form of the equation of state for which self-similar solutions will exist. The constitutive functions B, Γ and l can now be determined from the defining relations (2.5). From this we find

$$B = (p + p_0)F\left(\frac{(p + p_0)^\alpha}{\rho}, \frac{\lambda + \lambda_0}{(p + p_0)^{\alpha-1}}\right) \qquad \Gamma = G\left(\frac{(p + p_0)^\alpha}{\rho}, \frac{\lambda + \lambda_0}{(p + p_0)^{\alpha-1}}\right)$$

$$l = L\left(\frac{(p + p_0)^\alpha}{\rho}, \frac{\lambda + \lambda_0}{(p + p_0)^{\alpha-1}}\right). \tag{4.5}$$

Here, E is an arbitrary function while F, G and L are related to E and its derivatives through relations (2.5).

Note that the equation of state (4.4) assumes the Mie–Grüneisen form (see Zel'dovich and Raizer 1967) in special cases. In fact, take $\alpha = 0$, $p_0 = 0$ which, e.g., leaves invariant the initial conditions of the strong shock case and consider the inert case where λ is absent. Then (4.4) becomes

$$e - e_0 = (p/\rho)E(\rho). \tag{4.5i}$$

The Mie–Grüneisen form is

$$p - f'(\rho) = \rho\Gamma(\rho)(e - f(\rho)). \tag{4.5ii}$$

Requiring forms (4.5) to coincide gives

$$(\rho\Gamma(\rho))^{-1}(p - f'(\rho)) + f(\rho) = (p/\rho)E(\rho) + e_0.$$

Taking $E(\rho) = 1/\Gamma(\rho)$ then gives a linear differential equation for $f(\rho)$, namely

$$f'(\rho) - \rho\Gamma(\rho)f(\rho) = -e_0\rho\Gamma(\rho).$$

Thus

$$f(\rho) = \frac{\int e_0\rho\Gamma(\rho)\Phi(\rho)\,\mathrm{d}\rho + c}{\Phi(\rho)} \tag{4.5iii}$$

where

$$\Phi(\rho) = \exp\left(-\int \rho \Gamma(\rho)\, d\rho\right)$$

and c is an arbitrary constant. Thus (4.5ii) with $f(\rho)$ given by (4.5iii) gives forms of the Mie–Grüneisen equation of state under which similarity solutions can be found.

Let us return to the self-similar reduction of the ZND equations. By standard methods (see Bluman and Cole 1974), knowledge of the transformation group permits the calculation of the similarity variable and self-similar solutions. Here, we have similarity variables

$$s = r/(t+1)^{\xi+1} \tag{4.6}$$

where

$$\xi = (\alpha - 1)/2\beta = a/b \tag{4.7}$$

(without loss of generality we have taken $t_0 = 1$). The resulting self-similar forms of the solution are

$$\rho = (t+1)^{\eta}\bar{R}(s) \qquad\qquad u = (t+1)^{\xi}\bar{U}(s)$$
$$p + p_0 = (t+1)^{2\xi+\eta}\bar{P}(s) \qquad \lambda + \lambda_0 = (t+1)^{2\xi}\bar{\Lambda}(s) \tag{4.8}$$

where

$$\eta = -\alpha/\beta = c/b \qquad (\beta \neq 0). \tag{4.9}$$

The shock front and shock velocity are given by

$$r = (t+1)^{\xi+1} \qquad\qquad D = (\xi+1)(t+1)^{\xi}. \tag{4.10}$$

Notice that in the planar case ($\nu = 0$) the equations admit the transformation $\bar{r} = e^{a+b}(r+r_0) - r_0$ because the divergence term in the continuity equation vanishes. Hence the similarity variable will be in the planar case

$$s = (r+r_0)/(t+t_0)^{\xi+1}. \tag{4.11}$$

The requirement that the shock conditions be invariant further restricts the group (4.1). It is easy to see that (3.7a) forces $c = 0$. Hence $\alpha = \eta = 0$. The invariance of (3.7b) forces $p_0 = 0$, i.e. the strong shock condition. Similarly, invariance of (3.7c) forces $\lambda_0 = 0$; hence, for the self-similar solution all chemical reactions take place behind the shock front.

Therefore, in summary, under the strong shock assumption, the similarity variable is given by (4.6) and, upon introduction of

$$U = \frac{\bar{U}}{s(\xi+1)} \qquad R = \bar{R} \qquad P = \frac{\bar{P}}{s^2(\xi+1)^2} \qquad \Lambda = \frac{\bar{\Lambda}}{s^2(\xi+1)^2}, \tag{4.12}$$

the self-similar forms of the solution are

$$\rho = R(s) \qquad\qquad u = [r/(t+1)](\xi+1)U(s)$$
$$p = [r(\xi+1)/(t+1)]^2 P(s) \qquad \lambda = [r(\xi+1)/(t+1)]^2\Lambda(s). \tag{4.13}$$

Substitution of these quantities into the partial differential equations (3.2)–(3.5) gives

a system of ordinary differential equations in the quantities sR', sU', sP' and $s\Lambda'$:

$$\begin{bmatrix} U-1 & R & 0 & 0 \\ 0 & U-1 & 1/R & 0 \\ 0 & FP & U-1 & 0 \\ 0 & 0 & 0 & U-1 \end{bmatrix} \begin{bmatrix} sR' \\ sU' \\ sP' \\ s\Lambda' \end{bmatrix}$$

$$= \begin{bmatrix} -(\nu+1)RU \\ -U\left(U-\dfrac{1}{\xi+1}\right)-2P/R \\ -2P\left(U-\dfrac{1}{\xi+1}\right)-(\nu+1)FPU+k_ek_tP^{1-1/2\xi}s^{-1/\xi}(\xi+1)^{-1-1/\xi} \\ -2\Lambda\left(U-\dfrac{1}{\xi+1}\right)+k_t(P/R)P^{-1/2\xi}H(\xi+1)^{-1-1/\xi}s^{-1/\xi} \end{bmatrix}. \tag{4.14}$$

The initial conditions are obtained from (3.7) in the strong shock case while using (4.13) to get three relations

$$U(1)=1-1/R(1) \qquad P(1)=U(1) \qquad \Lambda(1)=0.$$

The fourth condition follows from (3.7d) when the equation of state is known. In the polytropic case where $e=p/\rho(\gamma-1)-\lambda q^2$, we have

$$R(1)=\frac{\gamma+1}{\gamma-1} \qquad U(1)=\frac{2}{\gamma+1} \qquad P(1)=\frac{2}{\gamma+1} \qquad \Lambda(1)=0. \tag{4.15}$$

5. The case $\beta=0$, reduction to phase-plane analysis

When $\beta=0$ in (4.2) or equivalently, $b=0$ in (4.1), the similarity variable becomes

$$s=r\exp(-t) \tag{5.1}$$

and the self-similar forms of the solution are

$$\rho=R(s) \qquad u=rU(s) \qquad p=r^2P(s) \qquad \lambda=r^2\Lambda(s). \tag{5.2}$$

The partial differential equations give rise, in the case $F=\gamma$, $G=\gamma-1$, $H=L=1$, to the following system of ordinary differential equations:

$$\begin{bmatrix} U-1 & R & 0 & 0 \\ 0 & U-1 & R^{-1} & 0 \\ 0 & \gamma P & U-1 & 0 \\ 0 & 0 & 0 & U-1 \end{bmatrix} \begin{bmatrix} sR' \\ sU' \\ sP' \\ s\Lambda' \end{bmatrix} = \begin{bmatrix} -(\nu+1)UR \\ -U^2-2P/R \\ -P[2U+(\nu+1)\gamma U-k(\gamma-1)] \\ -2U\Lambda+k_tP/R \end{bmatrix} \tag{5.3}$$

where $k=k_ek_t$.

This special case is important because it is the only case when the problem can be reduced to a phase-plane analysis, and it is equivalent to the case where the reaction rate is proportional to the internal energy $pv/(\gamma-1)$.

Using Cramer's rule and some algebraic manipulation, we may write (5.3) as

$$(U-1)DsR' = -R[(\nu+1)UD+A] \qquad DsU' = A$$

$$(U-1)DsP' = -P\{[(2+\gamma(\nu+1))U - k(\gamma-1)]D + \gamma A\} \qquad (5.4)$$

$$(U-1)s\Lambda' = -2U\Lambda + k_t P/R$$

where

$$A = -U^2(U-1) + \gamma P/R[(\nu+1)U + (2/\gamma)(1 - \tfrac{1}{2}k(\gamma-1))] \qquad (5.5)$$

and

$$D = (U-1)^2 - \gamma P/R. \qquad (5.6)$$

The qualitative behaviour of a system of nonlinear ordinary differential equations such as (5.4) may be determined from its critical points, where each of the derivatives becomes indeterminate. The key to physical interpretation of the critical-point analysis of equations (5.4) is the introduction of sound speed as a new variable and investigation into the characteristics of the original system of partial differential equations. So, let us define the sound speed C by $C^2 = \gamma P/R$. Using the relation $R'/R = P'/P - 2C'/C$ to eliminate R'/R from (5.4a), then using (5.4c), we obtain the system

$$(U-1)DsC' = B(U,C)C \qquad DsU' = A(U,C)$$

$$(U-1)DsP' = M(U,C)P \qquad (U-1)s\Lambda' = -2U\Lambda + C^2 k_t/\gamma \qquad (5.7)$$

where

$$D = (U-1)^2 - C^2 \qquad\qquad A = -U^2(U-1) + C^2[(\nu+1)U + z]$$

$$B = -\tfrac{1}{2}[(aU-b)D + (\gamma-1)A] \qquad M = -\{[(2+\gamma(\nu+1))U - b]D + \gamma A\} \qquad (5.8)$$

and where

$$z = (1/\gamma)[2 - k(\gamma-1)] \qquad a = 2 + (\nu+1)(\gamma-1) \qquad b = k(\gamma-1). \qquad (5.9)$$

The initial conditions given at the shock front ($s = 1$) are

$$U(1) = \frac{2}{\gamma+1} \qquad C(1) = \frac{[2\gamma(\gamma-1)]^{1/2}}{\gamma+1} \qquad P(1) = \frac{2}{\gamma+1} \qquad \Lambda(1) = 0. \qquad (5.10)$$

We notice that the first two equations in (5.7) are uncoupled from the remaining two, thus making a phase-plane analysis in the UC plane possible. The ratio of (5.7a) and (5.7b) gives the single equation

$$dC/dU = B(U,C)C/A(U,C)(U-1). \qquad (5.11)$$

Hence the problem has been reduced to a phase-plane ordinary differential equation plus three quadratures. See, e.g., Courant and Friedrichs (1948) for a similar reduction in the inert case.

6. Some remarks on characteristics

Before proceeding with a critical-point analysis of (5.11) we present some results which will relate our analysis to the physical system as well as the characteristic

structure of the flow. The results in this section are independent of the geometry (value of ν) chosen.

First, the system of partial differential equations (3.2)–(3.5) can be written in characteristic form (see Whitham 1976, p 116) as

$$\frac{du}{dt} \pm \frac{1}{\rho c}\frac{dp}{dt} = \mp\frac{\nu uc}{r} \pm \frac{\gamma-1}{\gamma}k\frac{Q}{c} \qquad \text{along } \frac{dr}{dt} = u \pm c \qquad (6.1)$$

$$dp/dt - c^2\,d\rho/dt = k(\gamma-1)\rho Q \qquad \text{along } dr/dt = u \qquad (6.2)$$

$$d\lambda/dt = k_t Q \qquad \text{along } dr/dt = u \qquad (6.3)$$

where $c^2 = \gamma p/\rho$.

The connection between the Mach (or sonic) lines defined by $dr/dt = u \pm c$, the particle paths defined by $dr/dt = u$, and the similarity variables can be summarised as follows:

(I) s = constant is a particle path if, and only if, $U = 1$;

(II) s = constant is a Mach line if, and only if, $D = 0$.

In other words, a phase trajectory in the UC plane which enters the line $U = 1$ must represent a particle path at that point, and the intersection with $D = 0$ must be a Mach point in the flow. (I) follows from the fact that

$$dr/dt|_{s=\text{constant}} - u = r(1 - U) \qquad (6.4)$$

and (II) follows from

$$(dr/dt|_{s=\text{constant}} - u)^2 - c^2 = r^2 D. \qquad (6.5)$$

From (5.4) we note that if a phase trajectory crosses a Mach line $D = 0$, then the derivatives will be undefined unless $A = 0$.

In this vein, we make the following remark:

(III) if $D = 0$ for a certain value of s and if the characteristic equations (6.1) hold, then $A = 0$.

The proof of (III) follows from writing the characteristic equations in terms of the similarity variables. To this end,

$$0 = \frac{du}{dt}\bigg|_{s=\text{constant}} \pm \frac{1}{\rho c}\frac{dp}{dt}\bigg|_{s=\text{constant}} \pm \frac{\nu uc}{\gamma} \mp \frac{\gamma-1}{\gamma}k\frac{Q}{c} = r[U \pm C(\nu U + z)]. \qquad (6.6)$$

Since A is given in (5.8), and $D = 0$ implies $U \pm C = 1$, it follows that

$$A = -U^2(U-1) + C^2[(\nu+1)U + z] = \pm U^2 C + C^2 U + C^2(\nu U + z)$$

$$= CU(C \pm U) + C^2(\nu U + z) = CU + C^2(\nu U + z)$$

on an outgoing characteristic for positive particle velocity. Hence $A = 0$ follows from (6.6), to confirm (III). Finally the third relation of (5.8) implies that $B = 0$ provided that $A = D = 0$.

In summary, if a phase trajectory in the UC phase-plane (figure 1) crosses the Mach line $D = 0$ then it must cross at a critical point (where $A = 0$ and $B = 0$) in order to have the characteristic equations satisfied. If it does not cross at a critical point then the characteristic equations will not be satisfied on the Mach line and the solution must end there with a singularity.
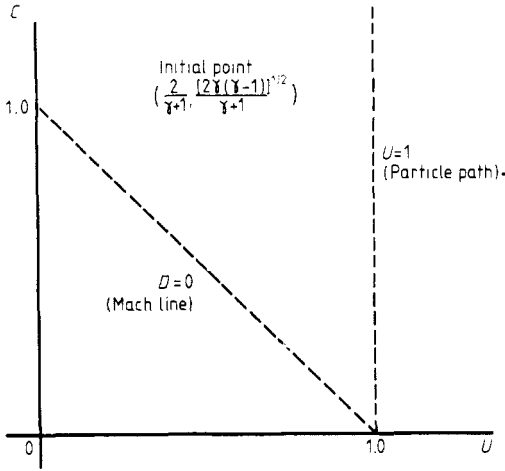
Figure 1. UC phase plane. U is the particle velocity and C is the sound speed.

7. Planar geometry

For planar geometry $(\nu = 0)$ and in the special case of a polytropic gas with $\gamma = 3$ it can be shown analytically that the critical point on the Mach line $D = 0$ is a focal point or a nodal point.

Eliminating C from the equations $D = 0$ and $A = 0$ (see (5.8)) gives the coordinates of the critical point which lies on the Mach line; these are

$$U_0 = (k - 1)/(k + \tfrac{1}{2}) \qquad C_0 = (3/2)/(k + \tfrac{1}{2}).$$

We can classify this critical point by translating it to the origin via the transformation

$$\bar{U} = U - U_0 \qquad \bar{C} = C - C_0$$

and then linearising the system (5.11). A long but straightforward calculation shows that linearised (5.11) becomes

$$d\bar{C}/d\bar{U} = (\alpha_1\bar{U} + \beta_1\bar{C})/(\alpha_2\bar{U} + \beta_2\bar{C})$$

where

$$\alpha_1 = -3(8k^2 + 2k + 17)/[8(k + \tfrac{1}{2})^3] \qquad \beta_1 = -3(k^2 - \tfrac{1}{2}k + 4)/[2(k + \tfrac{1}{2})^3]$$

$$\alpha_2 = 3(4k^2 - 20k + 7)/[8(k + \tfrac{1}{2})^3] \qquad \beta_2 = 3(k - 1)^2/(k + \tfrac{1}{2})^3.$$

It follows that

$$p \equiv -(\alpha_2 + \beta_1) = [\tfrac{27}{8}(k + \tfrac{1}{2})^{-3}](2k + 1) > 0$$

and

$$q \equiv \alpha_2\beta_1 - \alpha_1\beta_2 = \tfrac{9}{8}(6k^4 - 3k^3 + \tfrac{9}{2}k^2 + \tfrac{39}{4}k + 3)/(k + \tfrac{1}{2})^6.$$

Consequently,

$$\Delta \equiv p^2 - 4q = (-27k^4 + \tfrac{27}{2}k^3 + \tfrac{405}{16}k^2 + \tfrac{27}{16}k - \tfrac{135}{64})/(k + \tfrac{1}{2})^6.$$

It is easy to see that
 (i) $\Delta < 0$ for $0 \leq k < \frac{1}{4}$ or $k > \frac{5}{4}$;
 (ii) $\Delta > 0$ for $\frac{1}{4} < k < \frac{5}{4}$.
Consequently, in case (i) the critical point is a focal point (spiral) and in case (ii) it is a nodal point (see Birkhoff and Rota 1969, p 132). In the exceptional cases $k = \frac{1}{4}$ or $k = \frac{5}{4}$, the critical point is a starlike point since $\Delta = 0$ and $q > 0$. When an integral curve of (5.11) crosses the sonic line $D = 0$, by computing dC/dU at $D = 0$ it is easily seen that it crosses with slope $(\gamma - 1)/2$.

A typical UC phase portrait for (5.11) with $k = \frac{3}{2}$ is shown in figure 2. In this case the critical point on the Mach line is a stable spiral and is located at $(\frac{1}{4}, \frac{3}{4})$. The curves $D = 0$, $A = 0$ and $B = 0$ are shown by broken curves.
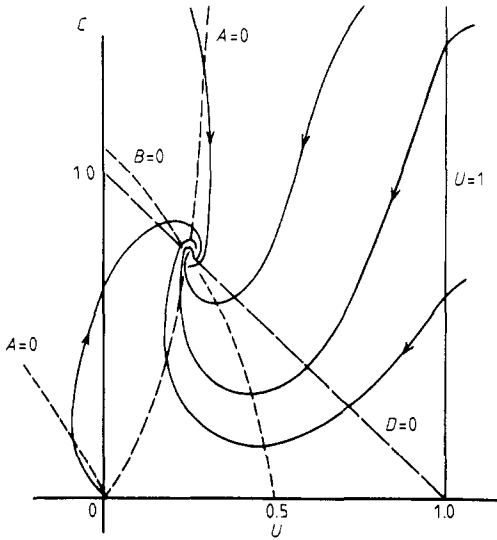

Figure 2. Phase portrait for (5.11) for $k = 1.5$, $\nu = 0$, and $\gamma = 3$. The critical point is a stable focus. Shown are loci $A = 0$ and $B = 0$.

However, (5.11) does not give a totally accurate description of the true phase trajectories. The actual equations are (5.7a, b),

$$\frac{dU}{ds} = \frac{A(U, C)}{sD(U, C)} \qquad \frac{dC}{ds} = \frac{CB(U, C)}{(U - 1)sD(U, C)} \tag{7.1}$$

with s running from $s = 1$ back to $s = 0$. The system (7.1) has a line of singularities at $D = 0$, which cancels out in (5.11).

Trajectories of (7.1) subject to the initial conditions (5.10a, b) are shown in figure 3. For $k = \frac{3}{2}$ the path begins at the initial point I and proceeds *away* from the critical point until it reaches the curve $U = 1$ which, by the results in § 6, is a particle path. This occurs at $s \approx 0.34$ and the solution becomes singular at that point (see (7.1b)).

For $k = 2.5$ the trajectory of (7.1) reaches the line $U = 0$ where, again, the solution becomes singular for a value s^* of s for which $s^* > 0$. For still larger values of k, e.g. $k = 5$, the trajectory goes up, then curls back to the Mach line $D = 0$ at $s = s^* > 0$ (see figure 3). Since the point of intersection is not a critical point, the solution becomes singular and must terminate.
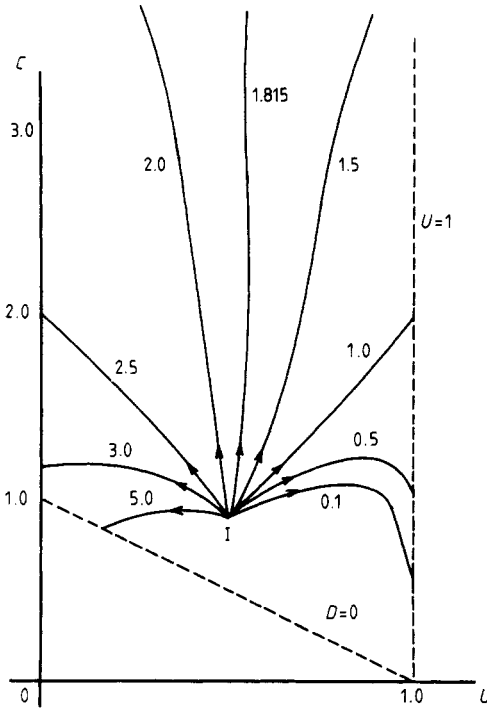
Figure 3. Solutions of (7.1) for $\nu = 0$, $\gamma = 3$ and various values of k which are labelled on the curves. All trajectories but one begin at the initial point I: $(0.5, 0.866)$ and end on the lines $D = 0$, $U = 0$ or $U = 1$ for a value of $s > 0$. The exception occurs when $k \doteq 1.815$ where the trajectory approaches $(\hat{U}, \infty)$ with $\hat{U} \doteq 0.55$ as $s \to 0$.

The following question therefore arises: is there a value of the modelling number k for which the similarity equations (5.7) have an analytic solution valid for all s in the interval $0 \leq s \leq 1$? Such a k cannot be determined analytically, but a numerical integration of (5.7) indicates that for a unique value $\bar{k}$ with $1.8156 < \bar{k} < 1.8162$, a non-singular solution exists. (The precision is sufficient for our present needs. The numerical calculations were performed on a microcomputer using a fourth-order Runge–Kutta routine.) For this special case $C \to \infty$, $U \to \hat{U} \approx 0.55$, and $P \to \infty$ as $s \to 0$. Consequently, one can regard (5.7) as a nonlinear eigenvalue problem where values of the eigenvalue k are sought for which the solution exists over the entire interval $0 \leq s \leq 1$.

8. Spherical geometry

The spherical case $(\nu = 2)$ has been treated in detail by Logan and Bdzil (1982). However, we are now able to give a physical interpretation to their results.

As in the planar case, there is a unique eigenvalue $k \approx 3.3515135$ in the spherical case for which equations (5.7) have a solution in the range $0 \leq s \leq 1$. In this case $C \to \infty$ and $U \to 0.5226$ as $s \to 0$. This corresponds to the integration to the saddle point in Logan and Bdzil. (We note that the xy Lie plane introduced in that paper is related to the UC plane in the present work via the transformations $y = U - 1$,

$x = SU' + U - 1$ and and $\tilde{P} = s^2 P$, where $\tilde{P}$ is their self-similar pressure. Their parameter a is equal to our modelling number k.) All other integrations end at singularities $U = 1$, $U = 0$, or $D = 0$, which represent characteristic curves (particle paths or Mach curves) for the original system of governing partial differential equations. Thus, in the rt plane, the solution must end at the curve $s = s^*$, precisely when that curve coincides either with a characteristic (or an envelope of characteristics) or with a particle line, e.g. a piston, or a contact discontinuity.

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