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Model solutions of the Wood–Kirkwood equations

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Abstract. The Wood-Kirkwood equations model ZND detonation waves in cylindrical geometry where the flow is restricted to the central stream tube. The entire class of self-similar solutions is obtained and in a special limit the governing equations are reduced to a single first-order non-linear equation. Solutions are obtained in the case in which the radial divergence of the flow is constant.

1. Introduction

One-dimensional ZND (Zeldovich-von Neumann-Doering) detonation waves have been discussed extensively in the literature (see Fickett and Davis 1979). Here we take into account two-dimensional effects and derive the class of self-similar motions in the Wood and Kirkwood (1954) model of slightly divergent flows, where the flow is restricted to a region near the axis of a cylindrical medium. One feature of this model is the coupling between the curvature of the reaction front and the divergence of the flow in the radial direction. The boundary effects caused by the walls of the cylinder enter only indirectly through a divergence term in the mass conservation equation. A perturbation solution about a planar shock front which couples directly to the boundary conditions has been obtained by Bdzil (1981) and Bdzil and Stewart (1986) in the case where the chemistry rapidly goes to completion. Similarity solutions for reacting flows have been discussed by several authors (e.g., Sternberg 1970, Cowperthwaite 1979, Logan and Perez 1980, Logan and Bdzil 1982, Holm and Logan 1983, Gardner 1983). Within the Wood-Kirkwood model the solution we obtain in this work will give insight into the nature of the coupling between the chemical reaction, shock curvature and radial divergence of the hydrodynamic flow.

2. The Wood–Kirkwood model

We consider a reactive medium in a quiescent state into which a shock is propagating. The shock initiates an irreversible chemical reaction $A \rightarrow B$ with reaction progress variable λ which measures the mass fraction of B. The reactive flow behind the shock is compressible, adiabatic and inviscid. By adiabatic we mean there is no heat flow between fluid elements; generally, in detonations, the hydrodynamic timescale is much faster than the timescale for heat conduction. Geometrically, the medium is a semi-infinitely long cylinder of finite radius into which we introduce a system of Eulerian coordinates with the z axis along the axis of the cylinder and r the radial distance

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from the axis. The origin of the z axis is the position at which a piston impacts the medium at time $t=0$. Behind the shock the governing equations are, in cylindrical symmetry,

$$\rho_t + u\rho_z + \omega\rho_r + \rho u_z + \rho\omega_r + \rho\omega/r = 0 \tag{1}$$

$$\rho u_t + \rho u u_z + \rho\omega u_r + p_z = 0 \tag{2}$$

$$\rho\omega_t + \rho u\omega_z + \rho\omega\omega_r + p_r = 0 \tag{3}$$

$$p_t + up_z + \omega p_r - (\gamma p/\rho)(\rho_t + u\rho_z + \omega\rho_r) = (\gamma-1)q\rho Q(\lambda, p, \rho) \tag{4}$$

$$\lambda_t + u\lambda_z + \omega\lambda_r = Q(\lambda, p, \rho) \tag{5}$$

where ρ, p, u and ω are the density, pressure, particle velocity in the z direction and particle velocity in the r direction, respectively. These equations are the usual conservation equations with (5) being the species equation with reaction rate Q depending on λ, p and ρ. This particular form of the energy equation (4) follows from the energy law $\mathrm{D}e/\mathrm{D}t = -p\mathrm{D}(1/\rho)/\mathrm{D}t$ along with the assumption that the reactant-product mixture obeys the equation of state

$$e = e_0 - \lambda q + p/\rho(\gamma - 1)$$

where e_0 is a constant and q is the specific heat of reaction (see Fickett and Davis 1979).

Following Wood and Kirkwood (1954) we specialise (1)-(5) to the axis or central stream tube. By symmetry

$$\lim_{r\to 0} \omega = 0 \qquad \lim_{r\to 0} p_r = 0$$

and from the definition of derivative

$$\lim_{r\to 0} \frac{\omega}{r} = \omega_r.$$

Hence, on the axis the governing equations become

$$\rho_t + u\rho_z + \rho u_z + 2\rho\omega_r = 0 \tag{6}$$

$$u_t + uu_z + (1/\rho)p_z = 0 \tag{7}$$

$$p_t + up_z - (\gamma p/\rho)(\rho_t + u\rho_z) = (\gamma - 1)q\rho Q(\lambda, p, \rho) \tag{8}$$

$$\lambda_t + u\lambda_z = Q(\lambda, p, \rho). \tag{9}$$

The function ω_r, the divergence of flow in the radial direction, is a function of t and z and is not known. We treat ω_r as a constitutive function which contains information concerning the boundary effects from the cylindrical walls. Generally, we assume

$$\omega_r = \omega_r(u, \lambda, \rho). \tag{10}$$

From the analysis we shall show that ω_r and Q must satisfy additional partial differential equations which permit their characterisation up to arbitrary functions.

As the shock propagates into the medium the Rankine-Hugoniot jump conditions apply across the shock front. At the axis those conditions are, assuming the strong shock condition,

$$\begin{aligned} &D = \tfrac{1}{2}(\gamma+1)u_1 \qquad \rho_1 = (\gamma+1)/(\gamma-1)\rho_0 \qquad p_1 = \tfrac{1}{2}\rho_0(\gamma+1)u_1^2 \\ &e_1 - e_0 = 1/(\gamma+1)(p_1/\rho_0) \qquad \lambda_1 - \lambda_0 = 0 \end{aligned} \tag{11}$$

where D is the shock velocity. The subscripts 0 and 1 denote states immediately in front of and immediately behind the shock, respectively. In summary, the mathematical problem is to general solutions of the differential equations (6)–(9) subject to the boundary conditions (11) which hold along the moving shock front. No *a priori* assumption can be made concerning the back boundary or piston path. Indeed, the similarity solution forces a back-boundary condition that must be satisfied for such solutions to exist.

3. Self-similar motions

A standard but lengthy similarity analysis (see, e.g., Logan 1987) leads to a class of invariant solutions of (6)–(9) and (11) under a local Lie group with operator

$$X = \tau\frac{\partial}{\partial t} + \zeta\frac{\partial}{\partial z} + \phi\frac{\partial}{\partial u} + \pi\frac{\partial}{\partial p} + \chi\frac{\partial}{\partial \rho} + \mu\frac{\partial}{\partial \lambda} \tag{12}$$

where the generators are given by

$$\begin{aligned} &\tau = at + c \qquad &&\zeta = bz + d \qquad &&\phi = (b-a)u \\ &\pi = 2(b-a)p \qquad &&\chi = 0 \qquad &&\mu = 2(b-a)\lambda \end{aligned} \tag{13}$$

where a, b, c and d are constants. For invariance the functions Q and ω_r are constrained to satisfy the partial differential equations

$$\pi\frac{\partial Q}{\partial p} + \mu\frac{\partial Q}{\partial \lambda} = (2b-3a)Q$$

$$\mu\frac{\partial \omega_r}{\partial \lambda} + \phi\frac{\partial \omega_r}{\partial u} = -a\omega_r.$$

The method of characteristics immediately yields

$$Q = p^{\beta} f(\lambda/p, \rho) \qquad \omega_r = u^{2-2\beta} g(\lambda/u^2, \rho) \tag{14}$$

where f and g are arbitrary functions and

$$\beta \equiv (2b-3a)/(2b-2a). \tag{15}$$

The forms of Q and ω_r given by (14) are necessary for self-similar motions of (6)–(9) and (11) to exist.

The similarity solution results from determining the integral curves of (12). The similarity variable is

$$s = (c_4 z + 1)/(c_3 t + 1)^{c_2} \tag{16}$$

where $c_2 = b/a$, $c_3 = a/c$ and $c_4 = b/d$. The shock path occurs at $s = 1$. The form of the self-similar solution is

$$\begin{aligned} &u(t, z) = (c_3 t + 1)^{c_2 - 1} u_i U(s) \qquad &&\rho(t, z) = \rho_i R(s) \\ &p(t, z) = (c_3 t + 1)^{2(c_2 - 1)} p_i P(s) \qquad &&\lambda(t, z) = (c_3 t + 1)^{2(c_2 - 1)} \Lambda(s) \end{aligned} \tag{17}$$

where u_i is the initial piston velocity and

$$p_i = \tfrac{1}{2}[\rho_0(\gamma+1)]u_i^2 \qquad \rho_i = (\gamma+1)/(\gamma-1)\rho_0. \tag{18}$$

When (17) is substituted into the partial differential equations (6)-(9) there results a system of ordinary differential equations for $U(s)$, $P(s)$, $R(s)$ and $\Lambda(s)$; this system (which we do not write down) can be integrated numerically for $s \leq 1$ subject to the initial conditions

$$U(1)=P(1)=R(1)=1 \qquad \Lambda(1)=0 \tag{19}$$

to determine the flow behind the shock, once the parameters β and c_4 and the functions Q and ω_r are chosen (note that $\frac{1}{2}(\gamma+1)u_i = c_2c_3/c_4$ and $c_2=(2\beta-3)/(2\beta-2)$).

4. Behaviour at the shock front

The form of the similarity solution (17) permits the calculation of various quantities at the shock front without knowing the flow behind. To compute the radius of curvature of the shock at the axis we consider the following kinematical argument. Let $\omega(\theta)$ and $u(\theta)$ denote the r and z components of the velocity vector at a point on the shock front, where θ is a small angle and σ is the radius of curvature (see figure 1). Then

$$\sigma \simeq \frac{r}{\theta} \simeq \frac{\omega(\theta)}{\omega_r(\theta)\theta} \simeq \frac{\omega(\theta)}{\omega_r(\theta)(\omega(\theta)/u(\theta))}.$$

Taking the limit as $\theta \to 0$ gives

$$\sigma \simeq \frac{u_1}{\omega_r(u_1, \lambda_1, \rho_1)}.$$

From (14) we obtain

$$\omega_r(u_1, \lambda_1, \rho_1) = \left(\frac{2D}{\gamma+1}\right)^{2-2\beta} g(0, \rho_1)$$

and so

$$\sigma \simeq \frac{1}{g(0,\rho_1)}\left(\frac{2D}{\gamma+1}\right)^{2\beta-1}. \tag{20}$$

Therefore, within the context of this solution the radius of curvature depends on the shock velocity D and the power of pressure β in the rate law.

The qualitative features of the similarity solution can also be determined at the shock front. From the fact that the shock velocity is

$$D = \tfrac{1}{2}(\gamma+1)u_i(c_3t+1)^{c_2-1}$$

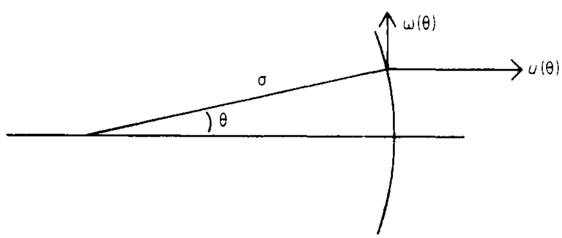

Figure 1. Geometry of the shock front.

and the pressure at the front is

$$p_1 = p_i(c_3 t + 1)^{2(c_2 - 1)}$$

we may draw the following conclusions based on the magnitude of the various constants. Six cases are distinguished.

(ia). $\beta > \frac{3}{2}$, $c_3 > 0$, $c_4 > 0$. In this case the shock is decelerating, and D, p_1 and σ all tend to zero as t tends to ∞. A comparession wave behind the shock will increase in distance from the shock front.

(ib). $\beta > \frac{3}{2}$, $c_3 < 0$, $c_4 < 0$. Here $0 < c_2 < 1$ and $(-1/c_4, -1/c_3)$ is a singular point. The shock is accelerating and both p_1 and σ are increasing to ∞ as t approaches $-1/c_3$. A compression wave behind the shock will overtake the shock front at $t = -1/c_3$.

(iia). $1 < \beta < \frac{3}{2}$, $c_3 > 0$, $c_4 < 0$. Since $c_2 < 0$ the shock is decelerating to zero and asymptotic to the line $z = -1/c_4$. Both p_1 and σ decrease along the shock.

(iib). $1 < \beta < \frac{3}{2}$, $c_3 < 0$, $c_4 > 0$. The shock is accelerating and asymptotic to $t = -1/c_3$. Along the shock p_1 and σ are increasing and compression waves behind the shock will overtake the shock as $t \to \infty$.

(iiia). $\beta < 1$, $c_3 > 0$, $c_4 > 0$. Here $c_2 > 1$ and the shock is accelerating. p_1 is increasing and σ is decreasing along the shock. Compression waves behind the shock will fall further behind.

(iiib). $\beta < 1$, $c_3 < 0$, $c_4 < 0$. The shock is decelerating to zero as $t \to -1/c_3$. The pressure p_1 decreases to zero and σ increases to ∞.

Several investigators (see, e.g., Kanel' and Dremin (1977)) have noticed that during the initiation stage many highly reactive materials have the property that the accelerating lead shock is overtaken from behind by a compression wave. This suggests that (ib) or (iib) is a possible model for detonation initiation. In the three where the shock is decelerating the solution will become invalid when the strong shock conditions cease to be a valid approximation.

5. A distinguished limit

A numerical integration of the ordinary differential equations resulting from the similarity analysis is always possible. However, one might ask under what assumptions can analytical progress be made. In the case of constant divergence of flow, a reaction rate proportional to the internal energy, and in the limit as $\beta \to 1^+$ the problem simplifies greatly. In this case the similarity variable (16) becomes

$$s = (c_4 z + 1)\exp[-\tfrac{1}{2}(\gamma + 1)u_i c_4 t] \tag{21}$$

and the form of self-similar motions is

$$\begin{aligned} u &= u_i \hat{U}(s)\exp[\tfrac{1}{2}(\gamma+1)u_i c_4 t] \qquad & \rho &= \rho_i R(s) \\ p &= p_i P(s)\exp[(\gamma+1)u_i c_4 t] \qquad & \lambda &= \Lambda(s)\exp[(\gamma+1)u_i c_4 t]. \end{aligned} \tag{22}$$

Taking $U \equiv \hat{U} - \frac{1}{2}(\gamma+1)s$ and

$$g(\Lambda/u_i^2\hat{U}^2, \rho_i R) = \Omega \qquad f(\Lambda/p_i P, \rho_i R) = k/[(\gamma+1)R\rho_i]$$

where Ω is a constant divergence rate and k is a rate constant for the chemical reaction, the partial differential equations (6)-(9) reduce to the system of ordinary differential equations for $0<s<1$:

$$\frac{U'}{U}+\frac{R'}{R}=-\frac{\nu}{U} \tag{23}$$

$$\frac{U'}{U}+(\gamma+1)\frac{1}{U}+\left(\frac{\gamma+1}{2}\right)^2\frac{s}{U^2}+\frac{\gamma-1}{2}\frac{1}{U^2}\frac{P'}{R}=0 \tag{24}$$

$$\frac{P'}{P}-\gamma\frac{R'}{R}=-\frac{\mu}{U} \tag{25}$$

$$\frac{\Lambda'}{\Lambda}+\frac{\gamma+1}{U}=\eta\frac{P}{R\Lambda U} \tag{26}$$

where

$$\nu\equiv\frac{\gamma+1}{2}+\frac{2\Omega}{u_i c_4} \qquad \mu\equiv\gamma+1-\frac{\gamma-1}{\gamma+1}\frac{qk}{u_i c_4} \qquad \eta=\frac{p_i k}{(\gamma+1)\rho_i u_i c_4}$$

and initial conditions are given at the shock front by

$$R(1)=P(1)=1 \qquad U(1)=\tfrac{1}{2}(1-\gamma) \qquad \Lambda(1)=0. \tag{27}$$

In (23)-(26) we observe the appearance of three dimensionless numbers ν, μ and η. The quantity η is the ratio of the energy of the hydrodynamic flow to the energy released by the chemical reaction. We can write $\nu=\frac{1}{2}(\gamma+1)+m_1$ and $\mu=\gamma+1-m_2$ where m_1 and m_2 are positive dimensionless modelling numbers which measure the ratio of the radial divergence of the flow to the normal velocity, and the ratio of the hydrodynamic and chemical timescales, respectively. The number c_4^{-1} is a length scale for the problem. Equations (23) and (25) may be integrated immediately; letting

$$\Sigma(s)=\exp\left(-\int_1^s\frac{d\xi}{U(\xi)}\right)$$

we obtain

$$R=\tfrac{1}{2}(1-\gamma)U^{-1}\Sigma^{\nu} \tag{28}$$

and

$$P=R^{\gamma}\Sigma^{\mu} \tag{29}$$

which give R and P directly in terms of U and integrals of U. The species equation (26) is linear in Λ and may be solved easily in terms of U. Thus it remains to determine a single equation for U. To this end we introduce the sound speed C defined by $C^2=\gamma P/R$. Clearly

$$\frac{R'}{R}=\frac{P'}{P}-2\frac{C'}{C} \tag{30}$$

and substituting this expression into (23) and (25) and then subtracting gives

$$2\frac{C'}{C}+(\gamma-1)\frac{U'}{U}=\frac{\nu(1-\gamma)-\mu}{U}. \tag{31}$$

Using (30) to eliminate P'/R from (24) gives

$$\frac{U'}{U}+\frac{\gamma+1}{U}+\left(\frac{\gamma+1}{2}\right)^2\frac{s}{U^2}+\frac{\gamma-1}{2\gamma}\frac{C^2}{U^2}\left(2\frac{C'}{C}-\frac{U'}{U}-\frac{\nu}{U}\right)=0. \tag{32}$$

It is straightforward but tedious to use (31) along with the definition of C to eliminate C from (32) and thereby obtain a single non-linear differential equation for the reduced particle velocity U. The idea is to solve (32) for $\Sigma(s)$ and then logarithmically differentiate.

Much insight can be gained by examining a special case. We assume that the system is tuned in such a way that $\nu(1-\gamma)=\mu$. This constraint still permits many reasonable configurations, and it forces the linear relationship $(1-\gamma)m_1+m_2=\frac{1}{2}(\gamma+1)^2$ on the modelling numbers, which are ratios of velocities and timescales. In this case (31) may be integrated directly to obtain

$$U=\tfrac{1}{2}\gamma^{1/(\gamma-1)}(1-\gamma)C^{2/(1-\gamma)}.$$

If $\gamma=3$ we have

$$C=-\sqrt{3}/U$$

where U satisfies the first-order equation

$$U'=(\nu-4U^4-4sU^3)/(U^4-3) \qquad U(1)=-1 \tag{33}$$

where $\nu=2+2\Omega/(u_i c_4)$ and $0<s<1$. We further have

$$\hat{U}=U+2s \qquad R=-U^{-1}\Sigma^{\nu} \qquad P=-U^{-3}\Sigma^{\nu}$$

and the species equation becomes

$$\Lambda'+4\Lambda/U=\eta/U^3$$

which has solution

$$\Lambda(s)=\eta\Sigma^4(s)\int_1^s \frac{\mathrm{d}\xi}{U^3(\xi)\Sigma^4(\xi)}.$$

Thus the problem has been reduced to a simple integration of (33). Sketches of the solution are shown in figure 2 in the case $\nu=3$, $\eta=1$. Although the similarity solution exists for all s in the range $0<s\leqslant 1$, there is a value $s=s_0$ when $\lambda=1$ and the chemical reaction is completed; thus the self-similar motion is valid only for $s_0\leqslant s\leqslant 1$. In general, this motion must be connected back to the piston by a time-dependent inert flow which will suffer a weak discontinuity at $s=s_0$.

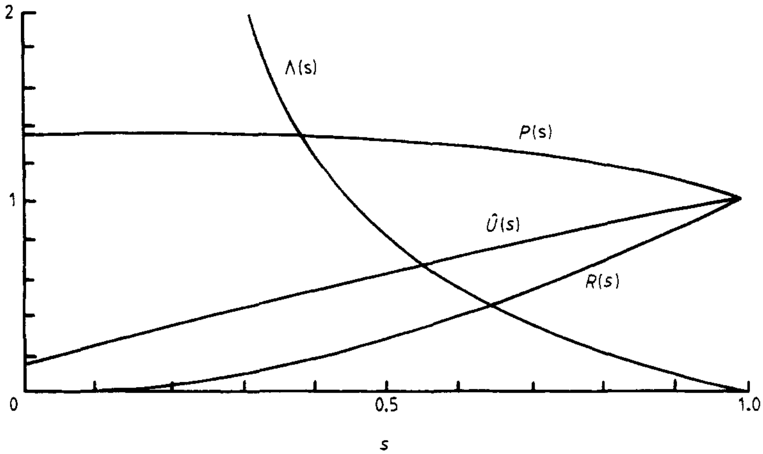

Figure 2. Graph of the self-similar particle velocity $\hat{U}$, pressure P, density R and progress variable Λ on $0\leqslant s\leqslant 1$. The behaviour of Λ near $s=0$ is $\Lambda\to+\infty$ as $s\to 0^+$.

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