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Weakly nonlinear reactive shocks with lateral divergence

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Abstract. Asymptotic equations are obtained in a weakly nonlinear limit of the Wood–Kirkwood equations for slightly divergent reactive flow. Specifically, in cylindrical symmetry the equations of reactive flow are restricted to the central stream tube, and the radial component of the velocity is assumed to be a function of wavespeed of a signal propagating through the medium. Asymptotic equations are obtained in the limit where the Mach number is close to unity and the components of the velocity are small in comparison; the heat release is assumed to be small, and two cases with different chemical kinetics are examined. In one case an Arrhenius-type reaction rate with large activation energy is considered, and in another case a depletion-type rate with no Arrhenius factor is considered. The asymptotic equations are compared to the Fickett analogue of detonation. Finally, the existence of ZND type waves within the context of the model asymptotic equations is examined in special cases.

1. Introduction

We consider waves propagating in a chemically reacting medium and derive a simplified asymptotic model when the flow is unidirectional with a slightly divergent component along the axis of propagation. The model equations are compared to the *ad hoc* detonation analogue equations proposed by Fickett (1985) for slightly divergent flows.

Geometrically, the medium is an infinitely long cylinder of finite radius. The flow is assumed to be cylindrically symmetric (no angular component) and dependent only upon the radial component r and the component x in the axial direction. The flow is then restricted to the axis (or central stream tube) by taking the limit of the reacting fluid equations as $r \rightarrow 0$. The resulting equations, for what is termed slightly divergent reactive flow, were obtained in a classic paper by Wood and Kirkwood (1954). The boundary effects from the walls of the cylinder enter into the equations indirectly through a divergence term in the continuity equation. The Wood–Kirkwood equations are discussed in Fickett and Davis (1979).

Using the slightly divergent flow equations as a base, we perform a weakly nonlinear analysis and examine the equations in a special asymptotic limit. In this limit waves propagate at a speed close to the sound speed in the material ahead and the particle velocity is small in comparison. Heat is released by the chemical reaction at the same order as the mean kinetic energy of the flow. In spite of these restrictive assumptions, which will be stated precisely in the subsequent analysis, the resulting asymptotic equations still admit a substantial nonlinear interaction between the chemical and fluid mechanical aspects of the flow.

The weakly nonlinear analysis is similar to that performed on the general, one-dimensional equations of reacting flow by Rosales and Majda (1983) (see also Fife

(1982) and Majda (1986)); here we include lateral divergence. As in these cases the weakly nonlinear model is a Burgers-like equation which couples the hydrodynamics and the chemistry, and a reaction rate equation that governs the reaction. When radial divergence is included the Burgers equation contains a term that accounts for this divergence phenomenon, and the term enters at leading order.

The general interest in slightly divergent flows arose from study of the diameter effect in high explosives. The diameter effect is the observation that the detonation velocity depends in a critical way upon the diameter of a charge, and below a certain 'failure diameter' self-sustaining detonation waves will not propagate. See Fickett and Davis (1979) for a complete discussion and bibliography up to 1979. More recently, 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. An article by Klein (1991) discusses the dynamics of weakly curved detonations and contains references of other recent work on multidimensional effects in combustion and detonation. A review article by Ledder and Logan (1992) discusses weakly nonlinear equations and analogues of detonation processes in a one-dimensional setting. Similarity solutions of the Wood-Kirkwood equations are discussed in Logan (1988).

The governing equations (continuity, momentum balances in the x and r directions, energy and chemical species) in cylindrical coordinates (r, x) with rotational symmetry are

$$\dot{\rho} + \rho u_x + \rho \omega_r + r^{-1} \rho \omega = 0 \quad (1.1)$$

$$\rho \dot{u} + p_x = 0 \quad (1.2)$$

$$\rho \dot{\omega} + p_r = 0 \quad (1.3)$$

$$c_p \rho \dot{T} - \dot{p} = Q \rho W(Z, T) \quad (1.4)$$

$$\dot{Z} = -W(Z, T) \quad (1.5)$$

with the equation of state given by $p = R\rho T$. Here, ρ is the density, p is the pressure, T is the temperature, u is the particle velocity in the x direction, ω is the particle velocity in the r (radial) direction and Z is the mass fraction of the reactant A in a model, irreversible, exothermic chemical reaction $A \rightarrow B$. The overdot denotes the material derivative

$$\frac{\partial}{\partial t} + u \frac{\partial}{\partial x} + \omega \frac{\partial}{\partial r}.$$

The constant c_p is the specific heat at constant pressure, Q is the heat of reaction, and R is the gas constant. The chemical reaction rate is $W(Z, T)$, and will be specified later. We do not include transport terms in (1.1)-(1.5) because we are ultimately interested in the propagation of shocks.

Following Wood and Kirkwood (1954) (see Fickett and Davis (1979) for a review) we specialize (1.1)-(1.5) to the x -axis (or central stream tube) by taking the limit as $r \rightarrow 0$. By symmetry,

$$\lim_{r \rightarrow 0} \omega(t, r, x) = 0$$

and it therefore follows that

$$\lim_{r \rightarrow 0} \frac{\omega(t, r, x)}{r} = \omega_r(t, x) \quad \lim_{r \rightarrow 0} p_r(t, r, x) = 0. \quad (1.6)$$

The first of the equations in (1.6) follows from the definition of derivative. Thus, the governing equations (1.1)–(1.5) are reduced to the four equations

$$D\rho/Dt + \rho u_x + 2\rho\omega_r = 0 \quad (1.7)$$

$$\rho Du/Dt + p_x = 0 \quad (1.8)$$

$$\rho c_p DT/Dt - Dp/Dt = Q\rho W(Z, T) \quad (1.9)$$

$$DZ/Dt = -W(Z, T) \quad (1.10)$$

where $D/Dt = \partial_t + u\partial_x$ and ρ , u , p , T and Z are functions of t and x .

The function $\omega_r(t, x)$ represents the radial component of the divergence of the flow field and is not known *a priori*. As noted above, the function ω_r contains the effects of the side boundaries, and the system (1.7)–(1.10) is not complete until ω_r is specified. Our approach will be to assume that ω_r is some function of the speed of a wavefront propagating in the medium; to leading order ω_r will be constant in the weakly nonlinear approximation. We refer to Fickett and Davis (1979, pp 199–204) for a thorough discussion of the role of the divergence term ω_r and how it couples to the boundaries of the vessel.

The chemical reaction rate $W(Z, T)$ is given by the Arrhenius law

$$W = k_1 Z \exp(-E/RT) \quad (1.11)$$

where k_1 is a constant, R is the gas constant, and E is the activation energy. With T_a being a reference temperature and $\theta \equiv E/RT_a$, we can write

$$W = \tilde{k} Z \exp[\theta(1 - T_a/T)] \quad (1.12)$$

where $\tilde{k} = k_1 \exp(-\theta)$. We assume $\theta \gg 1$ so that the chemical reaction will enter the equations in a significant way at leading order in the following analysis.

2. Non-dimensionalization

We assume a wave (any wave, not necessarily a shock) is propagating to the right into an undisturbed, quiescent medium with state

$$\rho_a, p_a, T_a, Z_a, u_a = 0 \quad c_a = \sqrt{\gamma RT_a}.$$

Here c_a is the sound speed in the medium ahead and γ is the ratio of specific heats and is related to R and c_p by the well known formula $\gamma - 1 = \gamma R/c_p$. The location of a reference point on the wave is given by a smooth function

$$x = s(t)$$

and the speed of the wave is

$$v(t) = s'(t) > 0.$$

We let L be a typical length scale in the quiescent material ahead and d be a typical length within the wave. We further let $t_{ac} = L/c_a$ be the acoustic time, i.e. the time required for a sound wave to travel a distance L , and we denote by t_{ch} the timescale for the chemical reaction. We also introduce the dimensionless parameters

$$\varepsilon \equiv \frac{d}{L} \quad q \equiv \frac{QZ_a}{T_a c_p} \quad k \equiv \tilde{k} t_{ch}.$$

The constant q is a heat release parameter, and k is the rate constant. We assume ε is small and that k is of order unity with respect to ε . Thus, our assumptions are

$$0 < \varepsilon \ll 1 \quad 0 < k = O(1).$$

We further assume

$$\theta = \varepsilon^{-1} \gg 1.$$

The orders of magnitude of the heat release q and the ratio $t_{\text{ch}}/t_{\text{ac}}$ will be chosen later so that the flow is weakly nonlinear, i.e. to leading order the flow is represented by a linear homogenous system, and the non-homogenities representing the chemical effects enter at the first correction level.

We now define dimensionless time and position variables by

$$\tau = \frac{t}{t_{\text{ac}}} \quad \xi = \frac{x - s(t)}{d}.$$

The coordinate ξ measures the distance to the wave location on the scale of the wave. New dimensionless dependent variables $\bar{\rho}$, \bar{p} , \bar{T} , \bar{u} , \bar{Z} are then defined by equations of the form

$$\bar{\psi}(\xi, \tau) = \psi_{\text{ref}}^{-1} \psi(x, t)$$

where ψ_{ref} is the appropriate quantity ρ_a , p_a , T_a , c_a or Z_a . The dimensionless wavespeed $\bar{v}(\tau)$ is defined by

$$\bar{v}(\tau) = c_a^{-1} v(t)$$

and the radial divergence $\omega_r(v)$ is scaled by

$$\bar{\omega}_r(\bar{v}) = \omega_{\text{ref}}^{-1} \omega_r(c_a \bar{v})$$

where ω_{ref} is the scale for ω_r and will be defined later when the equations are balanced to determine the weakly nonlinear form. The dimensioned quantities in equations (1.7)-(1.10) are now systematically replaced by the new dimensionless quantities. The chain rule gives

$$\partial_t = t_{\text{ac}}^{-1} \partial_\tau - cd^{-1} \partial_\xi \quad \partial_x = d^{-1} \partial_\xi$$

and so

$$\frac{D}{Dt} = t_{\text{ac}}^{-1} \partial_\tau + cd^{-1} (\bar{u} - \bar{v}) \partial_\xi.$$

For conciseness of notation we introduce the operator

$$H \equiv \varepsilon \partial_\tau + (\bar{u} - \bar{v}) \partial_\xi.$$

Then

$$\frac{D\psi}{Dt} = \frac{c_a}{d} \psi_{\text{ref}} H(\bar{\psi}).$$

Thus, the governing partial differential equations (1.7)-(1.10) take the form

$$H(\bar{\rho}) + \bar{\rho} u_\xi + 2\varepsilon t_{\text{ac}} \omega_{\text{ref}} \bar{\rho} \bar{\omega}_r(\bar{v}) = 0 \quad (2.1)$$

$$\bar{\rho} H(\bar{u}) + \gamma^{-1} \bar{p}_\xi = 0 \quad (2.2)$$

$$\bar{\rho} H(\bar{T}) - \frac{\gamma - 1}{\gamma} H(\bar{p}) = \varepsilon q t_{\text{ac}} t_{\text{ch}}^{-1} k \bar{\rho} \bar{Z} \exp(\theta[1 - \bar{T}^{-1}]) \quad (2.3)$$

$$H(\bar{Z}) = -\varepsilon k t_{\text{ac}} t_{\text{ch}}^{-1} \bar{Z} \exp(\theta[1 - \bar{T}^{-1}]). \quad (2.4)$$

These are the scaled mass, momentum, energy and chemical species equations, respectively.

3. Asymptotic expansion and balancing

We now assume forms for the state quantities which are power series in ε :

$$\begin{aligned}
 \bar{\rho}(\xi, t) &= 1 + \varepsilon\rho_0(\xi, \tau) + \varepsilon^2\rho_1(\xi, \tau) + O(\varepsilon^3) \\
 \bar{p}(\xi, \tau) &= 1 + \varepsilon p_0(\xi, \tau) + \varepsilon^2 p_1(\xi, \tau) + O(\varepsilon^3) \\
 \bar{T}(\xi, \tau) &= 1 + \varepsilon T_0(\xi, \tau) + \varepsilon^2 T_1(\xi, \tau) + O(\varepsilon^3) \\
 \bar{u}(\xi, \tau) &= \varepsilon u_0(\xi, \tau) + \varepsilon^2 u_1(\xi, \tau) + O(\varepsilon^3) \\
 \bar{Z}(\xi, \tau) &= Z_0(\xi, \tau) + O(\varepsilon) \\
 \bar{v}(\tau) &= v_0(\tau) + \varepsilon v_1(\tau) + O(\varepsilon^2).
 \end{aligned} \tag{3.1}$$

Here we remark that although $\bar{\rho}$, \bar{p} and \bar{T} are $O(1)$, the variations in these quantities are small. This assumption is at the core of the weakly nonlinear theory and leads to linear equations at leading order. Also, the particle velocity \bar{u} is taken to be small compared to the sound speed. We are careful to expand \bar{v} in a power series even though we are in a coordinate system that fixes the wave to all orders; velocities are measured with respect to the laboratory frame of reference rather than the frame attached to the wave.

For notational convenience we now define the operator G_0 by

$$G_0 \equiv \partial_\tau + (u_0 - v_1)\partial_\xi$$

whereupon we have

$$H(\bar{\psi}) = -\varepsilon v_0(\psi_{0\xi} + \varepsilon\psi_{1\xi}) + \varepsilon^2 G_0(\psi_0)$$

for $\psi = \rho$, T , u and p (but not Z , which must be treated separately). We first consider the species equation (2.4). When the expansions (3.1) are substituted we obtain

$$-v_0 Z_{0\xi} + O(\varepsilon) = -\varepsilon k t_{\text{ac}} t_{\text{ch}}^{-1} Z_0 \exp(T_0) + O(\varepsilon^2 t_{\text{ac}} t_{\text{ch}}^{-1}).$$

In order to bring in the chemical term at $O(1)$ we assume

$$t_{\text{ac}} t_{\text{ch}}^{-1} = \varepsilon^{-1} \gg 1. \tag{3.2}$$

Then, to leading order

$$v_0 Z_{0\xi} = k Z_0 \exp(T_0). \tag{3.3}$$

With the assumption (3.2) the energy equation (2.3) becomes

$$\bar{\rho} H(\bar{T}) - \frac{\gamma-1}{\gamma} H(\bar{p}) = q k \bar{\rho} \bar{Z} \exp[\theta(1 - \bar{T}^{-1})]$$

and substituting the expansions gives

$$\begin{aligned}
 (1 + \varepsilon\rho_0)(-v_0(T_{0\xi} + \varepsilon T_{1\xi})) + \varepsilon G_0(T_0) - \frac{\gamma-1}{\gamma} (-v_0 p_{0\xi} - \varepsilon v_0 p_{1\xi} + \varepsilon G_0(T_0)) \\
 = \varepsilon^{-1} q k Z_0 \exp(T_0) + O(q) + O(\varepsilon q).
 \end{aligned}$$

In order to introduce the energy release term at $O(\varepsilon)$, we are forced to assume

$$q = O(\varepsilon^2) = q_0 \varepsilon^2 \quad \dot{q}_0 = O(1).$$

Then, to leading order, the energy equation will be a linear homogeneous equation

$$O(1): \quad -v_0 T_{0\varepsilon} + v_0 \frac{\gamma-1}{\gamma} p_{0\varepsilon} = 0 \quad (3.4)$$

and at order $O(\varepsilon)$ we shall have

$$O(\varepsilon): \quad -v_0 \rho_0 T_{0\varepsilon} - v_0 T_{1\varepsilon} + G_0(T_0) + v_0 \frac{\gamma-1}{\gamma} p_{1\varepsilon} - \frac{\gamma-1}{\gamma} G_0(\rho_0) = q_0 k \bar{Z}_0 \exp(T_0). \quad (3.5)$$

The momentum equation (2.2) gives

$$O(1): \quad -v_0 u_{0\varepsilon} + \gamma^{-1} p_{0\varepsilon} = 0 \quad (3.6)$$

$$O(\varepsilon): \quad -v_0 u_{1\varepsilon} + \gamma^{-1} p_{1\varepsilon} + G_0(u_0) - \rho_0 v_0 u_{0\varepsilon} = 0. \quad (3.7)$$

The balancing of the terms in the continuity equation (2.1) will determine the order of ω_{ref} . Substituting the expansions (3.1) into (2.1) gives

$$\varepsilon v_0 (\rho_{0\varepsilon} + \varepsilon \rho_{1\varepsilon}) + \varepsilon^2 G_0(\rho_0) + (1 + \varepsilon \rho_0) (\varepsilon u_{0\varepsilon} + \varepsilon^2 u_{1\varepsilon}) + 2\varepsilon t_{\text{ac}} \omega_{\text{ref}} (1 + \varepsilon \rho_0) \bar{\omega}_r(\bar{v}) + O(\varepsilon^2 \omega_{\text{ref}}) + O(\varepsilon^2) = 0.$$

To bring in the radial divergence term at the correction stage, leaving a linear, homogeneous equation at leading order, we assume that

$$\omega_{\text{ref}} = O(\varepsilon).$$

Then we have the following equations:

$$O(1): \quad -v_0 \rho_{0\varepsilon} + u_{0\varepsilon} = 0 \quad (3.8)$$

$$O(\varepsilon): \quad -v_0 \rho_{1\varepsilon} + u_{1\varepsilon} + G_0(\rho_0) + \rho_0 u_{0\varepsilon} + \bar{\omega}_r(v_0) = 0 \quad (3.9)$$

where we have taken $\omega_{\text{ref}} \equiv \frac{1}{2} t_{\text{ac}}^{-1} \varepsilon$ and used Taylor's expansion for $\bar{\omega}_r(\bar{v})$;

$$\bar{\omega}_r(\bar{v}) = \bar{\omega}_r(v_0) + \varepsilon v_1 \bar{\omega}'_r(v_0) + \dots$$

In summary, we have assumed that the flow is weakly nonlinear, i.e. the state variables do not deviate substantially from their reference values, but they do deviate enough so that the model differs from the linear acoustical model. To leading order, the mass, momentum, and energy equations (equations (3.8), (3.6) and (3.4)) form a linear, homogeneous, hyperbolic system

$$\begin{pmatrix} 1 & -v_0 & v_0 \\ -v_0 & \gamma^{-1} & 0 \\ 0 & \gamma^{-1}(\gamma-1) & -1 \end{pmatrix} \begin{pmatrix} u_{0\varepsilon} \\ \rho_{0\varepsilon} \\ T_{0\varepsilon} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad (3.10)$$

where we have used the expanded equation of state

$$\rho_0 + \varepsilon p_1 = \rho_0 + T_0 + \varepsilon (\rho_1 + T_1 + \rho_0 T_0) + O(\varepsilon^2) \quad (3.11)$$

to eliminate $\rho_0 = p_0 - T_0$. The order of the radial divergence ω_r , the order of the heat release q , and the order of the ratio of timescales $t_{\text{ac}}/t_{\text{ch}}$, were chosen so that the inhomogeneities (radial divergence, energy released by the chemical reaction, and

chemical reaction rate) come in at the correction level. The ratio t_{ac}/t_{ch} is $O(\varepsilon^{-1})$ so that the principal cause for the change in the chemical composition Z in the wave is the chemical reaction. The assumption that the heat release parameter q is $O(\varepsilon^2)$ limits the effect of the energy liberated by the chemical reaction; the parameter q may be written as $q = Q/(T_a c_p/Z_a)$, and therefore the energy Q liberated by the reaction is much smaller than the thermal energy $T_a c_p/Z_a$ present in the flow ahead of the wave. Since q is $O(\varepsilon^2)$, this dimensionless heat release is the same order as the mean kinetic energy (proportional to \bar{u}^2) of the flow. Finally, the assumption that ω_r is $O(\varepsilon)$ brings in the radial divergence at the correction level, not at leading order. Orderwise, ω_r is the same as the flow velocity \bar{u} , which is small compared to the near Mach one wavespeed.

4. The weakly nonlinear equations

The system of leading order equations (3.10) has a non-trivial solution only if the coefficient matrix has non-zero determinant, i.e. when

$$v_0(\tau) = 1. \tag{4.1}$$

This condition therefore determines the leading order wavespeed. Equations (3.10) then become

$$p_{0\xi} = \frac{\gamma}{\gamma - 1} T_{0\xi} = \gamma u_{0\xi}. \tag{4.2}$$

Integrating and applying the condition that the perturbations p_0 , u_0 and T_0 vanish ahead of the wave, we obtain the leading-order solution

$$p_0 = \frac{\gamma}{\gamma - 1} T_0 = \gamma u_0 = \gamma \rho_0. \tag{4.3}$$

With (4.1), the chemical species equation (3.3) becomes

$$Z_{0\xi} = k Z_0 \exp T_0. \tag{4.4}$$

To complete the model it is necessary to obtain an equation for T_0 . Therefore we examine the $O(\varepsilon)$ correction equations given by (3.9), (3.7) and (3.5). Using (3.11) to eliminate ρ_1 ($\rho_1 = p_1 - T_1 - \rho_0 T_0$) and substituting the results (4.1) and (4.3) at leading order, these three $O(\varepsilon)$ equations become

$$\begin{aligned} u_{1\xi} - p_{1\xi} + T_{1\xi} &= -\frac{\partial}{\partial \xi} \left(\frac{1}{\gamma - 1} T_0^2 \right) - \frac{1}{\gamma - 1} G_0(T_0) - \frac{1}{(\gamma - 1)^2} T_0 T_{0\xi} - \bar{\omega}_r(1) \\ -u_{1\xi} + \gamma^{-1} p_{1\xi} &= \frac{1}{(\gamma - 1)^2} T_0 T_{0\xi} - \frac{1}{\gamma - 1} G_0(T_0) \\ \gamma^{-1}(\gamma - 1) p_{1\xi} - T_{1\xi} &= \frac{1}{\gamma - 1} T_0 T_{0\xi} + q_0 k Z_0 \exp(T_0). \end{aligned}$$

This non-homogeneous system has zero determinant and therefore there is a consistency condition, which can be found by adding the equations to obtain, after simplification,

$$T_{0r} - v_1 T_{0\xi} + \frac{\gamma - 1}{\gamma + 1} T_0 T_{0\xi} + \frac{1}{2}(\gamma - 1)\bar{\omega}_r(1) - \frac{1}{2}(\gamma - 1)q_0 k Z_0 \exp T_0 = 0. \tag{4.5}$$

Thus, we have the equations (4.4) and (4.5), which is a system of two equations for T_0 , Z_0 and v_1 .

We now perform a change of variables to eliminate v_1 . In (ξ, τ) coordinates the wave is stationary, and so travelling wave solutions of (4.5) must have speed zero. Meanwhile, equation (4.5) includes an unknown coefficient v_1 in a convective term. We now replace ξ with a new spatial coordinate η defined by

$$\eta = \xi + \int_0^\tau v_1(y) dy.$$

Then (4.5) becomes

$$U_\tau + UU_\eta + \frac{1}{2} \left(\frac{\gamma-1}{\gamma+1} \right)^2 \bar{\omega}_r(1) - \frac{1}{2} \frac{(\gamma-1)^2}{\gamma+1} q_0 k Z_0 \exp T_0 = 0 \quad (4.6)$$

where

$$U = \frac{\gamma-1}{\gamma+1} T_0.$$

In the new (η, τ) coordinate system the wave is on the path $\eta = \int_0^\tau v_1(y) dy$, and the wavespeed is $v_1(\tau)$. Since v_1 is yet to be determined, we are free to search for solutions in the new coordinate system that travel at any speed, and the speed v_1 will become like an eigenvalue when boundary conditions are imposed.

One final simplification will yield the weakly nonlinear equations. We define the constants

$$\alpha = \frac{1}{2} \left(\frac{\gamma-1}{\gamma+1} \right) \omega_r(1) \quad \beta = \frac{1}{2} \frac{(\gamma-1)^2}{\gamma+1} q_0.$$

Then (4.6) and (4.4) become

$$U_\tau + UU_\eta + \alpha - \beta Z_{0\eta} = 0 \quad (4.7)$$

$$Z_{0\eta} = k Z_0 \exp \left(\frac{\gamma-1}{\gamma+1} U \right). \quad (4.8)$$

Equations (4.7), (4.8) represent a system of quasilinear differential equations for the temperature perturbation U and the leading order chemical composition Z_0 . The radial divergence term enters as a constant α in the Burgers-like equation (4.7). Thus, we have obtained a simplified model in an asymptotic limit of the full nonlinear equations of reactive flow restricted to the central stream tube. In this weakly nonlinear limit the wavespeed is of the same order as the sound speed (i.e. it is near Mach one), and the particle velocity and radial divergence are small in comparison. Yet, there remains an interaction between the fluid dynamics and chemistry through the coupled nonlinear system (4.7), (4.8). One should not conclude that the general physical system in the non-asymptotic limit behaves according to (4.7), (4.8); the asymptotic equations would be expected to hold only under the given assumptions. The major deficiency in (4.7), (4.8) is that there are no negative characteristics to carry signals backwards into the flow in the general case. However, in spite of this deficiency, Fickett (1985) has reported that model equations like (4.7), (4.8) do mirror some physical aspects of general reactive flows.

It is interesting to now compare the analogue equations for laterally divergent detonations posed in an *ad hoc* manner by Fickett (1985, p 169). His analogue equations are

$$\rho_t + \rho\rho_x + \frac{1}{2}q_0\lambda_x = -\alpha \tag{4.9}$$

$$\lambda_t = r(\rho, \lambda) \tag{4.10}$$

where t is time and x is a Lagrangian particle label. Here, $\lambda = 1 - Z$ (the mass fraction of the product species) and r is the chemical reaction rate; the dependent variable ρ is interpreted as a density-like quantity. The constant q_0 is the heat release parameter, and $\alpha > 0$ is a ‘radial divergence’ term. Thus, there are some similarities between the Fickett analogue and the weakly nonlinear equations obtained rigorously in an asymptotic limit of the full fluid dynamical equations. One main difference is in the interpretation of the independent variables and the location of derivative with respect to those variables in the equations. The quantity ρ is indeed a density-like quantity (see (4.3)) since there is a linear relationship between the temperature T_0 and density ρ_0 in the asymptotic model. In (4.9), (4.10) an alternate interpretation might be that ρ is a ‘density perturbation’, and x is a coordinate moving with the wave. In any case, the weakly nonlinear analysis lends credence to the analogue equations (4.9), (4.10). However, in the sequel we shall observe that the analogue equations and the asymptotic equations give different conclusions regarding the diameter effect.

5. Non-Arrhenius kinetics

In much of the theoretical work on detonation theory (see Fickett and Davis 1979) the reaction rate is assumed to be of the form

$$W(Z) = k_1 Z^n$$

where $n > 0$ and k_1 is a constant. This rate law corresponds to n th-order kinetics with zero activation energy (compare (1.11)). In order to satisfy the cold boundary condition ahead of the wave (i.e. in order to have no reaction until the wave arrives), we more specifically take

$$W(Z, T) = k_1 Z^n \phi(T - T_a) \tag{5.1}$$

where ϕ is the Heaviside function which will turn on the reaction when the wave arrives ($\phi(y) = 0$ for $y \leq 0$ and $\phi(y) = 1$ for $y > 0$).

The weakly nonlinear analysis can be carried out in a similar manner as before with only minor changes; so we only outline the calculation. The same scalings as in section 2 apply except for those involving θ . The scaled mass and momentum equations (2.1) and (2.2) are unchanged, but the energy equation (2.3) and species equation (2.4) are changed to

$$\bar{\rho}H(\bar{T}) - \frac{\gamma-1}{\gamma} H(\bar{p}) = q\epsilon k_1 t_{ac} \bar{\rho} \bar{Z}_a^{n-1} \bar{Z}^n \phi(T_a(\bar{T}-1)) \tag{5.2}$$

$$\epsilon \frac{\partial \bar{Z}}{\partial T} + (\bar{u} - \bar{v}) \frac{\partial \bar{Z}}{\partial \xi} = -\epsilon t_{ac} k_1 Z_a^{1-n} \bar{Z}^n \phi(T_a(\bar{T}-1)). \tag{5.3}$$

In the Arrhenius case the activation energy θ determined the value of the small parameter ε and hence defined the length scale d of the wave. In the present case we take

$$k_1 t_{ac} \equiv \varepsilon^{-1}$$

which defines the length scale and brings in the chemistry at leading order. Again with the assumption that $q = q_0 \varepsilon^2$, so that the leading-order energy equation will be homogeneous, and with the ansatz (3.1), equation (5.3) gives to leading order

$$v_0 Z_{0\varepsilon} = Z_a^{n-1} Z_0^n \phi(T_a T_0 \varepsilon).$$

The energy equation (5.2) gives to $O(1)$ and $O(\varepsilon)$, respectively,

$$-T_{0\varepsilon} + \frac{\gamma-1}{\gamma} p_{0\varepsilon} = 0$$

$$-v_0 T_{1\varepsilon} + \frac{\gamma-1}{\gamma} v_0 p_{1\varepsilon} = \rho_0 v_0 T_{0\varepsilon} + \frac{\gamma-1}{\gamma} G_0(p_0) - G_0(T_0) + q_0 Z_a^{n-1} Z_0^n \phi(T_a T_0 \varepsilon).$$

The leading-order equations for mass, momentum, and energy are the same as (3.10) and so (4.1)–(4.3) follow. Substituting these results into the equations at the correction level finally yields, with a similar calculation as before, the asymptotic equations

$$U_\tau + UU_\eta + \alpha - \beta Z_{0\eta} = 0 \quad (5.4)$$

$$Z_{0\eta} = Z_0^n \phi(U) \quad (5.5)$$

where α , β and U are the same as before, and where we have set $Z_a = 1$ as the scale for Z , and we have noted that

$$\phi\left(\frac{\gamma+1}{\gamma-1} T_a U \varepsilon\right) = \phi(U).$$

6. Solution of the asymptotic equations

In this section we formulate and solve a boundary value problem (BVP) associated with the model equations (5.4), (5.5) in the zero activation energy case. We ask if the equations admit ZND (Zel'dovich–von Neumann–Doering) type waves (see Fickett and Davis 1979) where a constant velocity shock is propagating into an unperturbed reactive medium; in the shock it is assumed that no chemical reaction occurs, and the chemical energy is released behind the shock in a reaction zone between the shock and a piston that is supporting the flow from the rear. If the medium ahead of the shock is quiescent ($U = 0$, $Z = 1$), then it follows immediately from the conservation laws (5.4), (5.5) that the jump conditions (Rankine–Hugoniot conditions) across the shock are given by $U_s = 2D$, $Z_s = 1$ where D is the velocity of the shock and U_s and Z_s are the values of U and Z just behind the shock (see, for example, Whitham 1974). The rear boundary condition (at the unknown piston location) is taken to be $U = 0$. The motivation for this condition is that the products of the detonation will expand into an essentially infinite volume and thus return to an ambient state given by $\rho_0 = \gamma T_0 / (\gamma - 1) = 0$ (see (4.3)). We examine the case $n = 1$; other cases can be handled similarly.

Therefore, we consider the following BVP: determine a constant $D > 0$ and functions $U = U(\eta, \tau)$, $Z_0 = Z_0(\eta, \tau)$ satisfying:

$$U_\tau + UU_\eta + \alpha - \beta Z_{0\eta} = 0 \tag{6.1}$$

$$Z_{0\eta} = Z_0 \quad \tau \in R^1 \quad D\tau - \chi_0 < \eta < D\tau \tag{6.2}$$

with

$$U = 0 \quad Z_0 = 1 \quad \text{for } \eta > D\tau \tag{6.3}$$

$$U = 2D \quad Z_0 = 1 \quad \text{on } \eta = D\tau \tag{6.4}$$

$$U = 0 \quad \text{on } \eta = D\tau - \chi_0 \tag{6.5}$$

for some $-\infty \leq \chi_0 < 0$. The problem is shown schematically in the spacetime diagram in figure 1. Note that the constant state $U = 0, Z_0 = 1$ in the flow ahead is a solution to the PDEs (6.1), (6.2) since $\alpha = 0$ (because $\omega_r = 0$) ahead of the shock.

We therefore look for solutions of (6.1), (6.2) of the form

$$U(\eta, \tau) = u(\chi) \quad Z_0(\eta, \tau) = z(\chi) \tag{6.6}$$

where $\chi \equiv \eta - D\tau$. Using the lowercase u should cause no confusion with the same notation used in section 1. Substituting (6.6) into (6.1) and (6.5) gives the BVP

$$(u - D)u' + \alpha - \beta z' = 0 \tag{6.7}$$

$$z' = z \quad -\chi_0 < \chi < 0 \tag{6.8}$$

with

$$u(0) = 2D \quad z(0) = 1 \tag{6.9}$$

$$u(-\chi_0) = 0 \tag{6.10}$$

for D and for some $\chi_0 > 0$ still to be determined. Equations (6.8), (6.9) give $z = \exp \chi$, and then (6.7) can be solved for u . Thus, upon taking the plus sign on the radical when solving for u to meet the boundary condition,

$$z = \exp \chi \quad u = D + \sqrt{D^2 - 2\alpha\chi + 2\beta(e^\chi - 1)} \tag{6.11}$$

where we have evaluated the constant of integration using the shock condition $u(0) = 2D$. The shock velocity D , which is like an eigenvalue for this problem, is yet to be determined, and at the present it is unclear how the rear boundary condition can be satisfied since, in (6.11), $u \geq D$.

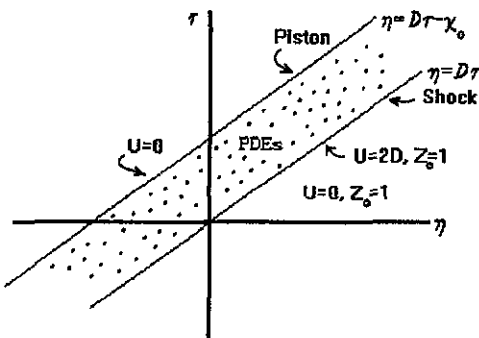


Figure 1. Spacetime diagram illustrating the domain of the boundary value problem (6.1)-(6.5).

To analyse the problem we write (6.7), (6.8) as a system of autonomous equations

$$z' = z \quad u' = \frac{\beta z - \alpha}{u - D} \tag{6.12}$$

which has a singular line at $u = D$; the phase diagram is shown in figure 2 with the ratio $\alpha/\beta < 1$. It is clear from (6.12) that if there is a path connecting the shock and the piston (on the $u = 0$ axis), then that path must pass through the singular line at the point C: $(\alpha\beta^{-1}, D)$, which is a saddlepoint for the desingularized system

$$\dot{z} = z(u - D) \quad \dot{u} = \beta z - \alpha \tag{6.13}$$

where the overdot is the derivative with respect to some other parameter along the integral curves. The phase plane for (6.13) is shown in figure 3. So the problem reduces to determining if a value of D exists for which a separatrix (the one dimensional unstable manifold W_u) from C connects to the shock point S (see figure 3).

The condition that the solution (6.11) pass through C is

$$\sqrt{D^2 - 2\alpha \ln\left(\frac{\alpha}{\beta}\right) + 2\beta\left(\frac{\alpha}{\beta} - 1\right)} = 0$$

or

$$D = \sqrt{2} (\alpha \ln(\alpha\beta^{-1}) - \alpha + \beta)^{1/2} \quad \alpha\beta^{-1} < 1 \tag{6.14}$$

which determines the eigenvalue, or shock velocity, D . We remark that $\alpha \ln(\alpha\beta^{-1}) - \alpha + \beta \geq 0$ for all $\alpha, \beta > 0$, so (6.12) is well defined. However, if $\alpha\beta^{-1} \geq 1$ then the critical point C lies to the right of S and there is no trajectory with $z \leq 1$ that connects S to the axis $u = 0, z \leq 1$.

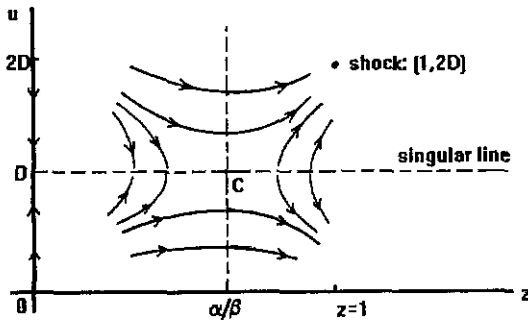


Figure 2. Direction field and trajectories for (6.12).

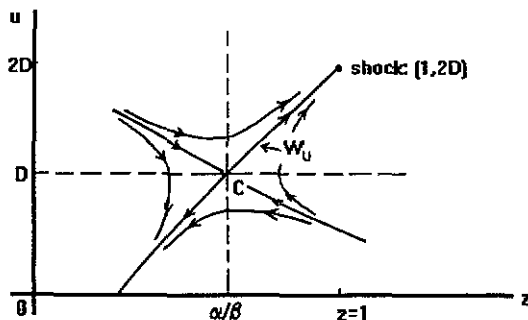


Figure 3. Phase diagram for the desingularized system (6.13).

Thus, the solution (6.11) is valid for $D \leq u \leq 2D$, with $\ln(\alpha\beta)^{-1} \leq \chi \leq 0$. To determine the solution in the range $0 \leq u \leq D$ we integrate (6.7), (6.8) to get

$$z = \exp \chi \quad u = D - \sqrt{D^2 - 2\alpha\chi + 2\beta(e^\chi - 1)} \quad (6.15)$$

where, when solving for u we take the minus sign on the radical. From (6.15) we observe that $u = 0$ when $\chi = -\chi_0$, where $-\chi_0$ is the negative root of the equation

$$\alpha\beta^{-1}\chi + 1 = \exp \chi. \quad (6.16)$$

We may now put together the preceding results in the following theorem.

Theorem. If $\alpha\beta^{-1} < 1$, then there exists a unique value of D given by (6.14) for which the BVP (6.1)–(6.5) has a solution. A solution is given by

$$Z_0(\eta, \tau) = \exp(\chi) \quad -\chi_0 \leq \chi \leq 0$$

$$U(\eta, \tau) = \begin{cases} D + \sqrt{D^2 - 2\alpha\chi + 2\beta(\exp \chi - 1)} & \ln(\alpha/\beta) \leq \chi < 0 \\ D - \sqrt{D^2 - 2\alpha\chi + 2\beta(\exp \chi - 1)} & -\chi_0 \leq \chi < \ln(\alpha/\beta) \end{cases}$$

where $\chi = \eta - D\tau$ and $-\chi_0$ is the negative root of (6.16).

A graph of $U(\chi)$ is shown in figure 4 in the case $\alpha = 1$ and $\beta = 2$. In this case $D = 0.783394$ and $\chi_0 = -1.59362$. Thus the reaction turns off at the cold piston when $Z = \exp(-1.59362) = 0.2032$, i.e. before all the reactant is depleted.

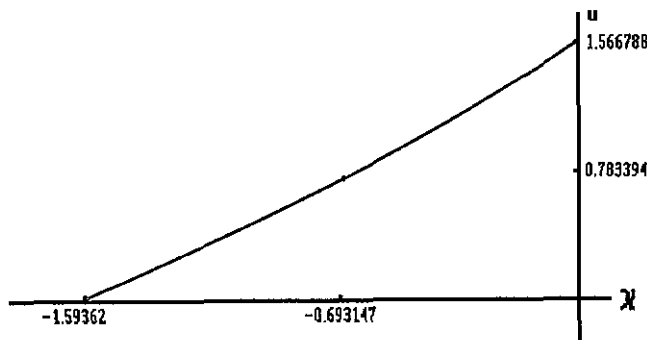


Figure 4. The calculated graph of $u = U(\chi)$ in the case $\alpha = 1$ and $\beta = 2$.

We make a few observations. For a fixed β (heat release), the shock velocity $D = D(\alpha)$ is a decreasing function of the radial divergence α , with $D(0) = \sqrt{2\beta}$ and $D(\beta) = 0$. For $\alpha > \beta$ there is no steady wave. This conclusion is physically plausible in that the heat release β supplies energy to the flow to sustain the wave; the radial divergence, on the other hand, dissipates energy through the coupling of the divergence to the lateral boundary conditions at the side of the tube. The narrower the tube, for example, the stronger the coupling, possibly through rarefactions propagated into the flow from the boundary. Thus, if $\alpha \geq \beta$ then the dissipation overcomes the energy released by the chemistry and a steady wave is impossible.

Although we do not present the details of the calculation, we remark that the Fickett analogue equations (4.9), (4.10) predict, for the simple rate law considered above ($r = k(1 - \lambda) = kZ$), that a steady wave can be propagated for any value of the divergence α . The reason for this difference is the t -derivative in (4.10), which introduces the

shock velocity D into the species equation. Thus, the asymptotic equations appear to reflect observed physical phenomena better than the analogue equations in the simple case.

7. Arrhenius rate law

We now present some numerical results showing the existence of an eigenvalue detonation, in this case the governing equations are given by (4.7), (4.8), with the Arrhenius rate law. The same boundary conditions (6.3)-(6.5) are imposed, as before. From (4.7), (4.8) we note that the travelling waveforms $U = u(\eta - D\tau)$, $Z_0 = z(\eta - D\tau)$ satisfy the system

$$z' = kz e^{2u} \tag{7.1}$$

$$u' = (\beta kz e^{2u} - \alpha)(u - D)^{-1} \tag{7.2}$$

where the derivative is with respect to $\chi \equiv \eta - D\tau$, and where we have fixed $\gamma = 3$. The value of $\gamma = 3$ is chosen for computational convenience; however, this value of γ (and even higher values of γ) is typical for the gaseous detonation products of solid explosives (see Fickett and Davis 1979). As in the non-Arrhenius case we observe that there is a singular line at $u = D$, and thus any trajectory connecting the shock S: ($z = 1$, $u = 2D$) to the cold piston (a point on $u = 0$) must pass through the singular line at the critical point C: ($z = (\alpha/\beta k) \exp(-2D)$, $u = D$) of the desingularized system

$$\dot{z} = kz(u - D) e^{2u} \tag{7.3}$$

$$\dot{u} = \beta kz e^{2u} - \alpha. \tag{7.4}$$

A necessary condition for such a trajectory to exist is that the critical point C must lie to the left of the shock point S, or

$$\frac{\alpha}{\beta k} e^{-2D} < 1. \tag{7.5}$$

The linearized matrix (Jacobian) corresponding to (7.3), (7.4) at the critical point C is

$$J = \begin{pmatrix} 0 & \alpha\beta^{-1} \\ \beta k e^{2D} & 2\alpha \end{pmatrix}.$$

Clearly, $\det J < 0$ and $\text{trace } J > 0$, and therefore C is a saddlepoint for all values $\alpha > 0$, $\beta > 0$, $k > 0$ of the parameters. Figure 5 shows a generic phase diagram. Contrary to the non-Arrhenius case discussed in section 6, it is not possible to analytically determine

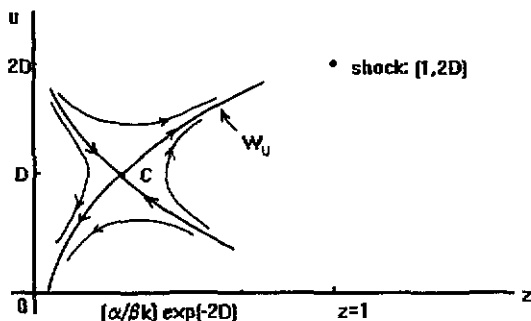


Figure 5. Phase diagram for the system (7.3), (7.4).

a condition on D that will ensure that the unstable manifold W_u (see figure 5) emanating from C will pass through the shock point S .

Therefore we resort to an argument based upon numerical calculations. Rather than perform an exhaustive parameter study (involving the four parameters k , α , β and D), we confine the analysis to the special case $k = \beta = 1$, $\alpha = 2$; it is shown that there is a value of the shock velocity D such that W_u connects C to S . With all the other parameters fixed, the phase diagram is deformed continuously as a function of D . Figure 6 depicts the core of the argument. For $D = 1.15$ the unstable manifold W_u passes above the point S representing the shock; for $D = 1.20$, W_u passes below S . Because the vector field defined by (7.3), (7.4) is continuous, it follows by a standard argument (based upon the intermediate value theorem) that there exists a value of D with $1.15 < D_0 < 1.20$ such that the separatrix W_u intersects the point S . Numerically, using Phaseplane (Ermentrout (1990), a numerical ordinary differential equation solver), D_0 was computed to be $D_0 \approx 1.17$.

Figure 7 shows the phase plane in the case $D = 1.17$. In this case there is a trajectory connecting the a point P on the axis $u = 0$, where the piston is located, to the point S

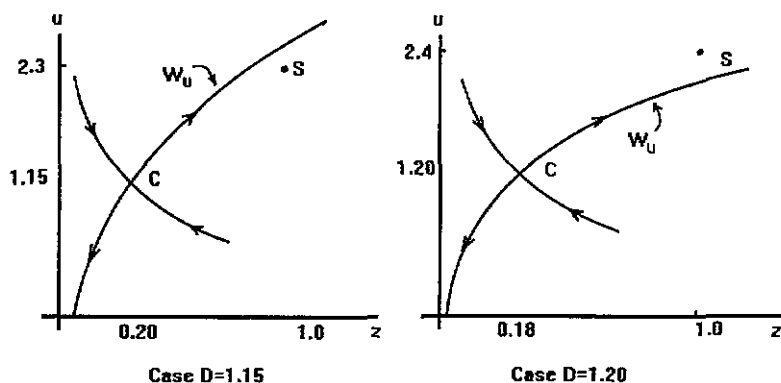


Figure 6. Phase diagrams for the system (7.3), (7.4) when $\alpha = 2$, $k = \beta = 1$. For $D = 1.15$ the unstable manifold W_u is above S ; for $D = 1.20$ it is below S .

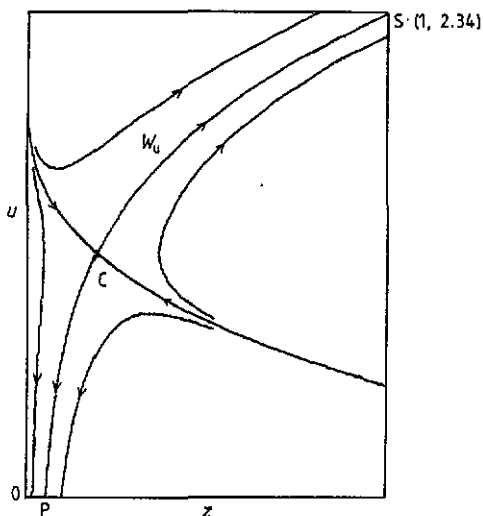


Figure 7. Actual computed phase diagram for (7.3), (7.4) in the case $\alpha = 2$, $k = \beta = 1$ and $D = 1.17$.

representing the shock (note that in the singular system (7.1), (7.2) the direction along the trajectory from P to C is opposite that shown in figure 7). This trajectory then represents a solution: a shock of strength $u = 2D$ and speed $D = 1.17$ followed by a reaction zone where u decays back to a cold piston $u = 0$ and where the reaction ceases without going to completion.

The problem studied in this section addresses the case where the reaction rate is temperature dependent, a problem posed by Fickett (1985, p 175). Although we have only examined one special case, it is noted that the Arrhenius factor forces changes in the conclusions; no longer is it required that the heat release β exceed the radial divergence α in order to have a steady wave, as in section 6. A complete parameter study would be required to determine if a steady wave exists in all cases where (7.5) is satisfied.

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References

- Bdzil J B 1981 *J. Fluid Mech.* **108** 195-226
 Bdzil J B and Stewart D S 1986 *J. Fluid Mech.* **171** 1-26
 Ermentrout B 1990 *Phaseplane* Version 3.0 (Pacific Grove, CA: Brooks-Cole)
 Fickett W 1985 *Introduction to Detonation Theory* (Berkeley, CA: University of California Press)
 Fickett W and Davis W C 1979 *Detonation* (Berkeley, CA: University of California Press)
 Fife P 1982 *Nonlinear Problems: Present and Future* ed A Bishop, D Campbell and B Nicolaenko (Amsterdam: North-Holland) pp 267-85
 Klein R 1991 *Dynamical Issues in Combustion Theory* ed P C Fife, A Linan and F Williams (New York: Springer) pp 127-66
 Ledder G and Logan J D 1992 *Int. J. Eng. Sci.* **30** (12) 1759-72
 Logan J D 1988 *J. Phys. A: Math. Gen.* **21** 643-50
 Majda A 1981 *SIAM J. Appl. Math.* **41** 70-93
 ——— 1986 *Reacting Flows: Combustion and Chemical Reactors* Part 1, ed G S S Ludford (Providence, RI: American Mathematical Society)
 Rosales R and Majda A 1983 *SIAM J. Appl. Math.* **43** 1086-118
 Whitham G B 1974 *Linear and Nonlinear Waves* (New York: Wiley-Interscience)
 Wood W W and Kirkwood J G 1954 *J. Chem. Phys.* **22** 1920