DETONATION WAVES AND DEFLAGRATION WAVES IN THE ONE DIMENSIONAL ZND MODEL FOR HIGH MACH NUMBER COMBUSTION

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DETONATION WAVES AND DEFLAGRATION WAVES IN THE ONE DIMENSIONAL ZND MODEL FOR HIGH MACH NUMBER COMBUSTION

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ABSTRACT. As a consequence of precise criteria for the existence of plane detonation and deflagration wave solutions to the Navier Stokes equations for a compressible fluid with a one step exothermic reaction, we are able to rigorously examine the limit of both types of wave as diffusion rates tend to zero, while the reaction rate remains constant. We call this limit the ZND model. We find that all strong ZND detonation waves are such limits. These waves are composed of an inert shock wave followed by a deflagration wave. There is also a continuous weak detonation with an unburned temperature equal to the ignition temperature. This wave is also the limit of viscous weak detonation waves. In addition, we find that continuous weak deflagration waves with unburned temperature equal to the ignition temperature are also limits of weak Navier Stokes deflagrations. We remark on the possibility of deflagrations in which the fuel is only partially burned.

1. INTRODUCTION. Exothermically reacting 'shock waves' are classified into two types: detonation waves, which are supersonic and compressive, and deflagration waves, which are subsonic and expansive. Because a chemical reaction depends on molecular collisions, the length scale for the chemical reaction in one of these waves is typically much larger than that for the shock wave which is associated with a detonation. Consequently the preferred inviscid model for high Mach number combustion is the ZND model [2, 4, 8], which for a one step exothermic reaction takes the following form in Eulerian coordinates:

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(1) $$(\rho u)_t + (\rho u)_x = 0,$$
$$(\rho u)_t + (\rho u^2 + p(\rho, T))_x = 0$$
$$(\rho(u^2/2 + e(\rho, T, Y)))_t + ((\rho(u^2/2 + e(v, T, Y)) + p(\rho, T))u)_x = 0,$$
$$(\rho Y)_t + (\rho u Y)_x = - k\rho Y\phi(T).$$

We assume that the mixture is an ideal gas in which the specific heats at constant volume, c_v, and at constant pressure, c_p, are constant and independent of the chemical composition. Then $p = R\rho T$ and $e = c_v T + qY$, where Y is the mass fraction of the reactant and q is the difference in heats of formation between the reactant and the product.

A brief discussion of Rankine Hugoniot conditions is in order. Suppose the reaction front has zero thickness. This is the Chapman Jouguet model for reaction shock waves. Because the reaction releases energy into the system, the classical Hugoniot curve of gas dynamics moves. See Fig. 1. For non-reacting, or inert shock waves, the Rankine Hugoniot conditions yield, typically, one possible wave for a given upstream state and given admissible speed. Waves which are subsonic upstream and supersonic downstream are ruled out by the second law of thermodynamics. For exothermically reacting shock waves, however, there may be two possible waves for a given admissible wave speed, as shown in Fig. 1. We have, thus, four distinct types of wave. Strong detonations are supersonic upstream and subsonic downstream. Weak detonations are supersonic upstream and downstream. Weak deflagrations are subsonic upstream and downstream. Strong deflagrations are subsonic upstream and supersonic downstream. Of these, only strong deflagrations can be ruled out by entropy considerations, and then only for purely exothermic reactions.

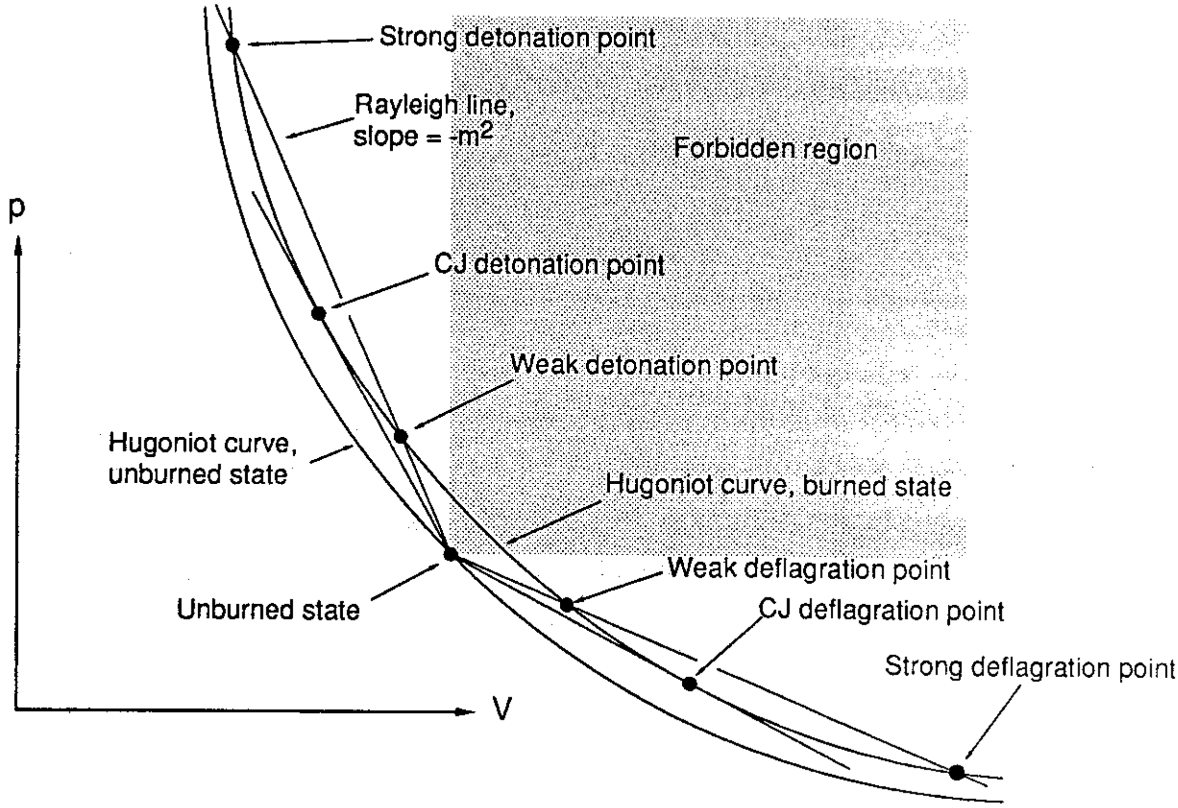

Fig. 1. The Chapman-Jouguet Diagram

2. EXISTENCE THEOREMS. In [6, 7] we have studied the existence and behavior of travelling wave solutions to the corresponding Navier Stokes model:

$$(2) \quad (\rho u)_t + (\rho u)_x = 0,$$

$$(\rho u)_t + (\rho u^2 + p(\rho, T))_x = (\mu u_x)_x$$

$$(\rho(u^2/2 + e(\rho, T, Y)))_t + ((\rho(u^2/2 + e(v, S, Y)) + p(\rho, T))u)_x = (\lambda T_x)_x + (q\rho D Y_x)_x + (\mu u u_x)_x$$

$$(\rho Y)_t + (\rho u Y)_x = (\rho D Y_x)_x - k\rho Y \phi(T).$$

By means of a Galillean transformation, the study of travelling wave solutions of this system reduces to the study of steady waves. For steady solutions the mass flux ρu must be constant; we denote its value by m. It is convenient to use m as a parameter for the speed of the wave. The reaction rate $\phi(T)$ is usually of the Arrhenius form:

$\phi(T) = exp(-E/RT)$; however a problem arises in studying steady or travelling waves with this form for ϕ because in this case the system of ordinary differential equations for the steady solutions has no unburned rest state. This is called the *cold boundary difficulty.* The standard way to resolve this difficulty is to modify ϕ for small T so that for some *ignition temperature* T_i, $\phi(T) = 0$ if and only if $T \le T_i$. In addition to this ignition temperature assumption we assume that ϕ is Lipschitz and monotone increasing.

For any variable U let U_- be the value of U at the unburned state, and let $U_\pm$ be the value of U at the burned state. Let U^* and U_* be the values of U at the specific burned states corresponding to a strong detonation point or a weak detonation point, respectively. Suppose that $\mu = \lambda/c_p$. Let $H = c_pT + u^2/2$ be the stagnation enthalpy, let $V = 1/\rho$ be the specific volume, and let $\varepsilon = (Y - \rho DY_x/m)$. Let y be a new space variable satisfying $(dy/dx) = mc_p/\lambda$. Then a steady solution to (2) must satisfy:

$$(3) \qquad V_y = (V - V_\pm)\left(1 - \frac{R}{2c_p}\right) + \frac{R}{m^2 c_p}\left(\frac{H}{V} - \frac{H_-}{V_-}\right)$$

$$H_y = H - H_\pm + q(\varepsilon - \varepsilon_\pm)$$

$$\varepsilon_y = -\frac{\lambda}{m^2 c_p} k\rho Y \phi(T)$$

$$Y_y = \frac{\lambda}{\rho D c_p}(Y - \varepsilon).$$

In order to state our existence results, we define the *Lewis number,* $L = \lambda/\rho Dc_p$, the *upper Lewis number,* $\Lambda^* = sup(L, 1)$, and the *lower Lewis number,* $\Lambda_* = inf(L, 1)$. For detonation waves, let Y_i be the greater of 0 or the maximum value of Y corresponding to an unburned rest state with $T = T_i$. Then, if $M^2 = u^2/\gamma RT$ is the square of the Mach number, let

$$\delta = (c_p - R/2)(T_i - T_-) + \frac{u_-^2}{4\gamma^2 M_-^4}\left(1 - \gamma^2 M_-^4 + \left(\gamma M_-^2 + 1\right)\sqrt{\left(\gamma M_-^2 + 1\right)^2 - 4\gamma M_-^2 \frac{T_i}{T_-}}\right).$$

Then $q(Y_- - Y_i) = max(\delta, qY_-)$. For deflagration waves, let $Y_i(T_-, Y_-) = Y_- - (c_p/q)(T_i - T_-)$. We have implicitly assumed, in both cases, that

$$\frac{T_i}{T_-} < \frac{\gamma}{4}\left(M_- + \frac{1}{M_-}\right)^2 .$$

This assures that the surface $T = T_i$ intersects the surface $V_y = 0$, and, in the case of deflagration waves, assures that there is an unburned state with $T = T_i$. For detonation waves we assume that $T_* > T_i$. By definition, $(Y_- - Y_i)$ is always positive. The principal result of [6] is the following theorem.

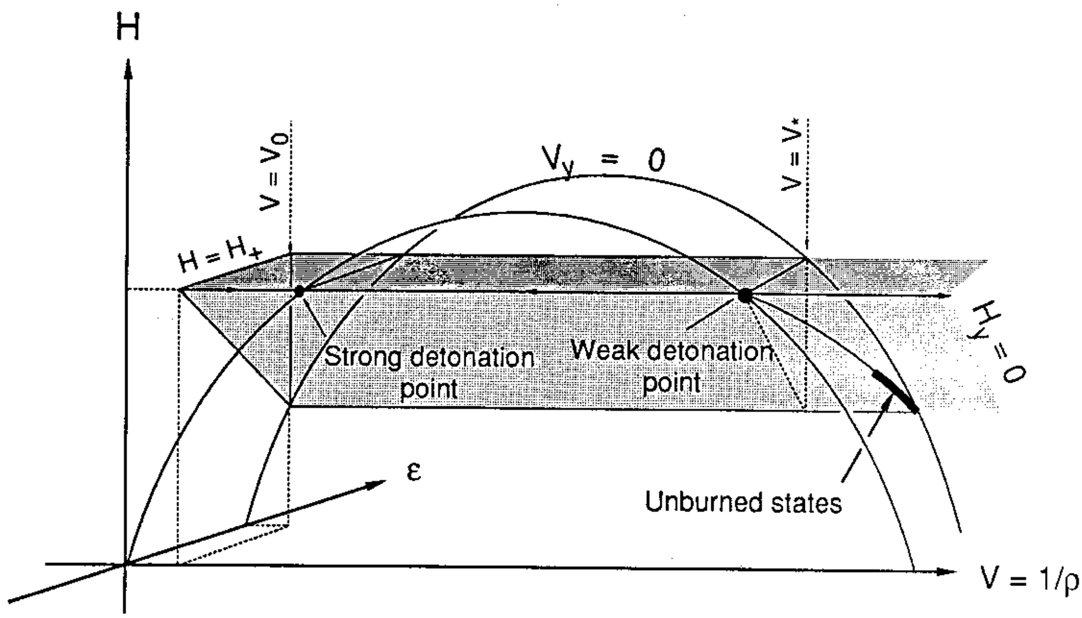

Fig. 2 The detonation flow

THEOREM 1. *Let (V_-, H_-, Y_-, Y_-) and $(V^*, H^*, 0, 0)$ be an unburned state and strong detonation state satisfying the Rankine Hugoniot conditions for a strong detonation with mass flux m, with $T_- < T_i$. Let $(V_*, H_*, 0, 0)$ be the corresponding weak detonation state. Then whenever*

$$(4) \qquad Y_- - Y_i > \left(\frac{2\gamma c_p}{(\gamma-1)m^2q^2V_*} \int_{T_i}^{T_*} \lambda k \Lambda^*(T_* - T)\,\phi(T)\,dT \right)^{\frac{1}{2}} .$$

there exists at least one solution of (3) connecting the unburned state at $y = -\infty$ to the strong detonation state at $y = +\infty$. If

$$Y_- < \left(\frac{2c_p}{m^2 q^2 V_-} \int_{T_-}^{T_- + qY_-/c_p} \lambda k \Lambda_* \left(T_- + \frac{qY_-}{c_p} - T \right) \phi(T)\, dT \right)^{\frac{1}{2}}.$$

then there is no such solution. For all of these solutions H, ε, *and* Y *are monotone. In addition, there exists one weak detonation solution with mass flux* m *and with an unburned state which does not satisfy condition (4).*

For deflagration waves, we need only consider the weak deflagration burned point. The existence result of [7] is:

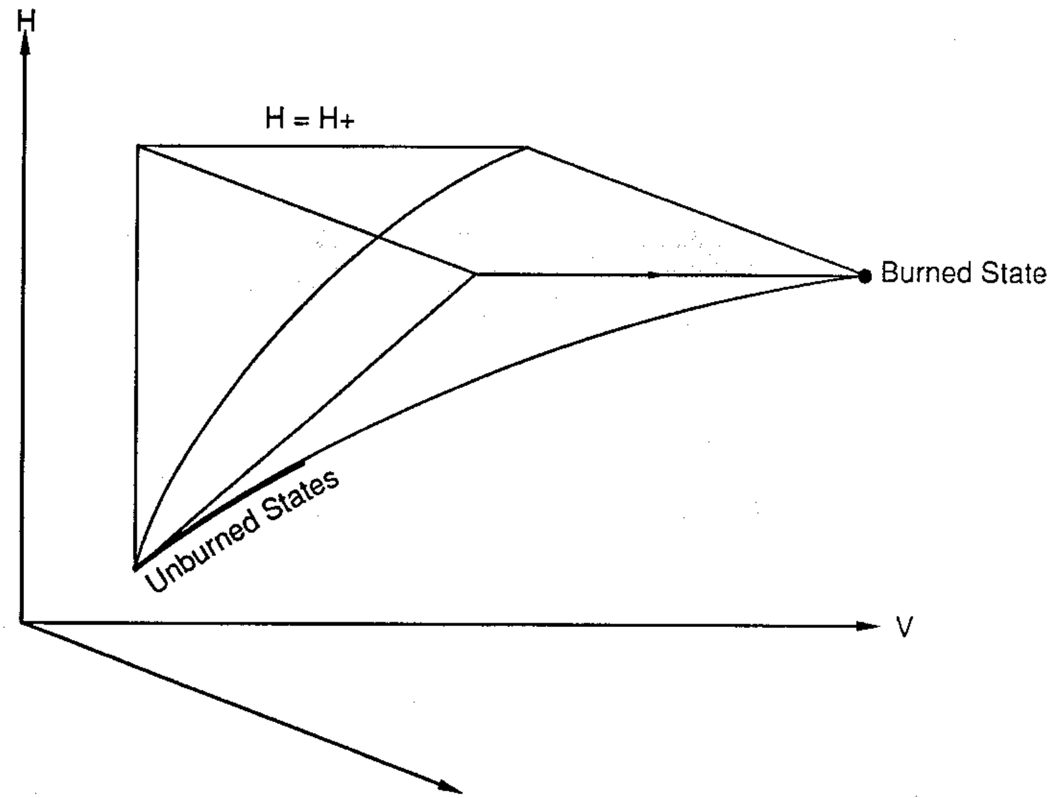

Fig. 3. The deflagration flow

THEOREM 2. *Let* (V_0, H_0, Y_0, Y_0) *and* $(V_+, H_+ 0, 0)$ *be an unburned state and weak deflagration state satisfying the Rankine Hugoniot conditions for a weak deflagration with mass flux* m, *with* $T_0 < T_i$. *Suppose also that the burned state is strongly subsonic, that is,* $\gamma M_+^2 < 1$, *and that*

$$Y_0 - Y_i(T_0, Y_0) = \left(\frac{2c_p}{m^2q^2V_-} \int_{T_-}^{T_-+qY_-/c_p} \lambda k \Lambda^*\left(T_- + \frac{qY_-}{c_p} - T\right)\phi(T)\,dT \right)^{\frac{1}{2}}.$$

There exists at least one solution of (3) connecting an unburned state (V_-, H_-, Y_-, Y_-) to (V_+, H_+, 0, 0) with mass flux m. Y_- satisfies

$$Y_0 > Y_- \geq \left(\frac{2c_p}{m^2q^2V_+} \int_{T_-}^{T_+} \lambda k \Lambda_*(T_+ - T)\,\phi(T)\,dT \right)^{\frac{1}{2}}.$$

All of the unknowns V, H, ε, and Y are monotone on this wave.

It is interesting to note the similarity of these results with those for premixed laminar flames [1, 3, 5].

3. THE ZND LIMIT. What happens to these solutions as the diffusion coefficients λ, μ, and D tend to zero? This question is not as simple as it would be for inert shock profiles, because the zeroth order term in the system (the reaction rate) ruins the self-similarity that is found in inert shock profiles. In fact the qualitative behavior, and even the existence of the solution varies with the diffusion coefficients and the reaction rate.

As λ, μ, and D tend to zero, every unburned detonation state with $T_- < T_i$ eventually satisfies the criteria given in Theorem 1 for the existence of a strong detonation profile. Consequently the unburned state for the weak detonation profile must tend to the unburned state with $T = T_i$. Similarly, by Theorem 2 the unburned state for the weak deflagration must tend to the unburned deflagration state with $T = T_i$. We proved in [6, 7] that for all of these solutions H, ε, and Y are monotone, and that V has at most one minimum (strong detonation waves usually do not have monotone V). Thus these solutions have bounded total variation independent of λ, μ, and D. By Helly's theorem we conclude that a suitable subsequence of these solutions converges pointwise a.e. to a weak solution of (1). Thus we find for detonation waves that *every strong ZND detonation with unburned temperature less than the ignition temperature is the limit of strong detonation solutions of (2). There is a continuous weak detonation solution of (1) with unburned temperature T_i, which is also the limit of weak* *detonation solutions of (2).* For weak deflagrations we find that *there is a weak deflagration solution of (1) which is continuous and has an unburned temperature T_i.*

REMARK. There is also a strong ZND detonation wave with unburned temperature equal to the ignition temperature. One can say, based on the results stated in section 2, that this solution is a limit of solutions of (2). These viscous profiles have unburned temperatures approaching the ignition temperature. There might also be a strong detonation solution of (2) with unburned temperature equal to the ignition temperature; however our techniques are not sufficiently precise to prove its existence.

Both the strong ZND detonation wave and the weak detonation wave with $T_- = T_i$ are probably essential parts of the ZND model. For the Chapman Jouguet model, this judgement may not be so easy to make. For the CJ model, a strong detonation wave is equivalent to a weak detonation immediately followed by an inert shock wave of the same speed.

4. PARTIALLY BURNED DEFLAGRATIONS. In our discussion of deflagrations, we assumed that the burned state was strongly subsonic, that is, $\gamma M_+^2 < 1$. The significance of this assumption comes from the fact that on the surface $V_y = 0$, the sign of (dT/dH) equals the sign of $(1 - \gamma M^2)$. Also, the sign of $(1 - \gamma M_+^2)$ determines the sign of T_y on solutions near the burned state [6]. While we cannot yet prove that this condition implies the monotonicity of T on the deflagration profile (except in the ZND limit), it is certain that when the burned state is not strongly subsonic then the temperature is strictly decreasing at the burned state.

For deflagration waves it is possible that the burned state temperature is actually below the ignition temperature. This is impossible for weak detonations, and unlikely for strong detonations because for a strong detonation to exist, the temperature at the *von Neumann point* (the subsonic inert shock state corresponding to the supersonic unburned state) the temperature must be above the ignition temperature. However for deflagration waves this is a real possibility. In this case we have a curve of burned, or partially burned rest states, as well as unburned rest states. In fact we might have a single curve of rest states. Each of these rest states has a one dimensional unstable manifold in (V, H, ε) space. If this orbit enters the region $T > T_i$, then combustion can take place. (This must happen if there is a rest state with $T = T_i$ and $\varepsilon < \varepsilon_-$.) Each rest state with $T < T_i$ also has a one dimensional stable manifold in

(V, H, ε) space. Since the rest states form a curve, or two curves, this curve has a two dimensional stable manifold and a two dimensional unstable manifold. Theorem 2 gives a condition which guarantees the intersection of these manifolds in a combustion solution. The value of ε at the point where this solution exits the region $T \geq T_i$ is the final mass fraction of the reactant. Further burning of this gas would require recompression to raise the temperature.

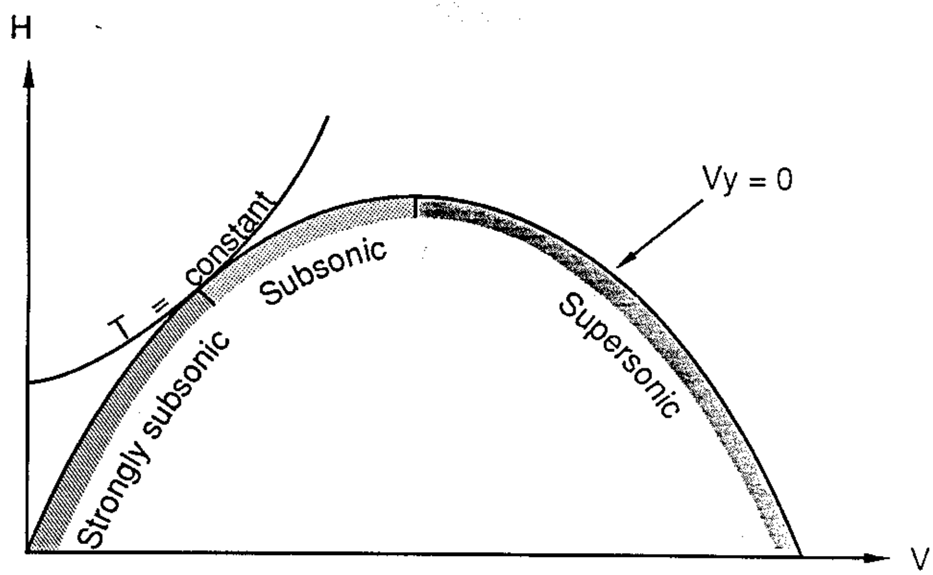

Fig. 4. Mach number and Temperature

In the ZND limit, a partially burned deflagration solution exists only if the curve defined by $V_y = 0$, $H_y = 0$ passes through the region $T > T_i$. In this case the solution must begin and end at rest states where $T = T_i$.

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