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THE EXISTENCE AND BEHAVIOR OF VISCOUS STRUCTURE FOR PLANE DETONATION WAVES*

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Abstract. A necessary condition and a sufficient condition are proved for the existence of steady plane wave solutions to the Navier–Stokes equations for a reacting gas. These solutions represent plane detonation waves, and converge to ZND detonation waves as the viscosity, heat conductivity, and species diffusion rates tend to zero. It is assumed that the Prandtl number is $\frac{3}{4}$, but arbitrary Lewis numbers are permitted. No assumption is made concerning the activation energy.

It is shown that the stagnation enthalpy and the entropy flux are always monotone for such solutions, and that the mass density and pressure are nearly always not monotone, as predicted by the ZND theory.

In certain parameter ranges, typically that of large diffusion, many of these waves have the appearance of a weak detonation followed by an inert shock wave. This confirms a phenomenon observed in numerical calculations and in a model system by Colella, Majda, and Roytburd.

Key words. shock waves, detonation waves, combustion

AMS(MOS) subject classifications. 76L05, 80A32, 80A25, 35L65

1. Introduction.

Detonation waves are compressive, exothermically reacting shock waves. One of the curiosities of combustion theory is that there also exist expansive "shock waves" known as *deflagration waves*, which will not be discussed in this paper. We will give a mathematically rigorous, but simple, discussion of the *viscous structure* of plane detonation waves.

We begin with a brief discussion of the inviscid theory, known as the Chapman–Jouguet (CJ) theory. By means of a Galilean transformation we may reduce the problem to one of studying steady plane waves. If we assume that the thickness of the reaction zone is zero, if we neglect all diffusion effects such as viscosity, heat conduction, and diffusion of species, and any external forces such as gravity, and if we look for steady plane waves, then we obtain the following system of differential equations:

$$(1.1)\qquad \begin{aligned} &(\mathrm{a}) && (\rho u)_x = 0, \\ &(\mathrm{b}) && \left[\rho u^2 + p(\rho, T)\right]_x = 0, \\ &(\mathrm{c}) && \left((\rho(u^2/2 + e(\rho, T, Y)) + p(\rho, T))u\right)_x = 0, \\ &(\mathrm{d}) && (\rho u Y)_x = -\rho u(Y_-)\delta(x - x_0). \end{aligned}$$

Here x is a space coordinate in the direction normal to the wave, x_0 is the location of the wave, and ρ, T, u, p, e, and Y are the mass density, temperature, x component of velocity, pressure, specific internal energy, and mass fraction of the reactant, respectively. Y_- is the unburned value of Y. As is standard practice, we have represented the extremely complicated chemical reaction by a simplified, one-step chemistry: reactant → product. From (1.1a) we see that the mass flux, ρu, has a constant value; we denote this value by m. The fluxes of momentum (1.1b) and energy (1.1c) are also constant; from this fact we obtain the *Rankine–Hugoniot conditions* for a shock wave, which

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in the inviscid theory is represented by a jump discontinuity in the unknowns. The difference between inert gas dynamics, and the exothermic reactive theory discussed here, lies in the fact that Y varies from a positive value on the unburned side of the wave, which we take to lie on the left side, to a zero value on the burned, or right side. Because the internal energy e depends on Y, the change in Y causes the classical Hugoniot curve (the solution locus of (1.1c)) of gas dynamics to move. As a consequence, we find that, for a given value of m, a given shock state on the left may now be connected by a shock wave to two possible states on the right, except for certain critical values of m for which there is a unique burned state — the *Chapman–Jouguet point* — see Fig. 1. In addition, the curve of possible burned states, parameterized by m, has two components. One component, corresponding to compressive waves, is called the detonation branch, and the other component, corresponding to expansive waves, is called the deflagration branch. By way of contrast, in an inert gas, for a given value of m, a state is usually connected to only one state on the right, and the curve of possible terminal shock states is usually connected.

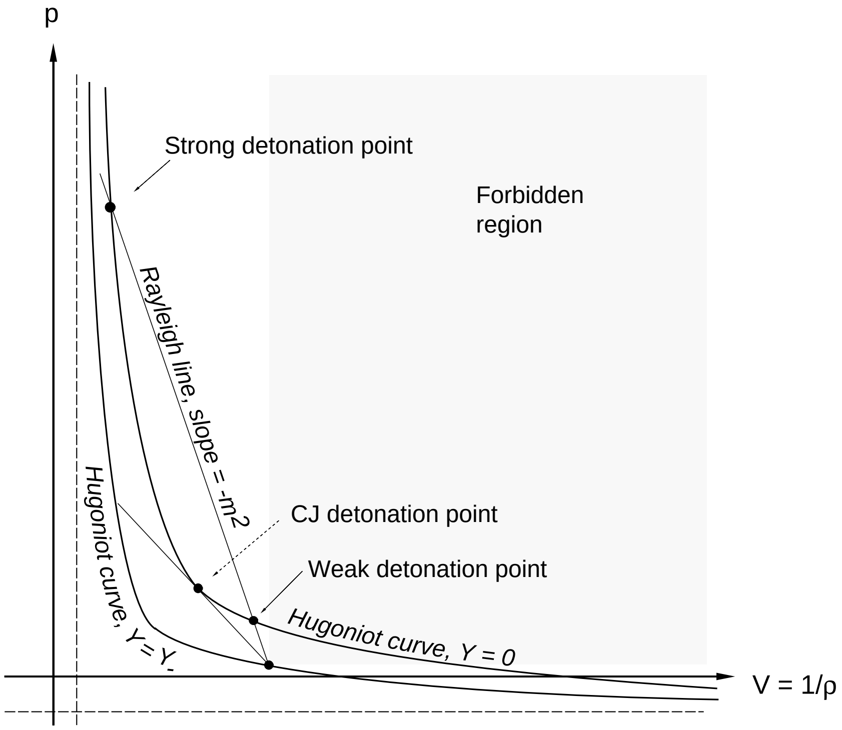

FIG. 1. *The Chapman–Jouguet diagram.*

The combustive shock waves of the CJ theory are classified as follows. A wave connecting the unburned state to the closer detonation point is called a *weak* detonation wave, and a connection to the farther detonation point is called a *strong* detonation. A detonation wave terminating at the Chapman–Jouguet point is called a *Chapman–Jouguet* detonation. Deflagration waves are similarly classified. For the exothermic, irreversible reactions considered here, strong deflagrations violate the second law of thermodynamics and are unphysical, and weak detonations are rare. If we permit an endothermic region then strong deflagrations and weak detonations are possible and perhaps even probable [FD].

The CJ theory for detonation waves is useful for deriving the Rankine–Hugoniot conditions, and for classifying the types of wave. However, this theory is physically flawed, because in reality the reaction zone is much thicker than the shock layer. This is due to the fact that the chemical reaction depends on molecular collisions and requires a distance much longer than the mean free path to achieve significant completion. The shock layer, however, has been experimentally observed to be several mean free paths thick. Consequently the appropriate inviscid model is the one developed independently by Zel'dovich, von Neumann, and Döring [Z], [ZK], [N1], [N2], [D], and which is known as the ZND model. In this model equation (1.1d) is replaced by a similar equation, but with a finite reaction rate:

$$(\rho u Y)_x = -r(\rho, Y, T) \tag{1.1d$'$}$$

For our purposes it is reasonable to assume that the reaction rate function r is continuous, nonnegative, and monotone in each variable. Our mathematical treatment will require that we assume that r vanishes whenever the temperature T is less than a given *ignition temperature* T_i. For a known reaction rate r (1.1a–c, d$'$) can be solved explicitly; the only detonation wave solutions are strong or CJ detonations. These waves, which are known as ZND waves, begin with a jump discontinuity which is an inert shock wave. This shock wave heats the gas above the ignition temperature; the reaction proceeds, with the velocity and temperature following a curve of equilibrium states for (1.1b, c), parameterized by Y. One of the interesting features of these waves is the peak in the pressure and density which is known as the *von Neumann spike*. By way of contrast, in inert shock waves the pressure and density are usually monotone [Gi].

The equations of inert, inviscid, non-heat-conducting gas dynamics are an example of a nonlinear hyperbolic system of conservation laws. In the theory for such systems it is standard practice to set admissibility criteria to distinguish physical from unphysical shock waves. One of the criteria in which much faith is put is to accept a shock wave as physical if it is *structurally stable.* A shock wave is structurally stable if it is the limit of solutions to models which include more physical effects, such as viscosity and heat conduction, as these models tend to the original inviscid model in which these effects are neglected. For steady plane detonation waves the effects of viscosity, heat conduction, and species diffusion may be considered to obtain the (steady) *reacting compressible Navier–Stokes equations*:

$$(1.2)\quad \begin{array}{ll}
\text{(a)} & (\rho u)_x = 0, \\
\text{(b)} & \left(\rho u^2 + p(\rho, T)\right)_x = (\mu u_x)_x\,, \\
\text{(c)} & \left[\left(\rho\left(u^2/2 + e(\rho, T, Y)\right) + p(\rho, T)\right) u\right]_x = (\lambda T_x)_x + (\mu u u_x)_x + (q\rho D Y_x)_x\,, \\
\text{(d)} & (\rho u Y)_x = (\rho D Y_x)_x - r(\rho, T, Y).
\end{array}$$

Here μ is the coefficient of viscosity, λ is the heat conductivity, D is the diffusion rate for the reactant, and q is the difference in the heats of formation of the reactant and the product [Wi].

In this paper we prove a necessary condition and a sufficient condition for the existence of heteroclinic solutions of (1.2) which extend from an unburned state at $x = -\infty$ to the strong detonation point at $x = \infty$. These conditions also apply to the Chapman–Jouguet detonation. See (4.8) and (5.3). For simplicity we restrict our attention to the case where the *Prandtl number* is $\frac{3}{4}$ $(\mu = \lambda/c_p)$. In the limit as λ, μ, and D tend to zero (with other parameters fixed) these solutions tend to the ZND wave. Thus the ZND wave is structurally stable to this particular perturbation of the model.

For all of these solutions the *stagnation enthalpy* $H = c_pT + u^2/2$ is monotone, as is the *entropy flux*: $mS - \lambda T_x/T$. For most of the strong detonation waves the density and the pressure attain their maxima in the interior of the wave; this corresponds to the von Neumann spike which occurs in the ZND wave. However, for a certain parameter range, namely whenever

$$\frac{L}{2}\left(1 - \sqrt{\frac{1 + 4Dk\phi(T^*)}{u^{*2}}}\right) > \frac{1}{\gamma}\left(1 - M^{*-2}\right),$$

where $L = \lambda/\rho D c_p$ is the *Lewis number*, M^* and T^* are the Mach number and temperature at the strong detonation point, and $k\phi(T^*)$ is the reaction rate as defined in (2.9), there exists a continuum of solutions which look like a weak detonation followed by a gas dynamic shock wave. For these waves the pressure and temperature are monotone. This pathological behavior has been noted before in [Wo2], [FD], [LL], [HoSt], and in numerical computations of solutions of the time-dependent Navier–Stokes equations for a reacting gas [CMR]. In these numerical computations it was observed that the weak detonation-shock wave solutions are dynamically stable as solutions of the time-dependent equations in one space dimension.

Since Zel'dovich, von Neumann, and Döring [Z], [N1], [N2], [D] described the typical plane detonation heuristically as an inert shock wave followed by a deflagration, there have been a number of papers on the structure problem for plane detonations. A common assumption has been that the Prandtl number is $\frac{3}{4}$ and that the Lewis number is 1. Under these assumptions Hirschfelder and Curtiss gave a good analysis of the behavior of structure profiles [HC], and Wood proved the existence of structure for "small" reaction rates [Wo1]. The approach taken here has much in common with Wood's, except that we have been more precise in our analysis, our results are stronger and more general, and we give explicit and fairly sharp statements of just how small the rate parameter must be.

A typical expression for the reaction rate is given by the Arrhenius law:

$$r(\rho, T, Y) = k\rho \cdot Y e^{-\theta/T}, \tag{1.3}$$

where θ is the activation energy E/R. In mathematical combustion theory it is standard practice to simplify models such as (1.2) by taking an appropriate distinguished limit as k and θ tend to infinity. This has the effect of reducing the thickness of the reaction zone to zero. Bush and Fendell [BF] gave a description of CJ detonations using asymptotic expansions in the limit of infinite activation energy. Stewart and Holmes proved the existence of viscous structure for (1.2), assuming a large, finite activation energy [HoSt]. Lu and Ludford gave a simplified analysis of weak, strong, and CJ detonations in the infinite activation energy limit [LL].

It is desirable to understand the existence of structure for plane detonation waves with no assumptions concerning activation energy, independent of any desire for mathematical generality. Because (under the ZND hypothesis) the reaction zone is much thicker than the shock layer, this problem should be studied for activation energies that are small compared to the reciprocals of the heat conductivity, viscosity, and species diffusion rate.

Gardner proved the existence of travelling plane detonation wave solutions to the Lagrangian reacting compressible Navier–Stokes equations [Ga]. He made no assumption on the Lewis and Prandtl numbers. However, he omitted the species diffusion term from the energy balance equation, and this term is not usually neglected. It may be that the effect of this term on the solution is very small. However, we will demonstrate in this paper that inclusion of this term permits a much more natural treatment of the problem and better bounds on the solution.

The remainder of the paper is organized as follows. In §2 we explain our assumptions in more detail, and we show that under these assumptions, and the assumption that the Lewis number is 1, that (1.2) is reduced to a system of three differential equations. This material has been extracted and specialized from [Wi]. It is included for clarity and completeness of exposition. In §3 we present the simple topological argument that proves the existence of viscous structure for steady plane detonation waves. In §4 we prove the estimate that makes the topological argument work, and we conclude this section with a sufficient condition for the existence of structure. In §5 we prove, using simple energy estimates on the stagnation enthalpy, a necessary condition for the existence of structure; if this condition is not satisfied then viscous structure does not exist. In §6 we give the generalization to arbitrary Lewis numbers. In §7 we discuss the behavior of the solutions for various parameter values. In §8 we present a rigorous discussion of the ZND limit. We conclude, in §9, with a proof that the entropy flux is monotone.

2. Reduction to three equations.

We make the basic thermodynamic assumption that both the reactant and product satisfy the same ideal gas law, and differ only in their heats of formation. Thus the pressure is independent of Y:

$$p = R\rho T. \tag{2.1}$$

We further assume that the internal energy depends linearly on Y, so that we have:

$$e = c_v T + qY, \tag{2.2}$$

where c_v is the specific heat at constant volume. These assumptions are probably not essential to the results that follow, and they could probably be replaced with more qualitative conditions similar to Weyl's conditions for the equation of state for an inert gas. However, these assumptions are essential to the simplifications that follow.

Observe that (1.2) can be integrated once to yield $\rho u = m = \textit{constant}$. If for any unknown U we let $U_\pm$ be the limit of U as x tends to $\pm\infty$, we have:

$$\begin{aligned}
&\text{(a)}\quad \mu u_x = m(u-u_\pm) + p - p_\pm\\
&\text{(b)}\quad \lambda T_x + \mu u u_x + q\rho D Y_x\\
&\qquad\qquad = m\left[c_v\left(T-T_\pm\right) + q\left(Y-Y_\pm\right) + \frac{1}{2}\left(u^2-u_\pm^2\right) + R\left(T-T_\pm\right)\right]\\
&\text{(c)}\quad (\rho D Y_x)_x = mY_x + r(\rho, Y, T)
\end{aligned} \tag{2.3}$$

Let $H = c_p T + u^2/2$ be the stagnation enthalpy. Here $c_p = c_v + R$ and is the specific heat at constant pressure. Then (2.3b) may be rewritten as:

$$(\lambda/c_p)H_x + (\mu - \lambda/c_p)\left(\frac{u^2}{2}\right)_x = m\left(H - H_\pm + q(\epsilon - \epsilon_\pm)\right), \tag{2.4}$$

where $\epsilon = Y - \rho D Y_x / m$ is a *reaction progress variable.* When the Prandtl number is $\frac{3}{4}$, then $\mu = \lambda / c_p$ and we have:

$$\left(\frac{\lambda}{m c_p}\right) H_x = H - H_\pm + q\,(\epsilon - \epsilon_\pm)\,. \tag{2.5}$$

It is convenient to let y satisfy

$$\frac{dy}{dx} = \frac{m c_p}{\lambda}, \tag{2.6}$$

so that the left-hand side of (2.5) becomes H_y. The system (2.3) reduces to a system of four first-order equations:

$$\begin{aligned} &\text{(a)} \quad m u_y = m\,(u - u_\pm) + mR\left(\frac{T}{u} - \frac{T_\pm}{u_\pm}\right) \\ &\text{(b)} \quad H_y = H - H_\pm + q\,(\epsilon - \epsilon_\pm) \\ &\text{(c)} \quad \epsilon_y = -\frac{\lambda}{m^2 c_p} r(\rho, Y, T) \\ &\text{(d)} \quad Y_y = \frac{\lambda}{\rho D c_p}(Y - \epsilon). \end{aligned} \tag{2.7}$$

Note that

$$(H - H_+)_y + \frac{\rho D c_p}{\lambda} q Y_y = H - H_+ + qY. \tag{2.8}$$

Thus if the *Lewis number*, $L = \lambda / \rho D c_p$, is 1, we see that the quantity $H - H_+ + q(Y - Y_+)$ satisfies the differential equation $f' = f$ and can be bounded only if it is identically zero. As we are interested only in bounded solutions, we may, in this case, restrict our attention to the plane $H - H_+ + q(Y - Y_+) = 0$, and (2.7) reduces to a system of three equations: (2.7a–c) with Y replaced by $(H_+ - H)/q$. We will not actually need to assume that the Lewis number is 1, however, this case is easier to understand.

Some of the results concerning this system are easier to interpret if we replace u by the *specific volume* $V = 1/\rho = u/m$. In this case (2.7a) becomes:

$$V_y = V - V_\pm + \frac{R}{m^2}\left(\frac{T}{V} - \frac{T_\pm}{V_\pm}\right). \tag{2.7a$'$}$$

With the exception of our discussion of entropy, we will restrict our attention to the system (2.7a$'$, b–d) = (2.7) for the remainder of this paper.

Following standard practice, we will resolve the *cold boundary difficulty* by means of an *ignition temperature* assumption. The cold boundary difficulty consists of the fact that the Arrhenius reaction rate (1.3) does not vanish, but is merely very small, at the unburned state. Thus no solution of (2.7) can tend to the unburned state as $x \to \infty$. Clearly this problem stems more from our unphysical, infinite domain than from any flaw in the reaction rate. However, as is customary, we will resolve this problem by modifying r so that it is zero for $T < T_i$, where T_i is the *ignition temperature*, and is chosen to be greater than the unburned temperature T_-.

Accordingly we will consider reaction rates of the form:

$$r(\rho, Y, T) = k \rho Y \phi(T), \tag{2.9}$$

where ϕ is a nonnegative Lipschitz monotone function of T, which vanishes for $T < T_i$.

In the next three sections we will usually assume that the Lewis number is 1, for ease of understanding. In §6 we will explain how to generalize to arbitrary Lewis numbers.

3. A picture is worth .... We now describe a region in (V, H, ϵ) space. The topological properties of the flow for (2.7) in this region will imply the existence of the desired structure profiles and will yield other properties as well.

For any bounded solution of (2.7) on which some quantity is strictly monotone, (V, H, ϵ) must tend to a rest state of (2.7) as y tends to $\pm\infty$. From (2.7c) we see that $r(\rho, Y, T)$ must vanish at any rest state. For our modified kinetics this can only happen if $Y = 0$ or $T < T_i$. Rest states satisfying $Y = 0$ are possible *burned states*; those satisfying $T < T_i$ are possible *unburned*, or *fresh gas* states. By (2.7d), ϵ is decreasing, so that the unburned state is at $y = -\infty$ and the burned state is at $y = +\infty$. Thus $Y_+ = 0$ and $\epsilon_+ = (Y - \rho D Y_x/m)_+ = 0$. Note that our choice of the coordinate y, and of V, makes the system (2.7) independent of the sign of $m = \rho u$.

At the unburned state, Y has a given value, Y_-, which, since Y is a mass fraction, is naturally bounded by 1. Since $\epsilon_- = Y_-$, we have, by (2.7b), $H_+ - H_- = qY_-$, which is the total heat per unit mass released by the reaction. Then (2.7a$'$) yields

$$\begin{aligned} &V_+ - V_- + \frac{R}{m^2}\left(\frac{T_+}{V_+} - \frac{T_-}{V_-}\right) \\ &= (V_+ - V_-)\left(1 - \frac{R}{2c_p}\right) + \frac{R}{m^2 c_p}\left(\frac{H_- + qY_-}{V_+} - \frac{H_-}{V_-}\right) = 0. \end{aligned} \tag{3.1}$$

Let γ be the ratio of specific heats, $c_p/c_v = c_p/(c_p - R)$. Then (3.1) becomes:

$$V_+^2 - \left(V_- + \frac{2(\gamma - 1)H_-}{m^2(\gamma + 1)V_-}\right) V_+ + \frac{2(\gamma - 1)}{m^2(\gamma + 1)}(H_- + qY_-) = 0. \tag{3.2}$$

If we solve this for V_+ we obtain

$$V_+ = \frac{V_-}{\gamma + 1}\left(\left(\gamma + \frac{1}{M_-^2}\right) \pm \sqrt{\left(1 - \frac{1}{M_-^2}\right)^2 - \frac{2(\gamma^2 - 1)qY_-}{u_-^2}}\right), \tag{3.3}$$

where

$$M^2 = \frac{u^2}{c^2} = \frac{u^2}{(\gamma p/\rho)}$$

is the square of the Mach number, and c is the sound speed. Note that if

$$\left(1 - \frac{1}{M_-^2}\right)^2 < \frac{2(\gamma^2 - 1)qY_-}{u_-^2} \tag{3.4}$$

then (3.1) has no solution. The two values of M^2 where equality holds in (3.4) correspond to exactly one burned state each. These burned states are the Chapman–Jouguet points; see Fig. 1.

For values of M^2 greater than the Chapman-Jouguet detonation value, there are two possible burned states. The flow at the unburned state is supersonic, as is the case for the upstream side of a nonreacting shock wave. At the strong detonation state the flow is subsonic, which corresponds to the downstream side of a nonreacting shock wave. However, at the weak detonation state the flow is supersonic, and this violates the nonreacting shock wave entropy condition.

The effect of the Mach number on the flow pattern for (2.7) at a burned state is as follows. The linearization of (2.7) at a burned state has the following eigenvalues:

$$(3.5)\quad \begin{aligned} &\text{(a)} \quad \sigma_1 = 1 - \frac{R}{2c_p} - \frac{RH_+}{m^2 V_+^2 c_p} = \frac{2(u_+^2 - \gamma p_+/\rho_+)}{2\gamma u_+^2} = \frac{1}{\gamma M_+^2}(M_+^2 - 1) \\ &\text{(b)} \quad \sigma_2 = 1 \\ &\text{(c)} \quad \sigma_{3,4} = \frac{L}{2}\left[1 \pm \sqrt{1 + 4Dk\phi(T_+)u_+^2}\right]. \end{aligned}$$

Thus, the strong detonation state has a two-dimensional stable manifold, and the weak detonation state has a one-dimensional stable manifold. From this simple fact it is already clear that although a weak detonation may be possible, a strong detonation is much more likely. The eigenvectors corresponding to $\sigma_1, \sigma_2, \sigma_3, \sigma_4$ are as follows.

$$\begin{aligned} \sigma_1 : &\quad X_1 = (1,\ 0,\ 0,\ 0), \\ \sigma_2 : &\quad X_2 = ((\gamma - 1),\ m^2\gamma V_+(1 - \sigma_1),\ 0,\ 0), \\ \sigma_3 : &\quad X_3 = \left(\frac{q(\gamma - 1)}{\gamma m^2 V_+(\sigma_3 - \sigma_1)},\ q,\ \sigma_3 - 1,\ \frac{L(\sigma_3 - 1)}{L - \sigma_3}\right), \\ \sigma_4 : &\quad X_4 = \left(\frac{q(\gamma - 1)}{\gamma m^2 V_+(\sigma_4 - \sigma_1)},\ q,\ \sigma_4 - 1,\ \frac{L(\sigma_4 - 1)}{L - \sigma_4}\right). \end{aligned}$$

From (2.7b) we note that $H_y > 0$ if $H - H_+ + q\epsilon > 0$. On the surface $H - H_+ + q\epsilon = 0$ we have that

$$(3.6)\qquad (H - H_+ + q\epsilon)_y = -\frac{q\lambda}{m^2 c_p} r \leq 0.$$

Therefore the region where $H_y \geq 0$ is *negatively invariant*, that is, the flow for (2.7) can only exit this region; it cannot enter. On the surface $V_y = 0$ (or $u_y = 0$) we have

$$(3.7)\qquad V_{yy} = \frac{\gamma - 1}{m^2 \gamma V_+} H_y.$$

Thus, inside the region $H_y \geq 0$, the region $V_y \leq 0$ is negatively invariant. Also the region $H \leq H_+$ is negatively invariant within $H_y \geq 0$.

All of the solutions that we find will lie in the region $H_y \geq 0$, $H \leq H_+$. However, detonation waves that are close to ZND waves will exit the region $V_y \leq 0$, attain a minimum value of V (or u) and maximum values of p and ρ, and then tend to the strong detonation state. To prove the existence of these waves, we need another boundary of the form $V = constant$. A natural choice is

$$(3.8)\qquad V = V_0 = \frac{(\gamma - 1)H_-}{(\gamma + 1)m^2 V_-}.$$

V_0 is the value of V at the end state of a nonreacting shock wave with initial state (V_-, H_-); this is the minimum value of V for a ZND detonation. The part of this

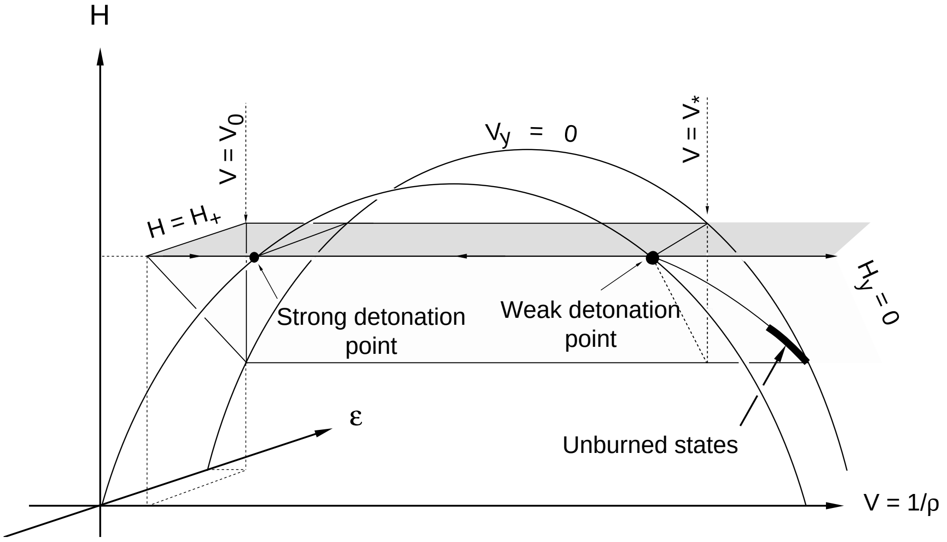

FIG. 2

surface lying within $H_y \geq 0$, $\epsilon < \epsilon_-$, also lies within $V_y \geq 0$. Therefore the region $V \geq V_0$ is positively invariant within the region $H_y \geq 0$, $\epsilon < \epsilon_-$.

Let $(V_*,\ T_*)$ be the value of $(V,\ T)$ at the weak detonation state, and let $(V^*,\ T^*)$ be the value at the strong detonation state. Consider the region W defined by $H_y \geq 0$, $\epsilon \leq \epsilon_-$, $H \leq H_+$, $V_0 \leq V \leq V_*$ (see Fig. 2). The flow for (2.7) enters W through a connected part of the boundary, namely, the union of the surfaces $V = V_*$, $\epsilon = \epsilon_-$, $V = V_0$. The flow leaves W through two components, $H_y = 0$, and $H = H_+$, which are separated by the positively invariant set P defined by $H_y = 0 = H - H_+$, $V_0 \leq V \leq V_*$. The following theorem of Wazewski [Wz1], [Wz2], which we quote from [C], implies that the set of all points in W which eventually flow out of W must also have two components.

DEFINITION 1. Let Γ be a topological space and let $\mathbb{R}$ denote the real numbers. Let a continuous function from $\Gamma \times R \to \Gamma$ be denoted by $(\gamma, t) \to \gamma \cdot t$. This function is called a *flow on* Γ if the following conditions are satisfied for all $\gamma \in \Gamma$ and $s, t \in \mathbb{R}$:

$$\text{(a)} \quad \gamma \cdot 0 = \gamma$$
$$\text{(b)} \quad \gamma \cdot (s + t) = (\gamma \cdot s) \cdot t.$$

If $\Gamma' \subset \Gamma$ and $U \subset \mathbb{R}$, let $\Gamma' \cdot U$ be the set of points $\gamma \cdot t$ such that $\gamma \in \Gamma'$ and $t \in U$.

DEFINITION 2. If $W \subset \Gamma$, let W° be the set of points $\gamma \in W$ such that, for some positive t, $\gamma \cdot t \notin W$. Let W^- be the set of points $\gamma \in W$ such that for any positive t, $(\gamma \cdot (0, t)) \not\subset W$. The set W^- is contained in W and is called the exit set of W. The set W is called a *Wazewski set* if the following conditions are satisfied:

(a) If $\gamma \in W$ and $(\gamma \cdot [0, t]) \subset cl(W)$ then $(\gamma \cdot [0, t]) \subset W$,

(b) W^- is closed relative to W°.

THEOREM. *(Wazewski). If* W *is a Wazewski set then* W^- *is a strong deformation retract of* W° *and* W° *is open relative to* W^-.

The set W that we have described above is a Wazewski set, as is the union of W with the set Q described in the next section. Since W° is homotopic to W, which has two components, W° must also have two components.

What separates these two components is S, the stable manifold for the strong detonation state, because any point which is not in one of these components must stay in W as y tends to infinity. Because H is always increasing within W, this solution must tend to a rest state, namely the strong detonation state. One boundary of this stable manifold is P; another is F, the stable manifold for the weak detonation state.

If there is a connected set in W consisting of points that tend to an unburned state U, as y tends to $-\infty$, and this set intersects both components of the exit set of W, then at least one of these points must be in S. The orbit of such a point is a viscous structure profile for a strong detonation wave.

In the next section we give sufficient conditions for the existence of such a set of points.

4. Some simple estimates.

Orbits leaving an unburned state U which lies in $T < T_i$ will stay in the plane $\epsilon = \epsilon_-$ until the surface $T = T_i$ is reached. Consider the curve G given by $H_y \geq 0$, $T = T_i$, $\epsilon = \epsilon_-$, and $V_y \leq 0$. All of the points of G flow towards U as y tends to $-\infty$. The endpoints of G flow out of $H_y \geq 0$, $V_y \leq 0$, immediately. Our strategy is to add a tunnel from W to G so that the exit set of the extended set is still disconnected. The existence of such a tunnel will imply the existence of a viscous structure profile from U to the strong detonation state. The tunnel is:

$$Q = \{(V, H, \epsilon) : V \geq V_*,\ H_y \geq 0,\ V_y \leq 0,\ \epsilon_- \geq \epsilon \geq g(T), \text{ and } T \geq T_i\}$$

The function g will be chosen so that the flow enters Q through the boundary $\epsilon = g(T)$, and so that $g(T) \geq \epsilon_i$ for $T_i \leq T \leq T_*$, where

$$\epsilon_i = \min\left\{ \epsilon \;\middle|\; \begin{array}{l} \text{There exist } H \text{ and } V \text{ such that} \\ H_y(H, V, \epsilon) = V_y(H, V, \epsilon) = \phi(T) = \phi\left(\dfrac{(H - m^2V^2/2)}{c_p}\right) = 0 \end{array} \right\}.$$

so that

$$\begin{aligned} q(\epsilon_- - \epsilon_i) &= \left(c_p - \frac{R}{2}\right)(T_i - T_-) \\ &\quad + \frac{u_-^2}{4\gamma^2 M_-^4}\left(1 - \gamma^2 M_-^4 + (\gamma M_-^2 + 1)\sqrt{(\gamma M_-^2 + 1)^2 - 4\gamma M_-^2 \frac{T_i}{T_-}}\right) \end{aligned} \tag{4.1}$$

See Fig. 3. Note that $\epsilon_- - \epsilon_i > 0$ whenever $T_i > T_-$. Also note that the flow enters Q through $\epsilon = \epsilon_-$ and $T = T_i$, while it exits through $H_y = 0$ and $V_y = 0$. The two components of the exit set are separated by the point $H_y = V_y = 0$, $T = T_i$. In order to choose the function g, we note that within Q, we have that

$$\frac{d\epsilon}{dT} = \frac{\epsilon_y}{T_y} = \frac{-\lambda\rho K\left(c_p(T_* - T) + m^2\dfrac{(V_*^2 - V^2)}{2}\right)\phi(T)}{qm^2\left(c_p(T - T_*) - m^2\dfrac{(V - V_*^2)}{2} + q\epsilon - R\left(T - T_*\dfrac{V}{V_*}\right)\right)}. \tag{4.2}$$

The right-hand side of (4.2) is monotone in V within Q. To see that the denominator is monotone in V for $V_* \leq V \leq V_-$, replace (V_*, T_*) by (V_-, T_-) and differentiate with respect to V, holding T constant. This denominator is also monotone in H as a function of (H, V). In the numerator, we decrease V to V_*. In the denominator, we decrease V, holding T constant, until we reach a value V_1 which satisfies either $H = H_+ - q\epsilon$ or $V_1 = V_*$. In the first case we obtain:

$$\left|\frac{d\epsilon}{dT}\right| \leq \frac{\lambda K c_p (T_* - T)\phi(T)}{-m^2 q V_* \left(m^2(V_1^2 - V_1 V_*) - R(T - T_* V_1/V_*)\right)}\ . \tag{4.3}$$

Then $T = (H_+ - q\epsilon - m^2 V_1^2/2)/c_p$, and we have that:

$$\left|\frac{d\epsilon}{dT}\right| \leq \frac{\lambda k c_p^2 (T_* - T)\phi(T)}{R m^2 q^2 V_* (\epsilon - f(V_1))}. \tag{4.4}$$

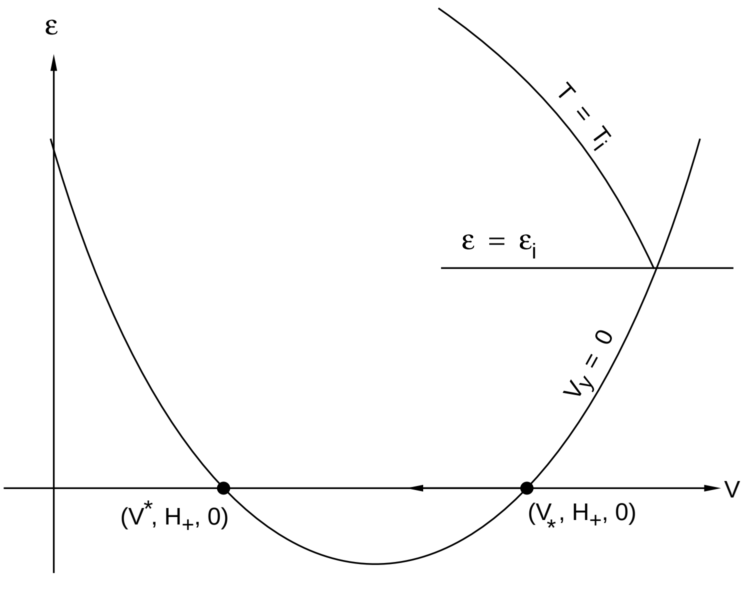

FIG. 3. *The plane* $H_y = H - H_+ + q\epsilon = 0$.

In the second case, we decrease the denominator further by decreasing H while holding $V = V_*$, until we reach $H = H_+ - q\epsilon$. This again yields (4.3), with $V_1 = V_*$ and a smaller value of T in the denominator; however, this value of T equals $(H_+ - q\epsilon - m^2 V_*^2/2)/c_p$. We still obtain (4.4), with $V_1 = V_*$.

Suppose $g(T) \geq \epsilon_i$ for $T_i \leq T \leq T_*$. Then $\epsilon \geq \epsilon_i$ within Q. Furthermore, $f(V_1) \leq \epsilon_i$ within Q (see Fig. 3). Let

$$g'(T) = \frac{\lambda k c_p^2}{R m^2 q^2 V_*} \frac{(T_* - T)\phi(T)}{g(T) - \epsilon_i}, \quad g(T_i) = \epsilon_-. \tag{4.5}$$

Then the flow enters Q through $\epsilon = g(T)$ as long as $g(T) \geq \epsilon_i$. If we solve (4.4), we find that along $\epsilon = g(T)$ we have:

$$(\epsilon - \epsilon_i)^2 = (\epsilon_- - \epsilon_i)^2 - \frac{2\gamma c_p}{(\gamma - 1) m^2 q^2 V_*} \int_{T_i}^{T} \lambda k (T_* - T)\phi(T) dT. \tag{4.6}$$

Since we need to have $\epsilon > \epsilon_i$ for $T_i \leq T \leq T_*$, we require

$$\epsilon_- > \epsilon_i + \left(\frac{2\gamma c_p}{(\gamma - 1)m^2 q^2 V_*} \int_{T_i}^{T_*} \lambda k (T_* - T)\phi(T) dT \right)^{1/2} . \tag{4.7}$$

Thus, (4.7) is a sufficient condition for the existence of a strong detonation structure profile. Since both λ and k can depend on T [Wi], it is important to keep them inside the integral.

For a CJ detonation wave, $(V_*, T_*) = (V^*, T^*)$. Condition (4.7) still implies the existence of a structure profile.

As λ tends to zero, with the other parameters held constant, condition (4.7) must be satisfied. In particular, since $\epsilon_- > \epsilon_i$ whenever $T_- < T_i$, we see that the strong and CJ detonations always have viscous structure when λ is sufficiently small. This is the limit of the "small rate parameter" considered by Wood [Wo1].

The region $(V_y < 0) \cap (H_y > 0) \cap (V > V_*) \cap (\epsilon < g(T))$ is negatively invariant, and contains the weak detonation point, and an interval of unburned states, including one corresponding to $\epsilon = \epsilon_i$, $T = T_i$, in its boundary. Since the exit set of this region is homotopic to a circle, and the region itself is contractible, another application of Wazewski's theorem shows that the one-dimensional stable manifold for the weak detonation point must be trapped in this region. Consequently one unburned state with $\epsilon = \epsilon_w$, $T = T_w$, $V = V_w$, which does not satisfy (4.7) must be connected to the weak detonation. Since this weak detonation is a boundary for the stable manifold of the strong detonation point, all unburned states with $\epsilon_- > \epsilon_w$ must be connected to the strong detonation point. As λ tends to zero, (ϵ_w, T_w, V_w) must tend to (ϵ_i, T_i, V_i).

5. A necessary condition. We obtain a necessary condition for the existence of viscous structure using energy estimates similar to those used in work on premixed laminar flames [BNS], [Ma], [Wg]. Observe that

$$H_{yy} = H_y - \frac{\lambda \rho k}{m^2 c_p}(H_+ - H)\phi(T). \tag{5.1}$$

If we multiply (5.1) by 1, H, and then H_y, and integrate each equation from $-\infty$ to $+\infty$, we obtain, using the fact that all derivatives tend to zero as y tends to $\pm\infty$:

$$\begin{aligned}
&\text{(a)} \quad H_+ - H_- = q\epsilon_- = \int_{-\infty}^{\infty} \frac{\lambda \rho k}{m^2 c_p}(H_+ - H)\phi(T)\, dy,\\
&\text{(b)} \quad \int_{-\infty}^{\infty} (H_y)^2\, dy = \int_{-\infty}^{\infty} \frac{\lambda \rho k}{m^2 c_p}(H_+ - H)H\phi(T)\, dy - \frac{H_+^2 - H_-^2}{2}.\\
&\text{(c)} \quad \int_{-\infty}^{\infty} (H_y)^2\, dy = \int_{-\infty}^{\infty} \frac{\lambda \rho k}{m^2 c_p}(H_+ - H)\phi(T) H_y\, dy\\
&\text{(d)} \quad \qquad\qquad\qquad \geq \int_{H_-}^{H_+} \frac{\lambda k}{m^2 c_p V_-}(H_+ - H)\phi\left((H - m^2 V_-^2/2)/c_p\right)\, dH.
\end{aligned} \tag{5.2}$$

Here we have used the fact that V_- is the maximum value of V on any detonation structure profile. Combining (5.2)(a–c) we find that:

$$\begin{aligned}
(H_+ - H_-)^2 m^2 c_p V_- &= (qY_- m)^2 c_p V_-\\
&\geq \int_{H_-}^{H_+} 2\lambda k (H_+ - H)\phi\left((H - m^2 V_-^2/2)/c_p\right)\, dH,\\
&= \int_{T_-}^{T_- + qY_-/c_p} 2\lambda k c_p \left(qY_- - c_p(T - T_-)\right)\phi(T)\, dT.
\end{aligned} \tag{5.3}$$

We may obtain a clearer interpretation of (5.3) with a little rearrangement and change of variables:

$$m^2 V_- \geq \int_0^1 2\lambda k c_p (1-\tau)\phi\left(T_- + \frac{qY_-\tau}{c_p}\right)\, d\tau. \tag{5.3$'$}$$

Thus, (5.3′) constitutes a necessary condition for the existence of a detonation structure profile. Note that if we replace V_- by V_+, then we also obtain a necessary condition for the existence of a deflagration structure profile. Also, (5.3′) is satisfied whenever $m^2 V_- \geq \lambda k \phi(T_- + qY_-/c_p)/c_p$.

6. **Arbitrary Lewis numbers.** When the Lewis number, $L = \lambda/\rho D c_p$, is not identically 1, then we must work with all four equations of (2.7). Consequently the region R must be extended to a region in $\mathbb{R}^4$. We require, therefore, additional boundaries for R, that is, upper and lower bounds for Y. It is interesting that we can obtain natural bounds for Y in terms of H, similar to the bounds that have been obtained for premixed laminar flames.

LEMMA. *Let*

$$\begin{aligned} \Lambda_* &= \inf(L,1) \\ \Lambda^* &= \sup(L,1) \end{aligned} \tag{6.1}$$

Then

$$\Lambda_*(H_+ - H) \leq qY \leq \inf(q\epsilon, \Lambda^*(H_+ - H)) \tag{6.2}$$

defines a negatively invariant region for (2.7).

Proof. We proceed exactly as in [Wg], using (2.8):

$$\begin{aligned} \frac{d}{dy}\left(H - H_+ + \frac{qY}{\Lambda_*}\right) &= (H - H_+)_y + \frac{q}{\Lambda_*}Y_y \\ &\leq (H - H_+)_y + \frac{q\rho D c_p}{\lambda}Y_y \\ &= H - H_+ + qY \\ &\leq H - H_+ + \frac{q}{\Lambda_*}Y. \end{aligned}$$

This last quantity is zero on the boundary of the region defined by

$$H - H_+ + \frac{q}{\Lambda_*}Y \geq 0.$$

Consequently this region is negatively invariant for (2.7). Similarly, the region defined by

$$H - H_+ + \frac{q}{\Lambda^*}Y \leq 0$$

is negatively invariant, within the region $Y \leq \epsilon$. This last condition is required to ensure that $Y_y \leq 0$. The region $Y \leq \epsilon$ is negatively invariant because on $Y = \epsilon$,

$$\begin{aligned} \frac{d}{dy}(\epsilon - Y) &= \epsilon_y - Y_y \\ &= \epsilon_y \leq 0. \end{aligned}$$

□

The topological argument is a little more sophisticated than the one given in §3. The region W is defined as before, with the additional inequality (6.2). The exit set for W is now connected; using the lemma we see that it is a union of four parts: $\Sigma_{out} = \Sigma_1 \cup \Sigma_2 \cup \Sigma_3 \cup \Sigma_4$, where

$$\Sigma_1 = \{(V,\ H,\ \epsilon,\ Y) \mid H = H_+,\ Y = 0,\ 0 < \epsilon \leq \epsilon_-,\ V_0 < V < V_*\}$$

$$\Sigma_2 = \left\{(V,\ H,\ \epsilon,\ Y) \middle| \begin{array}{l} qY = \min\left(q\epsilon,\ \Lambda^*(H_+ - H)\right),\ 0 < \epsilon \leq \epsilon_-, \\ V_0 < V < V_*,\ 0 \leq H_+ - H \leq q\epsilon \end{array}\right\}$$

$$\Sigma_3 = \{(V,\ H,\ \epsilon,\ Y) \mid H_+ - H = q\epsilon,\ \Lambda_*\epsilon \leq Y \leq \epsilon,\ 0 < \epsilon \leq \epsilon_-,\ V_0 < V < V_*\}$$

$$\Sigma_4 = \left\{(V,\ H,\ \epsilon,\ Y) \middle| \begin{array}{l} qY = \Lambda_*(H_+ - H),\ 0 < \epsilon \leq \epsilon_-, \\ V_0 < V < V_*,\ 0 \leq H_+ - H \leq q\epsilon \end{array}\right\}.$$

Note, however, that Σ_{out} is homotopic to a circle. The circle may be visualized as a path from Σ_1 to Σ_2 to Σ_3 to Σ_4 and back to Σ_1. This path cannot be contracted to a point within Σ_{out} because Σ_{out} does not contain the positively invariant line segment

$$P = \{(V,\ H,\ \epsilon,\ Y) : qY = H_+ - H = q\epsilon = 0, V_0 \leq V \leq V_*\}.$$

Again, Wazewski's principle implies that the set W_{out} of all points in W which eventually flow out of W must also be homotopic to a circle. The curve G of §4, given by $H_y \geq 0$, $T = T_i$, $\epsilon = \epsilon_-$, $V_y \leq 0$, is now extended, via (6.2), to a set G^* which is homeomorphic to a disk. The tunnel Q is also extended via (6.2). The estimates of §4 now show that the exit set of $W \cup Q$ is also homotopic to a circle. The boundary of G^* is homeomorphic to a circle and intersects the exit set of $W \cup Q$ with nonzero degree. Since a disk is not homotopic to a circle, at least one of the points of G^* must not exit W. This point must in fact tend to the strong detonation burned state. The sufficient condition (4.7) is now

$$\epsilon_- > \epsilon_i + \left(\frac{2\gamma c_p}{(\gamma - 1)m^2 q^2 V_*} \int_{T_i}^{T_*} \lambda k \Lambda^*(T_* - T)\phi(T)dT\right)^{1/2}. \tag{6.3}$$

7. Behavior. We have shown that strong or CJ detonation structure profiles exist if (4.7) is satisfied. From this we can see that the existence of these profiles depends on the values of λ, ϕ, and k, relative to m, q, and γ, between the unburned state and the weak detonation point. We will now show that the behavior of the solution depends strongly on the values of these parameters near the strong detonation point.

At the strong detonation point the linearization of (2.7) has two negative eigenvalues:

$$\text{(7.1)} \quad \begin{array}{ll} \text{(a)} & \sigma_1 = \dfrac{1}{\gamma}\left(1 - M^{*-2}\right) \\ \text{(b)} & \sigma_3 = \dfrac{L}{2}\left(1 - \sqrt{1 + \dfrac{4Dk\phi(T^*)}{u^{*2}}}\right). \end{array}$$

The relative sizes of σ_1 and σ_3 determine the node structure of the flow for (2.7) at the strong detonation point. If $Dk\phi(T^*)/u^{*2}$ is very small, or if L is very small (which would be physically unusual), so that $0 > \sigma_3 > \sigma_1$, then the flow has a node tangent to the eigenvector

$$X_3 = \left[\frac{q(\gamma-1)}{\gamma m^2 V^*(\sigma_3-\sigma_1)},\ q,\ \sigma_3-1,\ \frac{L(\sigma_3-1)}{L-\sigma_3}\right].$$

Thus, all but one of the structure profiles approaches the strong detonation state tangent to X_3. The one orbit that approaches tangent to X_1 is the purely nonreacting shock profile which connects the weak detonation state to the strong detonation state. The $(V,\ H,\ \epsilon)$ components of X_3 have the signs $(+,\ +,\ -)$. Thus, at the end of the wave, V and H are increasing and ϵ, which must be monotone, is decreasing. Since $V^* < V_-$, V cannot be monotone throughout the entire solution. Once the solution leaves the region $V_y < 0$, it cannot reenter, because H is monotone increasing. Hence V attains its minimum value at a single point of the solution. This minimum value must be greater than V_0, the minimum value for a ZND detonation.

The pressure must also attain an extremum in this case:

$$\begin{aligned}\frac{dp}{dy} &= \frac{R}{V}\frac{dT}{dy} - \frac{RT}{V^2}\frac{dV}{dy}\\ &= \frac{R}{c_p}\left(\frac{H_y}{V} - m^2\left(1 + \frac{c_pT}{u^2}V_y\right)\right).\end{aligned}$$

Since the flow is tangent to X_3 at the strong detonation state, we have, as the solution approaches that point,

$$\begin{aligned}\frac{dp}{dy} &= \frac{RH_y}{c_pV^*}\left(1 - \frac{\gamma-1+M^{*-2}}{\gamma(\sigma_3-\sigma_1)}\right)\\ &= \frac{RH_y}{c_pV^*(\sigma_3-\sigma_1)}\left(\frac{L}{2}\left(1-\sqrt{1+\frac{4Dk\phi(T^*)}{u^{*2}}}\right)-1\right)\\ &< 0.\end{aligned}$$

Since p is increasing when $V_y < 0$, p must attain a maximum in the interior of the wave.

The temperature behaves differently. Near the strong detonation state, we have

$$\begin{aligned}\frac{dT}{dy} &= \frac{1}{c_p}\left(H_y - m^2VV_y\right)\\ &= \frac{1}{c_p}\left(\frac{\gamma m^2V^*(\sigma_3-\sigma_1)}{\gamma-1} - m^2V^*\right)V_y\\ &= \frac{m^2V^*}{c_p(\gamma-1)}\left(\frac{\gamma L}{2}\left(1-\sqrt{1+\frac{4Dk\phi(T^*)}{u^{*2}}}\right)+M^{*-2}-\gamma\right)V_y.\end{aligned}$$

Thus, if M^{*-2} is less than γ, we see that T decreases near the burned state. Consequently T must attain a maximum value in the interior of the wave. This is consistent with the behavior of the ZND wave corresponding to this case; see [Wi, p. 194–197].

If M^{*-2} is greater than γ, then T decreases near the burned state if $\sigma_3 - \sigma_1$ is sufficiently small, but positive. In the inviscid limit for this case, as D, λ, and μ tend to zero, σ_3 tends to zero and T must increase near the burned state. It is a natural conjecture that T is monotone throughout the wave in this case. We say, therefore, that the flow is *strongly subsonic* near the burned state if $\gamma M^{*2} < 1$. If this condition is satisfied, then the maximum value of the temperature on the surface $V_y = 0$ (the Rayleigh line) occurs at a value of H higher than H_+, for on the surface $V_y = 0$,

$$\frac{dT}{dV} = \frac{T}{V}\left(1 - \gamma M^2\right).$$

and

$$\frac{dH}{dV} = \frac{Vm^2}{\gamma - 1}\left(1 - M^2\right),$$

whereas

$$\frac{d\left(M^2\right)}{dV} = \frac{M^2}{V}\left(1 + \gamma M^2\right) > 0.$$

(See [Wi]). As a consequence, the corresponding ZND wave, which follows the intersection of the surface $V_y = 0$ and the plane $H_y = 0$, must have a monotone temperature whenever the burned state is strongly subsonic.

This phenomenon may be explained by noting that M_* depends on the total heat released per unit mass, qY_-, and increases as qY_- increases with other parameters, particularly m, held constant. Thus the strong detonation burned state is strongly subsonic if the heat release is too weak, relative to the strength of the wave, to create a temperature spike. In experiments (see [Wi, §6.2.1] and references cited therein), strong detonation waves are observed principally when a piston, or other external force, is used to overdrive the wave; in this respect strong detonation waves resemble inert shock waves. Detonation waves that are not overdriven will decay to a Chapman–Jouguet detonation. Chapman–Jouguet detonations may be thought of as reacting shock waves that are driven by the reaction with no external force. Thus these waves are "pure" reacting shock waves, and qY_- is a parameter between inert shock waves with monotone temperature profiles and Chapman–Jouguet waves with temperature spikes.

As M^* tends to 1, σ_1 tends to zero, which leads us to the next case. If $Dk\phi(T^*)/u^{*2}$ is very large, or if L is very large, or if M_* is very close to 1, so that $0 > \sigma_1 > \sigma_3$, then the flow forms a node tangent to the eigenvector

$$X_1 = (1,\ 0,\ 0,\ 0).$$

In this case the solution may behave in an unusual manner. Detonations with Y_- close to ϵ_i, (T_- close to T_i) will follow the trajectory of the weak detonation, and then turn near the weak detonation burned state, and approach the strong detonation point along the trajectory of the inert shock profile. Thus these structure profiles look like a weak detonation followed by an inert shock wave. See Fig. 4, where a heuristic picture of the flow in the stable manifold is presented.[1] Similar observations have been made in [Wo2], [FD], [LL], and most recently for numerical calculations and for a simpler model in [CMR], where it was noted that these pathological waves are actually numerically stable as solutions of the time-dependent reacting compressible

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[1] Note that we have not proved that the stable manifold has no folds, so that V and e are global coordinates for the stable manifold, or that there is a monotone relationship between Y_- and the solution curves, such as depicted in Fig. 4. For a proof of such monotonicity for premixed laminar flames with $L > 1$, see [Ma].

Navier–Stokes equations. These authors also observed (numerically) an interesting phenomenon, namely that if the turning point of these solutions is sufficiently close to the weak detonation state, that is, if the spatial separation between the weak detonation and the inert shock wave is sufficiently large, then a bifurcation occurs wherein these two waves decouple and the inert shock moves slower than the weak detonation as predicted in [Wo2]. In this sense, a weak detonation can be observed. Weak detonations are also observed experimentally [FD], as a consequence of very complicated chemistry, change in equation of state, and endothermic or reversible reactions. A more significant point, made in [CMR], is that since $k\phi(T^*)/u^{*2}$ can be significantly large, it is important, in making machine calculations, to use an approximation scheme which does not add too much artificial diffusion, because this can radically change the character of the solution.

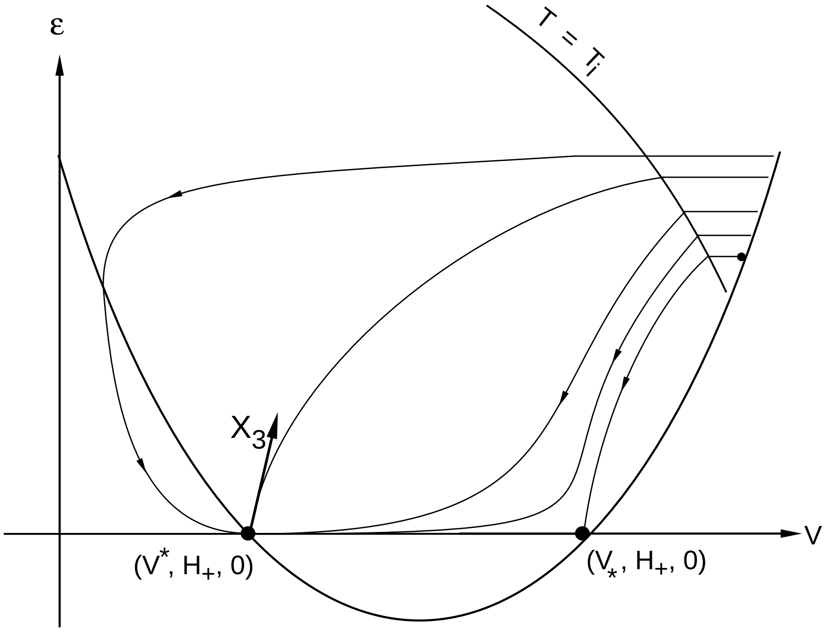

FIG. 4. *The flow in the stable manifold when* $0 > \sigma_1 > \sigma_3$.

For larger values of Y_-, there will be one wave which approaches the strong detonation state tangent to X_3, and others which approach tangent to X_1 but with V increasing. For the singular wave tangent to X_3 all quantities will be monotone, but for the others the pressure and density will attain maximum values. Since $H = c_pT + (m/\rho)^2/2$ is constant along X_1, the existence of a density peak in these waves implies the existence of a temperature peak.

For the CJ detonation, the burned state Mach number is 1, so that the above remarks apply to the behavior of this wave. All but one of the CJ detonation structure profiles must approach tangent to the eigenvector $\pm(1,0,0,0)$. However solutions cannot approach along $+(1,0,0,0)$ (the right side) because $V_y > 0$ there. Consequently there is one monotone CJ structure profile (presumably the one with minimum heat release) and the rest have peaks in pressure, density, and temperature.

8. The ZND limit. We have noted that as λ tends to zero (or λ and D, with L constant), then the sufficient condition (4.7), or (6.3), must be satisfied. The structure profiles satisfy natural a priori bounds, namely

$$\begin{gathered} V_0 \leq V \leq V_-, \\ H_- \leq H \leq H_+, \\ 0 \leq \Lambda_* \epsilon \leq Y \leq \epsilon \leq Y - . \end{gathered}$$

Thus, for any sequence $\lambda_n \to 0$, there is a corresponding sequence $(V_n,\ H_n,\ \epsilon_n,\ Y_n)$ of structure profiles with fixed end states, and which are uniformly bounded. Since H, ϵ, and Y are monotone, and V has at most one minimum, these profiles are also uniformly bounded in total variation. By Helly's theorem, some subsequence of this sequence must converge to a limit in L^1_{loc}. Taking a further subsequence we obtain convergence almost everywhere. The limit function is therefore a weak solution to (1.1a–c, d′). If $T_- < T_i$ then the limit is a ZND strong or CJ detonation. If $T_- = T_i$ then the limit is a continuous weak detonation which follows the curve $(H_y = 0) \cap (V_y = 0) \cap (\epsilon = Y)$ from $(V_i,\ H_i,\ \epsilon_i,\ Y_i)$ to $(V_*,\ H_*,\ 0,\ 0)$.

9. **The second law of thermodynamics.** In several shock structure problems, and particularly in MHD [CS1], [CS2], [Ge], the entropy flux has played an important role. In MHD the structure equations take the form

$$\frac{du}{dx} = B \nabla P(u)$$

where B is a positive diagonal matrix and P is the entropy flux. The gradient like structure that this gives to the problem is essential to our understanding of the solution to this very complicated system. In other areas it is useful to postulate that the entropy flux must be monotone [HaSe1],[HaSe2]; the inequality expressing this monotonicity is called the *Clausius–Duhem inequality.* We show here, assuming only that the reaction is exothermic and irreversible $(r(\rho, Y, T) \geq 0)$, that the entropy flux is monotone along a viscous structure profile for a plane steady detonation or deflagration wave. We have not used this fact in the above discussion, although it would have proved useful if we had not already known that H must be monotone.

The entropy flux is

$$P = mS - \lambda T_x / T.$$

Using Gibb's law: $TdS = de + pdV - qdY$ [Wi], we find that

$$\frac{dP}{dx} = \frac{m}{T}\left(\frac{de}{dx} + p\frac{dV}{dx} - q\frac{dY}{dx}\right) + \frac{\lambda T_x^2}{T^2} - \frac{(\lambda T_x)_x}{T}.$$

Using (1.2), we have

$$\begin{aligned} \frac{dP}{dx} = \frac{\lambda T_x^2}{T^2} - \frac{1}{T}&\left(\left[\left[\rho\left(u^2/2 + e(\rho, T, Y)\right) + p(\rho, T)\right] u\right]_x - (\mu u u_x)_x - (q\rho D Y_x)_x\right) \\ &+ \frac{m}{T}\left(\frac{de}{dx} + p\frac{dV}{dx} - q\frac{dY}{dx}\right) \\ = \frac{\lambda T_x^2}{T^2} &+ \frac{\mu u_x^2}{T} + \frac{qr}{T} \geq 0. \end{aligned}$$

Note that dP/dx only vanishes at rest points of (1.2). However, (1.2) is not gradient-like with respect to P, because

$$dP = -\frac{\lambda T_x}{T} dT + \frac{q d\epsilon}{T} - \frac{\mu u_x}{T} du;$$

since q/T does not vanish, neither does the gradient of P. This may be an anomaly which is due to the simple representations of the chemistry and the reaction rate which are used here.

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