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Author

Teng, Zhen-huan

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Zhen-huan Teng, Alexandre Joel Chorin, and Tai-Ping Liu

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RIEMANN PROBLEMS FOR REACTING GAS, WITH APPLICATIONS TO TRANSITION*

Zhen-huan Teng
Peiking University
and
Department of Mathematics
University of California
Berkeley, California 94720

Alexandre Joel Chorin
Department of Mathematics and Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

Tai-Ping Liu
Department of Mathematics
University of Maryland
College Park, Maryland 20742

January 1981

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RIEMANN PROBLEMS FOR REACTING GAS, WITH APPLICATIONS TO TRANSITION

Abstract

We analyze the Riemann problem for reacting gas flow, under conditions where detonations and deflagrations can occur. We show that for a given deflagration velocity law, a Riemann solution which involves a deflagration may fail to exist but a Riemann solution involving a detonation may exist instead. We use our results to study an idealized model of transition from deflagration to detonation, using the Glimm (random choice) method. Numerical and asymptotic results are given, which compare well with certain experimental data. The broader usefulness of the results is indicated. One of the most interesting features of our model is the indication it provides that no transition occurs if the flame is laminar, and thus in particular, if the flow is purely one dimensional.

1. Introduction

Riemann solutions are the building blocks of several numerical methods for solving the equations of gas dynamics (see e.g. [3],[6],[9],[10],[20]) as well as of theoretical analyses of these equations. Riemann solutions involving detonations have been described and used in a numerical calculation in [4]. The goal of the present paper is to extend this analysis to the cases in which deflagrations can appear. One of the striking facts about the solutions of the extended Riemann problem is that a solution with a deflagration with given velocity law may fail to exist and must be replaced by a solution with a detonation. This fact provides us with a simple method for analyzing the transition from deflagration to detonation whenever the flow can be idealized as one-dimensional and the deflagration as being infinitely thin. The results agree well with experimental data both qualitatively and quantitatively. In particular, within the class of flame laws considered, no transition occurs from a laminar flame, and the contrasting cases of open and half-closed tubes are well described. We display both numerical and asymptotic results.

The value of our solution extends beyond this idealized case. It is expected that a good numerical description of transition from deflagration to detonation -- in complex geometry and in cases where chemical kinetics, turbulence, and diffusion are considered in some detail -- will require a numerical method capable of resolving waves sharply and, on the basis of recent experience, is likely to require a good Riemann solution. We offer our solver as a step in that

direction.

We begin by defining a Riemann problem and by describing the random choice method briefly. Consider the hyperbolic system of equations

$$\underline{u}_t = (\underline{f}(\underline{u}))_x, \quad \underline{u}(x,0) \text{ given}, \quad (1.1)$$

where $\underline{u}$ is the solution vector, and subscripts denote differentiation. A Riemann problem for (1.1) is a problem in which $\underline{u}(x,0)$ has the form

$$\underline{u}(x,0) = \begin{cases} \underline{u}_r & \text{for } x < 0 \\ \underline{u}_l & \text{for } x > 0 \end{cases},$$

where $\underline{u}_r, \underline{u}_l$ are constant states. In the random choice method these Riemann problems are used as follows: The time t is divided into intervals of length k . Let h be a spatial increment. The solution is to be evaluated at the points (ih, nk) and $((i+1/2)h, (n+1/2)k)$, $i = 0, \pm 1, \pm 2, \dots$, $n = 1, 2, \dots$. Let $\underline{u}_i^n$ approximate $\underline{u}(ih, nk)$, and $\underline{u}_{i+1/2}^{n+1/2}$ approximate $\underline{u}((i+1/2)h, (n+1/2)k)$. The algorithm is defined if $\underline{u}_{i+1/2}^{n+1/2}$ can be found when $\underline{u}_i^n, \underline{u}_{i+1}^n$ are known. Consider the following Riemann problem:

$$\underline{w}_t = (\underline{f}(\underline{w}))_x, \quad t > 0, \quad -\infty < x < +\infty,$$

$$\underline{w}(x,0) = \begin{cases} \underline{u}_{i+1}^n & \text{for } x \geq 0, \\ \underline{u}_i^n & \text{for } x < 0. \end{cases}$$

Let $w(x,t)$ denote the solution of this problem. Let θ_i be a value of a variable θ , $-1/2 \leq \theta \leq 1/2$. Let P_i be the point $(\theta_i h, k/2)$, and let

$$\tilde{w} = w(P_i) = w(\theta_i h, k/2)$$

be the value of the solution w of the Riemann problem at P_i . We set

$$u_{i+1/2}^{n+1/2} = \tilde{w}.$$

In other words, at each time step, the solution is first approximated by a piecewise constant function; it is then advanced in time exactly, and new values on the mesh are obtained by sampling. Other ways of using Riemann solutions can be found in, e.g., [20],[21].

An earlier attempt to solve a problem similar to ours was made by Kurylo [10].

2.1 The Riemann problem for the equations of gas dynamics

For the sake of completeness, we begin by describing the Riemann problem for nonreacting gas dynamics, using notations and constructions that we shall use later in the reacting case (for more detail, see [3],[6]). Consider the gas dynamics equations

$$\begin{aligned} \rho_t + (\rho v)_x &= 0 \\ (\rho v)_t + (\rho v^2 + p)_x &= 0 \\ e_t + (ev + pv)_x &= 0 \end{aligned} \tag{2.1}$$

where ρ , v , ρv , e , and p , respectively, denote the density, velocity, momentum, internal energy, and pressure of the gas, and

$$e = \rho \epsilon + \frac{1}{2} \rho v^2 \quad (2.2)$$

is the total energy of the gas. For polytropic gases ϵ is given by the constitutive relation

$$\epsilon = \frac{1}{\gamma - 1} \frac{p}{\rho} \quad (2.3)$$

where γ is a constant larger than one. Let $\underline{u} \equiv (\rho, \rho v, e)$ and write (2.1) as

$$\underline{u}_t + \underline{F}(\underline{u})_x = 0 \quad .$$

The Riemann problem for (2.1) will have the initial data

$$\underline{u}(x, 0) = \begin{cases} \underline{u}_l & \text{for } x < 0 \\ \underline{u}_r & \text{for } x > 0 \end{cases} , \quad (2.4)$$

where $\underline{u}_l, \underline{u}_r$ are constant states. It is well-known that the solution consists of a left wave joining $\underline{u}_l$ and a constant state $\underline{u}_{II}$, a contact discontinuity joining $\underline{u}_{II}$ with a constant state $\underline{u}_I$, and a right wave joining $\underline{u}_I$ with $\underline{u}_r$, see [3],[6]. The right and left waves may be shock waves or rarefaction waves. The case where the left wave is a shock wave and the right wave is a rarefaction wave is depicted in Figure 2.1. When the right wave is a shock wave, it satisfies the jump conditions:

$$v_I = v_r + (p_I - p_r) \frac{\sqrt{(1 - \mu^2) \tau_r}}{\sqrt{p_I + \mu^2 p_r}}, \quad p_I > p_r \quad (2.5.1)$$

$$\tau_I = \tau_r - \frac{(v_I - v_r)^2}{p_I - p_r}, \quad \tau \equiv \frac{1}{\rho} \quad (2.5.2)$$

It propagates with speed

$$\sigma(\underline{u}_I, \underline{u}_r) = \frac{\rho_I v_I - \rho_r v_r}{\rho_I - \rho_r} \quad (2.6)$$

Here $\tau = \rho^{-1}$ is the specific volume of the gas and

$$\mu^2 = \frac{\gamma - 1}{\gamma + 1}.$$

When the right wave is a rarefaction wave, the right Riemann invariant is constant:

$$v_I = v_r + \frac{\sqrt{1 - \mu^2}}{\mu^2} \tau_r^{1/2} p_r^{1/2} (p_I^{(\gamma-1)/2\gamma} - p_r^{(\gamma-1)/2\gamma}), \quad p_I < p_r \quad (2.7)$$

Thus a state $\underline{u}$ is connected to $\underline{u}_r$ by a right wave only if

$$v = v_r + \varphi(p; p_r, \rho_r), \quad (2.8.1)$$

$$\varphi(p; p_r, \rho_r) \equiv \begin{cases} (p - p_r) \frac{\sqrt{(1 - \mu^2) \tau_r}}{\sqrt{p + \mu^2 p_r}}, & p \geq p_r \\ \frac{\sqrt{1 - \mu^2}}{\mu^2} \tau_r^{1/2} p_r^{1/2} (p^{(\gamma-1)/2\gamma} - p_r^{(\gamma-1)/2\gamma}), & p < p_r \end{cases}$$

Similarly if $\underline{u}$ is connected to $\underline{u}_l$ by a left wave then

$$v = v_f - \phi(p; p_f, \rho_f) \quad (2.8.2)$$

Two states $\underline{u}_{II}$ and $\underline{u}_I$ are connected by a contact discontinuity if

$$v_I = v_{II} \equiv v^* \quad , \quad p_I = p_{II} \equiv p^* \quad (2.9)$$

and the speed of the discontinuity is

$$\sigma(\underline{u}_{II}, \underline{u}_I) = v^* \quad (2.10)$$

Thus the states $\underline{u}_I$ and $\underline{u}_{II}$ represent a single point in the (p, v) -plane. One can verify that $\phi(p; p_f, \rho_f)$ is a strictly increasing function of p . Thus the curves (2.8.1) and (2.8.2) have a unique point of intersection in the (p, v) -plane (see Figure 2.2). At the point of intersection $(v, p) = (v^*, p^*)$ of (2.9). The states $\underline{u}_I$ and $\underline{u}_{II}$ are then defined by (2.5.2) and (2.7.2). This solves the Riemann problem for (2.1). An iteration method for actually locating the solution can be found in [3], [20], as well as below.

3. Detonation and deflagration waves

Our purpose in this section is to describe combustion waves in a hyperbolic model, in a form appropriate for use in later sections. (See also [4].) The chemical reaction zone is assumed to be infinitely thin, and an energy of formation q is released instantaneously when the chemical reaction takes place. The process is assumed to exothermic (i.e. release energy). Let the subscript 0 refer to unburned gas (i.e., gas which has not undergone the chemical reaction)

and 1 refer to burned gas. The unburned gas is on the right and the burnt gas on the left. We have, in place of (2.3),

$$\epsilon_1 = \frac{1}{\gamma_1 - 1} \frac{p_1}{\rho_1} + q_1$$

$$\epsilon_0 = \frac{1}{\gamma_0 - 1} \frac{p_0}{\rho_0} + q_0 .$$

For the sake of simplicity, we assume that $\gamma = \gamma_1 = \gamma_0$. The reaction is exothermic when

$$\Delta = q_1 - q_0 < 0 .$$

Let V be the velocity of the reaction zone. The speeds relative to the gas in front of the zone and behind the zone are

$$w_0 \equiv v_0 - V , \quad w_1 \equiv v_1 - V .$$

Conservation of mass and momentum is expressed by

$$\rho_1 w_1 = \rho_0 w_0 \equiv -M , \tag{3.1}$$

$$\rho_1 w_1^2 + p_1 = \rho_0 w_0^2 + p_0 . \tag{3.2}$$

Conservation of energy is expressed by

$$H \equiv H(\tau_1, p_1; \tau_0, p_0) \equiv \epsilon_1 - \epsilon_0 + \frac{\tau_0 - \tau_1}{2} (p_1 + p_0) = 0 .$$

or, equivalently,

$$p_0(\tau_0 - \mu^2 \tau_1) - p_1(\tau_1 - \mu^2 \tau_0) - 2\mu^2 \Delta = 0 . \tag{3.3}$$

This gives the locus of points in the (p, τ) -plane, which can be

connected to (p_0, τ_0) by a combustion wave (Figure 3.1). The omitted portion of the hyperbola corresponds to the unphysical events in which $M^2 < 0$. The upper portion of the curve corresponds to detonation waves; the lower portion to deflagration waves. These curves are further divided by the Chapman-Jouguet points S_1 and S_2 , which are the points of tangency of $H = 0$ and lines through (τ_0, p_0) .

We noticed in the previous section that it is convenient to use the (p, v) -plane to solve the Riemann problem for the gas dynamics equations. We now derive the velocity-pressure relations for combustion waves. From (3.1) and (3.2) we have

$$M = \frac{p_1 - p_0}{v_1 - v_0}, \quad M^2 = \frac{p_0 - p_1}{\tau_1 - \tau_0}. \quad (3.4)$$

Equations (3.3) and (3.4) yield

$$\frac{p_1 - p_0}{v_1 - v_0} = [p_0 \rho_0 \left(\frac{\gamma - 1}{2} + \frac{(\gamma + 1)p_1}{2p_0} \right) / (1 + (\gamma - 1)\rho_0 \Delta (p_1 - p_0)^{-1})]^{1/2}.$$

This shows that the locus of burned states $\underline{u}$ in the (p, v) -plane which can be related to the fixed unburned state $\underline{u}_0$ on the right by a combustion wave is given by (Figure 3.2),

$$v = v_0 + (p - p_0) \left[\frac{(1 - \mu^2)\tau_0 - 2\mu^2 \Delta (p_0 - p)^{-1}}{\mu^2 p_0 + p} \right]^{1/2}. \quad (3.5)$$

In the remainder of this section we investigate the Chapman-Jouguet (CJ) waves, i.e., combustion waves that correspond to the CJ point. A CJ wave moves with the speed of sound with respect to the

burned gas [7]. This information is sufficient to determine the state behind the wave. We deduce from (3.4) that when the right wave is a CJ wave, then

$$\frac{p_1 - p_0}{\tau_1 - \tau_0} = - \rho_1^2 \frac{\gamma p_1}{\rho_1} = - \frac{\gamma p_1}{\tau_1}$$

or, equivalently,

$$\tau_1(p_1(1 + \gamma) - p_0) = \gamma \tau_0 p_1 \quad (3.6)$$

Here we note that the sound speed is $c = \sqrt{\frac{\gamma p}{\rho}}$. The value $p_1 = p_{CJ}$ can be calculated from (3.3) and (3.6) by

$$p_1^2 + 2a p_1 + b = 0 \quad ,$$

$$a \equiv -p_0 + \Delta(\gamma - 1)\rho_0$$

$$b \equiv p_0^2 - 2\mu^2 \rho_0 p_0 \Delta \quad .$$

Since $\gamma > 1$ and $\Delta \leq 0$, we have $a^2 - b \geq 0$, and so

$$p_{CJ} = p_0 \pm (\gamma - 1)\rho_0 \Delta \left[1 - \sqrt{1 - \frac{2\gamma p_0}{(\gamma^2 - 1)\rho_0 \Delta}} \right] \quad (3.7)$$

where the plus sign (or minus sign) corresponds to CJ-detonation (or CJ-deflagration). The values of v_{CJ} and ρ_{CJ} are in turn obtained from (3.5) and (3.6), respectively,

$$v_{CJ} = v_0 + (p_{CJ} - p_0) \left[\frac{(1 - \mu^2)\tau_0 - 2\mu^2 \Delta (p_0 - p_{CJ})^{-1}}{\mu^2 p_0 + p_{CJ}} \right]^{1/2} \quad (3.8)$$

$$\rho_{CJ} = \frac{\rho_0(p_{CJ}^{(1+\gamma)} - p_0)}{\gamma p_{CJ}} \quad (3.9)$$

The speed of CJ-deflagration is determined by (3.1), (3.6)-(3.9):

$$v_{CJ} = v_0 + c_0 \sqrt{\gamma T_0} \left[\sqrt{-\frac{(\gamma^2+1)\Delta}{2} + \gamma T_0} + \sqrt{-\frac{(\gamma^2+1)\Delta}{2}} \right]^{-1} \quad (3.10)$$

where $T_0 = p_0/\rho_0$ is the temperature and $c_0 = \sqrt{\gamma p_0/\rho_0}$ the sound speed of the unburned gas.

4. The Riemann problem for reacting gas

We are interested in solving the Riemann problem (2.1), (2.4) when the solution contains combustion waves. Thus at least one of the states $\underline{u}_l$ and $\underline{u}_r$ contains unburned gas. For simplicity we assume that $\underline{u}_l$ is the burned state and $\underline{u}_r$ is the unburned state. Our purpose in the present section is to investigate possible wave patterns which relate $\underline{u}_l$ to $\underline{u}_r$.

We begin with the simpler situation where the wave pattern contains a right detonation wave (cf. [4]). In this case, our basic assumption is that only CJ detonations and strong detonations are admissible. Since a weak detonation is supersonic with respect to the gas behind it, it does not satisfy the linear stability criterion for the hyperbolic model. When dissipation effects are taken into consideration, our assumption in general holds qualitatively (cf. [7]). We now construct the wave pattern based on the above

assumption. Since the combustion wave is a right wave, there exist states $\underline{u}_I$ and $\underline{u}_{II}$ such that the wave connecting $\underline{u}_I$ and $\underline{u}_{II}$ is a left (nonreacting) wave, the wave connecting $\underline{u}_{II}$ and $\underline{u}_I$ is a contact discontinuity, and $\underline{u}_I$ is related to $\underline{u}_r$ by a right detonation and by right gas waves. When the detonation wave is a CJ detonation, it is sonic with respect to the gas behind it, and so $\underline{u}_I$ may be related to a right rarefaction wave connecting $\underline{u}_I$ and $\underline{u}_{CJ}$ and $\underline{u}_{CJ}$ may be connected to $\underline{u}_r$ by a CJ detonation (Figure 4.1). Note that in this case $\underline{u}_{CJ}$ is uniquely determined by $\underline{u}_r$ ((3.7)-(3.9)). On the other hand, when the detonation wave is a strong detonation, it is supersonic (resp. subsonic) with respect to the gas in front of (resp. behind) it, and so $\underline{u}_I$ can only be related to $\underline{u}_r$ by a single strong detonation wave (Figure 4.2).

The discussions above, along with identities (2.8), (3.5)-(3.10), show that the states $\underline{u} = \underline{u}_I$, which can be related to $\underline{u}_r$ on the right by a detonation wave with possibly a rarefaction wave, form a 1-parameter family whose projection on the (p, v) -plane is given by

$$v = v_r + \Psi(p; p_r, \rho_r) \quad , \quad (4.1)$$

$$\Psi(p; p_r, \rho_r) = \begin{cases} (p - p_r) \left[\frac{(1 - \mu^2) \tau_r - 2\mu^2 \Delta(p_r - p)^{-1}}{\mu^2 p_r + p} \right]^{1/2} , & \text{for } p > p_{CJ} \\ (p_{CJ} - p_r) \left[\frac{(1 - \mu^2) \tau_r - 2\mu^2 \Delta(p_r - p_{CJ})^{-1}}{\mu^2 p_r + p_{CJ}} \right]^{1/2} + \\ \frac{\sqrt{1 - \mu^2}}{\mu^2} \tau_{CJ}^{1/2} p_{CJ}^{1/2} (p^{(\gamma-1)/2 - \gamma} - p_{CJ}^{(\gamma-1)/2 \gamma}) , & \text{for } p \leq p_{CJ} \end{cases}$$

$$p_{CJ} = p_r + (\gamma-1)p_r\Delta \left[1 - \sqrt{1 - \frac{2\gamma p_r}{(\gamma-1)\rho_r\Delta}} \right],$$

$$\tau_{CJ} = \frac{\gamma \tau_r p_{CJ}}{p_{CJ}(1+\gamma) - p_r}.$$

A straightforward calculation shows that $\psi(p; p_r, \rho_r)$ is a strictly increasing function of p . Thus the wave pattern relating $\underline{u}_l$ and $\underline{u}_r$ is uniquely determined by locating the unique intersection point of the wave curves (2.8.2) and (4.1).

We now turn to deflagration waves. One can show that strong deflagration waves are not admissible ([5],[7]). In contrast to the case of detonation waves, wave patterns containing weak deflagration waves are not uniquely determined by $\underline{u}_l$ and $\underline{u}_r$. This is so because a deflagration wave is subsonic with respect to the gas in front of it and thus forms an internal boundary whose velocity can be prescribed (see [7]). A deflagration wave may be preceded by either a right rarefaction wave or a right shock wave. Moreover, the strength of these right waves is arbitrary. Thus a criterion is needed to determine the physical admissibility of weak deflagration waves so as to eliminate the arbitrariness of the wave pattern. There exist experimental data which relate the flame speed to the conditions in front of the flame (see, e.g., [1],[2],[11]). For the sake of simplicity we consider the family of flame velocity laws

$$v = v_0 + K T_0^Q \tag{4.2}$$

$$= v_0 + K (p_0/\rho_0)^Q, \quad K, Q \text{ constants}.$$

These flame laws are qualitatively similar to the experimental ones. A crude theory (see [12]) leads us to consider that $Q = 1/2$ for a laminar flame and $Q > 1/2$ for a turbulent flame (see, e.g., [1],[2]). The form (4.2) is chosen because it allows the laminar case to be done analytically. The major conclusions below are independent of the detailed form of the flame law.

The speed $(V-v_0)$ has to be less than the speed of CJ-deflagration, (3.10):

$$K(p_0/\rho_0)^Q \leq c_0 \sqrt{\gamma T_0} \left[\sqrt{-\frac{(\gamma^2+1)\Delta}{2} + \gamma T_0} + \sqrt{-\frac{(\gamma^2+1)\Delta}{2}} \right]^{-1} \quad (4.3)$$

Suppose that the wave pattern relating $\underline{u}_l$ and $\underline{u}_r$ contains a deflagration wave preceded by a right gas wave (Figure 4.3). As in Section 2, the crucial step in locating appropriate states $\underline{u}_0$, $\underline{u}_I$, and $\underline{u}_{II}$ is to find the locus of points $u = \underline{u}_I$ in the (p,v) -plane which can be related to $\underline{u}_r$ by a weak deflagration wave and a right gas wave. We have from (4.2)

$$w_0 = -K(p_0/\rho_0)^Q.$$

We have, by eliminating w_1 from (3.1) and (3.2),

$$\rho_0 w_0 = - \sqrt{\frac{\mu^2 p_0 + p_1}{(1-\mu^2)\tau_0 - \frac{2\mu^2 \Delta}{p_0 - p_1}}}.$$

This and (4.3) yield the value of p_1 in terms of $\underline{u}_0$; the value of v_1

is then obtained from (3.5):

$$p_1 = p_0 \left[\frac{1}{2} (1-\mu^2)(1-M_0^2) - 1/2 \sqrt{(1+\mu^2)^2(1-M_0^2)^2 + 8\mu^2 \frac{1+\mu^2}{1-\mu^2} M_0^2 \frac{\Delta}{T_0}} \right] \quad (4.4)$$

$$v_1 = v_0 + \frac{4\mu^2(1+\mu^2)M_0^2 \Delta}{(1-\mu^2) \sqrt{\gamma}} \left[\sqrt{T_0(1+\mu^2)(1-M_0^2) + (1+\mu^2)^2(1-M_0^2)^2 T_0} + 8\mu^2 \frac{(1+\mu^2)}{(1-\mu^2)} M_0^2 \Delta \right]^{-1/2} \quad (4.5)$$

where $M_0 = -\frac{w_0}{c_0}$ is the Mach number of the deflagration wave with respect to the unburned state $\underline{u}_0$. From (4.2) we have

$$M_0 = \frac{K}{\sqrt{\gamma}} T_0^{Q-1/2} = \frac{K}{\sqrt{\gamma}} (p_0/\rho_0)^{Q-1/2} \quad (4.6)$$

Remember that $\underline{u}_0$ is related to the fixed state $\underline{u}_r$ by a right nonreacting wave. Thus v_0 is related to $\underline{u}_r$ by (2.8.1) in terms of the parameter $\alpha \equiv p_0$:

$$v_0 = v_r + \rho(\alpha; p_r, \rho_r) \quad (4.7)$$

$$p_0 \equiv \alpha \quad (4.8)$$

The quantity τ_0 is related to $\underline{u}_r$ in terms of the parameter α through the jump condition (2.5) if the right wave is a shock wave, and through the isentropic law $p_r \rho_r^{-\gamma} = p_0 \rho_0^{-\gamma}$ if the right wave is a rarefaction wave, i.e.,

$$\tau_0 = \begin{cases} \tau_r \left(\frac{p_r + \mu^2 \alpha}{\mu^2 p_r + \alpha} \right) , & \alpha \geq p_r , \\ \tau_r \left(\frac{p_r}{\alpha} \right)^{1/2} , & \alpha \leq p_r . \end{cases} \quad (4.9)$$

Finally, if we remember (4.6)-(4.9), the identities (4.4) and (4.5) represent the locus $\underline{u} = \underline{u}_I$ in the (p,v) -plane in terms of the parameter $\alpha = p_0$:

$$p = p_I(\alpha; \underline{u}_r) , \quad v = v_I(\alpha; \underline{u}_r) . \quad (4.10)$$

The crucial step in finding the states $\underline{u}_I$ and $\underline{u}_{II}$ is to locate the point of intersection (v^*, p^*) of the curves (2.8.2) and (4.10) in the (p,v) -plane:

$$\begin{aligned} v^* &= v_I = v_{II} , \\ p^* &= p_I = p_{II} . \end{aligned}$$

However, as we shall see, there may exist more than one such intersection point or none at all. Within the family of flame laws (4.2), $Q = 1/2$ corresponds to a laminar flame, and $M_0 = K_Y^{-1/2}$ becomes a constant. In this case, it follows from (4.4) and (4.5) that $p_I(\alpha, \underline{u}_r)$ and $v_I(\alpha, \underline{u}_r)$ are both functions of T_0 . Since $T_0 = p_0 \tau_0 = \alpha \tau_0$ is a strictly monotonic function of α by (4.9), a calculation shows that the functions $p_I(\alpha, \underline{u}_r)$ and $v_I(\alpha, \underline{u}_r)$ are strictly monotonic functions of α . Thus the wave pattern is uniquely and stably determined by $\underline{u}_l$ and $\underline{u}_r$ (Figure 4.4). (This is consistent with the well-known fact that laminar flames do not exhibit a transition to detonation, see below.) We now turn to the case of a turbulent flame, $Q > 1/2$, for example, $Q \geq 2$. In this case the

dependence of p_I and v_I on the parameter α is quite complicated, and we resort to numerical calculations to study the wave (4.10). In general the curve is not a monotonic curve. Depending on the relative position of $\underline{u}_l$ and $\underline{u}_r$, the intersection set of (4.10) and (2.8.2) may include no points, one point, or two points (Figure 4.5). The meaning of this phenomenon will be analyzed below. In summary, it is always possible to solve the Riemann problem if one allows only detonation waves as reacting waves, and after exclusion of weak detonations the solution is unique. If one allows deflagration waves with a given non-laminar velocity law, then the solution may become non-unique, and there may be one or more solutions involving a deflagration as well as the one involving a detonation. Under certain circumstances, there may only be the detonation solution.

5. An iteration method for solving Riemann problems

In this section, we present an iteration method for solving Riemann problems numerically. When the wave pattern contains no combustion waves or only detonation waves the Riemann problem can be solved as in [4]. Thus we will concentrate on determining whether it is possible for the solution to contain a weak deflagration wave, and, when it does, how to calculate the solution. We shall look for the weakest wave, i.e., the one with the smallest pressure jump across the reaction zone. Assume for simplicity that the right state $\underline{u}_r$ is unburned and the left state $\underline{u}_l$ is burned, so that the solution contains a right combustion wave. In order for the combustion wave to

be a weak deflagration wave, the two curves (2.8.1) and (4.10) must meet. They do so if there exist α_-^0 and α_+^0 such

$$v_I(\alpha_-^0; \underline{u}_r) - v_\ell + \varphi(p_I(\alpha_-^0, \underline{u}_r); p_\ell, \rho_\ell) < 0, \text{ and} \quad (5.1)$$

$$v_I(\alpha_+^0; \underline{u}_r) - v_\ell + \varphi(p_I(\alpha_+^0, \underline{u}_r); p_\ell, \rho_\ell) > 0. \quad (5.2)$$

To determine whether α_-^0 and α_+^0 exist, we start with the state $\underline{u}_r$ and determine the sign of

$$g(\alpha) \equiv v_I(\alpha; \underline{u}_r) - v_\ell + \varphi(p_I(\alpha; \underline{u}_r); p_\ell, \rho_\ell)$$

when $\alpha = p_r$. We only consider the more interesting case when $g(p_r) > 0$. Notice that, as α increases $g(\alpha)$ increases until α reaches a critical value and then $g(\alpha)$ decreases (c.f. Figure 4.5). The existence of α_-^0 and α_+^0 is guaranteed if $g(\alpha)$ is positive at this critical value. To check this condition, we try $\alpha = p_r, p_r + \Delta\alpha, p_r + 2\Delta\alpha, \dots$, where $\Delta\alpha$ is a given small number. There are two possibilities: If $g(p_r + k\Delta\alpha) > 0$ for some large k , we choose the minimum k with this property, $g(p_r + (k-1)\Delta\alpha) \leq 0$, and set

$$\alpha_-^0 \equiv p_r + (k-1)\Delta\alpha,$$

$$\alpha_+^0 \equiv p_r + k\Delta\alpha.$$

(Figure 5.1) It may happen that for some k ,

$$0 > g(p_r + k\Delta\alpha) > g(p_r + j\Delta\alpha), \text{ for } j = 1, 2, \dots, k-1$$

$$\text{and } g(p_r + (k+1)\Delta\alpha) < g(p_r + k\Delta\alpha).$$

If this happens we set $\Delta\alpha = \frac{\Delta\alpha}{2}$ and repeat the procedure. We do so until $\Delta\alpha < 10^{-6}$. When this value of $\Delta\alpha$ is reached, no point of intersection of (2.8)e and (4.10) exists (Figure 5.2). We now show how to solve the Riemann problem when the solution contains a weak deflagration wave (c.f. Figure 5.1). We construct by induction a sequence $\{\alpha^\nu, p_\star^\nu, v_\star^\nu, \alpha_-^\nu, \alpha_+^\nu, \nu = 0, 1, \dots\}$ as follows:

$$\alpha^{\nu+1} = \frac{\alpha_-^\nu + \alpha_+^\nu}{2}$$

$$p_\star^{\nu+1} = p_1(\alpha^{\nu+1}, \underline{u}_r)$$

$$v_\star^{\nu+1} = v_1(\alpha^{\nu+1}, \underline{u}_r)$$

$$\alpha_-^{\nu+1} = \alpha^{\nu+1}, \quad \alpha_+^{\nu+1} = \alpha_+^\nu \quad \text{when} \quad v_\star^{\nu+1} - v_\ell + \varphi(p_\star^{\nu+1}, \underline{u}_\ell) < 0$$

$$\alpha_-^{\nu+1} = \alpha_-^\nu, \quad \alpha_+^{\nu+1} = \alpha^{\nu+1} \quad \text{when} \quad v_\star^{\nu+1} - v_\ell + \varphi(p_\star^{\nu+1}, \underline{u}_\ell) > 0$$

The iteration is stopped when

$$|\alpha^{\nu+1} - \alpha^\nu| < \epsilon$$

(we usually pick $\epsilon = 10^{-6}$). One then sets $p^\star = p_\star^{\nu+1}$, $v^\star = v_\star^{\nu+1}$, $p_0 = \alpha^{\nu+1}$ (p_0 is the pressure just ahead of the deflagration).

6. Numerical prediction of transition from deflagration to detonation

Consider a flow which can be idealized as one dimensional, with a flame which can be idealized as being thin, moving according to a given velocity law. The class of such flows does not encompass all reacting flows (see e.g. the calculations in [8]), but one can exhibit flows for which these idealizations are plausible (see e.g. [18]). The conclusion we can draw from our work to date is that a turbulent flame in such a one-dimensional reacting gas must, under some conditions, eventually undergo a transition to detonation; this must occur at the latest when the Riemann problem which involves the assumed deflagration no longer has a solution with deflagration. Note that in our idealization, all turbulence effects, all chemical effects, and all the effects of the three dimensionality of physical space are described by the deflagration velocity law. Measured velocity laws are given, e.g., in [1],[2].

In the next section we shall discuss the asymptotic properties of the flow whose initial data contain a deflagration. In this section, we wish to answer the more precise question "When does the transition occur?".

Note that our problem does not in general have a unique solution. A Riemann solution with a detonation, and one or more with deflagration, may coexist. This is very natural in our context. A flow starting from rest may continue at rest or exhibit a deflagration depending on whether someone has or has not lit a match. Outside

disturbances on the tube in which the reacting flow takes place may affect its nature and render it more explosive. To remove this natural non-uniqueness we make the following assumption: In every situation, the solution picked will be the one in which the reaction wave has the smallest strength (as measured by the pressure ratio). The Riemann solution of the preceding section is this weakest solution. This may be a very reasonable assumption for flow in a pipe as long as no one kicks it too violently from the outside. The details of the transition process cannot of course be seen by our calculations; they need a theory along the lines of [15],[16]. Once the Riemann solution has a unique solution, we can apply the random choice method and obtain flow fields numerically.

We present two examples. One is an ignition problem; the other is a problem with an accelerating flame. In each example there are two cases: one where transition occurs, the other where it does not.

Assume the reaction takes place in a tube with a closed end. Let the origin 0 be the closed end, with the positive x axis pointing along the tube. The state of gas at rest is $\rho(x,0) = 1$, $p(x,0) = 1$, $v(x,0) = 0$ ($x > 0$). The boundary condition at the closed end is $v(0,t) = 0$. The deflagration speed form is $V - v_0 = K(T_0)^Q$, $Q = 2$, where the subscript 0 refers to conditions immediately ahead of the deflagration front.

In the ignition problem, the gas is ignited at $x = 8$. Here the thermodynamic parameters are $\Delta = -20$, $\gamma = 1.4$. The spatial step is $h = 1$, the time step $K = 0.6/\max(|v+c|, |v-c|)$. A time-space wave

diagram of the solution is presented in Figure 5.1. Here $K = .095$. A solution obtained under similar circumstances but with $K = .1$ is displayed in Figure 6.2. On both diagrams (also for Figure 6.3 and Figure 6.4 in the following), the thick dashed lines represent the trajectories of deflagrations, the solid lines refer to shocks, the thick solid line corresponds to detonation, and the thin broken lines indicate slip lines. At the beginning stage the wave patterns on both diagrams are symmetric around $x = 8$: a weak deflagration with a pre-shock to the left and another to the right. When the left shock is reflected from the closed end the symmetry of wave pattern breaks down.

In the first case, the initial flame speed is 0.94. When the reflection shock first hits the right deflagration, its speed increased to 1.98. The flame speed reduces to 1.485 while the flame reaches $x = 55$. There is no transition. The deflagration speed slowly approaches its final speed 0.94. The left flame dies out when it reaches the closed end at time $t = 2.116$.

In the second case the initial deflagration speed is 1.050; when the reflection shock first hits the right deflagration, transition occurs. This occurs at $x \approx 20$ and at time 1.578. The detonation propagates at a speed of 7.356.

For the accelerating flame problem, initial conditions are provided by a deflagration with a pre-shock starting from the origin (see Oppenheim and Stern [18]). When the deflagration propagates to $x = 5$, its speed coefficient K is suddenly increased by a finite

increment ΔK . The time-space wave diagrams of the solutions are presented in Figures 6.3 and 6.4. Here the parameters are $\Delta = -27$, $\gamma = 1.26$, $K = 0.03367$, and $Q = 2.6$. $\Delta K = 0.07333$ in Figure 6.3, and $\Delta K = 0.08667$ in Figure 6.4.

In the first case the propagation speed of the flame increase to 1.142 from its initial speed 0.2037, while the deflagration travels a distance of 70. In the second case, however, as demonstrated in Figure 6.4, the process escalates to a detonation, propagating finally at a speed of 147.4. The transition occurs at the point $x = 66$ and at time 9.335. We point out an important fact in Figure 6.4: the transition does not happen immediately after a shock hits the deflagration, but a short time later when the deflagration meets a weak slip line, i.e., a small perturbation can induce transition.

These diagrams strongly resemble the diagrams obtained numerically by Kurylo et al. [11], and the experimental results in Oppenheim [18]; the comparison cannot be made quantitative because we used an artificial flame velocity law and an invariant γ . The algorithm is certainly simpler than the one in [11]; the assumptions of constant γ and flame velocity proportional to T^Q are in no way essential. The uncertainty in the location of the waves is an intrinsic feature of the random choice method (see [3]); the nature of the waves is sharply defined.

7. Asymptotic behavior of a reacting gas

In view of the complexity of a gas flow which includes combustion waves, it is desirable to study the asymptotic form of the flow, and, in particular, to predict whether an eventual transition from deflagration wave to detonation wave should occur. In a reacting gas the waves tend to combine and cancel, and the asymptotic state of the flow consists of elementary waves which are uniquely determined by the value of the initial data at far right and far left (Liu [13],[14]).

Consider first an open tube $-\infty < x < \infty$. Suppose that the initial state is uniform with zero speed and that the gas is ignited so that combustion waves travel to the right and left. In this case the situation is that of the Riemann problem with equal states on the right and left. There are two possibilities: When the stable branch of the right wave curve (4.10) intersects the line $v = 0$ at (u^*, p^*) , with corresponding states $\underline{u}_I$ ($v_I = v^* = 0$, $p_I = p^*$) and $\underline{u}_0$ (c.f. Section 4), by symmetry, the solution consists of a left shock wave, a right deflagration wave, a right deflagration wave, and a right shock wave. When the right wave (4.10) does not intersect $v = 0$, then the solution contains a CJ-detonation wave followed by a rarefaction wave. These waves are determined by the intersection of the wave (4.1) and the line $v = 0$.

Consider next the one-sided closed tube, $x \geq 0$, filled with uniform gas as above. Suppose that the gas is ignited at $x = x_0 > 0$. For a small time, the behavior of the flow is the same as the above open tube case. However, as the left waves are reflected from the

wall, $x = 0$, they catch up with the right waves and nonlinear interaction occurs. Eventually, all the left waves are weakened and decay with time. Thus the asymptotic state of the flow consists of right waves and contact discontinuities only. These waves relate the state $\underline{u}_r$ on the right and a state with zero speed adjacent to the wall on the left. Thus, the asymptotic state consists either of contact discontinuities, weak deflagration, and a right shock, or of contact discontinuities, right rarefaction wave, and CJ-detonation. However, the present situation may be drastically different from the situation in the open tube case: Suppose that the state $\underline{u}_r$ is such that the right wave curve (4.10) intersects $v = 0$ so that it is possible for the asymptotic state to contain a deflagration wave. Unlike the open tube case, the interaction of the waves reflected off the wall with the right deflagration wave may cause a transition. When this happens, the asymptotic state contains a right CJ-detonation. When the left deflagration wave reflects off the wall, it becomes a right rarefaction wave, but this wave may not catch up with the deflagration wave to cool the gas before other disturbances have already caused the transition.

8. Conclusions

We have constructed the solution of the Riemann problem for a reacting gas (under certain stringent assumptions which make a hyperbolic model applicable). We have used these solutions to predict the asymptotic behavior of a one-dimensional gas and have incorporated them into a numerical algorithm. Our results indicate in particular that the laminar member of our family of flames will not induce a transition.

We expect that more interesting multi-dimensional physical situations will be analyzable by numerical methods that incorporate our Riemann solutions.

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XBL 811-137

Fig. 2.1

XBL 811-142

Fig. 2.2

XBL 811-139

Fig. 3.1

Fig. 3.2

XBL 811-145

Fig. 4.1

XBL 811-143

Fig. 4.2

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Fig. 4.3

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Fig. 4.4

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Fig. 5.1

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Fig. 6.4