JOURNAL OF COMPUTATIONAL PHYSICS 81, 70–101 (1989)

The Generalized Riemann Problem for Reactive Flows

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Received August 10, 1987; revised January 26, 1988

A generalized Riemann problem is introduced for the equations of reactive non-viscous compressible flow in one space dimension. Initial data are assumed to be linearly distributed on both sides of a jump discontinuity. The resolution of the singularity is studied and the first-order variation (in time) of flow variables is given in exact form. © 1989 Academic Press, Inc.

1. INTRODUCTION

Consider the Euler equations that model the time-dependent flow of an inviscid, compressible, reactive gas in one space dimension. Taking a model with no heat conduction or viscosity, the equations take the form

$$U_t + F(U)_x = G(U), \tag{1.1}$$

$$U = \begin{pmatrix} \rho \\ \rho u \\ \rho(e + \frac{1}{2}u^2) \\ \rho z \end{pmatrix}, \quad F(U) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u(e + \frac{1}{2}u^2) + pu \\ \rho z u \end{pmatrix}, \quad G(U) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -k(\rho, p, z) \cdot \rho \end{pmatrix}.$$

Here ρ is the density, u is the velocity, e is the specific internal energy, p is the pressure, and z is the mass fraction of unburnt gas. Thus $z = 1$ (resp. $z = 0$) represents the completely unburnt (resp. burnt) gas. In (1.1) we are assuming also that an equation-of-state of the form $p = p(e, \rho, z)$ is given (note that e is the "total" internal energy, including the contribution of "chemical" energy). The "reaction rate" function $k(\rho, p, z)$ is assumed to be non-negative, so that the reaction process is "irreversible."

In this paper we provide the analytical tools needed for a numerical high resolution scheme for the time-integration of (1.1). To be specific, we address the *generalized Riemann problem* (GRP) which can be formulated as follows.

* This work was partially supported by the Applied Mathematical Sciences Subprogram of the Office of Energy Research, U.S. Department of Energy under contract DE-AC03-76SF00098, and by the Office of Naval Research under Grant N00014-86-K-069, while the author was visiting UCLA.

0021-9991/89 $3.00

Let $U_{\pm}(x)$ be two linear distributions of the flow variables and consider the initial value problem for (1.1) *where,*

$$U(x, 0) = \begin{cases} U_+(x), & x > 0, \\ U_-(x), & x < 0. \end{cases}$$

Let $U(x, t)$ be the solution. Find,

$$\begin{aligned} &\text{(a)} \quad U(0, 0) = \lim_{t \to 0+} U(0, t), \\ &\text{(b)} \quad \frac{\partial U}{\partial t}(0, 0) = \lim_{t \to 0+} \frac{\partial}{\partial t} U(0, t). \end{aligned} \tag{1.2}$$

Observe that even in the case that $U_{\pm}(x)$ are *constant* states, the solution $U(x, t)$ is not "self-similar" (i.e., depending on x/t only) due to the presence of a non-vanishing right-hand side in (1.1). Thus, characteristic lines and discontinuity trajectories are not straight lines and there are no "Riemann invariants" as in the standard Riemann problem for compressible flows (see [5]). Furthermore, the dependence of e on z implies that the flow is not "adiabatic," namely, that entropy is not preserved along streamlines even in smooth regions of the flow (indeed, the concept of entropy in this case needs to be discussed. See next section).

The main building block in our solution of the GRP is a careful analysis of the structure of a centered rarefaction wave. This analysis enables us to "propagate" directional derivatives from the head of the rarefaction fan, where they are determined by the initial conditions, to the tail of the fan, where they can be translated into the desired time-derivatives. While the method is applied in the present work only to the evaluation of the first-order time-derivatives, it can easily be generalized to account for the time-derivatives of any order.

In solving the GRP we make essential use of a fact that enables us to determine limiting values at the singularity by first solving the *associated Riemann problem* (RP) which is the following.

Given the above initial conditions for the GRP, set

$$U_r = \lim_{x \to 0+} U_+(x), \qquad U_l = \lim_{x \to 0-} U_-(x),$$

and let $U_{RP}(x, t) = R(x/t)$ be the solution of

$$\begin{aligned} &\frac{\partial}{\partial t} U_{RP} + \frac{\partial}{\partial x} F(U_{RP}) = 0, \\ &U_{RP}(x, 0) = \begin{cases} U_r, & x > 0, \\ U_l, & x < 0. \end{cases} \end{aligned} \tag{1.3}$$

Our proposition is now.

PROPOSITION [7]. *Let $U(x, t)$ be the solution to the GRP and let $R(x/t)$ be the solution of the associated RP. Then, for every fixed direction $x/t = \lambda$,*

$$\lim_{t \to 0+} U(\lambda t, t) = R(\lambda). \tag{1.4}$$

Furthermore, the wave configuration for the GRP near the singularity is the same as that for the associated RP.

The last part of the above proposition implies that if the solution of the associated RP yields a shock travelling to the right, then this is the case also for the GRP, etc.

In order to put this work in the appropriate perspective of numerical applications, let us recall briefly the so-called "Godunov-type" numerical schemes (approximating (1.1)).

Suppose that we use equally spaced grid points $x_i = i\,\Delta x$ along the x-axis and equal time intervals of size Δt. By "cell i" we shall refer to the interval extending between the "cell-boundaries" $x_{i \pm 1/2} = (i \pm \frac{1}{2})\Delta x$. We let Q_i^n denote the average value of a quantity Q over cell i at time $n\,\Delta t$. Similarly, we denote by $Q_{i+1/2}^{n+1/2}$ the value of Q at the cell boundary $x_{i+1/2}$, averaged over the time interval $(n\,\Delta t, (n+1)\,\Delta t)$. Generally speaking, a "Godunov-type" (or "quasi-conservative") difference scheme for (1.1) is given by

$$U_i^{n+1} - U_i^n = -\frac{\Delta t}{\Delta x}\left[F(U_{i+1/2}^{n+1/2}) - F(U_{i-1/2}^{n+1/2})\right] + \Delta t \cdot G(U_i^{n+1/2}). \tag{1.5}$$

In this scheme one must still give an appropriate interpretation to the values of U at time $(n+\frac{1}{2})\,\Delta t$. A fundamental way of doing it was proposed by Goldunov [6] and may be described as follows. Assume that at time $n\,\Delta t$ the point $x_{i+1/2}$ separates two *constant* states U_i^n, U_{i+1}^n, and also that $G \equiv 0$. Solving the resulting Riemann problem, one takes $U_{i+1/2}^{n+1/2}$ to be the (constant) solution along $x = x_{i+1/2}$ (observe that even if this line represents a jump discontinuity the flux vector is still continuous there). The resulting scheme is of first-order accuracy and has relatively poor resolution properties. In order to upgrade this scheme (in terms of accuracy and resolution) we assume now that the values of U are *linearly* distributed in cells, with possible jumps at $x_{i+1/2}$, which gives rise to an initial value problem for (1.1). Indeed, locally at each cell boundary we have a GRP, and its solution (as in (1.2)) serves as a linear (in time) approximation to the values $U(x_{i+1/2}, t)$. Thus, using the obvious analog of the notation in (1.2), one takes

$$U_{i+1/2}^{n+1/2} = U_{i+1/2}^n + \frac{\Delta t}{2} \cdot \left[\frac{\partial}{\partial t} U\right]_{i+1/2}^n. \tag{1.6}$$

Further details of the numerical scheme along with a numerical example will be given in Section 7.

To relate this work to previous work on the subject (i.e., finite difference schemes for (1.1) using "Riemann problem approach" at singularities) we mention the works

of Chorin [3] and Colella, Majda, and Roytburd [4]. Both of these works are aimed at calculating travelling combustion waves. In the limit of "infinite reaction rate" (i.e. with z jumping from 1 to 0) it is well known [5] that the fluid-dynamical model yields a shock across which the total reaction takes place. In contrast to that, in the "finite reaction rate" model given by (1.1) the jump in z occurs *only* across a contact discontinuity. Thus, the "local Riemann problem" solutions differ from the "global" problem that they are supposed to approximate. Colella, Majda, and Roytburd use a split scheme, where the fourth equation of (1.1) is handled in a separate step. On a "local" basis, this amounts to convecting the discontinuities of z only along streamlines (i.e., contact discontinuities). On the other hand, Chorin [3] uses a "Riemann solver" for the full system (1.1) where, however, he allows jumps of z across both shocks and contact discontinuities. The remarkable results that he gets (see also [4]) have to be contrasted with the obvious fact that his "Riemann solver" violates the weak solution requirement imposed on (1.1). We are not quite sure that his scheme is yet fully understood.

The plan of the paper is the following. In Section 2 we introduce our notation, discuss the characteristic relations associated with (1.1) and switch to a Lagrangian formulation of the problem. In Section 3 we discuss the resolution of a centered rarefaction wave. which serves as a basis for the full Lagrangian solution given in Section 4. In Section 5 we provide the details needed for the completion of the solution in the Eulerian framework. In Section 6 we specialize to the case where the equation of state is given by a γ-law relation (see (6.1)) and a simplified Arrhenius model is used for the reaction equation (see (6.3)). This is the case treated in the works [3, 4] mentioned above. Here we are able to give fully explicit expressions for the various ingredients of the solution.

In Section 7 we give a few more details related to the numerical scheme (1.5). In particular, we discuss two different ways (labeled "explicit" and "implicit") of differencing the reaction equation (the fourth equation in (1.1)). As an example, we give the results of several computations for an ozone decomposition C-J detonation. This example is taken from [4]. Using the same mesh sizes in our schemes, we compare our results with those obtained there.

Finally, in a recent preprint, A. Bourgeade [8] has obtained results closely related to ours. His methods, however, are completely different.

We conclude by remarking that the present method can easily be extended in various directions. One that could be of particular interest is the inclusion of "source terms" in the fluid-dynamical part. This (without reactions) was done in [2] for the case of a variable cross section and could be incorporated here to study reactions in, say, cylindrical or spherical geometries.

2. Preliminaries and Notation

In what follows we shall address the GRP as presented in (1.2). Recall that the Riemann problem in (1.3) was labeled as the *Associated RP*. In addition to the

basic flow variables appearing in (1.1), we shall also make extensive use of the speed of sound c and the "Lagrangian" speed of sound $g = \rho c$. The definition of c in our case needs to be clarified. Indeed, for each *fixed* value of z we define the entropy $S(e, \rho, z)$ as usual by

$$T\,dS_z \equiv T\left(\frac{\partial S}{\partial e}\,de + \frac{\partial S}{\partial \rho}\,d\rho\right) = de + p\,d\left(\frac{1}{\rho}\right), \tag{2.1}$$

where $T = T(e, \rho, z)$ is the temperature. Solving for e we have $e = e(\rho, S, z)$ and substituting this in the equation of state we get $p = p(S, \rho, z)$. We then set

$$c^2 = \frac{\partial p}{\partial \rho}(S, \rho, z). \tag{2.2}$$

As a rule, we shall always indicate the independent variables when differentiating a thermodnamical function, as has been done in (2.2).

It can easily be checked that the first three equations of (1.1) yield the characteristic relation

$$\frac{de}{dt} + p\,\frac{d(1/\rho)}{dt} = 0 \qquad \text{along} \quad \frac{dx}{dt} = u. \tag{2.3}$$

Using (2.1) and the fourth equation in (1.1), this can be written as

$$\frac{dS}{dt} = \frac{\partial}{\partial z} S(e, \rho, z)\,\frac{dz}{dt} = -k(e, \rho, z)\,\frac{\partial}{\partial z} S(e, \rho, z) \equiv -f \qquad \text{along} \quad \frac{dx}{dt} = u. \tag{2.4}$$

We now transform the system (1.1), replacing the coordinate x by the Lagrangian coordinate ξ given by

$$d\xi = \rho\,dx, \qquad \xi(0) = 0. \tag{2.5}$$

Replacing the third equation of (1.1) by (2.4), the system can now be written as

$$V_t + \Phi(V)_\xi = \Psi(V), \tag{2.6}$$

$$V = \begin{pmatrix} \tau \\ u \\ S \\ z \end{pmatrix}, \qquad \Phi(V) = \begin{pmatrix} -u \\ p \\ 0 \\ 0 \end{pmatrix}, \qquad \Psi(V) = \begin{pmatrix} 0 \\ 0 \\ -f \\ -k \end{pmatrix}, \qquad \tau = \frac{1}{\rho}.$$

In deriving the characteristic relations for (2.6), we express p in terms of S, ρ, z, so that the momentum equation becomes

$$u_t + c^2\rho_\xi + p_S S_\xi + p_z z_\xi = 0.$$

Combining this equation with suitable multiples of the other equations, we obtain

$$u_t \pm \rho c u_\xi \pm \frac{c}{\rho}(\rho_t \pm \rho c \rho_\xi) \pm \frac{p_S}{\rho c}(S_t \pm \rho c S_\xi)$$

$$\pm \frac{p_z}{\rho c}(z_t \pm \rho c z_\xi) = \mp \frac{1}{\rho c}(p_S f + p_z k). \tag{2.7}$$

But from (2.4) we have

$$p_S f + p_z k = k \cdot \left(\frac{\partial}{\partial S} p(S, \rho, z) \cdot \frac{\partial}{\partial z} S(e, \rho, z) + \frac{\partial}{\partial z} p(S, \rho, z) \right)$$

$$= k(e, \rho, z) \frac{\partial}{\partial z} p(e, \rho, z),$$

so that (2.7) simplifies to

$$g\, du \pm dp = \mp k \frac{\partial}{\partial z} p(e, \rho, z)\, dt \qquad \text{along} \quad \frac{d\xi}{dt} = \pm g. \tag{2.8}$$

Finally, we introduce some notation for the treatment of the GRP for the system (2.6). We assume that initially $V(\xi, 0) = V_\pm(\xi)$ is piecewise linear with a jump at $\xi = 0$. This is justified by the fact (to be proved later) that the time derivatives at the singularity depend only on the *limiting* values (as $\xi \to 0$) of the initial conditions and their slopes. Hence we may replace x-derivatives by ξ-derivatives according to (2.5). Letting $V_l = \lim_{\xi \to 0-} V_-(\xi)$, $V_r = \lim_{\xi \to 0+} V_+(\xi)$, we denote by $R_L(\lambda; V_l, V_r)$, $\lambda = \xi/t$, the Lagrangian solution of the associated Riemann problem. Denoting by $V(\xi, t)$ the solution to the GRP for (2.6), our objective (in analogy with (1.2)) is to determine $(\partial/\partial t)V(0, 0) = \lim_{t \to 0+} (\partial/\partial t)V(0, t)$. Clearly, in this case the line $\xi = 0$ represents the contact discontinuity across which the variables ρ, S, z may be discontinuous, so that we must compute their time derivatives on both sides of this line.

We employ the following notation conventions:

Subscripts "r, l" denote limiting values as $\xi \to 0+$, $0-$, respectively.

An asterisk (*) is used for values at $t = 0+$ along $\xi = 0$ (along with "r, l" for discontinuous quantities).

Further details are given in Table I, where Q stands for any one of the flow variables (see also Fig. 1 in Section 3 below).

Remark. Note that if two limiting processes are implied, they must be carried out in the indicated order. For example $(\partial Q/\partial \xi)_r^*$ means that first the ξ-derivative is evaluated at $\xi = 0+$ and its limit is then taken as $t \to 0+$. On the other hand, $(\partial Q/\partial t)_r$ is computed by first taking the t-derivative at $t = 0$ and then letting $\xi \to 0+$.

TABLE I

Notations for the Lagrangian GRP

Symbol	Definition
Q_r, Q_l	$\lim Q(\xi, 0)$ as $\xi \to 0+, 0-$
$\left(\frac{\partial Q}{\partial \xi}\right)_r, \left(\frac{\partial Q}{\partial \xi}\right)_l$	constant slopes for $\xi > 0$, $\xi < 0$
$V = R_L(\lambda; V_l, V_r)$	Lagrangian solution of the associated RP, $\lambda = \xi/t$
V^*	$= R_L(0; V_l, V_r)$
Q_r^*, Q_l^*	right and left values for Q discontinuous across $\xi = 0$ (e.g., $Q = \rho$ or g)
$\left(\frac{\partial Q}{\partial t}\right)^*$	$\lim_{t \to 0+} \frac{\partial}{\partial t} Q(\xi, t)$ at $\xi = 0$
$\left(\frac{\partial Q}{\partial t}\right)_r^*, \left(\frac{\partial Q}{\partial t}\right)_l^*$	Right and left values of $\left(\frac{\partial Q}{\partial t}\right)^*$ for discontinuous Q
$\left(\frac{\partial Q}{\partial \xi}\right)_r^*$	$= \lim_{t \to 0+} \lim_{\xi \to 0+} \frac{\partial}{\partial \xi} Q(\xi, t)$
$\left(\frac{\partial Q}{\partial \xi}\right)_l^*$	$= \lim_{t \to 0+} \lim_{\xi \to 0-} \frac{\partial}{\partial \xi} Q(\xi, t)$
$\left(\frac{\partial Q}{\partial t}\right)_r, \left(\frac{\partial Q}{\partial t}\right)_l$	$= \lim_{\xi \to 0+} \frac{\partial}{\partial t} Q(\xi, t)\|_{t=0}, \lim_{\xi \to 0-} \frac{\partial}{\partial t} Q(\xi, t)\|_{t=0}$

Also note the meaning of the various groups of variables:

$Q_r, Q_l, (\partial Q/\partial \xi)_r, (\partial Q/\partial \xi)_l$	are the given initial data.
Q^*, Q_r^*, Q_l^*	result from the solution of the associated RP.
$(\partial Q/\partial t)_l, (\partial Q/\partial t)_r$	are time-derivatives which are evaluated from the initial data by (2.6).
$(\partial Q/\partial t)^*, (\partial Q/\partial \xi)_r^*, (\partial Q/\partial \xi)_l^*$	result from the solution of the GRP.

3. Resolution of a Centered Rarefaction Wave (CRW)

It is a well-known fact that a jump discontinuity in the initial data is resolved in terms of centered rarefaction waves or jump discontinuities. In the context of the GRP the latter are easily handled in terms of the associated jump conditions, as we shall show in the next section. However, the centered rarefaction wave (CRW) requires some further considerations. These considerations are discussed in detail in this section and, as in the other applications of the GRP scheme, constitute the basic analytical tool of the method.

The basic idea is to use characteristic coordinates throughout the CRW, so that the singularity is "blown up" into a "full segment" in the characteristic plane, where the CRW is now represented by a rectangular zone. The base of this rectangle corresponds to the singularity. The flow variables are smooth in the rectangle and their values at the base are derived from $R_L(\lambda; V_l, V_r)$, the solution of the associated RP. The first derivatives normal to the base correspond to directional derivatives in the (ξ, t) plane. It turns out that these derivatives satisfy simple differential equations along the base. Thus, knowing the derivatives at one endpoint enables us to determine their values at the other (a "propagation of singularities" argument).

To fix the ideas we shall assume henceforth that the wave configuration is as displayed in Fig. 1. Recall that our basic assumption is that the wave pattern is already determined by the associated RP. In this and the next section we work solely with the Lagrangian formulation (2.6).

Let $\Gamma^{\pm}$ be the characteristic families of (2.6) corresponding to the eigenvalues $\pm g = \pm \rho c$. At the singularity, the slopes of the Γ^- curves extend from $-g_l$ at the head to $-g_l^*$ at the tail of the rarefaction. We introduce characteristic coordinates (α, β) such that $\alpha = \text{const}$ (resp. $\beta = \text{const}$) corresponds to a Γ^+ (resp. Γ^-) curve and such that

$$\begin{aligned} &\beta = \text{normalized slope of } \Gamma^- \text{ at the origin,} \\ &\beta = 1 \text{ at the head characteristic.} \\ &\alpha = \text{value of } \xi \text{ at point of intersection} \\ &\quad \text{of } \Gamma^+ \text{ with the curve } \beta = 1. \end{aligned} \tag{3.1}$$

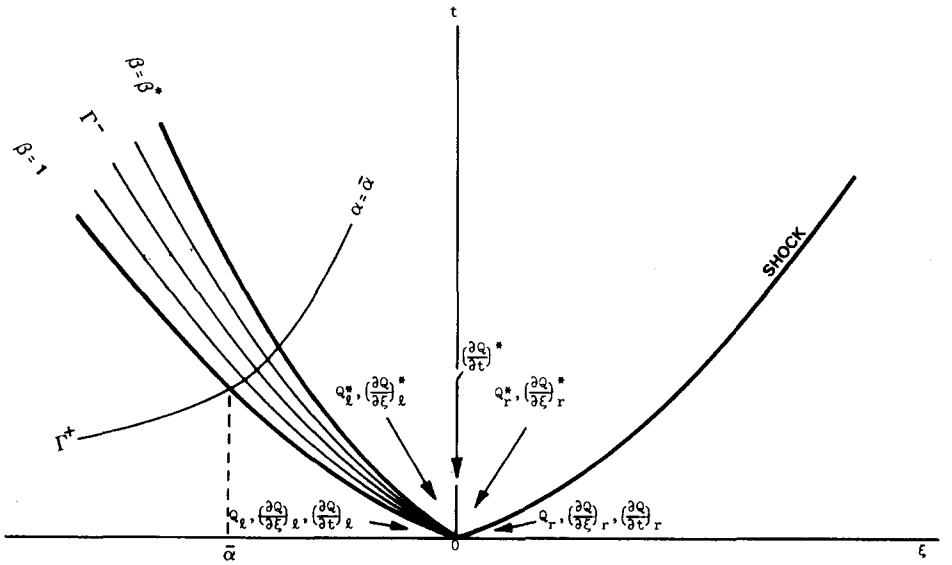

FIG. 1. Setup for the generalized Riemann problem.

In particular, the definition (3.1) implies that

$$\xi(\alpha, 1) = \alpha, \qquad g(0, \beta) = g_l \beta. \tag{3.2}$$

Thus, the CRW is now projected onto the rectangular region $-\alpha_0 \leqslant \alpha \leqslant 0$, $\beta^* \leqslant \beta \leqslant 1$, where $\beta^* = g_l^*/g_l$ and $\alpha_0 > 0$ is a fixed number. Any variable Q defined in this region (including ξ, t) is represented as $Q(\alpha, \beta)$. The values $V(0, \beta)$ are given in terms of the associated RP (with $\Psi \equiv 0$ in (2.6)),

$$V(0, \beta) = R_L(-g_l \beta; V_l, V_r). \tag{3.3}$$

In particular, we note that

$$S(0, \beta) \equiv S_l, \qquad z(0, \beta) \equiv z_l. \tag{3.4}$$

In the following proposition we give asymptotic expressions for $\xi(\alpha, \beta)$, $t(\alpha, \beta)$ (near $\alpha = 0$).

PROPOSITION 3.1. *We have*

$$\begin{aligned} \xi(\alpha, \beta) &= \alpha \beta^{1/2} + \varepsilon(\alpha, \beta) \cdot \alpha^2, \\ t(\alpha, \beta) &= -g_l^{-1} \alpha \beta^{-1/2} + \eta(\alpha, \beta) \cdot \alpha^2, \end{aligned} \tag{3.5}$$

where $\varepsilon(\alpha, \beta)$, $\eta(\alpha, \beta)$ are smooth functions.

Proof. From the definition (3.1) of α, β we get

$$\frac{\partial \xi}{\partial \alpha} = -g \frac{\partial t}{\partial \alpha}, \qquad \frac{\partial \xi}{\partial \beta} = g \frac{\partial t}{\partial \beta}. \tag{3.6}$$

Differentiate the first equation with respect to β, the second with respect to α and note that, at $\alpha = 0$, $\partial t/\partial \beta = 0$. Solving for $\partial t/\partial \alpha$, we have

$$2g(0, \beta) \frac{d}{d\beta} \left(\frac{\partial t(0, \beta)}{\partial \alpha} \right) + \left(\frac{d}{d\beta} g(0, \beta) \right) \cdot \frac{\partial t(0, \beta)}{\partial \alpha} = 0. \tag{3.7}$$

Also, from (3.2), (3.6), we get

$$\frac{\partial t}{\partial \alpha}(0, 1) = -g_l^{-1}, \qquad g(0, \beta) = g_l \beta.$$

Equation (3.7) now yields

$$\frac{\partial t}{\partial \alpha}(0, \beta) = -g_l^{-1} \beta^{-1/2}, \qquad \frac{\partial \xi}{\partial \alpha}(0, \beta) = \beta^{1/2},$$

from which (3.5) follows readily. Q.E.D.

Our objective in this section is to compute the derivatives $(\partial/\partial\alpha)\,Q(0,\beta)$ of all flow variables $Q(\alpha,\beta)$. Note that these derivatives vanish identically for the associated RP. As a first step, we compute $S_\alpha(0,\beta)$, $z_\alpha(0,\beta)$, the derivatives of the entropy S and the mass fraction z.

PROPOSITION 3.2. *Let f, k in Eqs. (2.6) be expressed in terms of the variables p, S, z. Then the functions $S_\alpha(0,\beta)=(\partial/\partial\alpha)S(0,\beta)$, $z_\alpha(0,\beta)=(\partial/\partial\alpha)z(0,\beta)$ satisfy*

$$\begin{aligned} &\text{(i)} \quad \frac{d}{d\beta}\left(\beta^{-1/2}S_\alpha(0,\beta)\right) = -g_l^{-1}\beta^{-2}f(p(0,\beta), S_l, z_l),\\ &\text{(ii)} \quad \frac{d}{d\beta}\left(\beta^{-1/2}z_\alpha(0,\beta)\right) = -g_l^{-1}\beta^{-2}k(p(0,\beta), S_l, z_l), \end{aligned} \tag{3.8}$$

which, together with the initial conditions,

$$\begin{aligned} &\text{(i)} \quad S_\alpha(0,1) = \left(\frac{\partial S}{\partial\xi}\right)_l + g_l^{-1}f(p_l, S_l, z_l),\\ &\text{(ii)} \quad z_\alpha(0,1) = \left(\frac{\partial z}{\partial\xi}\right)_l + g_l^{-1}k(p_l, S_l, z_l), \end{aligned} \tag{3.9}$$

determine completely $S_\alpha(0,\beta)$, $z_\alpha(0,\beta)$.

Proof. We prove for S. The proof for z is identical. From the chain rule and (2.4) we have

$$\frac{\partial}{\partial\xi}S(\xi,t)\cdot\frac{\partial\xi}{\partial\alpha}(\alpha,\beta) - f(p(\alpha,\beta), S(\alpha,\beta), z(\alpha,\beta))\frac{\partial t}{\partial\alpha} = \frac{\partial}{\partial\alpha}S(\alpha,\beta). \tag{3.10}$$

From (3.5) we see that $(\partial\xi/\partial\alpha)(\alpha,\beta)$ does not vanish near $\alpha=0$ so that (3.10) implies that the function

$$S'(\xi,t) = \frac{\partial}{\partial\xi}S(\xi,t), \tag{3.11}$$

is well defined and bounded as a function of (α,β). (Its smoothness depends on the smoothness properties of f. In the simplified model of Section 6 f will be discontinuous.) Letting $\alpha\to 0$ in (3.10) and using (3.4), (3.5) we have

$$S_\alpha(0,\beta) = S'(0,\beta)\cdot\beta^{1/2} + f(p(0,\beta), S_l, z_l)\cdot g_l^{-1}\beta^{-1/2}. \tag{3.12}$$

To evaluate $S'(0,\beta)$ we differentiate (3.11) with respect to t and use (2.4), (2.6) to get

$$\begin{aligned} \frac{\partial}{\partial t}S'(\xi,t) &= -\frac{\partial}{\partial\xi}f(p,S,z) = -f_p p_\xi - f_S S_\xi - f_z z_\xi\\ &= f_p u_t - f_S S' - f_z z_\xi. \end{aligned}$$

Next we view t as a function of (ξ, β) and multiply the last equation by $(\partial/\partial\beta)t(\xi, \beta)$. With ξ, β as independent variables we get

$$\frac{\partial}{\partial\beta} S'(\xi, \beta) = f_p \cdot \frac{\partial}{\partial\beta} u(\xi, \beta) - (f_S S' + f_z z_\xi) \frac{\partial}{\partial\beta} t(\xi, \beta).$$

The argument leading to the boundedness of $S'(\xi, t)$ near the singularity (see the paragraph following (3.10)) also implies the boundedness of z_ξ there. Hence, letting $\xi \to 0$ and noting that $\partial t/\partial\beta \to 0$ (and 3.4)), we get

$$\frac{d}{d\beta} S'(0, \beta) = f_p(p(0, \beta), S_l, z_l) \cdot \frac{d}{d\beta} u(0, \beta). \tag{3.13}$$

Going back to (3.12) it follows that

$$\begin{aligned}
\frac{d}{d\beta}(\beta^{-1/2} S_\alpha(0, \beta)) &= \frac{d}{d\beta}(S'(0, \beta)) + g_l^{-1} \frac{d}{d\beta}(\beta^{-1} f(p(0, \beta), S_l, z_l)) \\
&= f_p(p(0, \beta), S_l, z_l) \cdot \frac{d}{d\beta} u(0, \beta) \\
&\quad + g_l^{-1} \beta^{-1} f_p(p(0, \beta), S_l, z_l) \cdot \frac{d}{d\beta} p(0, \beta) \\
&\quad - g_l^{-1} \beta^{-2} f(p(0, \beta), S_l, z_l) \\
&= \left[\frac{d}{d\beta} u(0, \beta) + g(0, \beta)^{-1} \frac{d}{d\beta} p(0, \beta) \right] \cdot f_p(p(0, \beta), S_l, z_l) \\
&\quad - g_l^{-1} \beta^{-2} f(p(0, \beta), S_l, z_l).
\end{aligned}$$

But the expression in square brackets vanishes by the characteristic relation (2.8) (taken along the degenerate Γ^+-characteristic at $\alpha = 0$, where $\partial t/\partial\beta = 0$). This proves (3.8). The initial condition (3.9) is obtained from (3.12) by noting that $S'(0, 1) = (\partial S/\partial\xi)_l$. Q.E.D.

Our next result constitutes the main analytical tool of the method. We use the characteristic relation in order to derive an expression for $u_\alpha(0, \beta)$. To simplify notation, we introduce the function

$$\lambda = k(e, \rho, z) \frac{\partial}{\partial z} p(e, \rho, z). \tag{3.14}$$

As is the case with the other functions, we refer to λ as a function of α, β throughout the CRW. In fact, we shall need only the limiting values $\lambda(0, \beta)$, which are determined by the associated RP.

THEOREM 3.3. *Let* $a(\beta)=(\partial/\partial\alpha)u(0,\beta)$, *and let* $g=\rho c$ *be represented as* $g(p, S, z)$. *Then* $a(\beta)$ *satisfies*

$$\frac{d}{d\beta}a(\beta)=A(\beta), \qquad \beta^*\leqslant\beta\leqslant 1, \tag{3.15}$$

where

$$A(\beta)=-\frac{1}{2}g_l^{-2}\beta^{-1/2}\frac{d}{d\beta}(\beta^{-1}\lambda(0,\beta))$$
$$-\frac{1}{2}g_l^{-1}\beta^{-1}\cdot[g_S(0,\beta)\cdot S_\alpha(0,\beta)+g_z(0,\beta)\cdot z_\alpha(0,\beta)]\frac{d}{d\beta}u(0,\beta). \tag{3.16}$$

Equation (3.15) *is supplemented by the initial condition*

$$a(1)=\left(\frac{\partial u}{\partial\xi}\right)_l+g_l^{-1}\left(\frac{\partial p}{\partial\xi}\right)_l, \tag{3.17}$$

which, along with (3.8)–(3.9), *determines* $a(\beta)$ *completely.*

Proof. Write the characteristic relations (2.8) as

$$\begin{aligned} g\frac{\partial u}{\partial\alpha}-\frac{\partial p}{\partial\alpha}&=\lambda\frac{\partial t}{\partial\alpha},\\ g\frac{\partial u}{\partial\beta}+\frac{\partial p}{\partial\beta}&=-\lambda\frac{\partial t}{\partial\beta}. \end{aligned} \tag{3.18}$$

To eliminate p we differentiate the first equation in (3.18) with respect to β, the second with respect to α, add and evaluate at $\alpha=0$. Noting that $\partial t/\partial\beta=0$ at $\alpha=0$, we obtain

$$2g(0,\beta)a'(\beta)+a(\beta)\frac{d}{d\beta}g(0,\beta)+g_\alpha(0,\beta)\cdot\frac{d}{d\beta}u(0,\beta)$$
$$=\frac{d}{d\beta}\lambda(0,\beta)\cdot\frac{\partial t(0,\beta)}{\partial\alpha}. \tag{3.19}$$

Using the chain rule and (3.18) we have

$$g_\alpha(0,\beta)=g_p p_\alpha(0,\beta)+g_S S_\alpha(0,\beta)+g_z z_\alpha(0,\beta)$$
$$=g_p\left[ga(\beta)-\lambda\frac{\partial t(0,\beta)}{\partial\alpha}\right]+g_S S_\alpha+g_z z_\alpha. \tag{3.20}$$

Inserting this relation in (3.19) yields

$$2g(0,\beta)a'(\beta)+a(\beta)\left[\frac{d}{d\beta}g(0,\beta)+g_p g\frac{d}{d\beta}u(0,\beta)\right]$$
$$+\left[g_S S_\alpha+g_z z_\alpha-\lambda g_p\frac{\partial t(0,\beta)}{\partial\alpha}\right]\frac{d}{d\beta}u(0,\beta)=\frac{d}{d\beta}\lambda(0,\beta)\cdot\frac{\partial t(0,\beta)}{\partial\alpha}. \quad (3.21)$$

Observe that all quantities in the above equation are evaluated at $(0,\beta)$. In particular, by (3.4), $g(0,\beta)=g(p(0,\beta),S_l,z_l)$, so that, combined with (3.18),

$$g_l=\frac{d}{d\beta}g(0,\beta)=g_p\frac{d}{d\beta}p(0,\beta)=-g_p g\frac{d}{d\beta}u(0,\beta).$$

Also, by (3.5), $\partial t(0,\beta)/\partial\alpha=-g_l^{-1}\beta^{-1/2}$. Hence, we can write (3.21) in the form

$$2g_l\beta a'(\beta)+[g_S S_\alpha+g_z z_\alpha]\frac{d}{d\beta}u(0,\beta)-g_l^{-1}\lambda(0,\beta)\beta^{-3/2}$$
$$=-g_l^{-1}\beta^{-1/2}\frac{d}{d\beta}\lambda(0,\beta),$$

which is exactly (3.15), (3.16).

To establish (3.17) simply use the chain rule and (2.6), (3.5) to get

$$\frac{\partial u}{\partial\alpha}(0,1)=\left(\frac{\partial u}{\partial\xi}\right)_l\cdot\frac{\partial\xi}{\partial\alpha}(0,1)+\left(\frac{\partial u}{\partial t}\right)_l\frac{\partial t}{\partial\alpha}(0,1)=\left(\frac{\partial u}{\partial\xi}\right)_l+g_l^{-1}\left(\frac{\partial p}{\partial\xi}\right)_l. \quad \text{Q.E.D.}$$

The derivatives of the other flow variables are now obtained from the chararacteristic relation (3.18) and thermodynamic representations. In particular, expressing ρ, g in terms of p, S, z we get

COROLLARY 3.4. *The directional derivatives of p, p, g are given by*

$$\frac{\partial p}{\partial\alpha}(0,\beta)=g_l\beta_a(\beta)+g_l^{-1}\beta^{-1/2}\lambda(0,\beta),$$
$$\frac{\partial\rho}{\partial\alpha}(0,\beta)=c(0,\beta)^{-2}\frac{\partial p}{\partial\alpha}(0,\beta)+\rho_S S_\alpha(0,\beta)+\rho_z z_\alpha(0,\beta), \quad (3.22)$$
$$\frac{\partial g}{\partial\alpha}(0,\beta)=g_p\frac{\partial p}{\partial\alpha}(0,\beta)+g_S S_\alpha(0,\beta)+g_z z_\alpha(0,\beta).$$

4. THE LAGRANGIAN SOLUTION OF THE GRP

We continue the discussion of the previous section, assuming the configuration of Fig. 1. We seek here expression for time derivatives along the contact discontinuity

$\xi = 0$. Since the derivatives of S, z follow directly from (2.6) (see, e.g., (4.7) below), we need only compute $(\partial u/\partial t)^*$, $(\partial p/\partial t)^*$. As we shall see, these derivatives satisfy a pair of linear (algebraic) equations.

We have a shock travelling to the right. Using the notation introduced in Section 2 we let V_r (resp. V_r^*) be the pre-shock (resp. post-shock) values of V at the singularity (obviously, the subscript is suppressed in p^*, u^*). The (Lagrangian) shock speed W_r (i.e., the initial slope of the shock trajectory in the (ξ, t) plane) is given by the well-known jump condition

$$W_r = \frac{p^* - p_r}{u^* - u_r}. \tag{4.1}$$

We may now state the following theorem.

THEOREM 4.1. *Assume the configuration of Fig.* 1. *The derivatives* $(\partial p/\partial t)^*$, $(\partial u/\partial t)^*$ *are determined by a pair of linear equations,*

$$a_l\left(\frac{\partial u}{\partial t}\right)^* + b_l\left(\frac{\partial p}{\partial t}\right)^* = d_l, \tag{4.2}$$

$$a_r\left(\frac{\partial u}{\partial t}\right)^* + b_r\left(\frac{\partial p}{\partial t}\right)^* = d_r, \tag{4.3}$$

where, with $\beta^* = g_l^*/g_l$, $a(\beta)$ *as in Theorem* 3.3, *and* λ *as defined in* (3.14),

$$a_l = 1, \qquad b_l = (g_l^*)^{-1}, \qquad d_l = -(g_l g_l^*)^{1/2} a(\beta^*) - (g_l^*)^{-1}\lambda(0, \beta^*). \tag{4.4}$$

As for a_r, b_r, d_r, *they can be determined explicitly from the values of* V_r^*, V_r, $(\partial V/\partial \xi)_r$, *the Hugoniot* (u, p) *relation, and the reaction rate function. (Explicit expressions for a* γ*-law gas are given in Section* 6).

Proof. To establish (4.2) we note that the flow in the region $\xi(\alpha, \beta^*) \leqslant \xi \leqslant 0$ (i.e., between the tail characteristic of the rarefaction fan and the contact discontinuity) is smooth. Applying the chain rule along that characteristic we have

$$\frac{\partial p}{\partial \alpha}(0, \beta^*) = \left(\frac{\partial p}{\partial t}\right)^* \frac{\partial t(0, \beta^*)}{\partial \alpha} + \left(\frac{\partial p}{\partial \xi}\right)_l^* \frac{\partial \xi(0, \beta^*)}{\partial \alpha}.$$

From (2.6) we have $(\partial p/\partial \xi)_l^* = -(\partial u/\partial t)^*$. Using the expression (3.22) for $(\partial p/\partial \alpha)(0, \beta^*)$ and (3.5) for $(\partial t/\partial \alpha)(0, \beta^*)$, $(\partial \xi/\partial \alpha)(0, \beta^*)$ and noting that by (3.2), $g_l^* = g_l \beta^*$, we obtain (4.4).

Turning now to (4.3), we write the Hugoniot relation at $t > 0$ in the form

$$K(u, p, z, u_+, p_+, \rho_+) = 0, \tag{4.5}$$

where u_+, p_+, ρ_+ are the pre-shock values, u, p are the post-shock values, and z is the value at the shock (observe that for a weak solution of (1.1) z can be discon-

tinuous only acorss the contact discontinuity). The shock speed (in ξ, t) associated with the values in (4.5) is $W_+ = (p - p_+)/(u - u_+)$. Differentiating (4.5) in the shock direction we get

$$\left(\frac{\partial}{\partial t} + W_+ \frac{\partial}{\partial \xi}\right) K(u, p, z, u_+, p_+, \rho_+) = 0. \tag{4.6}$$

Consider now the limit of (4.6) as $t \to 0$. Then clearly $W_+ \to W_r$ and

$$(u, p, z) \to (u^*, p^*, z_r), \qquad (u_+, p_+, \rho_+) \to (u_r, p_r, \rho_r),$$
$$\frac{\partial u}{\partial t} \to \left(\frac{\partial u}{\partial t}\right)^* \qquad \frac{\partial p}{\partial t} \to \left(\frac{\partial p}{\partial t}\right)^*$$

and Eq. (4.6) reduces to the form (4.3). The details of this reduction procedure (which are needed also in the next section) are given in the following propositions, where the basic idea is to replace t-derivatives by ξ-derivatives ahead of the shock and ξ-derivatives by t-derivatives behind it. Q.E.D.

PROPOSITION 4.2. *The limits of time-derivatives behind the shock front are given by*

$$\left(\frac{\partial z}{\partial t}\right)_r^* = -k(e_r^*, \rho_r^*, z_r), \tag{4.7}$$

$$\left(\frac{\partial \rho}{\partial t}\right)_r^* = (c_r^*)^{-2}\left[\left(\frac{\partial p}{\partial t}\right)^* + \lambda(e_r^*, \rho_r^*, z_r)\right], \tag{4.8}$$

where λ is the function introduced in (3.14).

Proof. Equation (4.7) is just the fourth equation of (2.6). To establish (4.8), let us write ρ in terms of p, S, z, so that, along $\xi = \text{const}$,

$$\frac{\partial \rho}{\partial t} = \rho_p \frac{\partial p}{\partial t} + \rho_S \frac{\partial S}{\partial t} + \rho_z \frac{\partial z}{\partial t}$$
$$= c^{-2}\frac{\partial p}{dt} - k\left(\rho_S \frac{\partial S(e, \rho, z)}{\partial z} + \rho_z\right), \tag{4.9}$$

where we have used (2.2) and (2.4). Now, viewing S and p as functions of e, ρ, z and differentiating the identity

$$\rho = \rho(p(e, \rho, z), S(e, \rho, z), z)$$

with respect to z, we get

$$-\rho_p \frac{\partial p(e, \rho, z)}{\partial z} = \rho_S \frac{\partial S(e, \rho, z)}{\partial z} + \rho_z, \tag{4.10}$$

so that (4.9) becomes

$$\frac{\partial \rho}{\partial t} = c^{-2}\left(\frac{\partial p}{\partial t} + k\,\frac{\partial p(e, \rho, z)}{\partial z}\right) = c^{-2}\left(\frac{\partial p}{\partial t} + \lambda(e, \rho, z)\right).$$

Equation (4.8) is now obtained when we take the limit $t \to 0$ behind the shock. Q.E.D.

PROPOSITION 4.3. *The limits of time-derivatives ahead of the shock are given by*

$$\left(\frac{\partial u}{\partial t}\right)_r = -\left(\frac{\partial p}{\partial \xi}\right)_r, \qquad \left(\frac{\partial \rho}{\partial t}\right)_r = -\rho_r^2\left(\frac{\partial u}{\partial \xi}\right)_r, \tag{4.11}$$

$$\left(\frac{\partial p}{\partial t}\right)_r = -g_r^2\left(\frac{\partial u}{\partial \xi}\right)_r - \lambda(e_r, \rho_r, z_r). \tag{4.12}$$

Proof. Equations (4.11) follow directly from (2.6). As for (4.12), we repeat the argument of (4.9). So, expressing p in terms of ρ, S, z we have

$$\begin{aligned}\frac{\partial p}{\partial t} &= c^2\frac{\partial \rho}{\partial t} + p_S\frac{\partial S}{\partial t} + p_z\frac{\partial z}{\partial t}\\ &= -g^2\frac{\partial u}{\partial \xi} - k\left(p_S\frac{\partial S(e, \rho, z)}{\partial z} + p_z\right)\\ &= -g^2\frac{\partial u}{\partial \xi} - k\cdot\frac{\partial}{\partial z}\,p(e, \rho, z),\end{aligned}$$

which yields (4.12) in the limit $t \to 0$. Q.E.D.

Finally, we deal with the transformation of spatial derivatives to time derivatives behind the shock.

PROPOSITION 4.4. *The limits of spatial derivatives of flow variables behind the shock are given by*

$$\left(\frac{\partial p}{\partial \xi}\right)_r^* = -\left(\frac{\partial u}{\partial t}\right)^* \tag{4.13}$$

$$\left(\frac{\partial u}{\partial \xi}\right)_r^* = -(g_r^*)^{-2}\left[\left(\frac{\partial p}{\partial t}\right)^* + \lambda(e_r^*, \rho_r^*, z_r)\right], \tag{4.14}$$

$$\left(\frac{\partial z}{\partial \xi}\right)_r^* = \left(\frac{\partial z}{\partial \xi}\right)_r + W_r^{-1}\,[k(e_r^*, \rho_r^*, z_r) - k(e_r, \rho_r, z_r)], \tag{4.15}$$

$$\left(\frac{\partial \rho}{\partial \xi}\right)_r^* = 3\left(\frac{\partial u}{\partial t}\right)^* W_r^{-2}(\rho_r^*)^2$$

$$-\left(\frac{\partial p}{\partial t}\right)^* [(\rho_r^*)^2 W_r^{-3} + 3(c_r^*)^{-2} W_r^{-1}]$$

$$+3\left(\frac{\partial p}{\partial \xi}\right)_r W_r^{-2}(\rho_r^*)^2$$

$$\left(\frac{\partial u}{\partial \xi}\right)_r$$

$$+\left(\frac{\partial \rho}{\partial \xi}\right)_r \cdot \left(\frac{\rho_r^*}{\rho_r}\right)^2 - \lambda(e_r, \rho_r, z_r) W_r^{-3}(\rho_r^*)^2$$

$$-3\lambda(e_r^*, \rho_r^*, z_r) \cdot (c_r^*)^{-2} W_r^{-1}, \tag{4.16}$$

where, again, λ *is as in* (3.14).

Proof. Equation (4.13) follows from (2.6) and (4.14) is identical to (4.12) when pre-shock values are replaced by post-shock values. To obtain (4.15) we use the continuity of z across the shock which implies also the continuity of $(\partial/\partial t + W_r(\partial/\partial \xi))z$. Using (2.6) for the time derivatives we get (4.15). Finally, to extablish (4.16) we again differentiate a well-known identity [5] along the shock trajectory to get (compare (4.6)),

$$\left(\frac{\partial}{\partial t} + W_+ \frac{\partial}{\partial \xi}\right)\left[(p - p_+)\left(\frac{1}{\rho_+} - \frac{1}{\rho}\right) - (u - u_+)^2\right] = 0.$$

Letting $t \to 0$ and replacing post-shock ξ-derivatives (resp. pre-shock t-derivatives) by t-derivatives (resp. ξ-derivatives) in accordance with the previous results we get (4.16) as the limit of $\partial \rho / \partial \xi$. Q.E.D.

Remark. Note that by (4.6) the derivative $(\partial \rho/\partial \xi)_r^*$ is not needed for the Lagrangian solution. However, it will be needed in the Eulerian treatment.

5. The Eulerian Solution of the GRP

In this section we take up our main goal in this paper, the solution of the GRP for the Eulerian system (1.1), in the sense of (1.2).

We assume again the setup of Fig. 1, with the jump located initially at $x = 0$. As an auxiliary tool in the derivation we shall use the Lagrangian coordinate ξ defined by (2.5). As was demonstrated in the previous sections the time derivatives at the singularity depend only on the spatial slopes as $\xi \to 0$. Thus we are justified in

assuming that the initial values of flow variables are simultaneously piecewise linear in x and ξ, with slopes related by

$$\left(\frac{\partial Q}{\partial \xi}\right)_l = \rho_l^{-1}\left(\frac{\partial Q}{\partial x}\right)_l, \qquad \left(\frac{\partial Q}{\partial \xi}\right)_r = \rho_r^{-1}\left(\frac{\partial Q}{\partial x}\right)_r, \tag{5.1}$$

for any variable Q.

In addition to the notation introduced in Section 2 we use here the notation U_0, $(\partial U/\partial t)_0$ for the limiting values of $U(0, t)$ and its derivative as $t \to 0+$ (see (1.2)). Recall that U_0 is determined already by the associated RP (1.3), so we regard it as known in the present context, in complete analogy with V^* in the Lagrangian case. Thus, in this section we focus on the evaluation of $(\partial U/\partial t)_0$.

Using the Lagrangian transformation (2.5) and (5.1) we can now use the results of Theorem 4.1 and Proposition 4.2 in order to determine the time derivatives $(\partial Q/\partial t)^*$ of any flow variable Q along the contact discontinuity (including the discontinuous ones, for which we have right and left values of the derivative).

Let $\xi = \xi(t)$ be the Lagrangian representation of the line $x = 0$. It is easily seen that

$$\frac{d\xi}{dt} = -\rho(\xi(t), t) \cdot u(\xi(t), t), \qquad \xi(0) = 0. \tag{5.2}$$

Indeed, (5.2) follows by differentiating the identity $x(\xi(t), t) = 0$ and noting (2.5). Clearly, the value of the right-hand side in (5.2) at $t = 0$ is determined by U_0.

Suppose first that the line $x = 0$ (or, equivalently, $\xi = \xi(t)$) is *not* contained in the rarefaction fan. Then the chain rule and (5.2) imply, for any variable Q,

$$\left(\frac{\partial Q}{\partial t}\right)_0 = \lim_{t \to 0}\left(\frac{\partial}{\partial t} Q(\xi, t) - \rho_0 u_0 \frac{\partial}{\partial \xi} Q(\xi, t)\right) \qquad \text{along} \quad \xi = \xi(t). \tag{5.3}$$

Again, all derivatives in the right-hand side are known from U_0 and the results of Section 4. Indeed, the ξ-derivatives are treated in Proposition 4.4 (the expressions for $(\partial u/\partial \xi)_l^*$, $(\partial p/\partial \xi)_l^*$ are completely analogous to (4.13), (4.14), and the expression for $(\partial \rho/\partial \xi)_l^*$ is obtained by using the chain rule $(\partial \rho/\partial \alpha)(0, \beta^*) = (\partial \rho/\partial t)_l^* \cdot (\partial t/\partial \alpha)(0, \beta^*) + (\partial \rho/\partial \xi)_l^* \cdot (\partial \xi/\partial \alpha)(0, \beta^*)$ in conjunction with (3.22), (4.8)).

The fact that $x = 0$ is not contained in a rarefaction fan means that there is no characteristic curve (= "sonic signal") parallel to it, so that we can formulate our result as

THEOREM 5.1 (Non-sonic case). *In the non-sonic case the Eulerian solution to the GRP is given by the Lagrangian solution to the GRP (discussed in Section 4) and the chain rule (5.3).*

Next we discuss the *sonic* case. Here the line $x = 0$ is tangent at the origin to a curve of the Γ^--rarefaction fan (or, equivalently, coincides with a straight

Γ^--characteristic for the associated RP). The formula (5.3) is now meaningless since the involved derivatives blow up as we approach the singularity. We are forced, therefore, to replace the (ξ, t) representation by the more refined characteristic structure (α, β) which was introduced in Section 3.

Let $(\alpha(t), \beta(t))$ be the trajectory $x=0$ in the (α, β) plane. Our assumption that $x=0$ is sonic implies that

$$\alpha(0)=0, \qquad \beta(0)=\beta_0, \tag{5.4}$$

where

$$u(0, \beta_0)=c(0, \beta_0). \tag{5.5}$$

In (5.5) and throughout the rest of this section we are using the characteristic notation of Section 3.

The relation (5.5) determines β_0 uniquely and instead of (5.3) we have the formula

$$\left(\frac{\partial Q}{\partial t}\right)_0=\frac{\partial Q}{\partial \alpha}(0, \beta_0)\cdot\alpha'(0)+\frac{\partial Q}{\partial \beta}(0, \beta_0)\cdot\beta'(0). \tag{5.6}$$

We may now summarize the sonic case by the following theorem.

THEOREM 5.2 (Sonic case). *In the sonic case the Eulerian solution to the GRP is given by* (5.6), *where* β_0 *is determined in* (5.5), *the derivatives* $(\partial Q/\partial\beta)(0, \beta_0)$ *are evaluated from the associated RP, the derivatives* $(\partial Q/\partial\alpha)(0, \beta_0)$ *are obtained by* (3.8), (3.15) *and* (3.22), *and the slope* $(\alpha'(0), \beta'(0))$ *is given by*

$$\alpha'(0)=-g_l\beta_0^{1/2}, \tag{5.7}$$

$$\beta'(0)=\frac{1}{2}\beta_0^{1/2}\left[\frac{\partial g}{\partial \alpha}(0, \beta_0)-\frac{\partial(\rho u)}{\partial \alpha}(0, \beta_0)\right]. \tag{5.8}$$

(*The derivatives in* (5.8) *are given in* (3.22).)

Proof. To prove (5.7) we differentiate the identity $t=t(\alpha(t), \beta(t))$, using (3.5), and let $t\to 0$:

$$1=\frac{\partial t}{\partial \alpha}(0, \beta_0)\cdot\alpha'(0)+\frac{\partial t}{\partial \beta}(0, \beta_0)\cdot\beta'(0)=-g_l^{-1}\beta_0^{-1/2}\cdot\alpha'(0).$$

The proof of (5.8) is longer. First, we use the expressions (3.5) in $\partial\xi/\partial\alpha=-g(\partial t/\partial\alpha)$ and drop all terms which are $O(\alpha^2)$. We obtain

$$\beta^{1/2}+2\alpha\varepsilon(0, \beta)=-g(0, \beta)\cdot[-g_l^{-1}\beta^{-1/2}+2\alpha\eta(0, \beta)]+\frac{\partial g}{\partial \alpha}(0, \beta)\cdot(g_l^{-1}\beta^{-1/2})\cdot\alpha,$$

and since $g(0, \beta) = g_l \beta$ (see (3.2)), we get

$$\varepsilon(0, \beta) + g_l \beta \eta(0, \beta) = \frac{1}{2} g_l^{-1} \beta^{-1/2} \frac{\partial g}{\partial \alpha}(0, \beta). \tag{5.9}$$

Next, let $\xi = \xi(t)$ be the Lagrangian representation of $(\alpha(t), \beta(t))$. We have

$$\begin{aligned} \xi'(t) &= \frac{\partial \xi}{\partial \alpha} \alpha'(t) + \frac{\partial \xi}{\partial \beta} \beta'(t) \\ &= (\beta^{1/2} + 2\alpha\varepsilon(\alpha, \beta)) \cdot \alpha'(t) + \tfrac{1}{2}\alpha\beta^{-1/2}\beta'(t) + O(\alpha^2). \end{aligned} \tag{5.10}$$

On the other hand, using (5.2), (5.4) we have

$$\begin{aligned} \xi'(t) &= -\rho u(\xi(t), t) = -(\rho u)(0, \beta_0) - \frac{\partial}{\partial \alpha}(\rho u)(0, \beta_0) \cdot \alpha(t) \\ &\quad - \frac{\partial}{\partial \beta}(\rho u)(0, \beta_0) \cdot (\beta(t) - \beta_0) + O(t^2). \end{aligned} \tag{5.11}$$

But $(\partial/\partial\beta)(\rho u)(0, \beta_0) = 0$ by (5.5) and the characteristic relation $dp + g\, du = c^2\, d\rho + \rho c\, du = 0$ along $\alpha = 0$. Thus, equating first-order terms in (5.10), (5.11) we have

$$\alpha'(0)\beta'(0)\beta_0^{-1/2} + \beta_0^{1/2}\alpha''(0) + 2\varepsilon(0, \beta_0)\, \alpha'(0)^2 = -\alpha'(0) \cdot \frac{\partial}{\partial \alpha}(\rho u)(0, \beta_0). \tag{5.12}$$

Similarly, in analogy with (5.10)–(5.12), the identity $1 = (\partial t/\partial \alpha)\, \alpha'(t) + (\partial t/\partial \beta)\, \beta'(t)$ yields (taking first-order terms in t)

$$g_l^{-1} \cdot \alpha'(0)\, \beta'(0)\, \beta_0^{-3/2} + 2\alpha'(0)^2 \eta(0, \beta_0) - g_l^{-1} \alpha''(0)\, \beta_0^{-1/2} = 0. \tag{5.13}$$

Multiply (5.13) by $g_l \beta_0$ and add to (5.12) to obtain

$$2\alpha'(0)\, \beta'(0)\, \beta_0^{-1/2} + 2\alpha'(0)^2 [\varepsilon(0, \beta_0) + g_l \beta_0 \eta(0, \beta_0)] = -\alpha'(0) \frac{\partial}{\partial \alpha}(\rho u)(0, \beta_0).$$

The last equation, in conjunction with (5.7) and (5.9), implies (5.8). Q.E.D.

This concludes the discussion of the Eulerian solution to the GRP in all cases.

6. A Special Case: γ-Law Gas and a Simplified Arrhenius Model

In this section we specialize to the case that the equation of state is given by

$$p = (\gamma - 1)\, \rho(e - q_0 z), \qquad \gamma > 1, \quad q_0 > 0, \tag{6.1}$$

where the constant q_0 is the (chemical) energy released when a unit mass of unburnt gas is totally burnt. We take $\gamma > 1$ to be a given fixed constant.

Remark. In taking γ to be independent of z (and, in particular, the same for burnt and unburnt gas) we are following Chorin [3] and Colella, Majda, and Roytburd [4]. For a (presumably) more realistic model where $\gamma = \gamma(z)$ the entropy can still be taken as in (6.2) below and so is the speed of sound, but for the rest of the treatment one has to go back to the general discussion of the preceding sections.

It is immediate from our definition of entropy (2.1), combined with (6.1), that we can take

$$S = \frac{1}{\gamma - 1} \cdot \frac{p}{\rho^\gamma} = \rho^{1-\gamma}(e - q_0 z). \tag{6.2}$$

In addition to Eq. (6.1), and again following [3, 4], here we shall take a simplified Arrhenius model, where the reaction rate is a step function depending on temperature, which we take here as p/ρ. Thus, we assume

$$k = KzH(T - T_c), \qquad K > 0, \qquad T = p/\rho, \tag{6.3}$$

where

$$H(x) = \begin{cases} 1, & x > 0, \\ 0, & x \leqslant 0, \end{cases}$$

and T_c is a given ("critical") temperature. The function f in (2.4) is given now by

$$f = -Kq_0 \rho^{1-\gamma} z H(T - T_c), \qquad T = p/\rho, \tag{6.4}$$

and the function λ of (3.14) can be conveniently expressed in terms of ρ, p, z as

$$\lambda(\rho, p, z) = -(\gamma - 1)\, Kq_0 \rho z H(T - T_c). \tag{6.5}$$

In the rest of this section we give the explicit versions of the formulae appearing in the preceding sections when specialized to the present model. We start with the solution of the centered rarefaction wave for the associated RP (see Section 3).

PROPOSITION 6.1. *Let the coordinate β be defined by* (3.1). *For the γ-law case, the values at the singularity* ($\alpha = 0$) *are given by*

$$p(0, \beta) = p_l \beta^{2\gamma/(\gamma+1)}, \qquad \rho(0, \beta) = \rho_l \beta^{2/(\gamma+1)}, \qquad c(0, \beta) = c_l \beta^{(\gamma-1)/(\gamma+1)}, \tag{6.6}$$

$$u(0, \beta) = u_l + \frac{2c_l}{\gamma - 1}(1 - \beta^{(\gamma-1)/(\gamma+1)}). \tag{6.7}$$

Proof. The expressions in (6.6) follow from $g(0, \beta) = g_l \beta$ and the relations,

$$g = g_l \cdot \left(\frac{p}{p_l}\right)^{(\gamma+1)/2\gamma}, \qquad p = p_l \cdot \left(\frac{\rho}{\rho_l}\right)^\gamma,$$

which hold identically along $\alpha = 0$, where S and z are constant by (3.4). To obtain (6.7), write the characteristic relation (2.8) at the singularity (where $dt = 0$) as $du + (2/(\gamma - 1))\, dc = 0$. Q.E.D.

Next, we give the explicit versions of (3.8). By (6.6) we have

$$T(0, \beta) = \frac{p(0, \beta)}{\rho(0, \beta)} = T_l \cdot \beta^{2(\gamma-1)/(\gamma+1)}.$$

Corresponding to the "critical" temperature T_c we have β_c defined by

$$T(0, \beta_c) = T_c, \tag{6.8}$$

so that we have from (6.3)–(6.6),

$$\begin{aligned} &\text{(i)} \quad k(p(0, \beta), S_l, z_l) = K z_l H(\beta - \beta_c), \\ &\text{(ii)} \quad f(p(0, \beta), S_l, z_l) = -K q_0 z_l \rho_l^{1-\gamma} \beta^{-2(\gamma-1)/(\gamma+1)} H(\beta - \beta_c), \end{aligned} \tag{6.9}$$

$$\lambda(0, \beta) = -(\gamma - 1) K q_0 \rho_l z_l \cdot \beta^{2/(\gamma+1)} H(\beta - \beta_c). \tag{6.10}$$

Equation (3.8) now takes the form

$$\frac{d}{d\beta}(\beta^{-1/2} S_\alpha(0, \beta)) = K q_0 z_l g_l^{-1} \rho_l^{1-\gamma} \beta^{-4\gamma/(\gamma+1)} H(\beta - \beta_c),$$

$$\frac{d}{d\beta}(\beta^{-1/2} z_\alpha(0, \beta)) = -K g_l^{-1} z_l \beta^{-2} H(\beta - \beta_c),$$

which implies

$$S_\alpha(0, \beta) = \begin{cases} \beta^{1/2} S_\alpha(0, 1), & \beta_c \geqslant 1 \\ \beta^{1/2} \cdot \left\{ S_\alpha(0, 1) - \dfrac{\gamma + 1}{3\gamma - 1} K q_0 z_l g_l^{-1} \rho_l^{1-\gamma} (\beta^{(1-3\gamma)/(\gamma+1)} - 1) \right\}, & 1 > \beta \geqslant \beta_c, \\ \beta^{1/2} \cdot \beta_c^{-1/2} S_\alpha(0, \beta_c), & \beta < \beta_c < 1. \end{cases} \tag{6.11}$$

$$z_\alpha(0, \beta) = \begin{cases} \beta^{1/2} z_\alpha(0, 1) & \beta_c \geqslant 1, \\ \beta^{1/2} \cdot \{ z_\alpha(0, 1) + K g_l^{-1} z_l (\beta^{-1} - 1) \}, & 1 > \beta \geqslant \beta_c, \\ \beta^{1/2} \cdot \beta_c^{-1/2} z_\alpha(0, \beta_c), & \beta < \beta_c < 1, \end{cases} \tag{6.12}$$

along with the initial conditions (see (3.9)),

$$\begin{aligned} S_\alpha(0, 1) &= \left(\frac{\partial S}{\partial \xi} \right)_l - K q_0 z_l g_l^{-1} \rho_l^{1-\gamma} H(1 - \beta_c), \\ z_\alpha(0, 1) &= \left(\frac{\partial z}{\partial \xi} \right)_l + K z_l g_l^{-1} H(1 - \beta_c). \end{aligned} \tag{6.13}$$

Remark. Note that by (6.2) we obtain further,

$$\left(\frac{\partial S}{\partial \xi}\right)_l = \frac{1}{\gamma - 1}\left(\frac{\partial}{\partial \xi}\frac{p}{\rho^\gamma}\right)_l = \frac{1}{\gamma - 1}\left[\rho_l^{-\gamma}\left(\frac{\partial p}{\partial \xi}\right)_l - \gamma p_l \rho_l^{-\gamma - 1}\left(\frac{\partial \rho}{\partial \xi}\right)_l\right]$$

$$= \frac{1}{(\gamma - 1)\rho_1^\gamma}\left[\left(\frac{\partial p}{\partial \xi}\right)_l - c_l^2\left(\frac{\partial \rho}{\partial \xi}\right)_l\right]. \tag{6.14}$$

We can now proceed to provide the explicit solution for the CRW, corresponding to the general Theorem 3.3.

THEOREM 6.2. *For the γ-law case, the function $A(\beta)$ of* (3.16) *is given by*

$$A(\beta) = -\frac{1}{2} g_l^{-2}\left[\frac{d}{d\beta}(\beta^{-3/2}\lambda(0, \beta)) + \frac{1}{2}\beta^{-5/2}\lambda(0, \beta)\right]$$

$$-\frac{c_l}{2\gamma(\gamma + 1) S_l}\beta^{-2/(\gamma + 1)} S_\alpha(0, \beta). \tag{6.15}$$

Assuming the form (6.3) *for the reaction rate function, we obtain for $a(\beta)$ the following explicit form*:

$$a(\beta) = a(1) - \frac{c_l}{(3\gamma - 1)\gamma S_l}\left(\frac{\partial S}{\partial \xi}\right)_l \cdot (\beta^{(3\gamma - 1)/2(\gamma + 1)} - 1), \qquad \beta_c \geqslant 1,$$

$$a(\beta) = a(1) - \frac{\gamma(3\gamma - 5)}{(3\gamma - 1)^2} g_l^{-2}\lambda(0, 1)\cdot(\beta^{(1 - 3\gamma)/2(\gamma + 1)} - 1) \tag{6.16}$$

$$-\frac{\gamma - 1}{3\gamma - 1} g_l^{-1}\rho_l^\gamma\left[\left(\frac{\partial S}{\partial \xi}\right)_l + \frac{2}{3\gamma - 1} g_l^{-1}\rho_l^{-\gamma}\cdot\lambda(0, 1)\right]\cdot(\beta^{(3\gamma - 1)/2(\gamma + 1)} - 1),$$

$$1 > \beta \geqslant \beta_c, \tag{6.17}$$

$$a(\beta) = a(\beta_c + 0) + \frac{1}{2} g_l^{-2}\cdot\lambda(0, 1)\beta_c^{(1 - 3\gamma)/2(\gamma + 1)} - \frac{\gamma - 1}{3\gamma - 1} g_l^{-1} p_l^\gamma \beta_c^{-1/2} S_\alpha(0, \beta_c)$$

$$\cdot(\beta^{(3\gamma - 1)/2(\gamma + 1)} - \beta_c^{(3\gamma - 1)/2(\gamma + 1)}), \qquad \beta < \beta_c < 1. \tag{6.18}$$

Proof. It follows from (6.2) that

$$g = \rho c = (\gamma p \rho)^{1/2} = \gamma^{1/2}(\gamma - 1)^{-1/2\gamma} p^{(\gamma + 1)/2\gamma} S^{-1/2\gamma},$$

so that

$$g_S(0, \beta) = -\frac{1}{2\gamma}\frac{g(0, \beta)}{S_l} = -\frac{g_l \beta}{2\gamma S_l}, \qquad g_z \equiv 0.$$

Also, by (6.7) we have $(d/d\beta)u(0,\beta) = -(2c_l/(\gamma+1))\beta^{-2/(\gamma+1)}$. Inserting these expressions in (3.16), we get (6.15). The expressions (6.16)–(6.18) are now obtained by integrating $A(\beta)$, noting the expressions (6.10), (6.11) for $\lambda(0,\beta)$, $S_\alpha(0,\beta)$, respectively. Q.E.D.

Remark. Note that the assumption $\beta_c \geqslant 1$ means that no reaction takes place throughout the rarefaction wave, so that (6.16) coincides with the corresponding formula for the planar non-reactive case [1].

Finally we discuss the form assumed by (4.6) in the γ-law case, thus providing explicit expressions for a_r, b_r, d_r in (4.3).

THEOREM 6.3. *In the case of a γ-law equation of state, the coefficients a_r, b_r, d_r in* (4.3) *are given by, with* $\mu^2 = (\gamma-1)/(\gamma+1)$,

$$a_r = 2 - \frac{1}{2}\frac{p^* - p_r}{p^* + \mu^2 p_r}, \tag{6.19}$$

$$b_r = \frac{1}{2}\frac{u^* - u_r}{p^* + \mu^2 p_r} - (g_r^*)^{-2} W_r - W_r^{-1}, \tag{6.20}$$

$$d_r = L_u \cdot \left(\frac{\partial u}{\partial \xi}\right)_r + L_p \cdot \left(\frac{\partial p}{\partial \xi}\right)_r + L_\rho \left(\frac{\partial \rho}{\partial \xi}\right)_r + L_\lambda, \tag{6.21}$$

where

$$L_u = \frac{1}{2}(u^* - u_r)\left(\rho_r + \frac{\mu^2 g_r^2}{p^* + \mu^2 p_r}\right) + g_r^2 W_r^{-1} + W_r,$$

$$L_p = -2 - \frac{1}{2}\frac{\mu^2(p^* - p_r)}{p^* + \mu^2 p_r},$$

$$L_\rho = -\frac{1}{2}\frac{p^* - p_r}{\rho_r},$$

$$L_\lambda = \lambda_r W_r^{-1}\left(\frac{\mu^2}{2}\frac{p^* - p_r}{p^* + \mu^2 p_r} + 1\right) + (g_r^*)^{-2} W_r \lambda_r^*,$$

$$\lambda_r = \lambda(e_r, \rho_r, z_r), \qquad \lambda_r^* = \lambda(e_r^*, \rho_r^*, z_r).$$

Proof. As noted already, the Rankine–Hugoniot jump conditions for the system (1.1) imply that z is continuous across shocks. Thus, for the equation of state (6.1), the term $q_0 z$ is an additive constant, the same on both sides of the shock (this is definitely different from the way "sharp" detonation and deflagration waves are treated, as in [5]), Hence, the Hugoniot relation (4.5) has the same form as for the non-reactive case and is given by the well-known formula [5],

$$K(u, p, z, u_+, p_+, \rho_+) = u - u_+ - (p - p_+)\left[\frac{1-\mu^2}{\rho_+(p + \mu^2 p_+)}\right]^{1/2}. \tag{6.22}$$

Differentiating this expression as indicated in (4.6) and using the transformations between ξ-derivatives and t-derivatives as in Propositions 4.2–4.4 we obtain a linear relation of the type (4.3), with the coefficients given by (6.19)–(6.21). Q.E.D.

7. A Numerical Example

In the Introduction ((1.5), (1.6)) we have outlined a numerical scheme based on the analysis presented in this paper. Such a scheme (which we call a GRP-scheme) is indeed a straightforward implementation of the formulas derived here for the time derivatives of flow variables at cell boundaries. For the non-reactive case, including "quasi" one-dimensional flows, the GRP scheme was used successfully in a variety of test problems [1, 2].

The point we want to emphasize here is that the differencing of the reaction equation (the fourth equation in (1.1)) seems to be crucial in obtaining a stable "physical" solution. In fact, we shall show that rather small variations of the difference scheme lead to completely different weak solutions of the system (i.e., weak detonations followed by shocks as opposed to a C-J detonation).

We start by discussing the difference scheme (1.5), (1.6) in some more detail. First, using the explicit formulas in Theorem 4.1 and Proposition 4.2, we obtain the time-derivatives $(\partial\rho/\partial t)^n_{i+1/2}$, $(\partial p/\partial t)^n_{i+1/2}$, and $(\partial u/\partial t)^n_{i+1/2}$ (we are using the notation of (1.2)). This enables us to determine the fluxes for the first two equations in (1.1), thus obtaining ρ_i^{n+1} and u_i^{n+1}. Turning now to the last two equations of (1.1), we see that their fluxes depend on the evolution of the mass-fraction z (recall that e is a function of z). Let us now specialize to the simplified Arrhenius model, where k is given by (6.3).

If $\Delta t = t^{n+1} - t^n$, then $K \cdot \Delta t$ is (roughly) the amount by which z decreases in one time step (provided that $T > T_C$). Note that the CFL-condition for the system (1.1) does not depend on K. However, for a time step which is of the order of magnitude of K^{-1} or bigger, a conceivable "explicit" scheme would yield a detonation moving at a speed of one cell/time step. This can be a very high speed, manifesting itself as a "weak detonation," namely, a non-physical solution. Thus, in an attempt to avoid this situation, we have tried two different schemes for the solution of the last two equations of (1.1).

(a) *The "explicit" scheme.* Here $(\rho z)^{n+1/2}_{i+1/2}$ is evaluated explicitly as in (1.6). Similarly, using (6.3) we evaluate

$$(k\rho)_i^{n+1/2} = \tfrac{1}{2}K[(\rho z)^{n+1/2}_{i+1/2} + (\rho z)^{n+1/2}_{i-1/2}] \cdot H(T_i^n - T_C). \tag{7.1}$$

The fourth equation in (1.1) is now differenced as

$$(\rho z)_i^{n+1} - (\rho z)_i^n = -\frac{\Delta t}{\Delta x}[(\rho zu)^{n+1/2}_{i+1/2} + (\rho zu)^{n+1/2}_{i-1/2}] - \Delta t \cdot (k\rho)_i^{n+1/2}. \tag{7.2}$$

Combined with a similar explicit equation for e_i^{n+1}, one determines e_i^{n+1}, z_i^{n+1}. The procedure is then iterated once by modifying (7.1) as

$$(k\rho)_i^{n+1/2} = \frac{1}{2} K[(\rho z)_{i+1/2}^{n+1/2} + (\rho z)_{i-1/2}^{n+1/2}] \cdot H\left(\frac{T_i^{n+1} + T_i^n}{2} - T_c\right) \qquad (7.1)'$$

and then repeating (7.2).

(b) *The "implicit" scheme.* Here we are more specific about using the form (6.3) for k. The fluxes $(\rho zu)_{i+1/2}^{n+1/2}$ are calculated as before, but instead of (7.2) we get

$$(\rho z)_i^{n+1} - (\rho z)_i^n = -\frac{\Delta t}{\Delta x}[(\rho zu)_{i+1/2}^{n+1/2} - (\rho zu)_{i-1/2}^{n+1/2}]$$

$$-\frac{\Delta t}{2} \cdot K \cdot [(\rho z)_i^{n+1} H(T_i^{n+1} - T_c) + (\rho z)_i^n H(T_i^n - T_c)]. \qquad (7.3)$$

Together with the energy equation, we can solve for e_i^{n+1}, z_i^{n+1} (observe that p_i^{n+1}, and hence T_i^{n+1}, can be expressed by (6.1)) by iterations. In practice, we iterate only once. Note that essentially (7.3) contains a modification of the "source term" (7.1), but because it is iterated only once, the two schemes are quite close to each other (compare the "source terms" in (7.3) and (7.1)').

As a test case we have chosen the case of ozone decomposition C-J detonation discussed in [4]. The equation of state here is given by (6.1)–(6.3), where (in CGS units),

$$\gamma = 1.4, \qquad q_0 = 0.5196 \times 10^{10}, \qquad K = 0.5825 \times 10^{10}, \qquad T_c = 0.1155 \times 10^{10}.$$

The initial data was taken as the piecewise constant data defining a C-J detonation as a single wave (recall that in the Chapman–Jouguet model a C-J detonation corresponds to a sonic detonation, or, in other words, a sharp reaction wave that moves at minimal speed relative to the unburnt gas. See [5] for more details). The initial state was given by

$$(p, \rho, u, z) = \begin{cases} (p_0, \rho_0, 0, 1), & x > 50 \cdot \Delta x \\ (p_{cJ}, \rho_{cJ}, u_{cJ}, 0), & x < 50 \cdot \Delta x \end{cases}'$$

where $p_0 = 8.321 \times 10^5$, $\rho_0 = 1.201 \times 10^{-3}$, and $p_{cJ} = 6.270 \times 10^6$, $\rho_{cJ} = 1.945 \times 10^{-3}$, $u_{cJ} = 4.162 \times 10^4$.

Observe that the values p_{cJ}, ρ_{cJ}, u_{cJ} depend only on p_0, ρ_0, and q_0 (and not on K or T_c). The speed of the sharp front (in the Chapman–Jouguet theory) in this case is $D_{cJ} = 1.088 \times 10^5$.

If we take (following [4]) the atmospheric data as

$$p_{atm} = 1.0135 \times 10^6, \qquad \rho_{atm} = 1.29 \times 10^{-3},$$

then our C-J point is given by

$$p_{cJ} = 6.19 p_{atm}, \qquad \rho_{cJ} = 1.51 \rho_{atm}.$$

We mention that our C-J point is different from the one reported in [4]. This may be attributed to a discrepancy in p_0, ρ_0, or q_0. Thus, a full comparison is not possible. However, the main numerical phenomena seem to be the same.

Our calculations were made on an equally spaced mesh of 100 cells. To follow the moving wave, we keep eliminating mesh points at the left end and adding new mesh points at the right end, so as to keep the front always at (roughly) the middle point. Obviously, eliminating cells at the left poses a problem for the appropriate "in-flux boundary conditions." We have simply taken for these conditions the values at the last eliminated cell. Since this was done a large number of times during the course of one calculation, it might explain (at least partially) the appearance of oscillations in the flow profiles displayed below.

We now recall briefly the structure of a detonation wave in the Z-N-D model for the solution of (1.1) (see [4, 5] for more details). The wave (corresponding to a C-J sharp front in the Chapman–Jouguet theory) consists of a reaction zone of finite width moving at the C-J speed, across which the mass-fraction z varies from $z = 1$ to $z = 0$. The edge of the reaction zone facing the unburnt ($z = 1$) gas is a fluid-dynamical shock wave which raises the pressure and density to values significantly higher than the C-J values. We refer to this shock as the "Z-N-D spike." Following the spike, the pressure and density drop monotonically and continuously to their C-J values at the other edge of the reaction zone.

In our test-case the width of the reaction zone is approximately 5×10^{-5} cm and the Z-N-D spike values are approximately

$$p_{ZND} \approx 9.62 p_{atm}, \qquad \rho_{ZND} \approx 2.53 \rho_{atm}.$$

We ran the test case for the following values of Δx:

$$\Delta x = 5 \times 10^{-6}, \qquad 5 \times 10^{-5}, \qquad 5 \times 10^{-4}, \qquad 5 \times 10^{-1}.$$

These values correspond, respectively, to Figs. 8b, c, d, and e in [4] and should be compared with them.

In our results we display profiles of velocity, pressure, density, and the mass fraction z. Recall that we are using a frame of 100 cells, creating cells at the right and eliminating cells at the left, so as to capture the reaction zone at the middle.

Figure 2a gives the results for an explicit calculation with $\Delta x = 5 \times 10^{-6}$ cm, $\Delta t = 5 \times 10^{-12}$ s, after 2000 cycles. There are approximately 10 cells in the reaction zone, and the Z-N-D spike is clear and at its correct peak. In Fig. 2b we display the results for an implicit calculation again with $\Delta x = 5 \times 10^{-6}$ cm but $\Delta t = 10^{-11}$ s, after 1000 cycles. Thus, the implicit scheme allows for a time step which is twice as big as that needed for the explicit scheme.

In Figs. 3a, b we give the results for the explicit and implicit calculations, respectively, with $\Delta x = 5 \times 10^{-5}$ cm. Thus, the reaction zone is roughly of the same size

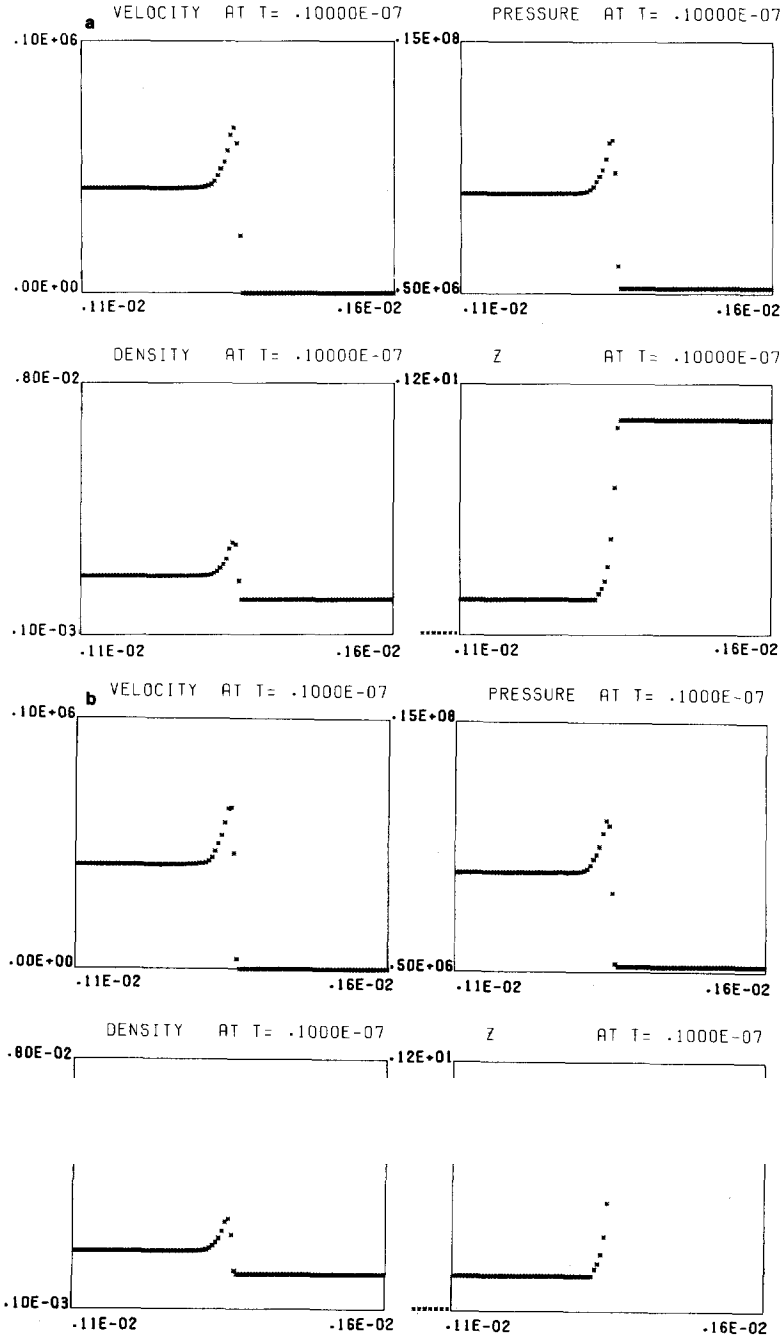

FIG. 2. (a) C-J wave, explicit scheme, reaction zone ≈ 10 cells; (b) C-J wave, implicit scheme, reaction zone ≈ 10 cells.

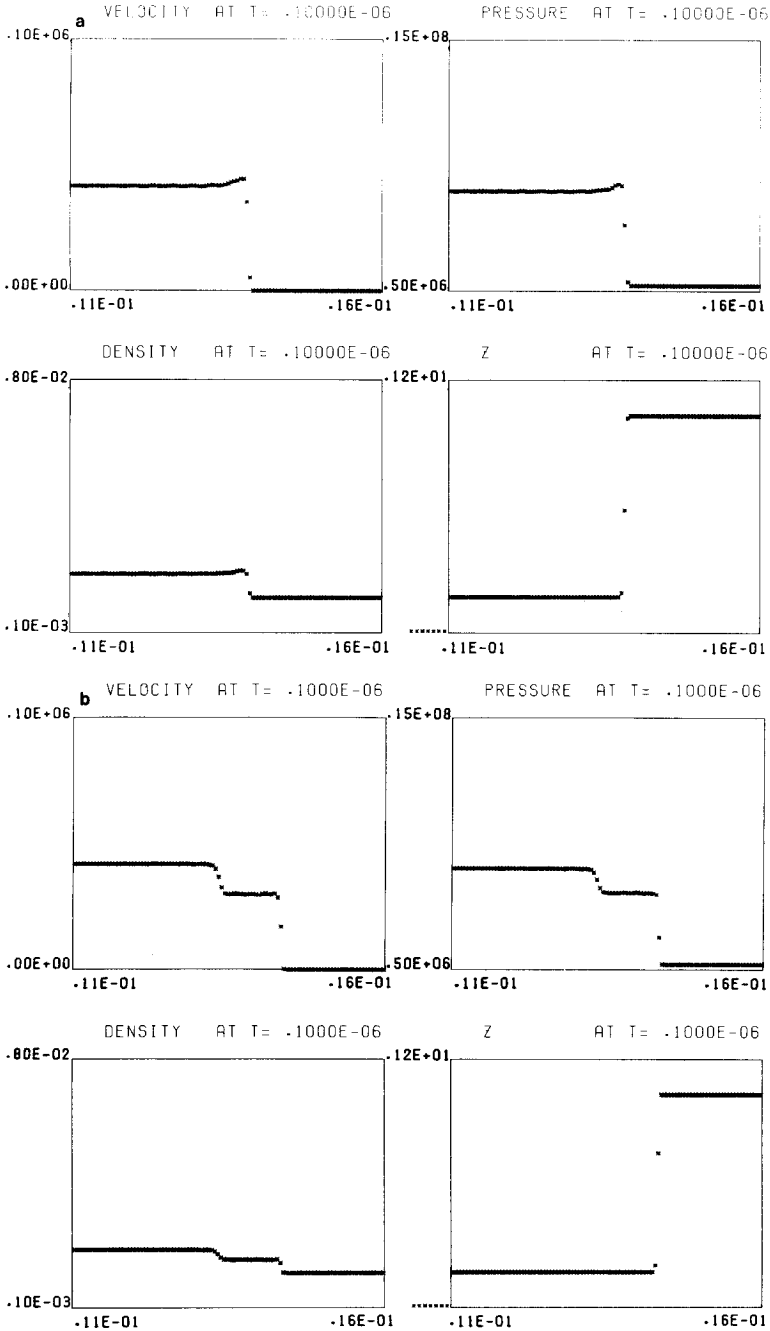

FIG. 3. (a) C-J wave, explicit scheme, reaction zone ≈ 1 cell; (b) C-J wave, implicit scheme, reaction zone ≈ 1 cell.

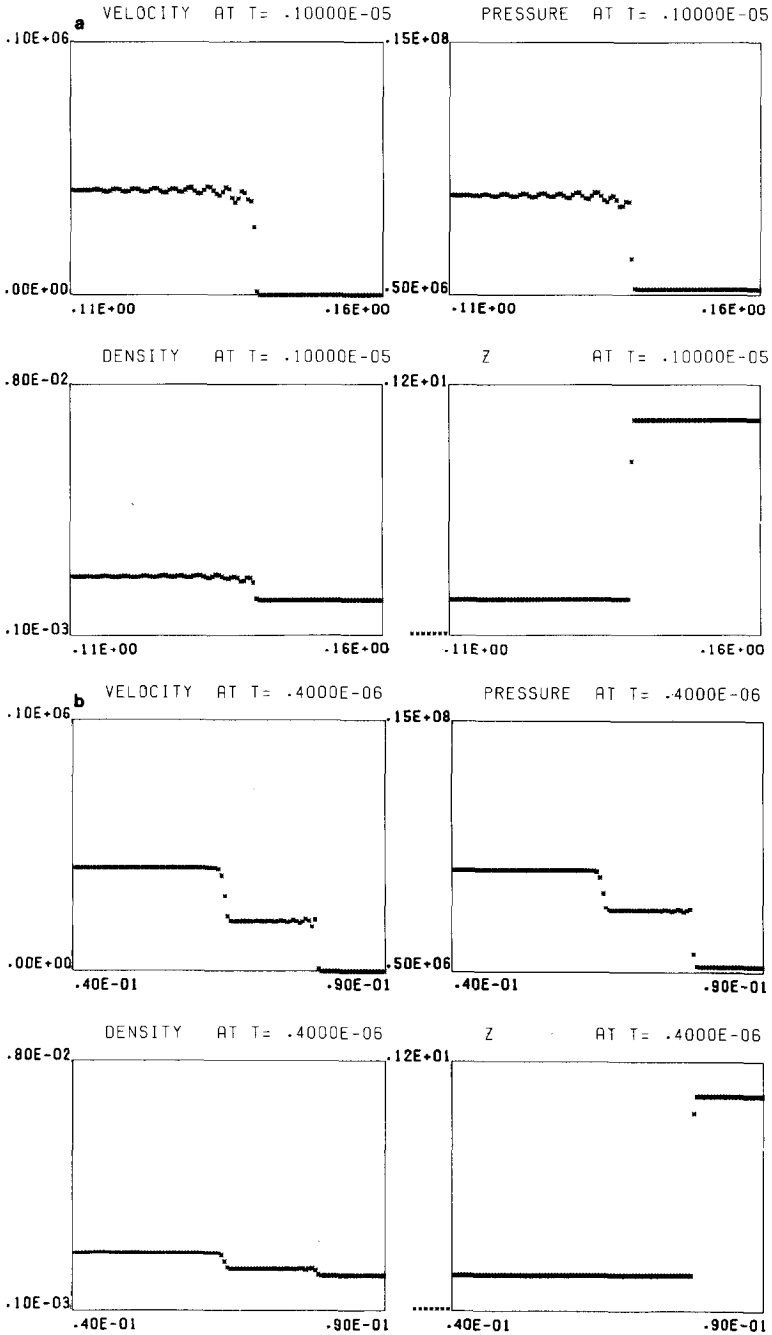

FIG. 4. (a) C-J wave, explicit scheme, reaction zone $\approx 1/10$ cell; (b) C-J wave, implicit scheme, reaction zone $\approx 1/10$ cell.

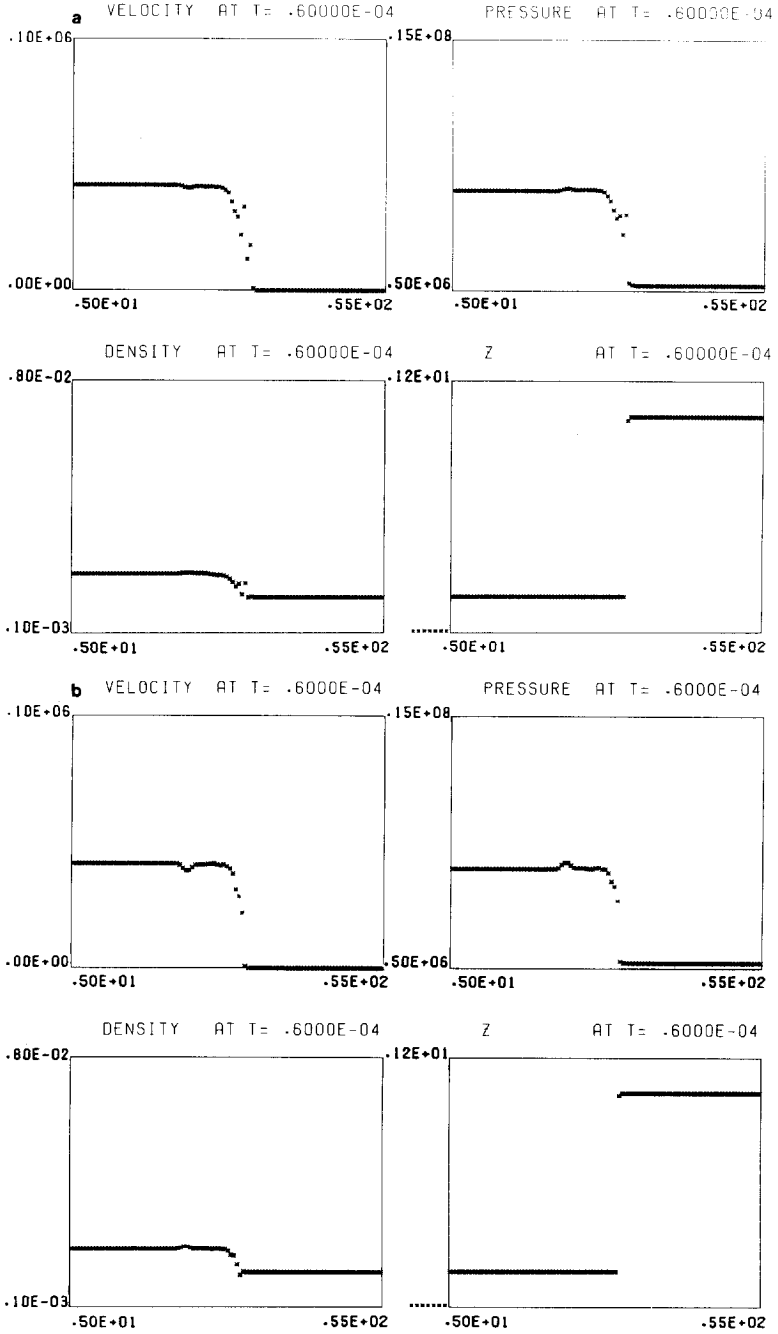

FIG. 5. (a) C-J wave, explicit scheme, reaction zone $\approx 10^{-4}$ cell; (b) C-J wave, implicit scheme, reaction zone $\approx 10^{-4}$ cell.

as one computational cell. To reach the time level $T = 10^{-7}$ s we need 2000 cycles for the explicit case but only 1000 cycles for the implicit case. However, the difference between the two results is truly amazing. While the explicit solution gives the physical C-J detonation, the implicit solution yields a weak detonation followed by a fluid dynamical shock wave in the burnt gas. This is exactly the solution obtained in [4]. In this case, one cannot expect the explicit solution to produce the correct value of the Z-N-D spike, since the whole reaction zone occupies only one computational cell.

Our next calculation was carried out with $\Delta x = 5 \times 10^{-4}$ cm, so that the reaction zone occupies roughly one tenth of a cell. The explicit scheme was run with $\Delta t = 10^{-10}$ s for 10,000 cycles, and the resulting profiles are shown in Fig. 4a. For the implicit scheme, we took $\Delta t = 10^{-9}$ s, and Fig. 4b shows the profiles after 400 cycles (so as to have the full structure within the frame). The discussion of Figs. 3a, b is applicable here too. (Note that the "non-physical" implicit profile is much smoother than the correct explicit profile. We cannot offer a simple explanation for that.)

Finally, we took the case $\Delta x = 5 \times 10^{-1}$ cm. Here the reaction zone is about 10^{-4} of one cell. And here is another surprise. Both the explicit and the implicit calculations proceeded smoothly and produced the correct C-J step. We used $\Delta t = 10^{-8}$ s for the explicit calculation and $\Delta t = 10^{-7}$ s for the implicit calculation. The results after 400 cycles are displayed in Figs. 5a, b.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge the numerous discussions I had with Professor Alexandre Chorin, who introduced me to the subject of this work and helped me understand some of the phenomena of combustion theory. I am indebted also to Dr. Joseph Falcovitz who made many improvements on the first version of this paper. The main part of this work was done while I was visiting the department of Mathematics and Lawrence Berkeley Laboratory at the University of California at Berkeley and the Department of Mathematics at UCLA. I thank these institutions and, in particular, Professors Paul Concus and Stanley Osher, for providing me with a stimulating and encouraging environment.

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