A Weak Formulation of Roe's Approximate Riemann Solver

I. TOUMI

Commissariat à l'Energie Atomique, Direction des Réacteurs Nucléaires, Département des Etudes Mécaniques et Thermiques,
Service d'Etude des Réacteurs et de Mathématiques Appliquées, Gif-sur-Yvette, 91191, France

This paper presents a weak formulation of Roe's approximate Riemann solver, based on a notion of weak solution to nonlinear hyperbolic systems in nonconservative form. This weak formulation is applied to the Euler equations for real gases and the homogeneous equilibrium two-phase flow model. Numerical results for a two-phase flow heat addition problem are given. © 1992 Academic Press, Inc.

1. INTRODUCTION

We consider numerical solutions of the intial-value problem for hyperbolic systems of conservation laws

$$\mathbf{u}_t + \mathbf{f}(\mathbf{u})_x = 0 \tag{1.1}$$

and

$$\mathbf{u}(x, 0) = u_0(x), \tag{1.2}$$

where $\mathbf{u}(x, t)$ is a column vector of m unknowns and the flux $\mathbf{f}(\mathbf{u})$ is some vector-valued function of $\mathbf{u}$, such that the Jacobian matrix given by

$$A(\mathbf{u}) \equiv \frac{\partial \mathbf{f}}{\partial \mathbf{u}} \tag{1.3}$$

has only real eigenvalues. Several upwind differencing schemes have been developed right from Godunov's original scheme [1]. Those schemes attempt to build the solution by solving a succession of Riemann problems. Recall that the Riemann problem is the initial-value problem for (1.1) with

$$\mathbf{u}(x, 0) \equiv u_L \ (x < 0); \qquad \mathbf{u}(x, 0) \equiv u_R \ (x > 0). \tag{1.4}$$

Numerical efficiency justifies the use of approximation of the exact solution of the Riemann problem. This paper concentrates on the linearized Riemann solver introduced by Roe [2], which exploits the fact that we can easily solve the Riemann problem for any linear system of equations. Roe therefore replaces (1.1) by the local linearization

$$\mathbf{u}_t + A(u_L, u_R) \mathbf{u}_x = 0, \tag{1.5}$$

where $A(u_L, u_R)$ is some average Jacobian matrix constructed to have the crucial property

$$\mathbf{f}(u_R) - \mathbf{f}(u_L) = A(u_L, u_R)(u_R - u_L). \tag{1.6}$$

Such a matrix is known as a Roe-averaged matrix and was first devised by Roe for the Euler equations with perfect gases [2].

Several extensions of Roe's linearization to an arbitrary equation of state have been proposed. Grossman and Walters [3] follow the original method that introduced a parameter vector $\mathbf{w}$ such that $\mathbf{u}$ and $\mathbf{f}(\mathbf{u})$ are both quadratic functions of $\mathbf{w}$, to obtain a Roe-averaged matrix. Glaister [4, 5] uses direct approximations of the eigenvalues and eigenvectors of $A(u_L, u_R)$ to provide linearizations valid for a general convex equation of state. The generalization by Vinokur [6] and Liou [7] assumes that $A(u_L, u_R)$ is the exact Jacobian matrix evaluated at some average state $\bar{\mathbf{u}}$, i.e.,

$$A(u_L, u_R) = A(\bar{\mathbf{u}}). \tag{1.7}$$

Surprisingly, an exact definition of a Roe-average for real gases not only exists but is actually not unique. All the methods cited above lead to a matrix $A(u_L, u_R)$ involving undefined coefficients, which are average pressure derivatives, e.g.,

$$\tilde{\chi} = \left(\frac{\partial \tilde{p}}{\partial \rho}\right)_\varepsilon; \qquad \tilde{\kappa} = \left(\frac{\partial \tilde{p}}{\partial \varepsilon}\right)_\rho, \tag{1.8}$$

where p is the pressure, ρ is the density, and ε is the specific internal energy. $\tilde{\chi}$ and $\tilde{\kappa}$ must satisfy a new condition

$$p_R - p_L = \tilde{\chi}(\rho_R - \rho_L) + \tilde{\kappa}(\varepsilon_R - \varepsilon_L). \tag{1.9}$$

Various ways of obtaining unique definitions of $\tilde{\chi}$ and $\tilde{\kappa}$ in terms of thermodynamic states u_L and u_R have been proposed. The various suggested solutions may not be justified if the equation of state is a non-convex function and the two states u_L and u_R are far apart.

It is to be noted that the average pressure derivatives will have a large effect on the accuracy and the general behavior of the approximate Riemann solver. Moreover, concerning two-phase flows such as mixtures of water and steam, the various formulas for $\tilde{\chi}$ and $\tilde{\kappa}$ suggested in [4, 6, 7] may lead to a nonhyperbolic matrix $A(u_L, u_R)$ because of additional difficulties due to the pressure derivatives discontinuity through the saturation curve. Then, a more careful and comprehensive study is needed. This is the main motivation of this paper.

In Section 2, we present a weak formulation of Roe's approximate Riemann solver based on a definition of a non-conservative product. We introduce a weak form of condition (1.6) involving a Lipschitz continuous path connecting u_L and u_R in $\mathbb{R}^m$, and we look at the effect of the path upon averaging. In Section 3, first, we identify the path that leads to the Roe-averaged state for an ideal gas, and then we construct a generalized Roe-averaged matrix for the Euler equations with real gases. We show also that the corresponding approximate Riemann solver preserves the hyperbolicity under some assumptions about the equation of state. In Section 4, we apply this weak formulation to a hyperbolic two-phase flow model and display numerical results for a standard two-phase flow heat addition problem involving two-phase flow instabilities.

2. WEAK FORMULATION OF ROE'S APPROXIMATE RIEMANN SOLVER

In this section we state a weak formulation of Roe's condition (1.6) based on a notion of weak solution to nonlinear hyperbolic systems under a nonconservative form. This section is inspired by recent works on nonconservative products but it is important to note that we are exclusively concerned by numerical solutions to systems of conservation laws.

2.1. Nonconservative Product

For smooth solutions we can write (1.1) in the equivalent nonconservative form

$$\mathbf{u}_t + A(\mathbf{u})\,\mathbf{u}_x = 0. \tag{2.1}$$

It is well known that the distribution theory is not suitable to define weak solutions of (2.1) when in the general case $A(\mathbf{u})$ is not the differential of a real-valued flux function $\mathbf{f(u)}$ (the product of two arbitrary distributions has no sense). Such nonconservative systems have been considered first by

Colombeau and Leroux [8, 9] and later on by Le Floch [10] and Dal Maso et al. [11].

In this paper, we are affected by the notion of entropy weak solution for nonlinear hyperbolic systems in nonconservative form introduced in [11]. This weak solution is based on a definition of nonconservative products of the form $g(u)(du/dx)$, where $g: \mathbb{R}^m \to \mathbb{R}^m$ is a smooth function and u is a function of bounded variation. Let us begin by a brief presentation of their definition. Then, we will indicate our application to approximate Riemann solvers.

From now on, we consider a fixed family of paths in $\mathbb{R}^m$, $\Phi: [0, 1] \times \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}^m$, satisfying the following properties of consistency and regularity:

For every states u_L and u_R in $\mathbb{R}^m$,

$$\Phi(0; u_L, u_R) = u_L, \qquad \Phi(1; u_L, u_R) = u_R. \tag{2.2a}$$

For every bounded set U of $\mathbb{R}^m$, there exists a constant $k > 0$ such that for every states u_L and u_R in U, $\qquad$ (2.2b)

$$\left| \frac{\partial \Phi}{\partial s}(s; u_L, u_R) \right| \leqslant k\,|u_L - u_R| \qquad \text{a.e.} \quad \text{in } [0, 1].$$

For every bounded set U of $\mathbb{R}^m$, there exists a constant $k > 0$ such that for every state (u_L, u_R) and (v_R, v_R) in U $\qquad$ (2.2c)

$$\left| \frac{\partial \Phi}{\partial s}(s; u_L, u_R) - \frac{\partial \Phi}{\partial s}(s; v_L, v_R) \right|$$

$$\leqslant k(|u_L - u_R| + |v_L - v_R|) \qquad \text{a.e.} \quad \text{in } [0, 1].$$

On the set where the function u is continuous, the product $g(u)(du/dx)$ is defined as a Borel measure. On the set of discontinuity points, which are at most countable, the path connecting the left and right values of u is used to define the measure $g(u)(du/dx)$.

PROPOSITION AND DEFINITION [11]. *Let u: $]a, b[\to \mathbb{R}^m$ be a function of bounded variation and let g: $\mathbb{R}^m \times [a, b] \to \mathbb{R}^m$ be a locally bounded Borel function. Then, there exists a unique bounded Borel measure μ on $]a, b[$ characterized by the two following properties:*

— *if u is continuous on a Borel set $\mathbf{B}$ of $]a, b[$, then*

$$\mu(\mathbf{B}) = \int_\mathbf{B} g(u(x), x) \left(\frac{du}{dx} \right)(x) \tag{2.3a}$$

— *if $x_0 \in \,]a, b[$, then*

$$\mu(x_0) = \int_0^1 g(\Phi(s; u(x_0-), u(x_0+)), x_0)$$

$$\times \frac{\partial \Phi}{\partial s}(s; u(x_0-), u(x_0+))\,ds. \tag{2.3b}$$

The nonconservative product of $g(u, \cdot)$ by du/dx is defined as the measure μ and is denoted by

$$\left[g(u, \cdot) \frac{du}{dx} \right]_\Phi = \mu. \qquad (2.4)$$

For the proof, see [11]. It should be observed that, except in the particular case of a conservative product, the nonconservative product (2.4) depends upon the path Φ. This definition has been applied to define weak solutions to the nonconservative system (2.1) and to get jump relations for discontinuous solutions.

PROPOSITION [11]. *The discontinuous function u given by*

$$u(x, t) = u_L \quad for \quad x - \sigma t < 0,$$
$$u_R \quad for \quad x - \sigma t > 0, \qquad (2.5)$$

with $\sigma \in \mathbb{R}$, is a weak solution to the system (2.1) if and only if the following generalized Rankine-Hugoniot condition holds

$$\int_0^1 (-\sigma I + A(\Phi(s; u_L, u_R))) \frac{\partial \Phi}{\partial s}(s; u_L, u_R) \, ds = 0. \qquad (2.6)$$

For the proof of this proposition and many other results, see [11]. We are now capable of giving what we may call a weak formulation of Roe's approximate Riemann solver for hyperbolic systems.

2.2. *Approximate Riemann Solver*

From now onwards, we consider approximate solutions to the Riemann problem (1.1)–(1.4) wich are exact solutions to the approximate linear problem,

$$\mathbf{u}_t + A(u_L, u_R)_\Phi \, \mathbf{u}_x = 0,$$
$$\mathbf{u}(x, 0) = \begin{cases} u_L & \text{if} \quad x < 0, \\ u_R & \text{if} \quad x > 0, \end{cases} \qquad (2.7)$$

where $A(u_L, u_R)_\Phi$ is a constant matrix depending on the data (u_L, u_R) and on the path $\Phi(s; u_L, u_R)$ which satisfies the list of properties:

$$\int_0^1 A(\Phi(s; u_L, u_R)) \frac{\partial \Phi}{\partial s}(s; u_L, u_R) \, ds$$
$$= A(u_L, u_R)_\Phi (u_R - u_L) \qquad (2.8a)$$

$$A(\mathbf{u}, \mathbf{u})_\Phi = A(\mathbf{u}) \qquad (2.8b)$$

$A(u_L, u_R)_\Phi$ has real eigenvalues and

a complete set of eigenvectors. (2.8c)

Once such a matrix has been constructed, its eigenvalues can be considered as the wavespeeds of the Riemann problem, and the projections of $u_R - u_L$ onto its eigenvectors (always possible because of (2.8c)) are the jumps which take place between intermediate constant states. The key property bestowed by (2.8a) is that the solution to the linearized problem (2.7) coincides with the solution (in the weak sense of [11]) of the exact nonconservative Riemann problem (2.1)–(1.4) whenever this involves merely a single shock or a single contact. By this we mean that if $u(x, t)$ is the discontinuous function given by (2.5) and if (u_L, u_R) satisfies the jump condition (2.6), then, thanks to (2.8a), σ is an eigenvalue of $A(u_L, u_R)_\Phi$. The projection of $u_R - u_L$ onto the eigenvectors of $A(u_L, u_R)_\Phi$ will be solely onto the eigenvector which corresponds to σ. Then, in this case, the solution of the Riemann problem will be exact.

We remark that the flux function $\mathbf{f}(\mathbf{u})$ does not appear explicitly in the condition (2.8a). Thereby, this weak formulation allows us to construct an approximate Riemann solver for hyperbolic nonconservative systems issued, for instance, on the theory of multiphasics flows [12]. For such systems, the choice of the path Φ will be crucial because both the exact solution and the approximate solver are strongly dependent from the path Φ. More research is still needed to clarify the choice of the family of paths introduced for the definition of a nonconservative product. Anyway, the finding of a satisfactory approximate Riemann solver for hyperbolic nonconservative systems is beyond the scoop of this paper.

On the other hand, concerning systems of conservation laws, the left-hand side of (2.8a) is independent of the path Φ,

$$\int_0^1 A(\Phi(s; u_L, u_R)) \frac{\partial \Phi}{\partial s}(s; u_L, u_R) \, ds$$

$$= \int_0^1 \frac{\partial \mathbf{f}}{\partial \mathbf{u}}(\mathbf{u}(\Phi(s; u_L, u_R))) \frac{\partial \Phi}{\partial s}(s; u_L, u_R) \, ds$$

$$= \mathbf{f}(\Phi(1; u_L, u_R)) - \mathbf{f}(\Phi(0; u_L, u_R))$$

$$= \mathbf{f}(u_R) - \mathbf{f}(u_L).$$

Thus, (2.8a) coincides exactly with Roe's condition (1.6). But, even in the context of conservation laws, this weak formulation may be useful because we expect that the family of paths Φ will given an efficient algorithm to construct a linearized Jacobian matrix $A(u_L, u_R)_\Phi$.

As a basic example, we introduce the canonical path which is the straight line linking u_L and u_R:

$$\Phi(s; u_L, u_R) = u_L + s(u_R - u_L), \qquad s \in [0, 1]. \qquad (2.9)$$

The corresponding Roe's matrix is given by

$$A(u_L, u_R)_\Phi = \int_0^1 (A(u_L + s(u_R - u_L))) \, ds. \qquad (2.10)$$

However, the integrals involved in (2.10) may not emerge in closed form, or the closed form may be expensive to compute. Since computational speed is a major requirement, we want to obtain analytical expressions for the eigenvalues and eigenvectors of $A(u_L, u_R)_\Phi$. By choosing more subtly the path Φ, an integrable matrix $A(u_L, u_R)_\Phi$ can be found.

2.3. Construction of $A(u_L, u_R)_\Phi$

We now present a way to construct a matrix $A(u_L, u_R)_\Phi$ satisfying conditions (2.8), which is very close to the concept of the parameter vector introduced by Roe. The main feature is the choice of the canonical path for a parameter vector w.

Let f_0 be a smooth function such that $f_0(w_L) = u_L$, $f_0(w_R) = u_R$, and $A_0(w) = \partial f_0/\partial w$ is a regular matrix for every state w. We consider the following path linking the two states u_L and u_R:

$$\Phi_0(s; u_L, u_R) = f_0(w_L + s(w_R - w_L)). \qquad (2.11)$$

Then

$$\int_0^1 A(\Phi_0(s; u_L, u_R)) \frac{\partial \Phi_0}{\partial s} (s; u_L, u_R) \, ds$$

$$= \int_0^1 A(f_0(w_L + s(w_R - w_L)))$$

$$\times A_0(w_L + s(w_R - w_L)) \, ds \cdot (w_R - w_L)$$

and

$$u_R - u_L = \int_0^1 A_0(w_L + s(w_R - w_L)) \, ds \cdot (w_R - w_L).$$

Thus, assuming that the matrix $\int_0^1 A_0(w_L + s(w_R - w_L)) \, ds$ is regular (which is true for $|w_R - w_L|$ small enough), we can define Roe's matrix by

$$\mathbf{A}(\mathbf{u_L}, \mathbf{u_R})_{\Phi_0} = \mathbf{C}(\mathbf{u_L}, \mathbf{u_R})_{\Phi_0} \mathbf{B}(\mathbf{u_L}, \mathbf{u_R})_{\Phi_0}^{-1} \qquad (2.12a)$$

with

$$\mathbf{B}(\mathbf{u_L}, \mathbf{u_R})_{\Phi_0} = \int_0^1 \mathbf{A_0}(\mathbf{w_L} + \mathbf{s}(\mathbf{w_R} - \mathbf{w_L})) \, \mathbf{ds} \qquad (2.12b)$$

$$\mathbf{C}(\mathbf{u_L}, \mathbf{u_R})_{\Phi_0} = \int_0^1 \mathbf{A}(\mathbf{f_0}(\mathbf{w_L} + \mathbf{s}(\mathbf{w_R} - \mathbf{w_L})))$$

$$\times \mathbf{A_0}(\mathbf{w_L} + \mathbf{s}(\mathbf{w_R} - \mathbf{w_L})) \, \mathbf{ds}. \qquad (2.12c)$$

It is clear that $A(u_L, u_R)_{\Phi_0}$ meets conditions (2.8a) and (2.8b). Condition (2.8c) is, in general, checked a posteriori.

2.4. Effect of the Path on Averaging

To provide a better understanding of the effect of the path Φ on the linearization of the exact Jacobian matrix, we study an example of nonconservative product. Let us consider the case where the function $g: \mathbb{R}^2 \to \mathbb{R}^2$ is given by

$$g(u) = (u_2, u_1), \qquad u = (u_1, u_2),$$

and $u \in \mathbb{R}^2$ is equal to the step function

$$u(x) = u_L + H(x)(u_R - u_L),$$

where $u_L = (u_1^L, u_2^L)$, $u_R = (u_1^R, u_2^R)$ are two vectors of $\mathbb{R}^2$ and H is the Heaviside function ($H(x) = 0$ if $x < 0$, $H(x) = 1$ if $x > 0$). Given any family of paths Φ, the definition of Section 2.1 shows that the product $g(u)(du/dx)$ is a multiple of the Dirac measure δ, concentrated at $x = 0$,

$$\left[g(u) \frac{du}{dx} \right]_\Phi = c\delta,$$

where c is given by

$$c = \int_0^1 g(\Phi(s; u_L, u_R)) \frac{\partial \Phi}{\partial s} (s; u_L, u_R) \, ds.$$

In fact, the function $g(u)$ is the differential of a real-valued function, $g(u) = (d/du)(u_1 u_2)$. Thus, the product $g(u)(du/dx)$ is trivially defined in the sense of the distributions, and c is equal to $u_1^R u_2^R - u_1^L u_2^L$, which clearly does not depend on the path Φ. But, as in the case of conservation laws where the left-hand side of (2.8a) is equal to the jump of the flux function between states u_R and u_L, we actually want to obtain the projection of c onto the plane $(\Delta u_1, \Delta u_2)$,

$$c = c_1 \Delta u_1 + c_2 \Delta u_2,$$

where $\Delta(\cdot) = (\cdot)_R - (\cdot)_L$ and the vector (c_1, c_2) is given by

$$(c_1, c_2) = \int_0^1 g(\Phi(s; u_L, u_R))$$

$$\times \int_0^1 \frac{\partial^2 \Phi}{\partial s \, \partial u} (s; u_L, u_L + \theta \, \Delta u) \, d\theta \, ds. \qquad (2.13)$$
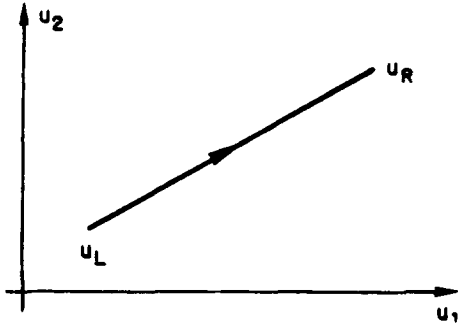
FIGURE 2.1

Let us now compare three different paths. First, using the canonical path defined by (2.9) (see Fig. 2.1), we obtain

$$(c_1, c_2) = \int_0^1 g(\Phi(s; u_L, u_R)) \, ds$$

$$= \int_0^1 (u_2^L + s(u_2^R - u_2^L), u_1^L$$

$$+ s(u_1^R - u_1^L)) \, ds$$

$$= \left(\frac{u_2^L + u_2^R}{2}, \frac{u_1^L + u_1^R}{2} \right).$$

Then, the canonical path leads to the linearization,

$$c = \Delta(u_1 u_2) = \bar{u}_2 \, \Delta u_1 + \bar{u}_1 \, \Delta u_2, \qquad (2.14)$$

where the overbar denotes the arithmetic mean value $\overline{(\cdot)} = \frac{1}{2}((\cdot)_L + (\cdot)_R)$.

Second, let us consider the path Φ_1 defined by

$$\Phi_1(s; u_L, u_R) = \begin{cases} (u_1^L + 2s(u_1^R - u_1^L), u_2^L) \\ \quad \text{for} \quad s \in [0, \frac{1}{2}] \\ (u_1^R, u_2^L + (2s-1)(u_2^R - u_2^L)) \\ \quad \text{for} \quad s \in [\frac{1}{2}, 1] \end{cases} \qquad (2.15)$$
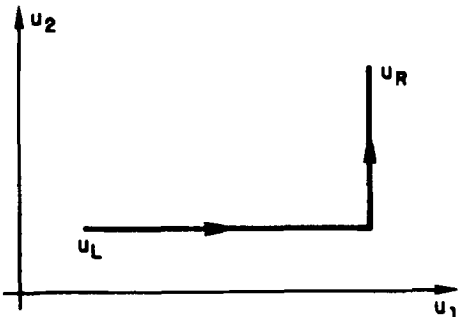

FIGURE 2.2

(see Fig. 2.2). We obtain

$$\frac{\partial \Phi}{\partial s}(s; u_L, u_R) = \begin{cases} 2(u_1^R - u_1^L, 0) & \text{for} \quad s \in [0, \frac{1}{2}] \\ 2(0, u_2^R - u_2^L) & \text{for} \quad s \in [\frac{1}{2}, 1] \end{cases}$$

and from (2.13)

$$(c_1, c_2) = \int_0^{1/2} g(\Phi(s; u_L, u_R)) \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix} ds$$

$$+ \int_{1/2}^1 g(\Phi(s; u_L, u_R)) \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix} ds$$

$$= \int_0^{1/2} (2u_2^L, 0) \, ds + \int_{1/2}^1 (0, 2u_1^R) \, ds$$

$$= (u_2^L, u_1^R).$$

Then, this path leads to the linearization:

$$\Delta(u_1 u_2) = u_2^L \, \Delta u_1 + u_1^R \, \Delta u_2. \qquad (2.16)$$

Third, if Φ_2 is the path, similar to Φ_1, defined by

$$\Phi_2(s; u_L, u_R) = \begin{cases} (u_1^L, u_2^L + 2s(u_2^R - u_2^L)) \\ \quad \text{for} \quad s \in [0, \frac{1}{2}] \\ (u_1^L + (2s-1)(u_1^R - u_1^L), u_2^R) \\ \quad \text{for} \quad s \in [\frac{1}{2}, 1] \end{cases} \qquad (2.17)$$

(see Fig. 2.3), again from (2.13), we obtain the following linearization:

$$\Delta(u_1 u_2) = u_2^R \, \Delta u_1 + u_1^L \, \Delta u_2. \qquad (2.18)$$

These very simple examples show that the linearization of nonlinear terms (in particular, quadratic terms) is closely related to the path Φ. From another standpoint, the formulas (2.14), (2.16), and (2.18) correspond to three different expressions for average partial derivatives of the function $u_1 u_2$ with respect to u_1 and u_2. Thus, the choice of a path Φ (or a vector parameter w with (2.11)) shall lead to a linearized Jacobian matrix $A(u_L, u_R)_\Phi$, completely deter-
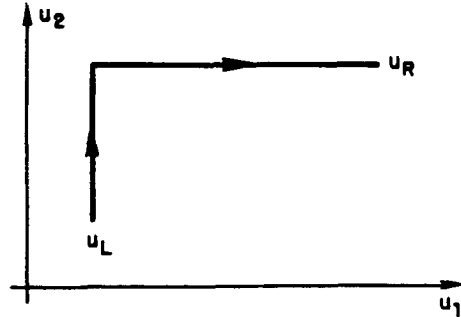

FIGURE 2.3

mined, and will give unique values of the average pressure derivatives $\bar{\chi}$ and $\bar{\kappa}$ in terms of the thermodynamic states u_R and u_L.

3. A GENERALIZED ROE'S APPROXIMATE RIEMANN SOLVER FOR THE EULER EQUATIONS

In this section we develop an approximate Riemann solver for the Euler equations in one dimension with any equation of state, using the weak formulation of Section 2. First, we identify the path that leads to the Roe-averaged matrix for an ideal gas [2]; then we use the same path for a real gas.

3.1. Equations of Flow and State

The Euler equations governing the flow of an inviscid, compressible fluid in one dimension may be written in conservation form as

$$\mathbf{u}_t + \mathbf{f}(\mathbf{u})_x = 0, \tag{3.1}$$

where

$$\mathbf{u} = (\rho, m, e)^T, \tag{3.2}$$

$$\mathbf{f}(\mathbf{u}) = (m, p + \rho u^2, u(e + p))^T, \tag{3.3}$$

together with

$$m = \rho u, \tag{3.4}$$

$$e = \rho H - p, \tag{3.5}$$

$$H = h + u^2/2, \tag{3.6}$$

where $\rho = \rho(x, t)$, $u = u(x, t)$, $m = m(x, t)$, $p = p(x, t)$, $h = h(x, t)$, $H = H(x, t)$, and $e = e(x, t)$ represent the density, velocity, momentum, pressure, specific enthalpy, total enthalpy, and the total energy, respectively, at a position x and time t. In order to complete the system we must specify an equation of state which is a thermodynamic relationship specific to each particular fluid. We will restrict ourselves to the gas in chemical equilibrium and assume that the equation of state can be written in the form

$$p = p(\rho, h). \tag{3.7}$$

Furthermore, we shall assume that $p(\cdot, \cdot)$ is a smooth function satisfying conditions which ensure that the system (3.1) is hyperbolic. For an ideal gas, Eq. (3.7) reduces to

$$p = \frac{\gamma - 1}{\gamma} \rho h, \tag{3.8}$$

where γ is the ratio of specific heat capacities of the fluid, and it is a constant. It will be convenient, in this section, to introduce the following dimensionless variables characterizing the equation of state,

$$\Gamma = -\frac{v}{T} \frac{\partial^2 \varepsilon}{\partial s \, \partial v} \tag{3.9a}$$

and

$$\gamma = \frac{v}{p} \left(\frac{\partial^2 \varepsilon}{\partial v^2} \right)_s, \tag{3.9b}$$

where $v = 1/\rho$ is the specific volume, T is the temperature, $\varepsilon = h - p/\rho$ is the specific internal energy, and s is the specific entropy. Here, γ is the adiabatic exponent, with $\gamma > 1$ for most materials and, in particular, for polytropic gases. Γ is called the Gruneisen coefficient, and it controls the mapping of isentropes into the p-v plane. In the case of an ideal gas, the Gruneisen coefficient Γ becomes $\gamma - 1$, which is a positive constant. Generally, thermodynamics plane no constraint on the sign of Γ. However, we will restrict ourselves to materials for which

$$\Gamma > 0. \tag{3.10}$$

This is the case when the material expands upon heating at constant pressure [13], which is true in most situations. But for some materials, Γ is negative in a portion of state space. A notable example is water, which contracts upon heating near $0°C$ and 1 bar. In order to prove the hyperbolicity of our approximate Riemann solver we introduce an extra condition to the equation of state, which is similar to those introduced by Smith [14] in analyzing the uniqueness of the Riemann problem:

$$\Gamma \leqslant (\gamma - \Gamma) \frac{pv}{\varepsilon}. \tag{3.11}$$

The above condition leads to some interesting relations on the pressure derivatives. For this purpose, let us recall various classical thermodynamics results.

The fundamental thermodynamic identity which follows from the first and second laws of thermodynamics, defines the pressure and the temperature as derivatives of ε:

$$d\varepsilon = T \, ds - p \, dv, \tag{3.12a}$$

In terms of the potential $h = \varepsilon + pv$, this identity is expressed as

$$dh = T \, ds + v \, dp. \tag{3.12b}$$

Moreover, it is shown in [13] that

$$\mathrm{v}\, dp = -\gamma p\, d\mathrm{v} + \Gamma T\, ds. \tag{3.12c}$$

Substituting for ds from Eq. (3.12a) and Eq. (3.12b) into Eq. (3.12c), gives

$$(1 + \Gamma)\,\mathrm{v}\, dp = -\gamma p\, d\mathrm{v} + \Gamma\, dh \tag{3.13a}$$

and

$$\Gamma\, d\varepsilon = (\gamma - \Gamma)\, p\, d\mathrm{v} + \mathrm{v}\, dp \tag{3.13b}$$

from which we deduce easily

$$\left(\frac{\partial p}{\partial h}\right)_\rho = \frac{\Gamma}{1 + \Gamma}\rho \tag{3.14}$$

and

$$\left(\frac{\partial \rho h}{\partial \rho}\right)_p = \frac{\varepsilon}{\Gamma}\left(\Gamma - (\gamma - \Gamma)\frac{p\mathrm{v}}{\varepsilon}\right). \tag{3.15}$$

Thus, if the inequalities (3.10) and (3.11) on the equation of state hold, $(\partial \rho h/\partial \rho)_p$ is nonpositive.

We now give the Jacobian $A(\mathbf{u})$, of the flux function $\mathbf{f}(\mathbf{u})$, since this matrix is needed to construct our approximate Riemann solver,

$$A(\mathbf{u}) = \begin{pmatrix} 0 & 1 & 0 \\ -u^2 + p_\rho & 2u + p_m & p_e \\ -Hu + up_\rho & H + up_m & u + up_e \end{pmatrix}, \tag{3.16}$$

where the notations

$$p_\rho = \left(\frac{\partial p}{\partial \rho}\right)_{m,e}, \qquad p_m = \left(\frac{\partial p}{\partial m}\right)_{\rho,e}, \qquad p_e = \left(\frac{\partial p}{\partial e}\right)_{\rho,m} \tag{3.17}$$

have been used.

3.2. Ideal Gas

The object of this section is to find a path $\Phi(s; \mathbf{u}_L, \mathbf{u}_R)$ such that the matrix $A(\mathbf{u}_L, \mathbf{u}_R)$, satisfying weak conditions (2.8), is exactly the averaged Jacobian matrix derived by Roe for an ideal gas [2],

$$\bar{A} = \begin{pmatrix} 0 & 1 & 0 \\ \dfrac{\gamma - 3}{2}\tilde{u}^2 & -(\gamma - 3)\tilde{u} & \gamma - 1 \\ \left(-\tilde{H} + \dfrac{\gamma - 1}{2}\tilde{u}^2\right)\tilde{u} & \tilde{H} - (\gamma - 1)\tilde{u}^2 & \gamma\tilde{u} \end{pmatrix}, \tag{3.18}$$

where

$$\tilde{u} = \frac{\sqrt{\rho_L}\, u_L + \sqrt{\rho_R}\, u_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}, \tag{3.19}$$

$$\tilde{H} = \frac{\sqrt{\rho_L} + \sqrt{\rho_R}\, H_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}. \tag{3.20}$$

In fact, $\bar{A}$ is equal to the exact Jacobian matrix for an average state $\bar{\mathbf{u}}(\mathbf{u}_L, \mathbf{u}_R)$:

$$\bar{A} = A(\bar{\mathbf{u}}). \tag{3.21}$$

$\bar{\mathbf{u}}$ is known as the Roe-averaged state and is given by the arithmetic mean value of the parameter vector $\mathbf{w}$:

$$\bar{\mathbf{u}} = \tfrac{1}{2}(\mathbf{w}_L + \mathbf{w}_R) \tag{3.22}$$

with

$$\mathbf{w} = \sqrt{\rho}\begin{pmatrix} 1 \\ u \\ H \end{pmatrix}. \tag{3.23}$$

Then, from Section 2.4, the canonical path for the parameter vector $\mathbf{w}$ seems to be a natural candidate for the path $\Phi_0(s; \mathbf{u}_L, \mathbf{u}_R)$. Specifically,

$$\Phi_0(s; \mathbf{u}_L, \mathbf{u}_R) = f_0(\mathbf{w}_L + s(\mathbf{w}_R - \mathbf{w}_L)), \qquad s \in [0, 1] \tag{3.24a}$$

with

$$\mathbf{w} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} = \sqrt{\rho}\begin{pmatrix} 1 \\ u \\ H \end{pmatrix} \tag{3.24b}$$

and

$$f_0(\mathbf{w}) = \begin{pmatrix} w_1^2 \\ w_1 w_2 \\ \dfrac{w_1 w_3}{\gamma} + \dfrac{\gamma - 1}{2\gamma}w_2^2 \end{pmatrix}. \tag{3.24c}$$

A straightforward computation yields

$$A_0(\mathbf{w}) \equiv f_0'(\mathbf{w}) = \begin{pmatrix} 2w_1 & 0 & 0 \\ w_2 & w_1 & 0 \\ \dfrac{1}{\gamma}w_3 & \dfrac{\gamma - 1}{\gamma}w_2 & \dfrac{1}{\gamma}w_1 \end{pmatrix} \tag{3.25}$$

and

$$A(\mathbf{u}(\mathbf{w}))\,A_0(\mathbf{w}) \equiv \begin{pmatrix} w_2 & w_1 & 0 \\ \dfrac{\gamma-1}{\gamma}\,w_3 & \dfrac{\gamma+1}{\gamma}\,w_2 & \dfrac{\gamma-1}{\gamma}\,w_1 \\ 0 & w_3 & w_2 \end{pmatrix}. \qquad (3.26)$$

The integrals involved in Eq. (2.12) can be calculated explicitly, for instance:

$$\int_0^1 (w_1^L + s(w_1^R - w_1^L))\,ds = w_1^L + \tfrac{1}{2}(w_1^R - w_1^L) = \bar{w}_1.$$

From Eqs. (3.24)–(3.26), together with the definition (2.12), we obtain

$$B(\mathbf{u}_L, \mathbf{u}_R)_{\Phi_0} = \begin{pmatrix} 2\bar{w}_1 & 0 & 0 \\ \bar{w}_2 & \bar{w}_1 & 0 \\ \dfrac{1}{\gamma}\,\bar{w}_3 & \dfrac{\gamma-1}{\gamma}\,\bar{w}_2 & \dfrac{1}{\gamma}\,\bar{w}_1 \end{pmatrix} \qquad (3.27)$$

and

$$C(\mathbf{u}_L, \mathbf{u}_R)_{\Phi_0} = \begin{pmatrix} \bar{w}_2 & \bar{w}_1 & 0 \\ \dfrac{\gamma-1}{\gamma}\,\bar{w}_3 & \dfrac{\gamma+1}{\gamma}\,\bar{w}_2 & \dfrac{\gamma-1}{\gamma}\,\bar{w}_1 \\ 0 & \bar{w}_3 & \bar{w}_2 \end{pmatrix}. \qquad (3.28)$$

Finally, a routine calculation shows that the matrix $C(\mathbf{u}_L, \mathbf{u}_R)_{\Phi_0}\,B(\mathbf{u}_L, \mathbf{u}_R)_{\Phi_0}^{-1}$ is equal to Roe's matrix (3.18) for an ideal gas.

3.3. Real Gas

We are now able to present our generalized approximate Riemann solver for a real gas described by the general equation of state (3.7). The previous section shows that the weak formulation, coupled with the canonical path for Roe's parameter vector $\mathbf{w}$, is equivalent to a search for an approximation to the Jacobian A with alternative approach used by Roe [2] and Vinokur [6] in the ideal gas case. A natural wish, for the real gas case, is to get a linearized Jacobian which has the same form as the one given by Roe for an ideal gas. Thus, we propose to keep the same path, i.e., the canonical path for the parameter vector $\mathbf{w}$. This path may be considered as the optimal choice as far as consistency. Therefore,

$$\Phi_0(s; \mathbf{u}_L, \mathbf{u}_R) = f_0(\mathbf{w}_L + s(\mathbf{w}_R - \mathbf{w}_L)), \qquad s \in [0, 1] \tag{3.29a}$$

with

$$\mathbf{w} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} = \sqrt{\rho} \begin{pmatrix} 1 \\ u \\ H \end{pmatrix} \tag{3.29b}$$

and

$$f_0(\mathbf{w}) = \begin{pmatrix} w_1^2 \\ w_1 w_2 \\ w_1 w_3 - p(w_1, w_2, w_3) \end{pmatrix}. \tag{3.29c}$$

The construction of $A(\mathbf{u}_L, \mathbf{u}_R)_{\Phi_0}$ involves the pressure $p(w_1, w_2, w_3)$ and its partial derivatives with respect to the variables w_i,

$$p_{w_1} = \left(\frac{\partial p}{\partial w_1}\right)_{w_2, w_3}, \qquad p_{w_2} = \left(\frac{\partial p}{\partial w_2}\right)_{w_1, w_3},$$

$$p_{w_3} = \left(\frac{\partial p}{\partial w_3}\right)_{w_1, w_2}. \tag{3.30}$$

By the chain rule for partial derivatives, we have

$$p_\rho = \frac{w_1 p_{w_1} - w_2 p_{w_2} - w_3 p_{w_3}}{2w_1(w_1 - p_{w_3})} \tag{3.31a}$$

$$p_m = \frac{p_{w_2}}{w_1 - p_{w_3}}, \tag{3.31b}$$

$$p_e = \frac{p_{w_3}}{w_1 - p_{w_3}}. \tag{3.31c}$$

Using the notations (3.30), Eq. (3.29c) yields the matrix

$$A_0(\mathbf{w}) \equiv f_0'(\mathbf{w}) = \begin{pmatrix} 2w_1 & 0 & 0 \\ w_2 & w_1 & 0 \\ w_3 - p_{w_1} & -p_{w_2} & w_1 - p_{w_3} \end{pmatrix}$$

and, using (2.12b), we obtain

$$B(\mathbf{u}_L, \mathbf{u}_R)_{\Phi_0} = \begin{pmatrix} 2\bar{w}_1 & 0 & 0 \\ \bar{w}_2 & \bar{w}_1 & 0 \\ \bar{w}_3 - \tilde{p}_{w_1} & -\tilde{p}_{w_2} & \bar{w}_1 - \tilde{p}_{w_3} \end{pmatrix}, \tag{3.32}$$

where $\bar{w}_i$ denotes again the arithmetic mean of w_i, and $\tilde{p}_{w_i}$ is an approximation of p_{w_i}, given by

$$\tilde{p}_{w_i} = \int_0^1 p_{w_i}(\mathbf{w}_L + s(\mathbf{w}_R - \mathbf{w}_L))\,ds. \tag{3.33}$$

In addition, we note that the approximations $\tilde{p}_{w_i}$ $(i = 1, 2, 3)$ are not independent, since

$$\Delta p = p_R - p_L = \int_0^1 \frac{d}{ds}\left(p(\mathbf{w}_L + s(\mathbf{w}_R - \mathbf{w}_L))\right) ds$$

$$= \int_0^1 \frac{dp}{d\mathbf{w}} \left(\mathbf{w}_L + s(\mathbf{w}_R - \mathbf{w}_L)\right) ds \,(\mathbf{w}_R - \mathbf{w}_L)$$

which gives the following necessary condition:

$$\Delta p = \tilde{p}_{w_1}\,\Delta w_1 + \tilde{p}_{w_2}\,\Delta w_2 + \tilde{p}_{w_3}\,\Delta w_3. \qquad (3.34)$$

To construct the matrix $C(\mathbf{u}_L, \mathbf{u}_R)_{\Phi_0}$ we begin by rewriting the flux $\mathbf{f}(\mathbf{u})$ as a function of $\mathbf{w}$:

$$\mathbf{f}(\mathbf{u}) = \begin{pmatrix} w_1 w_2 \\ p(w_1, w_2, w_3) + w_2^2 \\ w_2 w_3 \end{pmatrix}. \qquad (3.35)$$

From Eq. (3.35), we deduce

$$A(\mathbf{u}(\mathbf{w}))\, A_0(\mathbf{w}) = \begin{pmatrix} w_2 & w_1 & 0 \\ p_{w_1} & p_{w_2} + 2w_2 & p_{w_3} \\ 0 & w_3 & w_2 \end{pmatrix}$$

and

$$C(\mathbf{u}_L, \mathbf{u}_R)_{\Phi_0} = \begin{pmatrix} \bar{w}_2 & \bar{w}_1 & 0 \\ \tilde{p}_{w_1} & \tilde{p}_{w_2} + 2\bar{w}_2 & \tilde{p}_{w_3} \\ 0 & \bar{w}_3 & \bar{w}_2 \end{pmatrix}. \qquad (3.36)$$

Finally, using Eqs. (3.32)–(3.36), we obtain Roe's matrix associated with the path Φ_0,

$$A(\mathbf{u}_L, \mathbf{u}_R)_{\Phi_0} = \begin{pmatrix} 0 \\ -\dfrac{\bar{w}_2^2}{\bar{w}_1^2} + \dfrac{\bar{w}_1\,\tilde{p}_{w_1} - \bar{w}_2\,\tilde{p}_{w_2} - \bar{w}_3\,\tilde{p}_{w_3}}{2\bar{w}_1(\bar{w}_1 - \tilde{p}_{w_3})} \\ -\dfrac{\bar{w}_2 \bar{w}_3}{\bar{w}_1^2} + \dfrac{\bar{w}_2}{\bar{w}_1}\dfrac{\bar{w}_1\,\tilde{p}_{w_1} - \bar{w}_2\,\tilde{p}_{w_2} - \bar{w}_3\,\tilde{p}_{w_3}}{2\bar{w}_1(\bar{w}_1 - \tilde{p}_{w_3})} \end{pmatrix.$$

$$\left. \begin{matrix} & 1 & & 0 \\[2mm] & 2\dfrac{\bar{w}_2}{\bar{w}_1} + \dfrac{\tilde{p}_{w_2}}{\bar{w}_1 - \tilde{p}_{w_3}} & & \dfrac{\tilde{p}_{w_3}}{\bar{w}_1 - \tilde{p}_{w_3}} \\[3mm] & \dfrac{\bar{w}_3}{\bar{w}_1} + \dfrac{\bar{w}_2}{\bar{w}_1}\dfrac{\tilde{p}_{w_2}}{\bar{w}_1 - \tilde{p}_{w_3}} & & \dfrac{\bar{w}_2}{\bar{w}_1 - \tilde{p}_{w_3}} \end{matrix} \right).$$

$$(3.37)$$

In order to simplify these expressions, we focus our attention on the pressure derivatives given by Eq. (3.31) and we define the corresponding average (or approximations). A

number of choices can be made, but it is clear that the most natural choice is to take (see (3.31))

$$\tilde{p}_\rho = \frac{\bar{w}_1\,\tilde{p}_{w_1} - \bar{w}_2\,\tilde{p}_{w_2} - \bar{w}_3\,\tilde{p}_{w_3}}{2\bar{w}_1(\bar{w}_1 - \tilde{p}_{w_3})}, \qquad (3.38a)$$

$$\tilde{p}_m = \frac{\tilde{p}_{w_2}}{\bar{w}_1 - \tilde{p}_{w_3}}, \qquad (3.38b)$$

$$\tilde{p}_e = \frac{\tilde{p}_{w_3}}{\bar{w}_1 - \tilde{p}_{w_3}}. \qquad (3.38c)$$

It is easy to check that these average pressure derivatives satisfy the condition

$$\Delta p = \tilde{p}_\rho\,\Delta\rho + \tilde{p}_m\,\Delta m + \tilde{p}_e\,\Delta e. \qquad (3.39)$$

Now, substituting Eqs. (3.38) into Eq. (3.37), together with the identities

$$\tilde{u} = \frac{\bar{w}_2}{\bar{w}_1} \qquad \text{and} \qquad \tilde{H} = \frac{\bar{w}_3}{\bar{w}_1},$$

gives

$$A(\mathbf{u}_L, \mathbf{u}_R)_{\Phi_0} = \begin{pmatrix} 0 & 1 & 0 \\ -\tilde{u}^2 + \tilde{p}_\rho & 2\tilde{u} + \tilde{p}_m & \tilde{p}_e \\ -\tilde{H}\tilde{u} + \tilde{u}\tilde{p}_\rho & \tilde{H} + \tilde{u}\tilde{p}_m & \tilde{u} + \tilde{u}\tilde{p}_e \end{pmatrix}. \qquad (3.41)$$

We remark that the linearized Jacobian matrix $A(\mathbf{u}_L, \mathbf{u}_R)_{\Phi_0}$, given by Eq. (3.41), is equal to the exact Jacobian evaluated at some average state $\tilde{\mathbf{u}}$ defined by $\tilde{u}$, $\tilde{H}$, $\tilde{p}_\rho$, $\tilde{p}_m$, and $\tilde{p}_e$. The average velocity $\tilde{u}$ and the average total enthalpy $\tilde{H}$ have the same form as the perfect gas version, and the average pressure derivatives are those given by Eqs. (3.38).

To sum up, we found a Roe-averaged matrix for the Euler equations with an arbitrary equation of state, which is very similar to those obtained by other formulations, except for the definition of the averaged values of the derivatives of the pressure p. The derivation of these approximations, in our method, is more systematic than those of other investigators. The decisive advantage of this new formulation of Roe's approximate Riemann solver is to avoid the problem of finding average pressure derivatives $(\tilde{p}_\rho, \tilde{p}_m,$ and $\tilde{p}_e$ in our presentation or $\tilde{\chi}$ and $\tilde{\kappa}$ for Vinokur's approach [6]). However, the apparent drawback of this approach is the evaluation of the integrals in Eq. (3.33) which might be expensive to compute.

3.4. Hyperbolic Approximate Riemann Solver

While an exact definition of the coefficients $\tilde{p}_{w_i}$ is given by Eq. (3.33), for practical implementation, it is possible

to replace them by some approximations $\hat{p}_{w_i}$ as long as condition (3.34) is met precisely:

$$\Delta p = \hat{p}_{w_1} \Delta w_1 + \hat{p}_{w_2} \Delta w_2 + \hat{p}_{w_3} \Delta w_3. \qquad (3.42)$$

Let us begin by giving some preliminary results on the pressure derivatives. From Eq. (3.29b) we deduce

$$\rho = w_1^2,$$

$$u = \frac{w_2}{w_1},$$

$$h = \frac{w_3}{w_1} - \frac{w_2^2}{2w_1^2}.$$

Then,

$$p_{w_3} = \frac{1}{w_1} \left(\frac{\partial p}{\partial h} \right)_\rho$$

and, using Eq. (3.15), we obtain

$$p_{w_3} = \frac{\Gamma}{\Gamma + 1} w_1. \qquad (3.43)$$

Since the pressure is only a function of the thermodynamic variables ρ and h, we have

$$p_{w_2} = -u p_{w_3}. \qquad (3.44)$$

We note that, the above relations, while holding pointwise, do not necessarily hold for the average state quantities which are functions of two states. However, we shall choose approximations $\hat{p}_{w_i}$ such that

$$\hat{p}_{w_1} = (\tilde{H} + 2\tilde{\alpha}) \hat{p}_{w_3}, \qquad (3.45a)$$

$$\hat{p}_{w_2} = -\tilde{u} \hat{p}_{w_3}, \qquad (3.45b)$$

$$\hat{p}_{w_3} = \frac{\tilde{\Gamma}}{\tilde{\Gamma} + 1} \bar{w}_1, \qquad (3.45c)$$

where $\tilde{\Gamma}$ is the average Gruneisen coefficient defined by

$$\tilde{\Gamma} = \int_0^1 \Gamma(\mathbf{w}_L + s(\mathbf{w}_R - \mathbf{w}_L)) \, ds. \qquad (3.45d)$$

We also define the average adiabatic exponent $\tilde{\gamma}$ by

$$\tilde{\gamma} = \tilde{\Gamma} + 1. \qquad (3.45e)$$

The coefficient $\tilde{\alpha}$ in Eq. (3.45a) can be calculated from Eq. (3.42):

$$\Delta p = \hat{p}_{w_3} ((\tilde{H} + 2\tilde{\alpha}) \Delta w_1 - \tilde{u} \Delta w_2 + \Delta w_3)$$

$$= \frac{\tilde{\Gamma}}{\tilde{\Gamma} + 1} ((\bar{w}_3 + 2\tilde{\alpha}\bar{w}_1) \Delta w_1 - \bar{w}_2 \Delta w_2 + \bar{w}_1 \Delta w_3)$$

$$= \frac{\tilde{\Gamma}}{\tilde{\Gamma} + 1} (\tilde{\alpha} \Delta \rho + \Delta(\rho h)).$$

Thus, we have

$$\tilde{\alpha} = \frac{\tilde{\gamma}}{\tilde{\gamma} - 1} \frac{\Delta p}{\Delta \rho} - \frac{\Delta(\rho h)}{\Delta \rho} \qquad (3.45f)$$

(if $\Delta \rho = 0$, the operator Δ is replaced by the partial derivative). The coefficient $\tilde{\alpha}$ vanishes for an ideal equation of state and is positive, provided that conditions (3.10) and (3.11) hold (see Eq. (3.15)).

With these definitions, the averaged values of the derivatives of the pressure with respect to the conservative variables are given by

$$\tilde{p}_\rho = (\tilde{\gamma} - 1) \left(\alpha + \frac{\tilde{u}^2}{2} \right),$$

$$\tilde{p}_m = -(\tilde{\gamma} - 1)\tilde{u},$$

$$\tilde{p}_e = \tilde{\gamma} - 1.$$

Then, the Roe-averaged matrix $A(\mathbf{u}_L, \mathbf{u}_R)_{\Phi_0}$, given by Eq. (3.41) becomes

$$A(\mathbf{u}_L, \mathbf{u}_R)_{\Phi_0} = \begin{pmatrix} 0 & 1 & 0 \\ \frac{\tilde{\gamma} - 3}{2} \tilde{u}^2 + (\tilde{\gamma} - 1)\tilde{\alpha} & -(\tilde{\gamma} - 3)\tilde{u} & \tilde{\gamma} - 1 \\ \left(-\tilde{H} + \frac{\tilde{\gamma} - 1}{2} \tilde{u}^2 \right) \tilde{u} + (\tilde{\gamma} - 1)\tilde{u}\tilde{\alpha} & \tilde{H} - (\gamma - 1)\tilde{u}^2 & \tilde{\gamma}\tilde{u} \end{pmatrix}.$$

$$(3.46)$$

This matrix has a final form very similar to Roe's matrix for an ideal gas (3.18) and involves a unique integral (see Eq. (3.45d)) which can be evaluated by some approximate quadratures.

We turn now to examine the hyperbolicity of the

approximate Riemann solver (see condition (2.8c)). The equation for the eigenvalues is

$$(\tilde{u} - \lambda)\left((\tilde{u} - \lambda)^2 - (\tilde{\gamma} - 1)\left(\tilde{H} - \frac{\tilde{u}^2}{2} + \tilde{\alpha}\right)\right) = 0 \quad (3.47)$$

from which we obtain the eigenvalues $\tilde{u} - \tilde{a}$, $\tilde{u}$, $\tilde{u} + \tilde{a}$, where $\tilde{a}$ is an average sound speed given by the equation

$$\tilde{a}^2 = (\tilde{\gamma} - 1)\left(\tilde{H} - \frac{\tilde{u}^2}{2} + \tilde{\alpha}\right). \quad (3.48)$$

This expression of $\tilde{a}^2$ is positive if $\tilde{\gamma} > 1$ and $\tilde{\alpha} \geqslant 0$. These conditions are automatically satisfied for a perfect gas, but for a real gas it requires some additional assumptions about the equation of state. Then, Eqs. (3.10)–(3.11) are sufficient conditions to ensure real distinct eigenvalues for the matrix $A(\mathbf{u}_L, \mathbf{u}_R)_{\varPhi_0}$.

4. APPROXIMATE RIEMANN SOLVER FOR A TWO-PHASE FLOW MODEL

In order to show the ability of our formulation, we present in this section an approximate Riemann solver for two-phase flows such as mixtures of liquid and vapor.

4.1. Conservation Laws

Several sets of equations have been worked out for the modelling of two-phase flow. This section is devoted to the homogeneous equilibrium model, which has been widely used for the analysis of thermal–hydraulics transients. However, the results can be extended to more complex models incorporating unequal velocity for each phase and nonequilibrium thermodynamic effects [15].

The conservation equations for mass, momentum, and energy are

$$\partial_t(\alpha\rho_v + (1 - \alpha)\rho_l) + \partial_x(\alpha\rho_v u + (1 - \alpha)\rho_l u) = 0 \quad (4.1a)$$

$$\partial_t((\alpha\rho_v + (1 - \alpha)\rho_l)u) + \partial_x((\alpha\rho_v + (1 - \alpha)\rho_l)u^2 + p)$$
$$= -\tau - (\alpha\rho_v + (1 - \alpha)\rho_l)g \quad (4.1b)$$

$$\partial_t\left(\alpha\rho_v\left(h_v + \frac{u^2}{2}\right) + (1 - \alpha)\rho_l\left(h_l + \frac{u^2}{2}\right) - p\right)$$
$$+ \partial_x\left(\alpha\rho_v u\left(h_v + \frac{u^2}{2}\right)\right.$$
$$\left. + (1 - \alpha)\rho_l u\left(h_l + \frac{u^2}{2}\right)\right) = q + f_b. \quad (4.1c)$$

The v and l subscripts appearing in the system (4.1), refer to vapor and liquid phases respectively. The variables have the following meanings: α is the volume void fraction, $\rho_{v,l}$ is

the phasic density, $h_{v,l}$ is the phasic specific enthalpy, p is the pressure, and u is the common velocity. In the right-hand side, g is the gravity constant, τ represents the wall friction, q is a heat source and f_b represents some body forces. It will be useful to define the concentration

$$c = \frac{\alpha\rho_v}{\alpha\rho_v + (1 - \alpha)\rho_l} \quad (4.2)$$

and the mixture quantities

$$\rho = \alpha\rho_v + (1 - \alpha)\rho_l \quad (4.3)$$

$$h = ch_v + (1 - c)h_l. \quad (4.4)$$

The system (4.1) can be rewritten with the mixture variables ρ, u, and h as

$$\partial_t\mathbf{u} + \partial_x\mathbf{f}(\mathbf{u}) = s(\mathbf{u}), \quad (4.5a)$$

where

$$\mathbf{u} = \left(\rho, \rho u, \rho\left(h + \frac{u^2}{2}\right) - p\right)^{\mathrm{T}} \quad (4.5b)$$

$$\mathbf{f}(\mathbf{u}) = \left(\rho u, p + \rho u^2, \rho u\left(h + \frac{u^2}{2}\right)\right)^{\mathrm{T}} \quad (4.5c)$$

$$s(\mathbf{u}) = (0, -\tau - \rho g, q + f_b)^{\mathrm{T}}. \quad (4.5d)$$

The field equations for the homogeneous equilibrium model of two-phase flow is very similar to the Euler equations that represent a single-phase flow model. The differencies are mainly exhibited in the state functions and the source terms. The equation of state takes three forms according as we are in a single-phase region (liquid or vapor) or in a two-phase region. A general form for each of these equations is presented below; specific forms used in our computations are given in [16].

Liquid region. We assume that a relationship giving liquid density and liquid enthalpy as a function of the temperature and the pressure is available:

$$\rho = \rho_l(p, T) \quad \text{and} \quad h = h_l(p, T). \quad (4.6)$$

Vapor region. We assume again that

$$\rho = \rho_v(p, T) \quad \text{and} \quad h = h_v(p, T). \quad (4.7)$$

Two-phase region. Since the pressure p is a function of the temperature T, p and T are not appropriate independent variables. Also, we assume that the following relationships are available:

$$p = p_{\text{sat}}(T) \quad \text{or} \quad T = T_{\text{sat}}(p) \quad (4.8)$$

and

$$h = h_t(\rho, T).\qquad(4.9)$$

It is quite important for the construction of our approximate Riemann solver, to assume that whatever the case we can eliminate T to obtain an equation of state involving the mixture specific enthalpy, the mixture density, and the pressure of the form

$$h = h(\rho, p).\qquad(4.10)$$

Since the homogeneous equilibrium model provides only a single mixture mass equation and a single energy equation, additional thermal constraints are necessary. A variety of such constraints is possible, the simplest of which is the assumption that both vapor and liquid phases are at saturation in the two phase region:

$$\rho_{l,v} = \rho_{l,v}^{sat}(p) \equiv \rho_{l,v}(p, T_{sat}(p))\qquad(4.11)$$

$$h_{l,v} = h_{l,v}^{sat}(p) \equiv h_{l,v}(p, T_{sat}(p));\qquad(4.12)$$

$\rho_l^{sat}(p)$, $h_l^{sat}(p)$ and $\rho_v^{sat}(p)$, $h_v^{sat}(p)$ are the saturation densities and enthalpies for liquid and vapor, respectively. The vapor fraction volume in the two-phase region is given by

$$\alpha(\rho, p) = \frac{\rho - \rho_l^{sat}(p)}{\rho_v^{sat}(p) - \rho_l^{sat}(p)}.\qquad(4.13)$$

The phase of a state u is obtained from the quality

$$X = \frac{h - h_l^{sat}(p)}{h_v^{sat}(p) - h_l^{sat}(p)}.\qquad(4.14)$$

If $X \leqslant 0$ or $X \geqslant 1$, the state u is in a single-phase region, liquid or vapor. Otherwise, u belongs to the two-phase region. It should be observed that the global state function (4.10) is continuous through the saturation curve (4.8) (which is the boundary of the two-phase region) but its partial derivatives are discontinuous.

4.2. Choice of the Path Φ

The homogeneous equilibrium model has a great appeal because a complete analogy exists with the system of Euler equations. For the construction of a Roe-averaged matrix, we follow a procedure similar to the one used in Section 3. Thus, all we need to define our approximate Riemann solver is to describe the family of paths $\Phi(s; u_L, u_R)$ needed to construct the matrix $A(u_L, u_R)_\Phi$. To do this, we will consider two possibilities: whether the states u_L and u_R are in the same region or not.

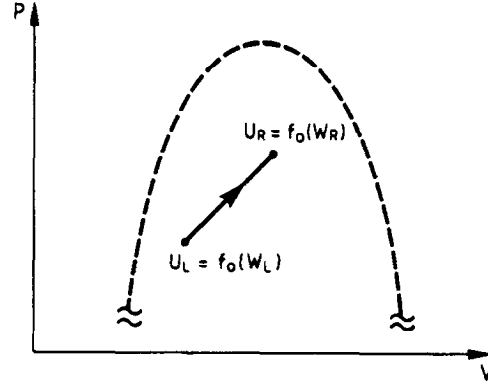**FIGURE 4.1**

If u_L and u_R are in the same region (liquid, vapor, or two-phase region) we are exactly in the same situation as with Euler equations with an arbitrary equation of state. Then, it is reasonable to keep in this case the same path Φ_0 given by Eq. (3.29), i.e., the canonical path for Roe's parameter vector w (Fig. 4.1).

On the other hand, if u_L and u_R are not in the same region, a more careful analysis is needed because the left and right states are not described by the same equation of state. In this case, the canonical path for Roe's parameter vector w leads to poor approximations of the pressure derivatives because of the discontinuity through the saturation curve. One can show that the average sound speed $\tilde{a}^2$ (Eq. (3.48)) could be negative if the pressure derivatives are poorly approximated.

To overcome the difficulties associated to a phase transition, we must introduce explicitly in the definition of the path Φ, an additional information which describes the transition from single-phase to two-phase flow. We now propose, a path $\Phi(s; u_L, u_R)$ which has so far worked each time that it has been used to compute a phase transition (vaporization as well as condensation).

Let us assume, for example, that $u_L(\rho_L, p_L, u_L)$ is in a liquid region ($X_L \leqslant 0$) and $u_R(\rho_R, p_R, u_R)$ is in a two-phase

FIGURE 4.2
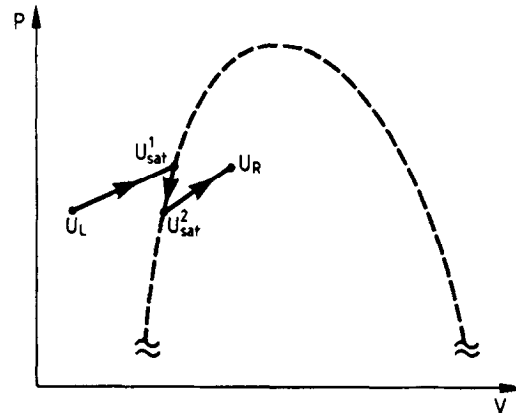
TABLE I

x (m)	Length (m)	K/L	q (W/m)
0.000–1.181	1.181	0	0
1.181–2.690	1.509	1.31	0
2.690–5.971	3.281	1.52	q
5.971–7.316	1.345	1.52	0

region $(X_R > 0)$. We take a path $\Phi(s; \mathbf{u}_L, \mathbf{u}_R)$ composed of three pieces: the first connects the state $\mathbf{u}_L$ to the state $\mathbf{u}_{sat}^1(\rho_f^{sat}(p_R), p_R, u_R)$ on the saturation curve, the second follows close on the saturation curve from $\mathbf{u}_{sat}^1$ to $\mathbf{u}_{sat}^2(\rho_f^{sat}(p_L), p_L, u_L)$, and the last links $\mathbf{u}_{sat}^2$ to $\mathbf{u}_R$ (Fig. 4.2).

Let $\mathbf{w}_L$, $\mathbf{w}_{sat}^1$, $\mathbf{w}_{sat}^2$, and $\mathbf{w}_R$ be the corresponding states for Roe's variables. The path $\Phi(s; \mathbf{u}_L, \mathbf{u}_R)$ can be written as

$$\Phi(s; \mathbf{u}_L, \mathbf{u}_R) = f_0(\psi(s; \mathbf{w}_L, \mathbf{w}_R)), \qquad (4.15)$$

where $f_0(\mathbf{w})$ is given by Eq. (3.24c) and

$$\psi(s; \mathbf{w}_L, \mathbf{w}_R) = \begin{cases} \mathbf{w}_L + 3s(\mathbf{w}_{sat}^1 - \mathbf{w}_L), \\ \qquad s \in [0, \tfrac{1}{3}] \\ \mathbf{w}_{sat}^1 + (3s - 1)(\mathbf{w}_{sat}^2 - w_{sat}^1), \\ \qquad s \in [\tfrac{1}{3}, \tfrac{2}{3}] \\ \mathbf{w}_{sat}^2 + (3s - 2)(\mathbf{w}_R - \mathbf{w}_{sat}^2), \\ \qquad s \in [\tfrac{2}{3}, 1]. \end{cases} \qquad (4.16)$$

Finally, the Roe-averaged matrix is defined by

$$A(\mathbf{u}_L, \mathbf{u}_R)_\Phi = C(\mathbf{u}_L, \mathbf{u}_R)_\Phi B(\mathbf{u}_L, \mathbf{u}_R)_\Phi^{-1}, \qquad (4.17)$$

where $B(\mathbf{u}_L, \mathbf{u}_R)$ and $C(\mathbf{u}_L, \mathbf{u}_R)$ are now given by

$$B(\mathbf{u}_L, \mathbf{u}_R)_\Phi \cdot (\mathbf{w}_R - \mathbf{w}_L) = \int_0^1 \frac{df_0}{d\mathbf{w}} (\psi(s; \mathbf{w}_L, \mathbf{w}_R))$$

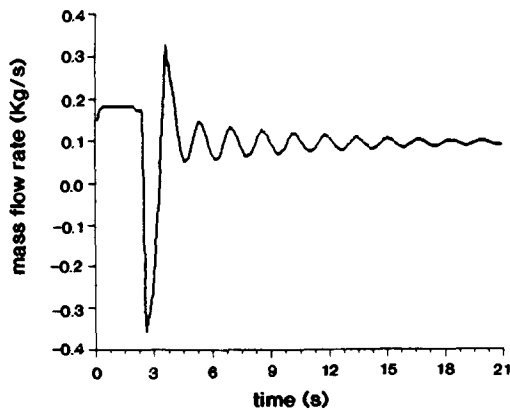$$\times \frac{\partial \psi}{\partial s} (s; \mathbf{w}_L, \mathbf{w}_R) \, ds \qquad (4.18)$$

FIGURE 4.3

$$C(\mathbf{u}_L, \mathbf{u}_R)_\Phi \cdot (\mathbf{w}_R - \mathbf{w}_L) = \int_0^1 \frac{d\mathbf{f}}{d\mathbf{w}} (\psi(s; \mathbf{w}_L, \mathbf{w}_R))$$

$$\times \frac{\partial \psi}{\partial s} (s; \mathbf{w}_L, \mathbf{w}_R) \, ds. \qquad (4.19)$$

4.3. Numerical Results on a Standard Problem

In this section we will give the numerical results obtained for a standard test problem in two-phase flow described in [16]. The purpose is to predict the transient resulting from heat addition to upward liquid flow in a smooth pipe. The smooth pipe is vertical, with the inlet at the bottom $(x = 0)$ and the outlet at the top $(x = 7.316 \text{ m})$ The cross-sectional area is uniform $(A = 0.000127 \text{ m}^2)$ as is the hydraulic diameter $(D = 0.00433 \text{ m})$. The pipe is divided into four sections, with the third section from the inlet being heated. The wall friction term may be calculated by the formula

$$\tau = \frac{1}{2} \rho u \, |u| \left(\frac{f}{D} + \frac{K}{L} \right),$$

where the friction factor f is a constant equal to 0.02 and the pipe loss factor per unit length K/L is specified in Table I. The heat source term is given by $q = q_0/A$ with

$$q_0 = \begin{cases} 0 & \text{for} \quad 0 \leqslant t < 2 \\ 18000(t - 2)/0.005 & \text{for} \quad 2 \leqslant t \leqslant 2.005 \\ 18000 & \text{for} \quad 2.005 < t. \end{cases}$$

Initial conditions at time $t = 0$ are

$$p(x, 0) = 7.102 + (6.984 - 7.102)(x/7.316)[MPa],$$

$$0 \leqslant x \leqslant 7.316$$

$$A\rho u(x, 0) = 806.3 \; [kg/m^2 s]$$

uniform along the pipe

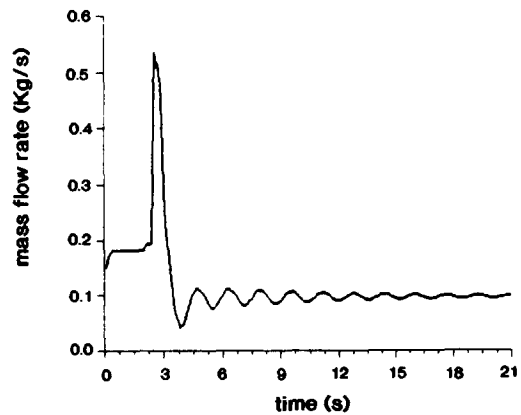$$h(x, 0) = 1.3 \; [MJ/kg] \qquad \text{uniform along the pipe.}$$
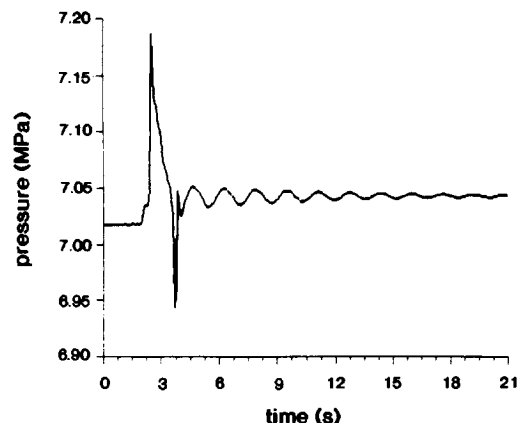

FIGURE 4.4

FIGURE 4.5

Boundary conditions applied throughout the transient are

$$p(0, t) = 7.102 \ [MPa], \qquad h(0, t) = 1.3 \ [MJ/\text{kg}],$$

$$p(7.316, t) = 6.984 \ [MPa].$$

The initial conditions do not represent a steady flow of water in the pipe, but steady flow is reached by the time heat is applied at 2 s. The flow parameters are such that the steady state reached after 18 s, is a two-phase flow in which a stationary boiling "front" is present. Therefore, during the transient there is a phase transition from single-phase to two-phase flow which was successfully handled by our approximate Riemann solver (with the path (4.16)).

There is no experimental data for this problem but converged reference solutions have been obtained with several codes [16]. Figures 4.3 and 4.4 give inlet and outlet mass flow rates time history. The time history of pressure at inlet to heated section is given in Figure 4.5. Figure 4.6 presents the time history of the flow quality defined by Eq. (4.14). All computations have been done using a first-order scheme with our generalized Riemann solver.
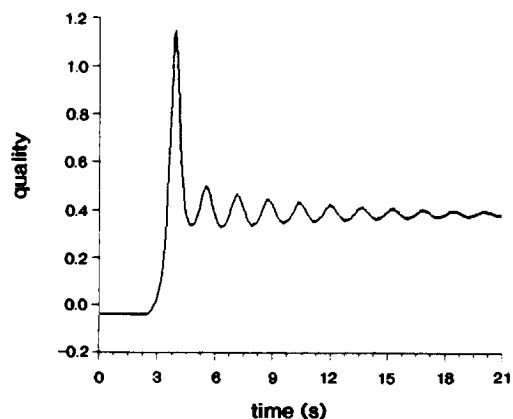

FIGURE 4.6

CONCLUSION

In this paper we have presented a weak formulation of Roe's approximate Riemann solver. Introducing a continuous path Φ in the state space, we described a new strategy for constructing a linearized Jacobian matrix. We have extended Roe's approximate Riemann solver for the Euler equations to incorporate a general equation of state that describes a real gas or a two-phase mixture, and we have seen that the choice of a path Φ leads to unique definitions for the averaged values of the pressure derivatives. In addition, the numerical results for a two-phase flow heat addition problem show the capacity of our approximate Riemann solver to handle very large discontinuities associated with the transition from single-phase to two-phase flow. We feel that this weak formulation may well have applications outside the context of conservation laws, for example, for nonconservative systems issued of the theory of multiphasics flows.

ACKNOWLEDGMENTS

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