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Generalized Flux-Vector Splitting and Roe Average for an Equilibrium Real Gas

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The flux-vector splittings of Steger–Warming and van Leer, and Roe's approximate Riemann solver are generalized to arbitrary equilibrium gas laws. Comparisons with other formulations are made.

INTRODUCTION

In extending upwind methods to hyperbolic systems of conservation laws, the most common approaches are based on either the flux-vector splittings of Steger and Warming [1] or van Leer [2], or the Roe approximate Riemann solver [3]. They all utilize the properties of the flux Jacobian matrix, and their original derivations relied on the algebraic simplicity of the perfect gas law. Many flows of current interest involve departure from a perfect gas due to vibrational excitation, dissociation, and ionization, although the assumption of thermodynamic and chemical equilibrium is still valid. The purpose of this paper is to present generalizations of these upwind methods to an arbitrary equilibrium gas law. Accurate numerical calculations for equilibrium air [4] show that the equation of state can be non-convex; i.e., the pressure derivatives can vary non-monotonically with density and internal energy. Consequently it is difficult to define optimum generalizations, valid for all gas laws and all numerical applications. Numerical calculations for some sample flows alone cannot be used to evaluate different generalizations. They can also be judged from theoretical considerations, by examining how well they satisfy basic physical principles. An obvious one for upwind methods is that the exact speed of sound is employed. Another that is less appreciated is that there is an

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arbitrary additive constant in the definition of the internal energy per unit mass. For those variables whose values are independent of that constant, the numerical algorithm should also preserve that independence, within roundoff errors. The relations presented here are based on these principles. For simplicity, the analysis is restricted to one-dimensional flow with a fixed grid. The corresponding relations for three-dimensional flow with time-varying grids are found in Refs. [5, 6]. The extension of these results to general, nonequilibrium flows is presented in Ref. [7].

The formulations of the two flux-vector splittings proposed by other investigators [8–12] either do not use the correct sound speed or do not satisfy the independence principle with respect to the energy constant. In order to obtain the proper generalizations of the two splittings, it is necessary to examine how they are related. Steger–Warming splitting is normally considered to result from the flux homogeneity property, while van Leer splitting results from the requirement that the split-flux Jacobians are continuous and possess a zero eigenvalue. Actually, they can be shown to be special cases of two general approaches to obtain flux-vector splitting for any hyperbolic system of conservation laws. Once this has been done, the way to generalize the two splittings becomes fairly clear.

In Roe's approximate Riemann solver, the flux Jacobian matrix is evaluated at an average state which results in the correct difference in flux between any two states. This Roe-averaged state refers only to those variables that appear *explicitly* in the Jacobian matrix. For a perfect gas, the elements of the matrix involve only variables per unit mass. Consequently, the density does not appear explicitly, and in Roe's original paper [3] an average density is not defined. Subsequently, many investigators *formally* defined an average density in order to express differences in conservative variables in terms of differences in primitive variables. While this slightly simplified the calculation of certain quantities, there is no *physical* basis for introducing such an average density. For an arbitrary equation of state, it is customary to consider the pressure as a function of density and internal energy per unit *mass* and to define derivatives with respect to these variables. This was done in the generalizations of the Roe average proposed by other investigators [11–13], and resulted in the presence of the density and the internal energy per unit mass, as well as the pressure derivatives, in the Jacobian matrix. In Refs. [12, 13], an average internal energy per unit mass was formally defined in a manner similar to the formal definition of an average density. Since the conservation laws are expressed in terms of conserved quantities per unit *volume*, it is actually physically more correct, in the present context, to treat the pressure as a function of density and internal energy per unit *volume*. If one does this, the Jacobian matrix will not explicitly contain the density or internal energy, thus obviating the need to define their averages in some artificial manner. This procedure is therefore followed in this paper. One must still obtain average values of the pressure derivatives. In the earlier stages of this work [6, 14, 15], and in Refs. [12, 13], it was established that only a linear relation exists between these two averages, so that a Roe-averaged state is not uniquely defined. Various methods for obtaining a unique state were proposed in those references. In the present paper, a new, exact definition of a unique

Roe-averaged state is given. Since its exact implementation may not always be practical, several approximations to the relations are also given.

The properties of the inviscid flux Jacobian matrix in one-dimensional flow are first obtained for an equilibrium gas satisfying an arbitrary equation of state. After a general discussion of flux-vector splitting for a hyperbolic system of conservation laws, the generalizations of Steger–Warming and van Leer flux splittings are derived. Their validity is examined by considering the special case of a thermally perfect gas. The generalized Roe average is presented next. Finally, comparisons are made with other formulations.

FLUX JACOBIAN MATRICES FOR AN EQUILIBRIUM GAS

The primitive variables defining a fluid state are the density ρ, velocity u, and the internal energy per unit mass ε, where there is an arbitrary additive constant in the definition of ε. The corresponding set of conservative variables U can be represented by the algebraic column vector

$$U=\begin{bmatrix}\rho\\ m\\ e\end{bmatrix}, \tag{1}$$

where $m=\rho u$ is the momentum per unit volume, $\tilde{\varepsilon}=\rho\varepsilon$ is the internal energy per unit volume, and $e=\tilde{\varepsilon}+\frac{1}{2}\rho u^2$ is the total energy per unit volume.

The set of inviscid flux components F is given by the algebraic column vector

$$F=\begin{bmatrix}M\\ P\\ E\end{bmatrix}=\begin{bmatrix}\rho u\\ mu+p\\ eu+pu\end{bmatrix}, \tag{2}$$

where M, P, and E are the flux of mass, momentum, and energy. The definition of e suggests that the equation of state for the pressure p be expressed as

$$p=p(\rho,\tilde{\varepsilon}). \tag{3}$$

The differential of p will be written as

$$dp=\chi\,d\rho+\kappa\,d\tilde{\varepsilon}, \tag{4}$$

where

$$\chi=\left(\frac{\partial p}{\partial\rho}\right)_{\tilde{\varepsilon}} \quad \text{and} \quad \kappa=\left(\frac{\partial p}{\partial\tilde{\varepsilon}}\right)_{\rho}. \tag{5}$$

If $h=(\tilde{\varepsilon}+p)/\rho$ is the specific enthalpy, the speed of sound c can then be expressed as

$$c^2=\chi+\kappa h. \tag{6}$$

Note that while the values of h and χ depend on the choice of arbitrary constant in the definition of ε, κ and c have well-defined values. It will also be convenient to define nondimensional parameters

$$\gamma = \frac{\rho c^2}{p} \quad \text{and} \quad \bar{\gamma} = 1 + \frac{p}{\tilde{\varepsilon}}. \tag{7}$$

We again note that the value of $\bar{\gamma}$ depends on the choice of arbitrary constant in the definition of ε.

An important special equation of state is that for a thermally perfect (but calorically imperfect) gas, which can be written in terms of properly normalized variables as

$$p = \rho T(\varepsilon), \tag{8}$$

where T is a dimensionless temperature. This law is valid for a dilute gas consisting of a single chemical species. For a diatomic gas with rotation fully excited, electronic excitation neglected, and vibration treated as a simple harmonic oscillator, the equation for $\varepsilon(T)$ is

$$\varepsilon(T) = \frac{5}{2}T + \frac{1}{e^{1/T} - 1}. \tag{9}$$

Equation (9) is a very good approximation for air below the temperature when oxygen starts to dissociate (approximately 2000 K). Using Eqs. (5)–(7) one can readily obtain for a thermally perfect gas the relations

$$p = \chi(\varepsilon)\rho + \kappa(\varepsilon)\tilde{\varepsilon} \tag{10}$$

and

$$\gamma = \kappa + 1, \qquad \bar{\gamma} = \gamma + \frac{\chi}{\varepsilon}. \tag{11}$$

If one further specializes Eq. (8) by letting $T(\varepsilon)$ be just a linear function of ε, one obtains the equation for a gas that is also calorically perfect—better known simply as a perfect gas. This law is valid for a gas consisting of structureless particles and is also a very good approximation for air at low temperatures. The derivatives χ and κ are now constants. It follows from Eqs. (10) and (11) that a great simplification is obtained if one chooses the arbitrary constant in the definition of ε so that $\chi = 0$ and $\bar{\gamma} = \gamma$. In fact, this choice is tacitly made in the usual definition of a perfect gas. It is therefore also customary to choose the arbitrary energy constant for a general gas so that χ approaches zero at low temperatures. This was already done in writing Eq. (9).

The differential expression $dF = A\,dU$ defines the flux Jacobian matrix operator A. Using Eq. (4), one can write A as

$$A = \begin{bmatrix} 0 & 1 & 0 \\ K_1 - u^2 & (2-\kappa)u & \kappa \\ (K_1 - H)u & H - \kappa u^2 & (1+\kappa)u \end{bmatrix}, \tag{12}$$

where $K_1 = \frac{1}{2}\kappa u^2 + \chi$ and $H = h + \frac{1}{2}u^2$ is the total enthalpy per unit mass. The three eigenvalues of A are readily found to be

$$\lambda_1 = u, \qquad \lambda_2 = u + c, \qquad \lambda_3 = u - c. \tag{13}$$

Note that while the elements of A are explicit functions of u, H, χ, and κ, the dependence on χ and κ in the eigenvalues is only through the linear combination in Eq. (6). The corresponding right eigenvector matrix R is

$$R = \begin{bmatrix} 1 & 1 & 1 \\ u & u+c & u-c \\ K_2 & H+cu & H-cu \end{bmatrix}, \tag{14}$$

where $K_2 = \frac{1}{2}u^2 - \chi/\kappa = H - c^2/\kappa$, while the left eigenvector matrix R^{-1} takes the form

$$R^{-1} = \begin{bmatrix} 1 - K_1/c^2 & \kappa u/c^2 & -\kappa/c^2 \\ \frac{1}{2}(K_1/c^2 - u/c) & -\frac{1}{2}(\kappa u/c^2 - 1/c) & \frac{1}{2}\kappa/c^2 \\ \frac{1}{2}(K_1/c^2 + u/c) & -\frac{1}{2}(\kappa u/c^2 + 1/c) & \frac{1}{2}\kappa/c^2 \end{bmatrix}. \tag{15}$$

The only difference between the expressions in Eqs. (12), (14), and (15) and the corresponding expressions for a perfect gas is the presence of χ in the terms K_1 and K_2, and the fact that κ is a variable instead of a constant. By writing K_1 and K_2 in terms of H and c^2, using Eq. (6), one can obtain expressions in which the only difference with the perfect gas expressions is the presence of the variable κ.

One can rewrite A in terms of its eigenvalues as

$$A = \sum_{i=1}^{3} \lambda_i P_i, \tag{16}$$

where the projection operators P_i are the tensor products

$$P_i = R_i R_i^{-1}. \tag{17}$$

From Eqs. (1), (2), and (12), one can also easily establish that

$$AU = F + (\gamma - 1 - \kappa)p \begin{bmatrix} 0 \\ 1 \\ u \end{bmatrix}. \tag{18}$$

It follows that the necessary and sufficient condition for the homogeneity property $F = AU$ is given by a thermally perfect gas (Eq. (8)). (This property is also true for a nonequilibrium mixture of thermally perfect gases if the density of each species is treated as a separate dependent variable [7].)

GENERAL FORMULATION OF FLUX-VECTOR SPLITTING

Before we derive the generalizations of flux-vector splitting to arbitrary, equilibrium gas laws, it is instructive to consider a general hyperbolic system of conservation laws $U_t + [F(U)]_x = 0$, for which the eigenvalues of A are all real. If the eigenvalues are all of one sign, then upwind differencing can be simply implemented. In flux-vector splitting methods, for the general case of eigenvalues of mixed sign, the flux F is written as

$$F = F^+ + F^-, \tag{19}$$

so that the split-flux Jacobian operators $A^\pm = \partial F^\pm / \partial U$ have the property that their eigenvalues $\lambda_i(A^\pm) \gtrless 0$ for all i. (In practice, one can permit some $\lambda_i(A^\pm) \lessgtr 0$ if they are sufficiently small in magnitude.) Then F^+ and F^- can each be differenced in an upwind manner.

Assume that the dependence of the eigenvalues $\lambda_i(A)$ on some variable u is such that there exist critical values of $u = \bar{u}^\pm$ for which all $\lambda_i \gtrless 0$ when $u \gtrless \bar{u}^\pm$. It follows that

$$F^\pm = F, \qquad F^\mp = 0 \qquad \text{for} \quad u \gtrless \bar{u}^\pm. \tag{20}$$

Let $\bar{u}_i$ denote the zero of each $\lambda_i(u)$, where the notation $\lambda_i(u)$ implies that other dependent variables are fixed. Then the $\bar{u}^\pm$ must satisfy

$$\bar{u}^+ = \max_i \bar{u}_i \qquad \text{and} \qquad \bar{u}^- = \min_i \bar{u}_i. \tag{21}$$

There are two general approaches to obtain a flux-vector splitting for $\bar{u}^- \leqslant u \leqslant \bar{u}^+$. One is based on the eigenvalues λ_i, and involves an expansion of the form

$$F = \sum_i F_i(u), \tag{22}$$

where each $F_i(u)$ is associated with an eigenvalue λ_i. Then $F^\pm$ is the sum of those F_i associated with all $\lambda_i \gtrless 0$. It follows that the resulting $A^\pm$ and $\lambda_i(A^\pm)$ are in general discontinuous at each of the zeros $\bar{u}_i$. For any choice of F_i one must still check whether the resulting $\lambda_i(A^\pm)$ are all of the correct sign. This type of splitting was first derived for the gasdynamic equations by Steger and Warming [1], and will therefore be referred to as generalized Steger–Warming flux-vector splitting.

The other approach is based only on the two limiting zeros $\bar{u}^+$ and $\bar{u}^-$, and involves the construction of interpolation functions for the interior range $\bar{u}^- \leqslant u \leqslant \bar{u}^+$ which connect the known forms of $F^\pm$ outside that region. Various continuity conditions can be imposed at $u = \bar{u}^+$ and $u = \bar{u}^-$, and the form of the interpolation functions can be based on the form and symmetries of $F(u)$. The final splitting formulas must again be checked for the correct signs of the $\lambda_i(A^\pm)$. This type of splitting was first derived for the gasdynamic equations by van Leer [2], and will therefore be referred to as generalized van Leer flux-vector splitting.

GENERALIZED STEGER–WARMING FLUX-VECTOR SPLITTING

For a thermally perfect gas, the first approach is suggested immediately, since Eqs. (16) and (18) can be combined to yield

$$F = \sum_{i=1}^{3} \lambda_i P_i U. \tag{23}$$

Using Eqs. (1), (11), (14), (15), and (17), one can then express F as

$$F = \sum_{i=1}^{3} F_i, \tag{24}$$

where the F_i are given by

$$F_1 = \frac{\lambda_1 \rho(\gamma - 1)}{\gamma} \begin{bmatrix} 1 \\ u \\ \frac{1}{2}u^2 + \varepsilon - \frac{c^2}{\gamma(\gamma-1)} \end{bmatrix}, \qquad F_{\substack{2\\3}} = \frac{\lambda_{\substack{2\\3}} \rho}{2\gamma} \begin{bmatrix} 1 \\ u \pm c \\ H \pm cu \end{bmatrix}, \tag{25}$$

and $\gamma = \gamma(\varepsilon)$. The special case of a perfect gas is obtained by letting γ be constant, and setting $\varepsilon - c^2/\gamma(\gamma - 1) = 0$. (While they explicitly stated that their approach was valid for a thermally perfect gas, Steger and Warming [1] only presented results for a perfect gas.) The total flux for the region $-c < u < c$ can then be split according to the signs of the eigenvalues. For $-c < u < 0$, we therefore have

$$F^+ = F_2 \qquad \text{and} \qquad F^- = F_1 + F_3, \tag{26}$$

while for $0 < u < c$,

$$F^+ = F_1 + F_2 \qquad \text{and} \qquad F^- = F_3. \tag{27}$$

To obtain a generalization for an arbitrary equilibrium gas, we follow a different procedure which is an extension of the work of Sanders and Prendergast [16]. The basic idea is the observation that the eigenvalues are three velocities. We can therefore associate with each eigenvalue λ_i a fictitious stream with velocity $u_i = \lambda_i$, density ρ_i, and internal energy per unit mass ε_i. Each stream can then be characterized by the column vector

$$U_i = \begin{bmatrix} \rho_i \\ \rho_i u_i \\ \rho_i \varepsilon_i + \frac{1}{2}\rho_i u_i^2 . \end{bmatrix}. \tag{28}$$

In order to obtain a form similar to that of Eq. (25), the fictitious flux due to each stream is assumed to be convective only, namely,

$$F_i = u_i U_i = \lambda_i U_i. \tag{29}$$

The six unknowns are determined from the conditions

$$U = \sum_{i=1}^{3} U_i \qquad \text{and} \qquad F = \sum_{i=1}^{3} F_i. \tag{30}$$

Since the first component of the equation for F gives the same relation as the second component of the equation for U, we are left with one degree of freedom. From the first two components of U and F one readily obtains

$$\rho_2 = \rho_3 = \frac{\rho}{2\gamma} \qquad \text{and} \qquad \rho_1 = \rho\left(1 - \frac{1}{\gamma}\right). \tag{31}$$

The third components of U and F result in the relations

$$\varepsilon_2 = \varepsilon_3 \qquad \text{and} \qquad \sum_{i=1}^{3} \rho_i \varepsilon_i = \rho\left(\varepsilon - \frac{c^2}{2\gamma}\right). \tag{32}$$

The relations in Eqs. (31) and (32) are consistent with solution (25) for a thermally perfect gas, but are now valid for an arbitrary γ defined by Eq. (7). In choosing the manner in which the remaining degree of freedom is parametrized, we use the principle that the solution should be independent of the arbitrary constant in the definition of ε. It follows that each $\varepsilon_i = \varepsilon +$ a term proportional to c^2, where the proportionality factor is independent of the arbitrary constant. A convenient choice is to let

$$\varepsilon_1 = \varepsilon - \frac{(1-\psi)c^2}{\gamma(\gamma-1)}. \tag{33}$$

The non-dimensional parameter ψ has been chosen so that $\psi = 0$ corresponds to solution (25) for a thermally perfect gas. Thus the solution derived from the homogeneity property $F = AU$ is seen to be just one member of a one-paramter family of flux-vector splittings. (In the earlier stages of this work, whose results are reported in Ref. [15], the parametrization $\rho_1 \varepsilon_1 = \psi\rho[\varepsilon - c^2/(2\gamma)]$ was chosen. This does not satisfy the independence principle concerning the arbitrary constant in the definition of ε, and the resulting analysis is therefore flawed.)

The dependence on ψ can be studied simply by first considering the perfect gas case for a constant ψ. The necessary condition for the split-flux Jacobian matrix A^+ to have eigenvalues that are all non-negative is that $\det A^+ \geqslant 0$. For the range $-c < u < 0$, one obtains

$$\det A^+ = \frac{(c+u)^3}{16\gamma^2}\left[3 - \gamma - 2\psi\,\frac{(\gamma-1)}{\gamma}\right]. \tag{34}$$

It follows from Eq. (34) that we must take $\psi \leqslant \frac{1}{2}\gamma(3-\gamma)/(\gamma-1)$. For the region $0 < u < c$, one can show that the minimum value of $\det A^+$ occurs when u approaches zero. This minimum value is

$$\det A^+ = \frac{c^3}{16\gamma^3}\left[5 - 3\gamma - 2\psi\,\frac{(3-\gamma)(\gamma-1)}{\gamma}\right]. \tag{35}$$

It follows from Eq. (35) that we must take $\psi \leqslant \frac{1}{2}\gamma(5-3\gamma)/[(3-\gamma)(\gamma-1)]$. For $1 < \gamma < 3$, this second condition on ψ automatically satisfies the previous inequality derived for $-c < u < 0$. In order to determine an optimum value of ψ, we note that in general the three eigenvalues of A^+ are discontinuous at $u = -c$, $u = 0$, and $u = c$. For $\psi = 0$, the two largest eigenvalues become continuous at $u = c$. It follows from Eq. (35) that we are limited to $\gamma \leqslant \frac{5}{3}$ when $\psi = 0$. Fortuitously, the maximum value of γ, corresponding to a gas consisting of structureless particles, is $\gamma = \frac{5}{3}$. One can further show from numerical calculations that all the eigenvalues of A^+ for $\psi = 0$ are real and non-negative in the range $-c < u < c$ when $\gamma \leqslant \frac{5}{3}$. For these reasons, $\psi = 0$, i.e., the Steger–Warming solution, is the optimum choice for a perfect gas. It has the interesting interpretation that all the internal energy is carried by streams 2 and 3. A plot of the three eigenvalues of A^+ for $\gamma = 1.4$ is shown in Fig. 1 as functions of the Mach number u/c. Note that the minimum eigenvalue increases monotonically with u, starting from 0 at $u = -c$. After undergoing a discontinuous drop at $u = 0$, it increases monotonically again, reaching its maximum value at $u = c$. For a thermally perfect gas satifying Eqs. (8) and (9), numerical calculations for a fixed temperature T based on solution (25) show the same qualitative behavior for the minimum eigenvalue as in Fig. 1. The critical value to examine is the one right after the discontinuous drop at $u = 0$. This is obtained from Eq. (27), evaluated at $u = 0$. The results are shown in Fig. 2, as a function of temperature. It is seen that it remains positive throughout the temperature range. Thus we have shown that, at least for Eq. (9), the choice $\psi = 0$ has the right eigenvalue behavior for a thermally perfect gas.

The choice of ψ for an arbitrary gas is still open. A reasonable choice is to let ψ be proportional to the quantity $\gamma - 1 - \kappa$, since it gives $\psi = 0$ for a thermally perfect gas. But this would introduce a second thermodynamic parameter, namely κ, into the solution. Since κ does not appear explicitly in U or the eigenvalues of A, the solution would not satisfy the simple notion of flux-vector splitting discussed previously. Furthermore, due to the general nature of the variation of γ and κ, it

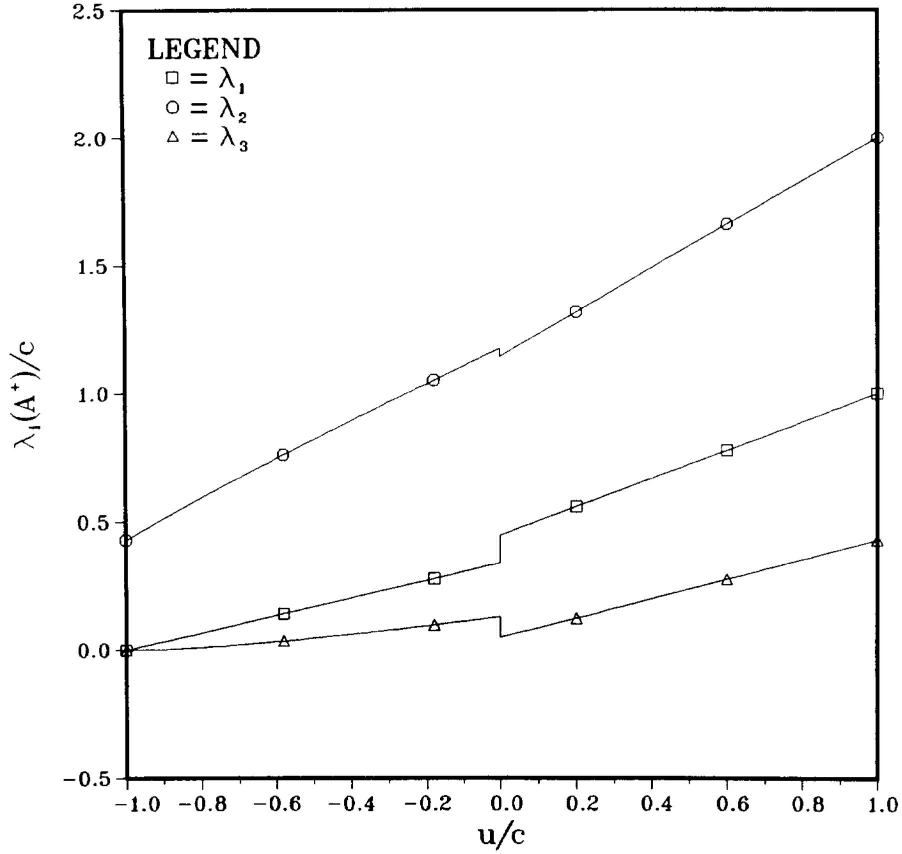

FIG. 1. Eigenvalues of A^+ for Steger–Warming flux-vector splitting. Perfect gas, $\gamma = 1.4$.

would be difficult to determine the proportionality factor in a simple manner. For these reasons, the simplest choice is to set $\psi = 0$ for an arbitrary gas. Thus Eqs. (25)–(27) also define the generalized Steger–Warming flux-vector splitting, with γ defined by Eq. (7) for an arbitrary gas.

GENERALIZED VAN LEER FLUX-VECTOR SPLITTING

In order to avoid the discontinuities of the Steger–Warming type of flux-vector splitting, one can use the second approach based on interpolation functions. van Leer [2] obtained a solution for a perfect gas which has the additional property that $E^{\pm}$ can be expressed as a function of $M^{\pm}$ and $P^{\pm}$ alone. It follows from this degeneracy condition that one of the eigenvalues of $A^{\pm}$ is identically zero. This results in a sharper capture of transonic shocks. Although one cannot expect

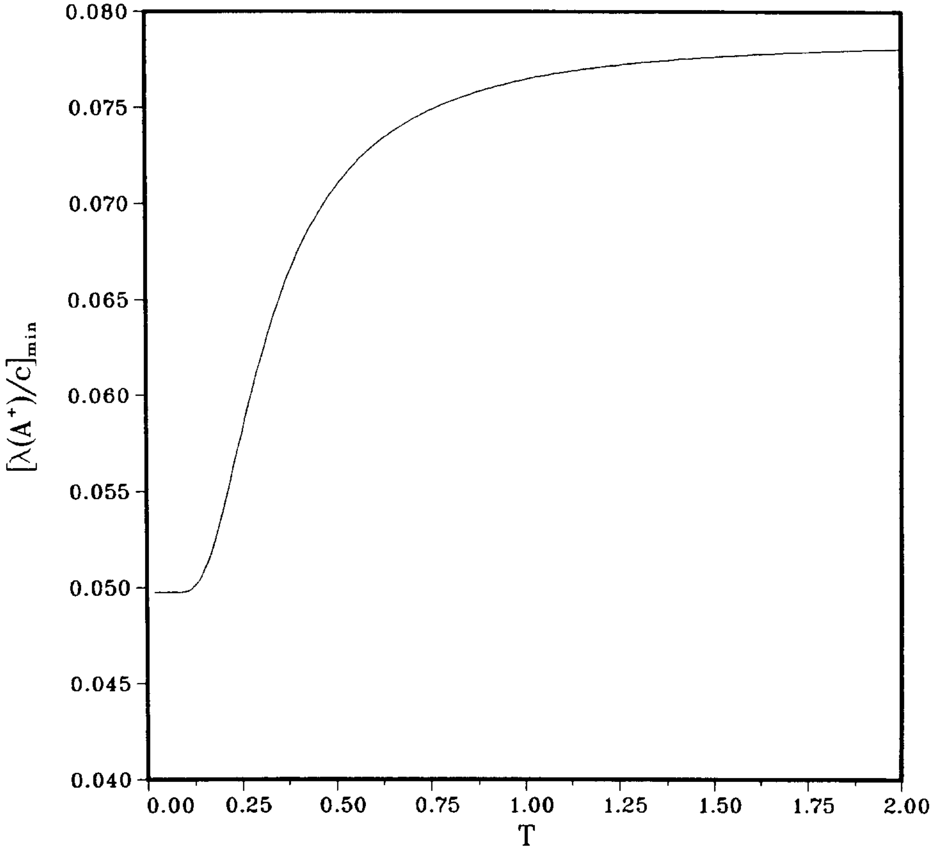

FIG. 2. Minimum eigenvalue of A^+ in the range $0 < u < c$ for Steger–Warming flux-vector splitting. Thermally perfect gas satisfying Eq. (12).

to maintain this property exactly for an arbitrary equilibrium gas, one can seek a solution that approximates it as closely as possible.

In terms of the nomenclature introduced earlier, the dependence of the eigenvalues on the velocity u is such that $\bar{u}^+ = -\bar{u}^-$. One can then easily demonstrate that for any $f(u)$ that is either an even or odd function of u,

$$f^+(u) = \pm f^-(u) \qquad \text{if} \quad f(u) = \pm f(-u). \tag{36}$$

Equation (36) certainly applies to the present case, since each of the components of $F(U)$ defined by Eq. (2) is either an even or odd function of u. (But it is easy to see that relation (36) can be applied to any *arbitrary* $F(U)$. The condition on $\bar{u}^+$ and $\bar{u}^-$ can always be satisfied if one defines a new variable $u' = u - (\bar{u}^+ + \bar{u}^-)/2$. Any component of $F(U)$ can then be expressed as a sum of an even and odd function of u'.)

As a function of u, all the components of $F(U)$ can be represented by at most the cubic polynomial

$$f(u) = a_0 + a_1 u + a_2 u^2 + a_3 u^3. \tag{37}$$

This suggests the use of polynomials in u for the interpolation functions. The requirement of continuous differentiability at $u = \pm c$ therefore necessitates a factor $(u \pm c)^2$ in the formulas for $F^{\pm}$. The lowest order polynomials for $f^{\pm}(u)$ satisfying Eqs. (19) and (36) can then be expressed as

$$f^{\pm}(u) = \frac{(u \pm c)^2}{4c} (a_0^{\pm} + a_1^{\pm} u), \tag{38}$$

where

$$a_0^{\pm} = \frac{2a_0}{c} \pm (a_1 - c^2 a_3) \tag{39a}$$

and

$$a_1^{\pm} = 2ca_3 \pm \left(a_2 - \frac{a_0}{c^2}\right). \tag{39b}$$

Using Eqs. (37)–(39), one obtains immediately for the mass and momentum flux the expressions

$$M^{\pm} = \pm \frac{\rho}{4c} (u \pm c)^2 \tag{40}$$

and

$$P^{\pm} = \frac{M^{\pm}}{\gamma} [(\gamma - 1)u \pm 2c]. \tag{41}$$

They are identical to those derived by van Leer for a perfect gas, except that γ is now a variable. One can similarly obtain a two-term expansion for $E^{\pm}$. But this would not reduce to van Leer's solution for a perfect gas in which $A^{\pm}$ has one zero eigenvalue. However, the function $\pm (u + c)^2 (u - c)^2$ satisfies the continuity conditions at $u = \pm c$, and such a term can be added to $E^{\pm}$ without affecting $E(u)$. We thus again have a one-parameter family of flux splittings. We seek a form for $E^{\pm}$ that reduces simply to van Leer's solution for a perfect gas. Guided by the form of Eq. (41), we express the additive function in such a way that $E^{\pm}$ can be written as

$$E^{\pm} = M^{\pm} \left[\frac{\{(\gamma - 1)u \pm 2c\}^2}{2(\gamma^2 - 1)} + \left\{ \varepsilon - \frac{c^2}{\gamma(\gamma - 1)} \right\} + \beta (u \mp c)^2 \right], \tag{42}$$

where β is an arbitrary non-dimensional parameter that is independent of the arbitrary constant in the definition of ε. (Note that when $\beta = 1/(\gamma + 1)$, $E^{\pm} = M^{\pm}H$. This choice of flux splitting, which pereserves the total enthalpy, was recommended for hight Mach number flows by Hänel *et al.* [17].)

For a perfect gas, the second term in $E^{\pm}$ vanishes. van Leer's condition of a vanishing eigenvalue for $A^{\pm}$ requires β to vanish also. One can show that the remaining eigenvalues are both of the proper sign for $1 \leqslant \gamma \leqslant 3$. The three eigenvalues of A^{+} for $\gamma = 1.4$ are plotted as a function of the Mach number in Fig. 3. For an arbitrary gas law, for which $\varepsilon \neq c^2[\gamma(\gamma - 1)]$, one requires the second term in $E^{\pm}$. Since γ is a variable, it is impossible to obtain the vanishing eigenvalue condition identically throughout the velocity range for any choice of β.

It is instructive to consider again the thermally perfect gas law (8). From physical considerations it follows that $\varepsilon'(T) > 0$. It is then easy to demonstrate that for the solution with $\beta = 0$, det A^{+} and $\varepsilon''(T)$ have opposite signs. Since $\varepsilon''(T) > 0$ for a gas

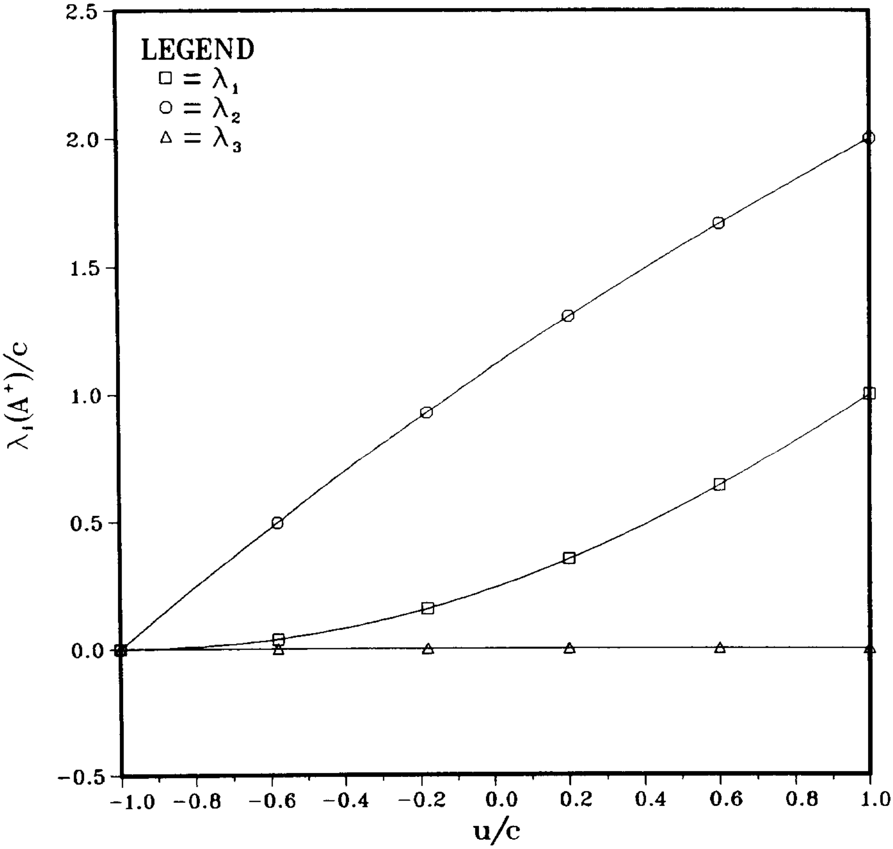

FIG. 3. Eigenvalues of A^{+} for van Leer flux-vector splitting. Perfect gas, $\gamma = 1.4$.

satisfying Eq. (9), one of the eigenvalues is *negative* in the whole subsonic velocity range for this case. Numerical calculations show that its minimum value is reached at a Mach number of 0.55. Figure 4 shows this minimum eigenvalue as a function of temperature. We see that the minimum value of $\lambda_i(A^+)/c$ is -0.0018, which is extremely small, so that the effect on a numerical scheme is not noticeable. In view of this fact and the general nature of the variation of γ, it is simplest to set $\beta = 0$ for an arbitrary gas. We therefore rewrite Eq. (42) as

$$E^{\pm} = M^{\pm}\left[\frac{\{(\gamma-1)u \pm 2c\}^2}{2(\gamma^2-1)} + \left\{\varepsilon - \frac{c^2}{\gamma(\gamma-1)}\right\}\right]. \tag{43}$$

In examining the forms of Eqs. (25), (40), (41), and (43), it is apparent that both of the splittings can be expressed in the following unified rule as modifications of the perfect gas formulas:

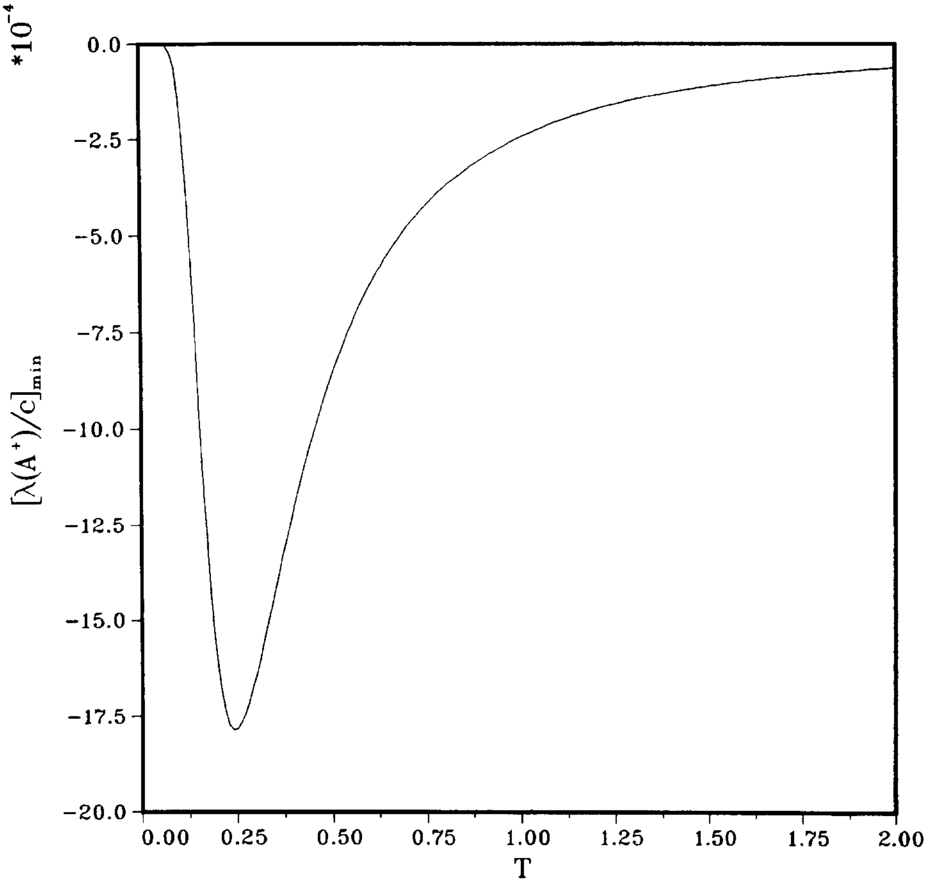

FIG. 4. Minimum eigenvalue of A^+ in the range $-c < u < c$ for van Leer flux-vector splitting. Thermally perfect gas satisfying Eq. (12).

1. Express the perfect gas flux-vector splittings in terms of u, ρ, c, and γ.

2. The generalized flux-vector splittings have the same form, with the constant γ replaced by the variable γ, except the split energy flux, which is given by

$$E^{\pm} = E^{\pm}_{\mathrm{PG}} + M^{\pm}_{\mathrm{PG}} \left[\varepsilon - \frac{c^2}{\gamma(\gamma-1)} \right]. \tag{44}$$

Generalized Roe Average

Among the various approximate Riemann solvers, the most common one uses the Roe average because of its simplicity and its ability to satisfy the jump conditions across discontinuities exactly. The derivation in Ref. [3] for a perfect gas employed parameter vectors. To obtain a generalization for an equilibrium gas, a different, more direct approach is used here.

In approximate Riemann solvers based on local linearization, the flux at a point separating two states U_L and U_R is based on the eigenvalues and eigenvectors of some average $\bar{A}$. The optimum choice for $\bar{A}$ is one satisfying

$$\Delta F = \bar{A}\, \Delta U, \tag{45}$$

where $\Delta(\cdot) = (\cdot)_R - (\cdot)_L$. This choice of $\bar{A}$ captures discontinuities exactly. One way of obtaining $\bar{A}$ is to seek an average state $\bar{U}$, such that

$$\bar{A} = A(\bar{U}). \tag{46}$$

The notation $\bar{U}$ implies only those variables that appear explicitly in Eq. (46). Such a state is known as a Roe-averaged state and was derived by Roe for a perfect gas. The generalization to an equilibrium gas is obtained by substituting Eqs. (1), (2), (12), and (46) into Eq. (45). The second component of Eq. (45) results in

$$\begin{aligned} \rho_R u_R^2 - \rho_L u_L^2 + \Delta p = {} & [(\tfrac{1}{2}\bar{\kappa} - 1)\bar{u}^2 + \bar{\chi}]\Delta\rho + (2 - \bar{\kappa})\bar{u}(\rho_R u_R - \rho_L u_L) \\ & + \bar{\kappa}\, \Delta\tilde{\varepsilon} + \tfrac{1}{2}\bar{\kappa}(\rho_R u_R^2 - \rho_L u_L^2). \end{aligned} \tag{47}$$

The average velocity $\bar{u}$ must be some linear combination of u_L and u_R. After expressing Eq. (47) in terms of u_L and u_R, the terms involving each of the products u_L^2, u_R^2, and $u_L u_R$ must satisfy the equation separately, since u_L and u_R can vary independently. One thus obtains [5] for $\bar{u}$ the relation

$$\bar{u} = \alpha u_L + (1 - \alpha) u_R, \tag{48}$$

where

$$\alpha = \frac{\sqrt{\rho_L}}{\sqrt{\rho_L} + \sqrt{\rho_R}}. \tag{49}$$

Equations (48) and (49) are the identical relations derived by Roe for a perfect gas. The remaining terms in Eq. (47) result in the new condition

$$\bar{\chi}\,\Delta\rho+\bar{\kappa}\,\Delta\tilde{\varepsilon}=\Delta p. \tag{50}$$

This is just the discrete form of Eq. (4), averaged between the two states. This last condition is automatically satisfied for a perfect gas. In a similar manner, the third component of Eq. (45) results in the additional relation

$$\bar{H}=\alpha H_L+(1-\alpha)H_R, \tag{51}$$

which is also true for a perfect gas. From the definition of H, Eqs. (48) and (51) can be combined to define the Roe-averaged specific enthalpy as

$$\bar{h}=\alpha h_L+(1-\alpha)h_R+\tfrac{1}{2}\alpha(1-\alpha)(\Delta u)^2. \tag{52}$$

Note that $\bar{h}$ is a function of the thermodynamic states L and R as well as the velocity difference Δu and could lie outside the range given by h_L and h_R if the magnitude of Δu is sufficiently large. The Roe-averaged sound speed is given by Eq. (6) as

$$\bar{c}^2=\bar{\chi}+\bar{\kappa}\bar{h}. \tag{53}$$

For a perfect gas, Eqs. (48), (49), (51)–(53) are sufficient to define uniquely $\bar{\lambda}_i$, $\bar{R}$, and $\bar{R}^{-1}$, since $\bar{\chi}=0$ and $\bar{\kappa}$ is a given constant.

For an arbitrary equilibrium gas, Eq. (50) provides only one relation for the variables $\bar{\chi}$ and $\bar{\kappa}$. We thus have the paradoxical situation that not only does a Roe-averaged state exist for an equilibrium gas, its precise value is not uniquely defined. For the special case in which state L and R are precisely those that satisfy the jump conditions across a discontinuity, Eqs. (48) through (53) are consistent with the exact Riemann solver, even though $\bar{\chi}$ and $\bar{\kappa}$ are not uniquely defined. For a shock wave, one can combine these equations to obtain [5]

$$\bar{h}=\frac{\Delta\tilde{\varepsilon}}{\Delta\rho}=\frac{\rho_L h_L+\rho_R h_R}{\rho_L+\rho_R}=\frac{(1-\alpha)^2 h_L+\alpha^2 h_R}{(1-\alpha)^2+\alpha^2} \tag{54}$$

and

$$\bar{c}^2=\Delta p/\Delta\rho. \tag{55}$$

It is easy to show that Eqs. (54) and (55) are also valid for a non-stationary shock wave. The values of $\bar{h}$ and $\bar{c}^2$ as given by Eqs. (54) and (55) will in general not be consistent with a thermally perfect gas law, except for the special case of a perfect gas.

It is clear from Eqs. (4) and (50) that unique values of $\bar{\chi}$ and $\bar{\kappa}$ must be defined in terms of the thermodynamic states L and R and cannot be functions of $\bar{h}$ or $\bar{c}^2$, since those average quantities also depend on the velocity difference Δu. Accurate numerical calculations for air [4] show that χ and κ can vary non-monotonically with ρ or $\tilde{\varepsilon}$ if the states L and R are far apart. A clue to a simple definition for the two average derivatives can be obtained by considering the special case $\tilde{\varepsilon}_L = \tilde{\varepsilon}_R$, i.e., $\Delta\tilde{\varepsilon} = 0$. Integrating Eq. (4) and substituting into Eq. (50) yields

$$\bar{\chi} = \frac{\Delta p}{\Delta \rho} = \frac{1}{\Delta \rho} \int_{\rho_L}^{\rho_R} \chi(\rho, \tilde{\varepsilon}_L)\, d\rho. \tag{56}$$

Thus $\bar{\chi}$ is the integrated average of χ along the straight-line path between states L and R in the $\rho - \tilde{\varepsilon}$ plane for this special case. Actually, there is an infinite set of paths that can be used to define $\bar{\chi}$, but the straight-line path is the simplest one that can be defined for an arbitrary function. Similarly, for $\Delta\rho = 0$ one obtains

$$\bar{\kappa} = \frac{\Delta p}{\Delta \tilde{\varepsilon}} = \frac{1}{\Delta \tilde{\varepsilon}} \int_{\tilde{\varepsilon}_L}^{\tilde{\varepsilon}_R} \kappa(\rho_L, \tilde{\varepsilon})\, d\tilde{\varepsilon}. \tag{57}$$

Let an arbitrary, smooth path between any two states L and R be defined parametrically by the functions $\rho(t)$ and $\tilde{\varepsilon}(t)$, where the parameter t is normalized so that $t_L = 0$ and $t_R = 1$. Integrating Eq. (4) along this path, one obtains

$$\Delta p = \int_0^1 \chi[\rho(t), \tilde{\varepsilon}(t)]\, \rho'(t)\, dt + \int_0^1 \kappa[\rho(t), \tilde{\varepsilon}(t)]\, \tilde{\varepsilon}'(t)\, dt. \tag{58}$$

The simplest choice is the straight-line path

$$\rho(t) = \rho_L + t\, \Delta\rho, \tag{59a}$$

$$\tilde{\varepsilon}(t) = \tilde{\varepsilon}_L + t\, \Delta\tilde{\varepsilon}. \tag{59b}$$

Substituting Eqs. (59) into Eq. (58), and comparing with Eq. (50), yields the general relations

$$\bar{\chi} = \int_0^1 \chi[\rho(t), \tilde{\varepsilon}(t)]\, dt, \tag{60a}$$

$$\bar{\kappa} = \int_0^1 \kappa[\rho(t), \tilde{\varepsilon}(t)]\, dt. \tag{60b}$$

Equations (59) and (60) give unique definitions of $\bar{\chi}$ and $\bar{\kappa}$ satisfying condition (50) for arbitrary values of $\Delta\rho$ and $\Delta\tilde{\varepsilon}$, including the limiting case $\Delta\rho = \Delta\tilde{\varepsilon} = 0$. From Eqs. (52) and (53) one sees that even if $\Delta u = 0$, $\bar{c}^2$ is not equal to the integrated average of c^2. Since h is a smoothly varying function (compared to χ and κ), it is reasonable to expect that $\bar{c}^2$ will always be positive. For a thermally perfect gas law obeying Eq. (8), and $\Delta\varepsilon \neq 0$, Eqs. (60a) and (60b) become

$$\bar{\chi} = \rho_L \rho_R \,\Delta\varepsilon \int_{\varepsilon_L}^{\varepsilon_R} \frac{(T - \varepsilon T')\, d\varepsilon}{(\Delta\tilde{\varepsilon} - \varepsilon\,\Delta\rho)^2}, \tag{61a}$$

$$\bar{\kappa} = \rho_L \rho_R \,\Delta\varepsilon \int_{\varepsilon_L}^{\varepsilon_R} \frac{T'\, d\varepsilon}{(\Delta\tilde{\varepsilon} - \varepsilon\,\Delta\rho)^2}. \tag{61b}$$

If $\Delta\varepsilon = 0$, these relations are replaced by $\bar{\kappa} = T'(\varepsilon_L)$ and $\bar{\chi} = T(\varepsilon_L) - \varepsilon_L \bar{\kappa}$.

Given an equation of state, or some piecewise analytic representation (such as Ref. [4]), the integrals in Eqs. (60) can be evaluated in principle for any two thermodynamic states L and R. In general, this will be an expensive operation. A piecewise representation of the results for all possible combinations L and R would require excessive storage, since one would have to fit functions of four independent variables. Practical computations therefore require some approximate procedure.

One method is suggested by the work of Glaister [13]. One can approximate Eqs. (60) by piecewise smooth paths consisting of straight-line segments $\rho =$ constant and $\tilde{\varepsilon} =$ constant. The resultant average pressure derivatives can then be expressed in terms of pressures at certain points. The simplest such relation is obtained in terms of the state A defined by $\rho_L, \tilde{\varepsilon}_R$, and the state B defined by $\rho_R, \tilde{\varepsilon}_L$. Then $\bar{\chi}$ and $\bar{\kappa}$ are defined as the arithmetic averages of the values resulting from integrating Eq. (4) via paths L–A–R and L–B–R, respectively. This results in

$$\bar{\chi} = \tfrac{1}{2}(p_B - p_L + p_R - p_A)/\Delta\rho, \tag{62a}$$

$$\bar{\kappa} = \tfrac{1}{2}(p_R - p_B + p_A - p_L)/\Delta\tilde{\varepsilon}. \tag{62b}$$

These are replaced by $\bar{\chi} = \frac{1}{2}(\chi_L + \chi_R)$ if $\Delta\rho = 0$, and $\bar{\kappa} = \frac{1}{2}(\kappa_L + \kappa_R)$ if $\Delta\tilde{\varepsilon} = 0$. It is easy to show that Eqs. (60) and (62) give the same results if p is a quadratic polynomial in ρ and $\tilde{\varepsilon}$. However, if the states L and R are far apart, and χ and κ vary non-monotonically, the introduction of the fictitious states A and B could give poor results. There is also the possibility that the states A or B could be outside the permissible range for the equation of state program.

A different method is to start with some approximations to Eqs. (60a) and (60b), which we call $\hat{\chi}$ and $\hat{\kappa}$ and which will not satisfy Eq. (50) exactly. One then finds values of $\bar{\chi}$ and $\bar{\kappa}$ satisfying Eq. (50) which are closest to $\hat{\chi}$ and $\hat{\kappa}$. This can be formulated geometrically as projecting the point $\hat{\chi}$, $\hat{\kappa}$ onto the straight line defined by Eq. (50). But in order for the Roe-averaged state to be independent of the arbitrary constant in the definition of ε, one must first recast the problem so that geometric relationships will not be affected by the choice of this constant. This can be accomplished if one first divides Eq. (50) by $\bar{\kappa}$. The slope of the straight line for the variables $1/\bar{\kappa}$ and $\bar{\chi}/\bar{\kappa}$ is now given by Δp and $\Delta\rho$, both of which are uniquely defined by states L and R. A further scale factor $\hat{s}$ with the dimension of $\bar{\chi}$ must be introduced, since $\bar{\chi}$ is not dimensionless. The projection on to the straight line is then defined by the relation

$$\frac{\hat{s}^2}{\bar{\kappa}}\,\Delta\rho + \frac{\bar{\chi}}{\bar{\kappa}}\,\Delta p = \frac{\hat{s}^2}{\hat{\kappa}}\,\Delta\rho + \frac{\hat{\chi}}{\hat{\kappa}}\,\Delta p. \tag{63}$$

If one introduces the error

$$\delta p = \Delta p - \hat{\chi}\,\Delta \rho - \hat{\kappa}\,\Delta \tilde{\varepsilon} \tag{64}$$

and the quantity

$$D = (\hat{s}\,\Delta \rho)^2 + (\Delta p)^2, \tag{65}$$

one can solve Eqs. (50) and (63) to obtain the final relations

$$\bar{\chi} = \frac{D\hat{\chi} + \hat{s}^2\,\Delta\rho\,\delta p}{D - \Delta p\,\delta p}, \tag{66a}$$

$$\bar{\kappa} = \frac{D\hat{\kappa}}{D - \Delta p\,\delta p}. \tag{66b}$$

A natural choice for the scale factor $\hat{s}$ is

$$\hat{s} = \widehat{c^2} = \hat{\chi} + \widehat{\kappa h}, \tag{67}$$

where the same quadrature approximation that was used to calculate $\hat{\chi}$ and $\hat{\kappa}$ is assumed. Note that the $\hat{s}$ given by Eq. (67) is guaranteed to be positive. This is not necessarily true of one defined $\hat{s} = \hat{\chi} + \hat{\kappa}\hat{h}$.

Let $\rho_M = (\rho_L + \rho_R)/2$ and $\tilde{\varepsilon}_M = (\tilde{\varepsilon}_L + \tilde{\varepsilon}_R)/2$ define the midpoint state M. Then possible approximate quadrature formulas for $\hat{\chi}$ are the midpoint rule

$$\hat{\chi} = \chi_M, \tag{68}$$

the trapezoidal rule

$$\hat{\chi} = (\chi_L + \chi_R)/2, \tag{69}$$

[redacted]

with analogous formulas for $\hat{\kappa}$ and $\widehat{c^2}$. Equations (68) and (69) are exact if p is a quadratic polynomial in ρ and $\tilde{\varepsilon}$, while Eq. (70) is exact if p is a cubic polynomial. While the expressions for $\bar{\chi}$ and $\bar{\kappa}$ given in Refs. [6, 14, 15] used approximation (69), they differ from the present results since Eq. (63) was written in terms of $\widehat{1/\kappa}$ and $\widehat{\chi/\kappa}$. If the states L and R are reasonably close, approximations (68) or (69) should be adequate. For large separation of the two states, Simpson's rule (70) may be required. The quantity D/p_L^2 is a useful nondimensional parameter measuring the separation of the two states. Actually, if one uses an efficient equation of state program, such as Ref. [4], to calculate p, the derivatives χ and κ can be obtained with little additional computational effort. The evaluation of $\bar{\chi}$ and $\bar{\kappa}$ using Eqs. (69), and (64)–(67) could then be more efficient as well as more accurate than the use of Eqs. (62).

While the above relations are all that are required to construct a Riemann solver using Roe's linearization, an additional algebraic simplicity can be achieved by expressing differences in conservative variables in terms of differences in primitive variables. If one *formally* defines

$$\bar{\rho} = \sqrt{\rho_L \rho_R}, \tag{71}$$

one obtains the identities

$$\Delta(\rho u) = \bar{\rho}\, \Delta u + \bar{u}\, \Delta\rho \tag{72}$$

and

$$\Delta(\rho u^2) = 2\bar{\rho}\bar{u}\, \Delta u + \bar{u}^2\, \Delta\rho. \tag{73}$$

An important quantity in the approximate Riemann solver is the column vector $R^{-1}\,\Delta U$. Its components are the jumps in the characteristic variables. Using Eqs. (50), (72), and (73), it can be expressed simply in terms of Δp, $\Delta\rho$, and Δu as

$$R^{-1}\,\Delta U = \begin{bmatrix} \Delta\rho - \Delta p/\bar{c}^2 \\ \frac{1}{2}(\Delta p/\bar{c}^2 + \bar{\rho}\,\Delta u/\bar{c}) \\ \frac{1}{2}(\Delta p/\bar{c}^2 - \bar{\rho}\,\Delta u/\bar{c}) \end{bmatrix}. \tag{74}$$

These expressions have the same form as for the perfect gas case. The quantities $\bar{\chi}$ and $\bar{\kappa}$ do not appear explicitly. Note that the introduction of $\bar{\rho}$ can be avoided by employing Eq. (72).

COMPARISONS WITH OTHER FORMULATIONS

The generalization of Steger–Warming flux-vector splitting for an equilibrium real gas given by Palmer [10] and Grossman and Walters [11] is obtained by replacing γ with $\tilde{\gamma}$ in Eqs. (7) and (25) and setting $\chi = 0$. Since accurate numerical calculations for air [4] show that γ and $\tilde{\gamma}$ can differ by more than 20%, the effective sound speed can differ from the true sound speed by more than 10%. This could give rise to errors in transonic regions. The formula of Montagné [8] is based on the analysis of this paper, except that the arbitrary parameter is chosen by assuming that the internal energy per unit mass of each stream is the same. This is equivalent to setting $\alpha = (3-\gamma)/2$, and does not reduce to the Steger–Warming flux-vector splitting for a perfect gas. The pseudo splitting formula of Liou *et al.* [12] is based on Eq. (18), with the homogeneous term treated in the manner of Steger and Warming, and the inhomogeneous term treated in a central difference manner. The solution explicitly involves the parameter κ, which we have already indicated to be inconsistent with the simple notion of flux-vector splitting. It also appears that their $F^{\pm}$ is discontinuous at $u = \pm c$ for an arbitrary gas law.

The generalization of van Leer flux-vector splitting given by Grossman and Walters [11] is again based on replacing γ by $\bar{\gamma}$ and does not use the true sound speed. Since $\bar{\gamma}$ is a variable, van Leer's condition of one zero eigenvalue can also not be obtained exactly in their formulation. For a thermally perfect gas, they also obtain one eigenvalue of the wrong sign. The formula of Montagné [9] differs from Eq. (57), involving both γ and $\bar{\gamma}$ in the first term, with the second term absent. His solution is internally inconsistent, since it does not satisfy Eq. (19). The formula of Liou *et al.* [12] is obtained from Eq. (42) by setting $\beta = (\bar{\gamma} - \gamma)/\{(\gamma + 1)[\gamma(\bar{\gamma} - 1) + 2\bar{\gamma}]\}$. This does not satisfy the principle that the solution should be independent of the arbitrary constant in the definition of ε.

The formulas for Roe's approximate Riemann solver described by Grossman and Walters [11] involve three approximations. They assume that (1) $\Delta\bar{\gamma}$ and $\Delta\gamma$ are small, (2) $\Delta\bar{\gamma}$ can be related to Δp via an isentropic formula, and (3) $\bar{\gamma}$ is nearly equal to γ. All these approximations can be poor if the two states are far apart. If one notes that

$$c^2 = \frac{(\bar{\gamma} - 1)}{\bar{\gamma}}\gamma h, \tag{75}$$

their final expressions are equivalent to setting $\chi = 0$, with $\bar{\gamma}$ and γ replaced by their arithmetic averages. The calculations of Ref. [4] show that setting $\chi = 0$ in the first eigenvector of Eq. (14) may not be justified.

Glaister [13] and Liou *et al.* [12] follow analyses similar to the present one for the generalized Roe average, except that their equation of state is expressed as

$$p = p(\rho, \varepsilon). \tag{76}$$

With the notation for the pressure derivatives defined by the differential relation

$$dp = p_\rho \, d\rho + p_\varepsilon \, d\varepsilon, \tag{77}$$

the results derived previously take the same form, except that Eqs. (50) and (53) are replaced by

$$\overline{p_\rho}\,\Delta\rho + \frac{\overline{p_\varepsilon}}{\bar{\rho}}\,[\Delta(\rho\varepsilon) - \bar{\varepsilon}\,\Delta\rho] = \Delta p \tag{78}$$

and

$$\bar{c}^2 = \overline{p_\rho} + \frac{\overline{p_\varepsilon}}{\bar{\rho}}\,(\bar{h} - \bar{\varepsilon}). \tag{79}$$

Note that one now needs to define $\bar{\rho}$ and $\bar{\varepsilon}$. Glaister [13] suggests that they satisfy the relation

$$\Delta(\rho\varepsilon) = \bar{\varepsilon}\,\Delta\rho + \bar{\rho}\,\Delta\varepsilon, \tag{80}$$

so that Eq. (78) reduces to the discrete form of Eq. (77), namely,

$$\overline{p_\rho}\,\Delta\rho+\overline{p_\varepsilon}\,\Delta\varepsilon=\Delta p. \tag{81}$$

Glaister also defines $\bar{\rho}$ by Eq. (71), in order to satisfy Eq. (72), even though the latter is not really required in the analysis. Combining Eq. (71) with Eq. (80) yields the relation

$$\bar{\varepsilon}=\alpha\varepsilon_L+(1-\alpha)\varepsilon_R \tag{82}$$

to define $\bar{\varepsilon}$. Actually, Eq. (82) can be derived purely from thermodynamic considerations. If one assumes that $\overline{p_\rho}$ and $\overline{p_\varepsilon}$ are both positive, then it follows from Eqs. (52) and (79) that defining $\bar{\varepsilon}$ by Eq. (82) guarantees that $\bar{c}^2$ will be positive. Equation (71) then follows from Eqs. (80) and (82). While it appears that Eqs. (52) and (82) are inconsistent in the limit of a perfect gas, one must recall that $\bar{h}$ is defined formally in terms of $\bar{H}$ and $\bar{u}$, and unlike $\bar{\varepsilon}$, it depends on the velocity difference Δu.

Glaister's solution for $\overline{p_\rho}$ and $\overline{p_\varepsilon}$ is analogous to Eqs. (62), in terms of the state A defined by ρ_L, ε_R and the state B defined by ρ_R, ε_L. It is easy to show that this does not reduce to Roe's solution for a perfect gas. In fact, the arithmetic averages used to obtain Eqs. (62) must be replaced by properly weighted averages in this case. The correct form of Glaister's solution is

$$\overline{p_\rho}=[\alpha(p_B-p_L)+(1-\alpha)(p_R-p_A)]/\Delta\rho, \tag{83a}$$

$$\overline{p_\varepsilon}=[\alpha(p_R-p_B)+(1-\alpha)(p_A-p_L)]/\Delta\varepsilon. \tag{83b}$$

These are replaced by $\overline{p_\rho}=\alpha(p_\rho)_L+(1-\alpha)(p_\rho)_R$, if $\Delta\rho=0$, and $\overline{p_\varepsilon}=\alpha(p_\varepsilon)_R+(1-\alpha)(p_\varepsilon)_L$, if $\Delta\varepsilon=0$. The weighted averages are necessary since the state C defined by $\bar{\rho}$, $\bar{\varepsilon}$, which appears explicitly in Eq. (79), does not lie on the straight-line path between states L and R in the $\rho-\varepsilon$ plane. (It actually lies on the straight-line path between states A and B.) The integral definitions analogous to Eqs. (60) must therefore also be modified, since one must integrate Eq. (77) along the piecewise smooth path L–C–R. The unique definitions of $\overline{p_\rho}$ and $\overline{p_\varepsilon}$ satisfying condition (81), which reduce to Roe's solution for a perfect gas, can be written as

$$\overline{p_\rho}=\alpha\int_0^1 p_\rho[\rho_1(t),\varepsilon_1(t)]\,dt+(1-\alpha)\int_0^1 p_\rho[\rho_2(t),\varepsilon_2(t)]\,dt, \tag{84a}$$

$$\overline{p_\varepsilon}=(1-\alpha)\int_0^1 p_\varepsilon[\rho_1(t),\varepsilon_1(t)]\,dt+\alpha\int_0^1 p_\rho[\rho_2(t),\varepsilon_2(t)]\,dt, \tag{84b}$$

where

$$\rho_1(t)=\rho_L+\alpha t\,\Delta\rho,\qquad \rho_2(t)=\bar{\rho}+(1-\alpha)t\,\Delta\rho, \tag{85a}$$

$$\varepsilon_1(t)=\varepsilon_L+(1-\alpha)t\,\Delta\varepsilon,\qquad \varepsilon_2(t)=\bar{\varepsilon}+\alpha t\,\Delta\varepsilon. \tag{85b}$$

One can easily show that Eqs. (83) and (84) give the same results if p is a quadratic polynomial in ρ and ε. From the definitions of states A, B, and C, it follows that as α approaches zero or one, the correct form of Glaister's solution (83) approaches the correct integral definition (84) for any gas law. Special forms of Eqs. (84) for a thermally perfect gas, analogous to Eqs. (61), can also be written.

As indicated earlier, if the states L and R are far apart, the introduction of the fictitious states A and B in Glaister's solution could give poor results, or may not be allowed by the equation of state program. The other approach is to choose some approximations p_ρ and $\widehat{p_\varepsilon}$ to Eqs. (84) and to find their projections onto Eq. (81). Liou *et al.* [12] suggest using

$$\widehat{p_\rho}=(p_\rho)_C, \qquad \widehat{p_\varepsilon}=(p_\varepsilon)_C, \tag{86}$$

which corresponds to Eq. (68). The appropriate relations corresponding to Eqs. (69) and (70) are

$$p_\rho=\alpha(p_\rho)_L+(1-\alpha)(p_\rho)_R, \qquad \hat{p}_\varepsilon=(1-\alpha)(p_\varepsilon)_L+\alpha(p_\varepsilon)_R \tag{87}$$

and

$$\begin{aligned}\widehat{p_\rho}&=\tfrac{1}{2}[\alpha(p_\rho)_L+(p_\rho)_C+(1-\alpha)(p_\rho)_R],\\ \widehat{p_\varepsilon}&=\tfrac{1}{2}[(1-\alpha)(p_\varepsilon)_L+(p_\varepsilon)_C+\alpha(p_\varepsilon)_R].\end{aligned} \tag{88}$$

Since the path L–C–R is not a straight-line path, the accuracy of these approximations is not as great as those of Eqs. (68)–(70). Thus Eqs. (86) and (87) are exact if p is a bilinear function of ρ and ε, while Eq. (88) is exact if p is a quadratic polynomial in ρ and ε. Note also that a polynomial in ρ and $\tilde{\varepsilon}$ is a higher order polynomial in ρ and ε. Liou *et al.* [12] recommend p_ρ/p_ε as the subfactor to make Eq. (81) dimensionless. However, in their numerical results, they employed the scale factor $\Delta\varepsilon/\Delta\rho$. As the authors themselves pointed out, this latter choice has a flaw, since the resultant formulas for $\overline{p_\rho}$ and $\overline{p_\varepsilon}$ break down when either $\Delta\rho$ or $\Delta\varepsilon$ approaches zero.

In summary, the use of ρ and ε instead of the more natural ρ and $\tilde{\varepsilon}$ as independent thermodynamic variables results in additional terms in the flux Jacobian matrix. This requires the definition of $\bar{\rho}$ and $\bar{\varepsilon}$ in formulating the Roe average. While plausible arguments can be used to define such a state, its presence results in more complex expressions to define the Roe-average pressure derivatives. From the examination of the respective relations, it would appear that under the most general conditions, the approximate evaluations of these pressure derivatives would be less accurate (and no more efficient) than those based on ρ and $\tilde{\varepsilon}$.

CONCLUDING REMARKS

We have shown that generalizations of the two flux-vector splittings and the Roe average to an arbitrary, equilibrium gas introduce one degree of freedom in each case. The particular forms we have chosen are believed to be the simplest that satisfy basic physical principles and are valid for the most general flow conditions and gas laws. They involve only minor modifications of the perfect gas formulas. Their accuracy and numerical efficiency depends on the representation of the equation of state. In particular, they can be computationally competitive with more approximate formulas when the pressure derivatives and sound speed are obtained with minimal additional effort once the pressure is determined.

The flux-vector splittings represent a simpler problem, since they involve a single thermodynamic state for each split-flux term. Only the pressure and sound speed, and not the individual pressure derivatives, need to be evaluated. Some confidence in the validity of the formulas is obtained from the calculation of the split-flux Jacobian eigenvalues for a thermally perfect gas satisfying Eq. (9). The fact that the general expressions for the splittings can be obtained from the perfect gas formulas by the same rule, even though the two splittings are derived from entirely different approaches, lends further confidence in their validity.

The generalization of the Roe average is more difficult to define, since it depends on two thermodynamic states—more specifically, the thermodynamic path between those states. The *theoretical* definition given by Eqs. (60), based on a linear path, is the simplest solution valid for a general gas law that is consistent with the Roe linearization. Since it involves an integration, it is not *computationally* practical, and some approximate method must be used. If the two states are sufficiently far apart, and the pressure derivatives have a highly non-monotonic behavior, any of the simple approximations discussed in the paper could give poor results. The use of ρ and ε as independent thermodynamic variables does not alleviate this problem and introduces additional complexity. Consequently, there would appear to be no particular advantage in using these variables.

The validation of our generalizations has been carried out in numerical calculations for a variety of one-dimensional Riemann problems in Ref. [14]. In steady state or explicit unsteady calculations, upwind methods serve to introduce numerical dissipation in a natural way. Yet the proper amount of dissipation in a given flow region is not a precisely defined quantity. Thus, unless the regions where very large gradients occur happen to lie in a part of thermodynamic space in which the equation of state deviates markedly from a locally perfect gas law, numerical calculations will not show significant variations in the results due to different generalizations. In fact, Glaister [13] obtained excellent agreement with the exact solutions of shock reflection problems for various equations of state, even though his formula for the Roe average is inconsistent with the perfect gas form. The search for an efficient, robust algorithm for arbitrary flows and general equations of state cannot be based on numerical calculations alone, but should also be guided by sound theoretical considerations. The formulas we propose follow these principles.

REFERENCES

1. J. L. STEGER AND R. F. WARMING, *J. Comput. Phys.* **40**, 263 (1981).
2. B. VAN LEER, "Flux-Vector Splitting for the Euler Equations," ICASE Report 82-30, Sept., 1982 (unpublished); Lecture Notes in Physics (Springer-Verlag, New York/Berlin, 1982), Vol. 170, p. 507.

3. P. L. Roe, *J. Comput. Phys.* **43**, 357 (1981).
4. Y. Liu and M. Vinokur, "Equilibrium Gas Flow Computations. I. Accurate and Efficient Calculation of Equilibrium Gas Properties," AIAA Paper 89–1736, June 1989 (unpublished).
5. M. Vinokur, "Flux Jacobian Matrices and Generalized Roe Average for an Equilibrium Real Gas," NASA CR-177512, December 1988 (unpublished).
6. M. Vinokur and Y. Liu, "Equilibrium Gas Flow Computations. II. An Analysis of Numerical Formulations of Conservation Laws," AIAA Paper 88–0127, Jan. 1988 (unpublished).
7. Y. Liu and M. Vinokur, *J. Comput. Phys.* **83**, 373 (1989).
8. J.-L. Montagné, La Recherche Aérospatiale English Edition, 1986-6, 45.
9. J.-L. Montagné, "Rapport de Synthèse finale," ONERA, 23/1285 AY, Dec. 1985 (unpublished).
10. G. Palmer, "An Implicit Flux-Split Algorithm to Calculate Hypersonic Flow Field in Chemical Equilibrium," AIAA Paper 87-1580, June 1987 (unpublished).
11. B. Grossman and R. W. Walters, *AIAA J.* **27**, 524 (1989).
12. M.-S. Liou, B. van Leer and J.-S. Shuen, *J. Comput. Phys.* **87**, 1 (1990).
13. P. Glaister, *J. Comput. Phys.* **74**, 382 (1988).
14. J.-L. Montagné, H. C. Yee, and M. Vinokur, *AIAA J.* **27**, 1332 (1989).
15. H. C. Yee, "Upwind and Symmetric Shock-Capturing Schemes," NASA TM 89464, May, 1987 (unpublished).
16. R. H. Sanders and K. H. Prendergast, *Astrophys. J.* **188**, 489 (1974).
17. D. Hänel, R. Schwane, and G. Seider, in "*Proceedings, AIAA 8th Computational Fluid Dyamics Conference, Honolulu, HI, 1987*, p. 42.