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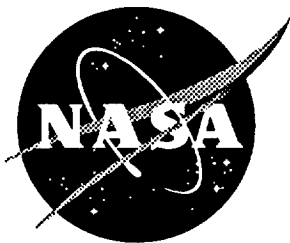
An Approximate Riemann Solver for Thermal and Chemical Nonequilibrium Flows

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AN APPROXIMATE RIEMANN SOLVER FOR
THERMAL AND CHEMICAL NONEQUILIBRIUM FLOWS

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Abstract

Among the many methods available for the determination of inviscid fluxes across a surface of discontinuity, the flux-difference-splitting technique that employs Roe-averagnd variables has been used extensively by the CFD community because of its simplicity and its ability to capture shocks exactly. This method, originally developed for perfect gas flows, has since been extended to equilibrium as well as nonequilibrium flows. Determination of the Roe-averaged variables for the case of a perfect gas flow is a simple task; however, for thermal and chemical nonequilibrium flows, some of the variables are not uniquely defined. Methods available in the literature to determine these variables, seem to lack sound bases. The present paper describes a simple, yet accurate, method to determine all the variables for nonequilibrium flows in the Roe-average state. The basis for this method is the requirement that the Roe-averaged variables form a consistent set of thermodynamic variables. The present method satisfies the requirement that the square of the speed of sound be positive.

Symbols

A	inviscid flux Jacobian
a, b	factors defined in Eqn. (5)
c	speed of sound
$C_{p,i}$	specific heat at constant pressure for species i
$C_{v,t,i}$	specific heat at constant volume for translational and rotational energy for species i
$C_{v,V,i}$	specific heat at constant volume for vibrational energy for species i
E	$=e + (u^2 + v^2)/2$, total energy (sum of internal and kinetic energies) per unit mass
e_{tr}	sum of translational, rotational, and formation energies per unit mass of the gas mixture
$e_{tr,i}$	sum of translational, rotational, and formation energies per mole of species i
e_V	vibrational energy per unit mass of the gas mixture

$e_{V,i}$ vibrational energy per mole of species i

F, G   inviscid flux vectors in x- and y-directions

f_i constants, 1.5 and 2.5 for atomic and molecular particles, respectively

H $=E + p/\rho$, total enthalpy of the gas mixture

n_x, n_y x- and y-components of the unit outward normal to an interface

p pressure

q $=(u^2 + v^2)/2$, kinetic energy

R universal gas constant

R, R^{-1} left- and right-eigenvector matrices of **A**

r $= \sqrt{\rho_R / \rho_L}$

T translational temperature

T_V vibrational temperature

T_{ref} reference temperature, zero Kelvin

t time

U   unknowns vector

u, v velocity components in x- and y-directions, respectively

W   vector of production terms

W_i molecular weight of species i

x_i mass fraction of species i

α_i $\partial p / \partial \rho_i$

β $\partial p / \partial (\rho E)$

γ specific heat ratio in ideal gas

$\Delta h_{f,i}$ heat of formation of species i at reference temperature

Λ vector of eigenvalues of matrix **A**

ϕ $\partial p / \partial [\rho e_V]$

ρ density of the gas mixture

ρ_i partial density of species i

Subscripts:

e electrons

i, j indices for chemical species

n normal to the interface

L left side of the interface

R right side of the interface

t translational mode

V vibrational mode

Introduction

In the numerical simulation of high speed flows, the flux-difference-splitting techniques have been successfully employed in the determination of the inviscid fluxes across a surface of discontinuity. Among these techniques, the one that uses the so-called Roe-averaged variables is popular among the researchers because of its simplicity and ability to capture shocks exactly. This is true for the case of perfect gases for which Roe [1] derived expressions for the necessary variables in the Roe-average state. The procedure has since been extended to equilibrium flows (see [2]-[5]), and to chemical and thermal nonequilibrium flows (see [6]-[8]). However, in all these extension the simplicity associated with a perfect gas case is lost. In addition, some of the Roe-averaged variables are not defined uniquely. This led to several methods for the determination of these variables, some of which are based on computational experience. However, these methods lacked sound bases in their approach.

The present paper addresses this issue, and describes a method for the determination of the Roe-averaged variables for thermal and chemical nonequilibrium flows. The method is simple, accurate, and requires no approximations. The basis for the present method is a requirement that the variables in the Roe-average state form a consistent set of thermodynamic variables. For the case of an air model with charged particles, the procedure requires the determination of a vibrational temperature for given values of vibrational energy and mixture composition. This, however, is a routine computation. For the case of a gas mixture with only inert particles, the method gets considerably simplified. Finally, it is important that any such method yield physically meaningful results in all cases, i.e., the square of speed of sound in the Roe-average state must be posi-

tive. The present method satisfies this requirement for all cases.

Analysis

Consider the Euler equations for two-dimensional flows written in conservation form:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0 \tag{1}$$

where

$$U = [\rho, \rho u, \rho v, \rho E]^T$$
$$F = [\rho u, p + \rho u^2, \rho u v, \rho u H]^T \tag{2}$$
$$G = [\rho v, \rho v u, p + \rho v^2, \rho v H]^T$$

We consider two-dimensional flows only for simplicity; the present analysis carries to three-dimensional flows without any loss of generality. If a computational domain is discretized into cells, and the unknowns are assumed to be discontinuous across the interface between two adjacent cells, then a question arises as to what is the flux across these surfaces of discontinuity? This is a classical Riemann problem for which several approximate solvers are available. Among these solvers, the one that uses Roe-averaged variables has been widely used by researchers in the CFD community. Determination of the Roe-averaged variables for the perfect gas case is simple, and these variables satisfy the jump conditions across normal shocks exactly. Adopting this approach, the numerical flux across a surface of discontinuity is written as

$$F_n = [F_{nL} + F_{nR} + |\bar{A}| (U_R - U_L)]/2 \tag{3}$$

where U_R and U_L are the unknowns in the left and the right cells, respectively, and F_{nL} and F_{nR} are the fluxes in the left and right cells normal to the common surface, respectively. The matrix $\bar{A}$ is the Jacobian of the inviscid fluxes, and is evaluated at the Roe-averaged state $\bar{U}$, which in turn is a function of U_L and U_R. The matrix $|\bar{A}| = \bar{R}|\bar{\Lambda}|\bar{R}^{-1}$ where the matrices $\bar{R}$ and $\bar{R}^{-1}$ are the left and the right eigenvector matrices of the matrix $\bar{A}$. Roe [1] identified the properties this matrix $\bar{A}$ should satisfy as the following:

(i) The matrix $\bar{A}$ constitutes a linear mapping from U to F.

(ii) As $U_L \to U_R \to U$, $\bar{A}(U_L, U_R) \to A(U)$, where $A = \partial F_n / \partial U$.

(iii) For any U_L and U_R, $\bar{A}(U_L, U_R) \cdot (U_L - U_R) = F_L - F_R$.

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(*iv*) The eigenvalues of $\overline{A}$ are linearly independent.

Roe determined the unknowns $\overline{U}$, and hence the matrix $\overline{A}$ that satisfies these properties. The unknowns that determine the matrix $\overline{A}$, its eigenvalues, and its eigenvectors are given by

$$\overline{u} = au_L + bu_R \qquad \overline{v} = av_L + bv_R \qquad \overline{H} = aH_L + bH_R \qquad (4)$$

where

$$a = \sqrt{\rho_L}/[\sqrt{\rho_L} + \sqrt{\rho_R}] = 1/(1+r) \qquad b = \sqrt{\rho_R}/[\sqrt{\rho_L} + \sqrt{\rho_R}] = r/(1+r) \qquad (5)$$

Note that $r = \sqrt{\rho_R/\rho_L}$ and $a + b = 1$. The speed of sound $\overline{c}$ is given by

$$\overline{c}^2 = (\gamma - 1)(\overline{H} - \overline{q}) \qquad (6)$$

where $\overline{q} = (\overline{u}^2 + \overline{v}^2)/2$. Computing the variables $\overline{u}, \overline{v}$, and $\overline{H}$ using Eqn. (4) has since become known as Roe-averaging. Flux difference splitting technique using Roe-averaged values has been successfully used by many researchers in solving high speed flows.

Nonequilibrium Flows

Consider the governing equations for thermal and chemical nonequilibrium flows in two-dimensions. The number of governing equations is $N = n_s + 2 + n_e$, where n_s is the number of chemical species considered in the chemistry model, and n_e is the number of energy equations. The other two equations come from conservation of x- and y-momentum. Gnoffo [6 & 9] considers a 11-species air model with two temperatures - translational and vibrational. In determining the flux across a surface of discontinuity, he employs the flux-difference-splitting technique. However, explicit expression for the variables in the Roe-average state are available for only some of the variables. In his analysis, Gnoffo [6] uses these expressions, and makes approximations for the remaining variables, based on his computational experience. Other approximate methods for the determination of these variables are available, (see Liu & Vinokur, [7], for example). In the present paper we examine Gnoffo's multi-species, two-temperature model, and present a method for the determination of the Roe-averages for all of the necessary variables without making any approximations.

As in the ideal gas case, we consider two-dimensional flows for simplicity. The governing equations for nonequilibrium flow of a multi-species, two-temperature gas written in conservation form as described by Gnoffo [9] are as follows:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \mathbf{W} \tag{7}$$

where

$$\mathbf{U} = [\rho_i, \rho u, \rho v, \rho E, \rho e_V]^T$$

$$\mathbf{F} = \left[\rho_i u, p + \rho u^2, \rho u v, \rho u H, \rho u e_V\right]^T \tag{8}$$

$$\mathbf{G} = \left[\rho_i v, \rho v u, p + \rho v^2, \rho u H, \rho v e_V\right]^T$$

Only the convective terms are considered. The quantity $\mathbf{W}$ Eqn. (7) is a vector of the production terms, and does not enter into the present analysis. Most of the analysis described here follows Gnoffo's analysis with minor changes in the notations.

There are n_s mass conservation equations - one for each chemical species considered, two momentum conservation equations, and two energy conservation equations - one for total energy and one for vibrational energy. The term H is the total enthalpy, and is equal to $E + p/\rho$ where E is the total energy given by $e_{tr} + e_V + q$. The quantity e_{tr} is the sum of translational, rotational, and formation energies of molecular and atomic particles, e_V is the sum of vibrational, electronic, and electron translational energies, and $q = (u^2 + v^2)/2$ is the kinetic energy. In the two-temperature model the translational temperature, T, describes e_{tr}, and vibrational temperature, T_V, describes e_V. Henceforth, we shall use the terms 'vibrational energy' to represent the sum of vibrational, electronic, and electron translational energies. Note that the temperatures do not appear explicitly in the governing equations. Also note that in the vibrational energy equation, the term corresponding to the work done by the electron pressure gradient has been moved over to the right hand side of the governing equations and lumped with the production terms. This has lead to some simplifications in the analysis.

Before proceeding to the determination of the Roe-averaged variables and computing the fluxes, it is useful to review the procedure for the determination of the energies. In the two-temperature model, the translational and rotational modes are assumed to be fully excited, and hence the heat capacities of these modes are independent of the temperature, and the internal energy is a linear function of the translational temperature, i.e.,

$$e_{tr,i}(T) = \int_{T_{ref}}^{T} C_{v,t,i}(T')\,dT' + \Delta h_{f,i} \qquad (9)$$

Without loss of generality we assume the reference temperature, T_{ref}, to be equal to zero Kelvin. Note that $C_{v,t,i}$ are constants (independent of temperature), and are equal to $2.5R/W_i$ for molecular species and $1.5R/W_i$ for atomic species. The quantity $\Delta h_{f,i}$ is the enthalpy of formation of species i at the reference temperature.

Unlike the translational-rotational modes, the vibrational and electronic energy modes are assumed to be only partially excited; hence the vibrational heat capacity depends on the vibrational temperature. The heat capacity for the vibrational mode of species i can be evaluated by utilizing the curve fits for the total heat capacity evaluated at T_V, and subtracting out the constant contribution from translational and rotational modes as follows:

$$C_{v,V,i}(T_V) = C_{v,i}(T_V) - C_{v,t,i} \qquad (10)$$

Note that $C_{v,i}(T_V) = C_{p,i}(T_V) - R/W_i$. Curve fits for $C_{p,i}$ in terms of T may be found in the literature (see e.g., Prabhu and Erickson [10]). Integrating $C_{v,V,i}$ from T_{ref} (equal to zero Kelvin) to the required temperature T_V we obtain $e_{V,i}$, i.e.,

$$e_{V,i}(T_V) = \int_{T_{ref}}^{T_V} C_{v,V,i}(T')\,dT' \qquad (11)$$

The energies per unit mass of the mixture are determined as follows:

$$e_{tr} = \sum_{i=1}^{n_s - 1} e_{tr,i} x_i \qquad e_V = \sum_{i=1}^{n_s} e_{V,i} x_i \qquad (12)$$

Note that the summation for translational energy is over all the species except the electrons; the electron translational energy is included in the vibrational energy. Equations (9) - (12) are relations between the two energies, their respective temperatures, and the mixture composition. For given values of the energies and the mixture composition, the translational and vibrational temperatures can be determined. Similarly, if the temperatures and the mixture composition are known, the energies can be computed. These are routine computations.

The component of flux normal to the common side between two cells is denoted by $\mathbf{F}_n$. The Jacobian matrix $\mathbf{A} = \partial \mathbf{F}_n / \partial \mathbf{U}$ can be evaluated (see Gnoffo [9]), and is given by

$$
A = \begin{bmatrix}
U(\delta_{ij} - x_i) & x_i n_x & x_i n_y & 0 & 0 \\
\alpha_j n_x - Uu & (1-\beta)un_x + U & (1-\beta)vn_x - V & \beta n_x & \phi n_x \\
\alpha_j n_y - Uv & (1-\beta)un_y + V & (1-\beta)un_y + U & \beta n_y & \phi n_y \\
(\alpha_j - H)U & Hn_x - \beta Uu & Hn_x - \beta Uv & (1+\beta)U & \phi U \\
-Ue_V & e_V n_x & e_V n_y & 0 & U
\end{bmatrix}
\tag{13}
$$

The eigenvalues of A can be determined, and are given by

$$
\Lambda = (U \text{ repeated } (n_s + 1) \text{ times, } U + c, U - c, \quad U)
\tag{14}
$$

Subscript i refers to species i and row i, and subscript j refers to species j and column j, and δ_{ij} is the Kronecker delta. The quantities $U = un_x + vn_y$ and $V = vn_x - un_y$ are the velocity components normal and parallel to the cell interface respectively, n_x and n_y are the x- and y-components of the unit outward pointing normal to the interface respectively, x_i are the mass fractions of the constituent species, and c is the speed of sound defined by

$$
c^2 = \sum_{i=1}^{n_s} \alpha_i x_i + \beta (H - 2q) + \phi e_V
\tag{15}
$$

The quantities α_i, $i = 1, \dots, n_s$, β, and ϕ are the partial derivatives of pressure, defined as follows:

$$
\alpha_i = \frac{\partial p}{\partial \rho_i} = \frac{RT'}{W_i} + \beta q - \beta e_i - \phi e_{V,i}
\tag{16}
$$

$$
\beta = \frac{\partial p}{\partial \rho E} = \frac{R}{C_{v,t}} \sum_{i=1}^{n_s - 1} \frac{x_i}{W_i}
\tag{17}
$$

$$
\phi = \frac{\partial p}{\partial \rho e_V} = \frac{R}{C_{v,V}} \frac{x_e}{W_e} - \beta
\tag{18}
$$

In Eqn. (16), $T' = T$ for heavy particles (atoms, molecules, and ions), and $T' = T_V$ for the electrons. Note that the quantities $C_{v,t}$ and $C_{v,V}$ are given by

$$
C_{v,t} = \sum_{i=1}^{n_s - 1} x_i C_{v,t,i} \qquad C_{v,V} = \sum_{i=1}^{n_s} x_i C_{v,V,i}
\tag{19}
$$

As noted earlier, $C_{v,t,i} = 2.5R/W_i$ for molecular particles and $1.5R/W_i$ for atomic particles

making $C_{v,t}$ dependant only on the mixture composition. Consequently, β also depends only on the mixture composition, and is easily determined if the mixture composition is known. The quantity ϕ, however, depends on the mixture composition and $C_{v,v}$, which is a function of the vibrational temperature.

The left- and right-eigenvector matrices of $\mathbf{A}$ corresponding to the eigenvalues in Eqn. (14) are denoted by $\mathbf{R}$ and $\mathbf{R}^{-1}$, and are given by

$$
\mathbf{R} = \begin{bmatrix}
c^2 \delta_{ij} - \alpha_j x_i & \beta u x_i & \beta v x_i & -\beta x_i & -\phi x_i \\
-V & -n_y & n_x & 0 & 0 \\
\alpha_j - Uc & cn_y - \beta u & cn_y - \beta v & \beta & \phi \\
\alpha_j + Uc & -cn_y - \beta u & -cn_y - \beta v & \beta & \phi \\
-\alpha_j e_V & \beta u e_V & \beta v e_V & -\beta e_V & c^2 - \phi e_V
\end{bmatrix}
\tag{20}
$$

$$
c^2 \mathbf{R}^{-1} = \begin{bmatrix}
\delta_{ij} & 0 & x_i & x_i & 0 \\
u & -c^2 n_y & [u + cn_x]/2 & [u - cn_x]/2 & 0 \\
v & c^2 n_x & [v + cn_y]/2 & [v - cn_y]/2 & 0 \\
[2\beta q - \alpha_j]/\beta & c^2 V & [H + cU]/2 & [H - cU]/2 & -\phi/\beta \\
0 & 0 & e_V/2 & e_V/2 & 1
\end{bmatrix}
\tag{21}
$$

The matrices $\bar{\mathbf{R}}$, $\bar{\mathbf{R}}^{-1}$, and the eigenvalues of $\bar{\mathbf{A}}$ defined by the Roe-averaged variables (denoted by an overline) are required for the determination of the flux. In order to determine the Roe-averaged variables, we start with the following necessary condition that $\bar{\mathbf{A}}$ must satisfy:

$$
\Delta (\mathbf{F}_n) = \bar{\mathbf{A}} \Delta (\mathbf{U})
\tag{22}
$$

where $\Delta ( ) = ( )_R - ( )_L$. We are seeking a set of variables that satisfies the above equation exactly. This equation has N components corresponding to the N governing equations. Of these N components, the first n_s components (corresponding to the species mass conservation equations) are satisfied, if we define

$$
\bar{x}_i = a (x_i)_L + b (x_i)_R \qquad \bar{u} = au_L + bu_R \qquad \bar{v} = av_L + bv_R
\tag{23}
$$

where, as in the ideal gas case, the quantities a and b are functions of densities in the left and right cells, and are defined in Eqn. (5). Note that

$$\sum_{i=1}^{n_s} \bar{x}_i = a \sum_{i=1}^{n_s} (x_i)_L + b \sum_{i=1}^{n_s} (x_i)_R = a + b = 1 \tag{24}$$

This is a necessary condition if $\bar{x}_i, i = 1, \ldots, 5$ are to retain the property of the mass fraction. Next, the components of Eqn. (22) corresponding to the momentum equations are satisfied provided the condition

$$\Delta(p) = \sum_{i=1}^{n_s} (\bar{\alpha}_i - \bar{\beta}\bar{q}) \Delta(\rho_i) + \bar{\beta}\Delta(\rho e) + \bar{\phi}\Delta(\rho e_V) \tag{25}$$

is satisfied. Note that $e = e_{tr} + e_V$. Finally, the components of Eqn. (22) corresponding to the total energy and the vibrational energy equations are satisfied, if we define

$$\bar{H} = aH_L + bH_R \qquad \bar{e}_V = a(e_V)_L + b(e_V)_R \tag{26}$$

Thus, we have determined the unknowns $\bar{x}_i, \bar{u}, \bar{v}, \bar{H}$, and $\bar{e}_V$ in terms of the corresponding quantities in the left and right cells, and the density ratio across the interface. Of these, the relations for $\bar{u}, \bar{v}$, and $\bar{H}$ are the same as in the ideal gas case. A condition similar to Eqn. (25) for the ideal gas case is satisfied identically.

It remains to determine the quantities $\bar{\alpha}_i, \bar{\beta}$, and $\bar{\phi}$ which are not defined explicitly. The only condition they must satisfy is the Eqn. (25). We describe here a simple method to compute these quantities. The basis for the present method is the requirement that these unknowns together with $\bar{x}_i$ and $\bar{e}_V$ form a consistent set of thermodynamic variables. We consider two cases - (1) a gas mixture containing charged particles and electrons, and (2) a gas mixture of only neutral particles. The first case is treated in detail. The second case is much simpler, and the results follow from the those of the first case.

Case 1: Gas mixture of charged particles and electrons:-

As noted earlier, β depends only on the mixture composition. Hence, we require that the Roe-averaged quantity, $\bar{\beta}$, depend only on the mixture composition at the Roe-average state, and be determined using a relation similar to Eqn. (19). Accordingly, we write

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$$\bar{\beta} = \frac{R}{\bar{C}_{v,t}} \sum_{i=1}^{n_s-1} \frac{\bar{x}_i}{W_i} \tag{27}$$

where, as in Eqn. (21), we note

$$\bar{C}_{v,t} = \sum_{i=1}^{n_s-1} \bar{x}_i \bar{C}_{v,t,i} = \sum_{i=1}^{n_s-1} \bar{x}_i C_{v,t,i} \tag{28}$$

Hence, $\bar{\beta}$ can be readily computed. Following a similar reasoning, we write for $\bar{\phi}$ as in Eqn. (20)

$$\bar{\phi} = \frac{R}{\bar{C}_{v,V}} \frac{\bar{x}_e}{W_e} - \bar{\beta} \tag{29}$$

Again, as in Eqn. (21) we note

$$\bar{C}_{v,V} = \sum_{i=1}^{n_s} \bar{x}_i \bar{C}_{v,V,i} (\bar{T}_V) \tag{30}$$

The value of $\bar{C}_{v,V,i}$, however, must be evaluated at an appropriate vibrational temperature, $\bar{T}_V$. Since $\bar{e}_V$ and the mixture composition $\bar{x}_i$ are known, we require that the appropriate vibrational temperature, $\bar{T}_V$, be consistent with $\bar{e}_V$ and $\bar{x}_i$. This temperature can be determined following a routine computation. Once $\bar{T}_V$ is determined, $\bar{\phi}$ can be evaluated.

Next, we proceed to the determination of α_i. Following the argument of the previous paragraph, we require $\bar{\alpha}_i$ to have the same functional relation with the other variables as in Eqn. (18), and write

$$\bar{\alpha}_i = \frac{R\bar{T}'}{W_i} + \bar{\beta}\bar{q} - \bar{\beta}\bar{e}_i - \bar{\phi}\bar{e}_{V,i} \tag{31}$$

In this equation, all the quantities except $\bar{e}_i$ and $\bar{T}'$ are known. For electrons, $\bar{T}' = \bar{T}_V$, which is known, and $\bar{e}_i = \bar{e}_{V,i} = 1.5R\bar{T}_V/W_i$. Hence $\bar{\alpha}_i$ for electrons is readily obtained, and may be expressed as follows:

$$\bar{\alpha}_e = R\bar{T}_V[1 - 1.5(\bar{\beta} + \bar{\phi})]/W_e + \bar{\beta}\bar{q} \tag{32}$$

For the heavy particles we have $\bar{T}' = \bar{T}$; hence we write

$$\bar{e}_i = \bar{e}_{tr,i} + \bar{e}_{V,i} = f_i R\bar{T}/W_i + \Delta h_{f,i} + \bar{e}_{V,i} \tag{33}$$

This equation together with Eqn. (31) provides a linear relation between $\bar{\alpha}_i$ and $\bar{T}$, which may be written as follows:

$$\bar{\alpha}_i = R\bar{T}[1 - f_i\bar{\beta}]/W_i + \bar{\beta}(\bar{q} - \Delta h_{f,i}) - (\bar{\beta} + \bar{\phi})\bar{e}_{V,i} \tag{34}$$

This equation alone is not sufficient to solve for $\bar{T}$ (or $\bar{\alpha}_i$). Moreover, we need to satisfy the condition in Eqn. (25). Hence we combine Eqns. (25), (32), and (34), and obtain the following:

$$\Delta(p) = R\bar{T} \sum_{i=1}^{n_s-1} \left[\left(1 - f_i\bar{\beta}\right)/W_i - \bar{\beta}\Delta h_{f,i} - (\bar{\beta} + \bar{\phi})\bar{e}_{V,i} \right] \Delta(\rho_i)$$
$$+ (\bar{\alpha}_e - \bar{\beta}\bar{q})\Delta(\rho_e) + \bar{\beta}\Delta(\rho e) + \bar{\phi}\Delta(\rho e_V) \tag{35}$$

Solving for the only unknown $\bar{T}$ in this equation, we find

$$\bar{T} = \frac{\left\{ \begin{array}{c} \Delta(p) - \beta\Delta(\rho e) - \phi\Delta(\rho e_V) - \alpha_e\Delta(\rho_e) \\ + \sum_{i=1}^{n_s-1} \left[\bar{\beta}\Delta h_{f,i} + (\bar{\beta} + \bar{\phi})\bar{e}_{V,i}\right]\Delta(\rho_i) - R\bar{T}_V[1 - 1.5(\bar{\beta} + \bar{\phi})]\Delta(\rho_e)/W_e \end{array} \right\}}{R \sum_{i=1}^{n_s-1} \Delta(\rho_i)\left[1 - f_i\bar{\beta}\right]/W_i} \tag{36}$$

Once $\bar{T}$ is determined, $\bar{\alpha}_i$ for the heavy particles can be computed using Eqn. (34). Although $\bar{T}$ does not occur explicitly in any of the matrices used in the determination of the fluxes, it is desirable that the value of $\bar{T}$ computed by Eqn. (36) is positive. In order to demonstrate this, we simplify Eqn. (36) and write it in the following form:

$$\bar{T} = aT_L + bT_R -$$

$$\frac{(\bar{\beta} + \bar{\phi})\left[\Delta(\rho e_V) - \sum_{i=1}^{n_s}\bar{e}_{V,i}\Delta(\rho_i)\right] + R\,\Delta\left[\rho x_e\left(T_V - \bar{T}_V\right)\right]/W_e}{R \sum_{i=1}^{n_s-1}\left[1 - f_i\bar{\beta}\right]\Delta(\rho_i)/W_i} \tag{37}$$

It has not been possible to further simplify Eqn. (37) so as to demonstrate that the values of $\bar{T}$ given by this equation are always positive. However, on the right-hand-side of this equation, the

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first two terms are positive and large, and the quantities in the numerator of the third term, being differences of similar quantities, are small. In all the numerical exercises we have performed, the third term has always been only a small fraction of the first two, and the value of $\bar{T}$ has been a positive quantity. In the freestream this term is indeterminate, and is set equal to zero. Once $\bar{T}$ is determined, $\bar{\alpha}_i$ for the heavy particles can be computed using Eqn. (34).

The Roe-averaged speed of sound may be determined using the following:

$$\bar{c}^2 = \sum_{i=1}^{n_s} \bar{\alpha}_i \bar{x}_i + \bar{\beta} [\bar{H} - 2\bar{q}] + \bar{\phi} \bar{e}_V \tag{38}$$

Thus, all the Roe-averaged values of the quantities $\bar{\alpha}_i$, $i = 1, ..., n_s$, $\bar{\beta}$, $\bar{\phi}$, and $\bar{c}$ required to compute the matrices $\bar{\mathbf{A}}$, $\bar{\mathbf{R}}$, and $\bar{\mathbf{R}}^{-1}$ are determined. These quantities satisfy the necessary condition given by Eqn. (25) exactly. Together with $\bar{x}_i$, $\bar{e}_V$, $\bar{T}$, and $\bar{T}_V$, they form a consistent set of thermodynamic variables, which is the basis for the method of determining these quantities described here. The method is simple, and makes no approximations. The only additional computation required is the determination of the vibrational temperature, $\bar{T}_V$ for the given values of vibrational energy, $\bar{e}_V$, and the mixture composition, $\bar{x}_i$; however, this is a routine computation.

It is necessary that the value of the square of the speed of sound computed by Eqn. (38) be positive. To demonstrate that $\bar{c}^2$ computed by Eqn. (38) is always positive, we start with the definition of $\bar{H}$

$$\bar{H} = aH_L + bH_R = ah_L + bh_R + \bar{q} + \delta \tag{39}$$

where $\delta = \frac{ab}{2} \left[(u_R - u_L)^2 + (v_R - v_L)^2 \right] \geq 0$. Next, we substitute $h = e_{tr} + e_V + p/\rho$ in the above equation, and obtain the following:

$$\bar{H} = \bar{e}_{tr} + \bar{e}_V + \overline{p/\rho} + \bar{q} + \delta \tag{40}$$

where $\bar{e}_{tr} = a (e_{tr})_L + b (e_{tr})_R$ and $\overline{p/\rho} = a (p/\rho)_L + b (p/\rho)_R$.

Next, in Eqn. (38), we substitute for $\bar{\alpha}_i$ from Eqns. (32) and (34), and for $\bar{H}$ from Eqn. (40), and simplify to obtain

$$\bar{c}^2 = \bar{\beta} [\bar{\varepsilon} + (\overline{p/\rho}) + \delta] + R\bar{T}_V \bar{x}_e / W_e \tag{41}$$

where $\bar{\varepsilon} = a\varepsilon_L + b\varepsilon_R$, and

$$\varepsilon = RT \sum_{i=1}^{n_s-1} f_i x_i / W_i \tag{42}$$

All the terms on the right hand side of equation (41) are greater than or equal to zero, proving that the square of the speed of sound, $\bar{c}^2$, is always positive.

Case 2: Gas mixture of only neutral particles:-

The procedure described above is simplified when electrons are absent in the gas mixture. The governing equations are the same as in Eqns. (7) and (8), and the thermodynamic relations given in Eqns. (9), (10), (11), (12), and (14)-(19) as well as the matrices $\bar{A}$, $\bar{R}$, and $\bar{R}^{-1}$ given in Eqns. (13), (20), and (21) are also applicable.

The Roe-averaged quantities defined in Eqn. (23), (24), and (26) are applicable without any changes. The necessary condition given in Eqn. (25) remains the same as well. Equation (27) for the quantity $\bar{\beta}$ is applicable. However, since electrons are absent, the quantity $\bar{\phi}$ is given by

$$\bar{\phi} = \bar{\beta} \tag{43}$$

and there is no need to determine the quantity $\bar{T}_V$. With $\bar{\beta} + \bar{\phi} = 0$, the expression for $\bar{\alpha}_i$, given in Eqn. (34), can be written as follows:

$$\bar{\alpha}_i = R\bar{T}\left[1 - f_i\bar{\beta}\right]/W_i + \bar{\beta}\left(\bar{q} - \Delta h_{f,i}\right) \tag{44}$$

The temperature, $\bar{T}$, is determined following a similar procedure, and is given by

$$\bar{T} = \left[\Delta(p) - \bar{\beta}\Delta(\rho e_{tr}) + \bar{\beta}\sum_{i=1}^{n_s}\Delta(\rho_i)\Delta h_{f,i}\right] / R\sum_{i=1}^{n_s-1}\left[1 - f_i\bar{\beta}\right]\Delta(\rho_i)/W_i \tag{45}$$

This equation for $\bar{T}$ can be simplified and may be written in the following elegant form:

$$\bar{T} = aT_L + bT_R \tag{46}$$

This also demonstrates that the temperature $\bar{T}$ is always positive, and lies in between T_L and T_R. After computing $\bar{T}$, $\bar{\alpha}_i$ can be determined using Eqn. (44).

The speed of sound given in Eqn. (38) is still applicable and can be written as

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$$\bar{c}^2 = \sum_{i=1}^{n_s} \bar{\alpha}_i \bar{x}_i + \bar{\beta} \, [\bar{H} - 2\bar{q} - \bar{e}_V] \tag{47}$$

This can be further simplified, and written in the following form:

$$\bar{c}^2 = \bar{\beta} \, (\bar{\epsilon} + \overline{(p/\rho)} + \delta) \tag{48}$$

again proving that the square of speed of sound determined by this method is always positive.

Conclusion

A new method is presented to determine the Roe-averaged variables required to determine the inviscid fluxes in chemical and thermal nonequilibrium flows. These variables form a consistent set of thermodynamic variables, and satisfy the necessary condition. The method is simple, and does not make any approximations. The only additional computation required in determining the Roe-averaged variables for gas mixtures with electrons, is the computation of vibrational temperature for given values of the vibrational energy and the mixture composition. This, however, is only a routine computation. A logical requirement that the square of the speed of sound be positive is satisfied.

Acknowledgments

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Among the many methods available for the determination of inviscid fluxes across a surface of discontinuity, the flux-difference-splitting technique that employs Roe-averaged variables has been used extensively by the CFD community because of its simplicity and its ability to capture shocks exactly. This method, originally developed for perfect gas flows, has since been extended to equilibrium as well as nonequilibrium flows. Determination of the Roe-averaged variables for the case of a perfect gas flow is a simple task; however, for thermal and chemical nonequilibrium flows, some of the variables are not uniquely defined. Methods available in the literature to determine these variables, seem to lack sound bases. The present paper describes a simple, yet accurate, method to determine all the variables for nonequilibrium flows in the Roe-average state. The basis for this method is the requirement that the Roe-averaged variables form a consistent set of thermodynamic variables. The present method satisfies the requirement that the square of the speed of sound be positive.

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