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1 ABSTRACT

A multi-species solver for plasma at thermodynamical equilibrium is developed. A numerical scheme, based on Roe’s, is implemented with some modification regarding the average quantities. A perfect gas treatment is carried out for validations, and a quasi-real gas treatment is also presented. The latter takes into account the changes in the composition of the gas caused by fluctuations in temperature and density.

2 INTRODUCTION

Over the last 40 years, numerous numerical methods have been developed for the solution of compressible flows. Among these methods, the scheme proposed by Roe [1] has proven to be very robust and its use is widespread among the practitioners of computational fluid dynamics. While the original model was developed by Roe [1] in 1980 for an ideal gas, Glaisier [2] suggested in 1987 a variant of Roe’s scheme to solve non-perfect gases with a general equation of state law of the form \( P = f(e, \rho) \).

Following these ideas, in this paper we consider the numerical simulation of the unidimensional Euler equations for multi-species flows. In the treatment of these equations, thermal equilibrium is always assumed. The contribution of this work in this field of study is the development of a dimensionless form of the governing equations devoted to multispecies, as well, the development and implementation of Roe’s average for multispecies and finally, coupling the current development with a general equation of state module. The latter is not based on an equation of state, but rather on a parametric form suited to the treatment of multispecies.

3 GOVERNING EQUATIONS

The Euler system of equations describing multispecies flows can be written according to Mehlman [3].

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = 0
\]

with

\[
\mathbf{U} = \begin{pmatrix}
\rho_1 \\
\rho_2 \\
\vdots \\
\rho_n \\
\rho_n u \\
\rho_n p \\
\rho_n E
\end{pmatrix} \quad \mathbf{F} = \begin{pmatrix}
\rho_1 u \\
\rho_2 u \\
\vdots \\
\rho_n u \\
\rho_n u + P \\
\rho_n u E + P \end{pmatrix}
\]

where the subscript \( n \) indicates the number of species and \( E = e + \frac{1}{2} u^2 \) is the total energy. A key aspect to the multi-species treatment is to consider that the pressure and the density are given by the sum of the partial pressure and the sum of the relative densities for each of the \( n \) species (Dalton’s Law) respectively. That is:

\[
P = \sum_{i=1}^{n} P_i \quad \rho = \sum_{i=1}^{n} \rho_i
\]

The pressure is evaluated from the computed variables, using an equation of state.

\[
P = f(e, \rho)
\]

Enthalpy is evaluated as follows:

\[
H = e + \frac{P}{\rho} + \frac{u^2}{2} = E + \frac{P}{\rho}
\]

The expression used to describe the sound velocity is also used:

\[
c^2 = \frac{P}{\rho^2} \frac{\partial P}{\partial \epsilon} + \frac{\partial P}{\partial \rho}
\]
4 ROE'S METHOD

Roe's method uses the linearized form of equation (1), which is:

\[ \frac{\partial U}{\partial t} + A \frac{\partial U}{\partial x} = 0 \] (7)

where \( A = \frac{\partial F}{\partial W} \) is the Jacobian matrix. In order to obtain this matrix, it is useful to express both vectors, \( F \) and \( U \), as functions of a conservative vector \( W \), as follows:

\[ U(W) = W = \begin{pmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \rho_n \end{pmatrix} \]

\[ F(W) = \begin{pmatrix} \frac{w_1}{\sum_{i=1}^{n} w_i} \\ \frac{w_2}{\sum_{i=1}^{n} w_i} \\ \vdots \\ \frac{w_{n+1}}{\sum_{i=1}^{n} w_i} \end{pmatrix} \]

(8)

(9)

In this form, \( F \) can easily be differentiated with respect to \( W \), and the Jacobian matrix, \( A(W) \), can thus be constructed. The only quantities that cannot be obtained explicitly are the pressure and its partial derivatives with respect to \( w_i \), since a definition of the equation of state has not yet been given. The treatment of the pressure terms is presented in the following section.

4.1 Pressure terms

Since the pressure is defined as \( P = P(\rho_1, \rho_2, \ldots, \rho_n, c) \), the partial derivatives of the pressure with respect to the \( w_i \) variables are:

\[ \frac{\partial P}{\partial w_i} = \frac{\partial P}{\partial \rho} \frac{\partial \rho}{\partial w_i} + \frac{\partial P}{\partial e} \frac{\partial e}{\partial w_i} \] (10)

We can now express each partial derivative in a conservative way. Because \( \rho = \sum_{i=1}^{n} w_i \), it follows that:

\[ \frac{\partial \rho}{\partial w_1} = \frac{\partial \rho}{\partial w_2} = \ldots = \frac{\partial \rho}{\partial w_n} = 1 \]

\[ \frac{\partial \rho}{\partial w_{n+1}} = 0 \quad \frac{\partial \rho}{\partial w_{n+2}} = 0 \]

Also, the relation \( c = E - \frac{u^2}{2} = \frac{w_1}{\sum_{i=1}^{n} w_i} - \frac{w_2^2}{2 (\sum_{i=1}^{n} w_i)^2} \) leads to:

\[ \frac{\partial e}{\partial w_1} = \frac{\partial e}{\partial w_2} = \ldots = \frac{\partial e}{\partial w_n} = \frac{u^2 - E}{\rho} \] (11)

\[ \frac{\partial e}{\partial w_{n+1}} = \frac{u}{\rho} \quad \frac{\partial e}{\partial w_{n+2}} = \frac{1}{\rho} \] (12)

With these results, and defining \( P_e = \frac{\partial P}{\partial e} \), equation (10) yields:

\[ \frac{\partial P}{\partial w_i} = c^2 - \frac{P_e}{\rho} (H - u^2) \quad i = 1, n \] (13)

\[ \frac{\partial P}{\partial w_{n+1}} = \frac{u}{\rho} \quad \frac{\partial P}{\partial w_{n+2}} = \frac{P_e}{\rho} \] (14)

4.2 Jacobian matrix

Using the expressions found in section (4.1), the Jacobian matrix can

\[ A = \frac{\partial F}{\partial U} \]

4.3 Eigenvectors

The eigenvalues of the Jacobian matrix are calculated according to the expression \( |A - \lambda I| = 0 \), and they are:

\[ \lambda_1 = u - c \]

\[ \lambda_2 = \lambda_3 = \ldots = \lambda_{(n+1)} = u \]

(15)

\[ \lambda_{(n+2)} = u + c \]

Using the relation \( (A - \lambda I) \epsilon_i = 0 \), one gets the matrix \( S \), formed by the \( \epsilon_i \) eigenvectors. That is,

\[ S = \begin{pmatrix} \epsilon_1 & 1 & 0 & \ldots & 0 \\ \epsilon_2 & 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \epsilon_n & 0 & 0 & \ldots & 1 \\ u - c & u & u & \ldots & u + c \end{pmatrix} \]

(16)

In this matrix, \( u^2 - \theta_k \) (\( k = 1, 2, \ldots, n \)) are the most important terms when dealing with real gases. This term comes from the expression \( H - \frac{c^2 \rho}{P_e} \) and has been obtained as follows.

Using equation (6) we re-write the above expression:

\[ H - \frac{c^2 \rho}{P_e} = E - \rho \frac{P_e}{P} \]

When equations (14) are inserted into the chain
derivative of $P_\rho = f(\rho_1, \rho_2, \ldots, \rho_n, \rho E)$, the following expression is found:

$$P_\rho = \sum_{i=1}^{n} \frac{\partial P}{\partial \rho_i} + P_2 \left( \frac{E - u^2}{\rho} \right)$$

Thus,

$$H - \frac{c_\rho}{P_c} = E - \rho \frac{\partial P}{\partial \rho_c} = E + n^2$$

$$u^2 - \frac{\partial P}{\partial \rho_c} = u^2 - \theta_k$$

With $S$ being fully defined, the Jacobian matrix can now be constructed according to:

$$\Delta \mathbf{F} = \mathbf{A} \Delta \mathbf{U}$$

where $\mathbf{D} = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_{n+2})$ is the diagonal matrix of eigenvalues. In order to numerically evaluate the fluxes, the Jacobian is approximated by,

$$\mathbf{A} \approx \frac{\partial \mathbf{F}}{\partial \mathbf{U}} \approx \frac{\Delta \mathbf{F}}{\Delta \mathbf{U}}$$

which translates into $\Delta \mathbf{F} = \mathbf{A} \Delta \mathbf{U}$. Considering the local left $(l)$ and right $(r)$ states of a fluid on the corresponding sides of an element and with $\mathbf{D} = \frac{\mathbf{D} + |\mathbf{D}|}{2}$, the well-known upwind formula for vector equations is obtained:

$$\mathbf{F} = \frac{1}{2} (\mathbf{F}_l + \mathbf{F}_r) - \frac{1}{2} \mathbf{S} |\mathbf{D}| \mathbf{S}^{-1} \Delta \mathbf{U} \quad (17)$$

where $|\mathbf{D}| = \text{diag}(|\lambda_1|, |\lambda_2|, \ldots, |\lambda_{n+2}|)$. Roe's approximation implies the replacement matrix (16) by a mean-value matrix $\mathbf{A} = \mathbf{A} (\mathbf{U}_l, \mathbf{U}_r)$, where $\mathbf{U}_l$ and $\mathbf{U}_r$ are the left and right states, respectively, of the fluid at a given side. In other words,

$$\frac{\partial \mathbf{U}}{\partial \mathbf{U}} + \mathbf{A}(\mathbf{U}_l, \mathbf{U}_r) \frac{\partial \mathbf{U}}{\partial \mathbf{U}} = 0$$

The three principal mean-quantities in $\hat{\mathbf{A}}$ are:

$$\hat{\rho}_n = \frac{\rho_n \sqrt{\rho_n} + \rho_r \sqrt{\rho_r}}{\sqrt{\rho_n} + \sqrt{\rho_r}}$$

$$\hat{u} = \frac{u_l \sqrt{\rho_l} + u_r \sqrt{\rho_r}}{\sqrt{\rho_l} + \sqrt{\rho_r}}$$

$$\hat{H} = \frac{H_l \sqrt{\rho_l} + H_r \sqrt{\rho_r}}{\sqrt{\rho_l} + \sqrt{\rho_r}}$$

It is to be noted that the current form of the expression for the mean value of the density differs from the original form proposed by Roe ($\hat{\rho}_n = \sqrt{\rho_n \rho_r}$). This choice is justified by necessity. An expression for each $\hat{\rho}_i$ was required, which would preserve its form as it is summed up to obtain $\hat{\rho}$. From the previous expressions, one obtains:

$$\hat{\rho} = \sum_{i=1}^{N} \hat{\rho}_i = \frac{\rho_l \sqrt{\rho_l} + \rho_r \sqrt{\rho_r}}{\sqrt{\rho_l} + \sqrt{\rho_r}}$$

and $\hat{\rho}_n = \hat{\rho}_n / \hat{\rho}$. For both constant $R$ and $c_v$, their mean values are:

$$\hat{R}_c = \frac{R_l \sqrt{\rho_l} + R_r \sqrt{\rho_r}}{\sqrt{\rho_l} + \sqrt{\rho_r}}$$

$$\hat{c}_v = \frac{c_{v_l} \sqrt{\rho_l} + c_{v_r} \sqrt{\rho_r}}{\sqrt{\rho_l} + \sqrt{\rho_r}}$$

With these average quantities, we can address the elements of $\mathbf{A} \approx \mathbf{A}(\mathbf{U}_r, \mathbf{U}_l)$.

### 5 Perfect Gas Treatment

For the sake of simplicity and validation, a perfect gas development is carried out. Using this relation and its partial derivatives, it is possible to evaluate the missing quantities from matrix (16). However, before doing so, some simple definitions and relations are specified:

- Energy-temperature relation: $e_i = e_v, T$ \quad (18)

- Coefficient $k$: $k = \sum_{i=1}^{n} \kappa_i y_i e_v$ \quad (19)

- Mass fraction definition: $y_i = \rho_i / \rho$ \quad (20)

#### 5.1 Energy

Due to relation (3), the equation of state (4) can be expressed in the following form:

$$P = \kappa p e = \sum_{i=1}^{n} \kappa_i y_i e_v$$

If the latter is rearranged, and inserting relations (19) and (20):

$$e = \frac{(\sum_{i=1}^{n} \kappa_i y_i e_v) (\sum_{i=1}^{n} y_i c_v)}{\sum_{i=1}^{n} \kappa_i y_i c_v} \quad (21)$$

The differentiated form of this equation, with respect to $e_i$, will be required, hence:

$$\frac{\partial e_i}{\partial e} = \frac{\kappa_i y_i (\sum_{i=1}^{n} y_i c_v)}{\sum_{i=1}^{n} \kappa_i y_i c_v} \quad (22)$$

By introducing relation (18) into (21) one obtains:

$$e = T \sum_{i=1}^{n} y_i c_v \quad (23)$$

#### 5.2 Pressure

The equation of state (24) can also be expressed as a function of $T$, using equation (23) and relation (19):

$$P = \rho T \sum_{i=1}^{n} \kappa_i y_i c_v \quad (24)$$

Expressions for the partial derivatives of $P = \kappa p e$ will also be required:

$$P_e = \frac{\partial P}{\partial e} = \kappa p \quad (25)$$
5.3 Sound Velocity

By inserting the equation of state (24) and its derivative (25) into equation (6), we obtain:

\[ c^2 = \kappa \rho \varepsilon + \kappa \varepsilon \quad (26) \]

Using relation (19) and equation (23), we obtain the expression for the velocity of sound:

\[ c^2 = (\kappa + 1) \left( \sum_{i=1}^{n} y_i \kappa_i c_{vi} \right) T \quad (27) \]

5.4 The \( \theta_k \) term

Using the previous developments, it is possible to evaluate \( \theta_k \):

\[ \theta_k = \rho \left( \frac{\delta P}{\delta \rho} \right) \quad (28) \]

which, with equations (13) and (14), results in:

\[ \theta_k = \frac{\rho}{\delta \rho} \left( c^2 - \frac{\delta P}{\delta \rho} (H - u^2) \right) \quad (29) \]

Finally, inserting equations (5), (26) and (25), we obtain:

\[ \theta_k = \frac{u^2}{2} \quad (30) \]

6 DIMENSIONLESS FORM

For the sake of simplicity, each of the computed variables are transformed into their nondimensional forms. The reference values, \( T_o \) and \( \rho_o \), are selected at initialization, and the reference length \( L_o \) is set to the length of the domain. The establishment of a reference value for constants with dimensions is also a necessity. To preserve the structure of equation (2), the relation \( \frac{\rho_o \theta_o \theta_o}{L_o} = 1 \) must be satisfied.

7 EQUATION OF STATE AND QUASI-REAL GAS

During processes where low-temperature gases are transformed in high-temperature plasma, as, for example, is the case for circuit-breakers arcs (see [4] for further details), the perfect gas equation of state cannot be applied blindly. During these types of transformations, the composition of the gas dramatically changes (due to dissociation, recombination, ionisation, etc.) and the thermodynamic properties that take into account these new species have to be determined. A numerical method, developed by Godin and Trépanier [5], calculates the chemical evolution of the gas at a specific temperature. It is to be noted that real gas phenomena that occur at very low temperatures, such Van der Waals forces are neglected. Also, the real gas effect of high ionisation conditions and high pressure are not taken into account because they have little to no effect on the end results (as stated by Godin and Trépanier [5]).

In the present development, all the relations (Equations (23) and (24)), for example) between thermodynamic variables are evaluated with two parameters: \( c_v \) and \( R \). In a standard perfect gas development, we consider these two parameters to be constant values to be used in the equation of state. In the quasi-real gas development, this structure for the equation of state is still used, but new values for these two parameters \( c_v \) and \( R \) are evaluated according to the newly formed species in the plasma. With this approach, the sound velocity given by equation (27) is no longer valid, and equation (6) has to be used. This treatment demands the computation of two new values: \( P_o \) and \( P_p \). These values will also be used in equation (28), which can no longer be simplified to (30). These two quantities are evaluated in the same manner as \( c_v \) and \( R \), except that, apart from temperature and density, they also depend on the concentration of each species.

Figures (1) shows the variation of one of these variables \( c_v \) for varying temperatures and densities for \( \text{N}_2 \). As demonstrated, both variables are reasonably constant for temperatures between 300 K and 5000 K. But beyond that, they have variations of more than 500%.

8 RESULTS AND VALIDATIONS

8.1 Two species

This validation has been made in order to compare the current solver with the solution given by Larrouin [6] and an analytical solution. The initial conditions are Nitrogen at 300 K and 1.1769 kg/m³ on the left side, and CO₂ at 240 K and 0.14711 kg/m³ on the right side. The simulation runs for 0.7037 milliseconds, the grid contains 101 nodes and
the CFL number is 0.75. This last value was used in order to reproduce the conditions given by [6]. The results are presented in figure (2).

8.2 Air as a multispecies gas

For the next case, air treated as a uniform gas is compared with air treated as a combination of different gases. The initial conditions of the multispecies air are shown in Table (1). For air treated as a single species, with $\gamma = 1.399$ and $R = 287.05$, values for temperature, density and velocity are also taken from Table (1). For this validation, the grid is set to 1001 points, the CFL number is 1 and the time simulated is 0.7037 milliseconds. Figure (3) shows that the numerical solution is quite close to the analytical one. It also shows that the two numerical solutions (for monospecies and multispecies) coincide, which shows the validity of the current multispecies treatment.

8.3 Shock generated by different gas

In this last validation, the quasi-real gas features of the code are fully exploited. Two different gases are put on either side of the tube. Both gases are at
Table 1: Initial conditions of the multispecies air, for validation 3.

<table>
<thead>
<tr>
<th>Species</th>
<th>Initial Temperature (K)</th>
<th>Initial Density (kg/m³)</th>
<th>Initial Velocity (m/s)</th>
<th>Initial YN₂</th>
<th>Initial YO₂</th>
<th>Initial YCO₂</th>
<th>Final YN₂</th>
<th>Final YO₂</th>
<th>Final YCO₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>N₂</td>
<td>300</td>
<td>330.0</td>
<td>0.5884</td>
<td>0.0769</td>
<td>0.1251</td>
<td>0.2648</td>
<td>0.0769</td>
<td>0.1251</td>
<td>0.2648</td>
</tr>
<tr>
<td>O₂</td>
<td>28000</td>
<td>330.0</td>
<td>0.5884</td>
<td>0.0769</td>
<td>0.1251</td>
<td>0.2648</td>
<td>0.0769</td>
<td>0.1251</td>
<td>0.2648</td>
</tr>
<tr>
<td>CO₂</td>
<td>29000</td>
<td>330.0</td>
<td>0.5884</td>
<td>0.0769</td>
<td>0.1251</td>
<td>0.2648</td>
<td>0.0769</td>
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</tr>
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<td>0.1251</td>
<td>0.2648</td>
<td>0.0769</td>
<td>0.1251</td>
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</tr>
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</table>

REFERENCES


9 CONCLUSION

A multi-species solver for plasma at thermodynamical equilibrium has been developed. A numerical scheme, based on Roe’s, has been implemented with some modification regarding the average quantities. A perfect gas treatment has been realized for validation, and a quasi-real gas treatment has also been presented. The latter takes into account the changes in the composition of the gas caused by fluctuations in temperature and density.