Numerical Solution of Compressible Euler Equations for Gas Mixture Applications

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A computer code, based on Euler Equations in generalized curvilinear coordinates, has been developed to resolve binary perfect gas mixture flows. The capability of modeling various mixture effects is built in the algorithm and the computer code. The Roe's numerical scheme is used to discretize the convective terms of the governing fluid flow equations, while a simple upwinding method is applied for the equation of continuity of species. Some applications of binary gas mixture flows, including nozzle cooling and thrust vectoring, are investigated and the role of mixing phenomenon in these flows is classified. Additionally, the influences of using different gases on flow fields are evaluated, especially in two-dimensional thrust-vectoring problems.

INTRODUCTION

Recent years have witnessed a growing interest in developing suitable numerical methods for computing the mixture of fluid flows and their efficient implementation in studying complex flow phenomena (e.g., [1-10]). In 1996, a quasi conservative algorithm was developed by Abgrall [6] to prevent pressure oscillations in multicomponent flows. In 1997, Jenny, Mueller and Thomann [11] showed that conservative Euler solvers for gas mixtures produce numerical errors and oscillations near to contact discontinuities.

For a mixture of perfect gases, a simple correction of the total energy per unit volume was proposed by Jenny, Mueller and Thomann [11] to avoid errors and oscillations found near contact discontinuities. Ivings, Causon and Toro [12] developed a hybrid high resolution upwind algorithm for multicomponent inviscid flows. Then, Shyue [8] developed a fluid mixture type algorithm for compressible multicomponent flow with the Van der Waals equation of state.

Also, Abgrall and Karni [9] proposed a simple algorithm for multimaterial flows consisting of pure fluids separated by material interfaces to remove the oscillations generated at material interfaces. Marquina and Mulet [10] developed a conservative extension of the Euler equations for gas dynamics in Cartesian coordinates to reduce the oscillations near to gas interfaces.

Most recent works have focused on the problems consisting of pure fluids separated by material interfaces (e.g., [1,2,9,13-16]). Understanding the dynamics of fluids consisting of several interpenetrating fluid components is also of great interest in a wide range of physical flows, as well as in industrial applications. For this purpose, in the present study, Euler equations, for the mixture and conservation of the species, are solved using Roe's method. Some typical flows are considered in this study, which give rise to both theoretically and computationally challenging problems.

In the present work, the influences of using different sets of binary mixtures of gas are studied in the context of a converging-diverging supersonic nozzle problem. This paper focuses on proper modeling and the appropriate numerical method for interpenetrating a mixture of perfect gases.

MULTICOMPONENT FLOW EQUATIONS

For simplicity of exposition, the dynamics of a mixture of two gases in two space dimensions will be considered. An extension to more components or more dimensions can be directly carried out. Let \( \rho \) denote the density of the mixture and \( c \) the mass fraction of the first component. Therefore, \( 1-c \) is the mass fraction of the second component. Both components of gases are assumed to be in thermal equilibrium and are calorically perfect gases. \( c_{v1}, c_{v2}, c_{p1}, c_{p2}, \gamma_1 \) and \( \gamma_2 \) are the specific heat at constant volume, specific

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heat at constant pressure and ratio of specific heat of gas components, respectively. By standard thermodynamic arguments [10], the ratio of the specific heat of a mixture of gases is:

$$\gamma(c) = \frac{c_p}{c_v} = \frac{c_{p1}c + c_{p2}(1 - c)}{c_{v1}c + c_{v2}(1 - c)}$$  \hspace{1cm} (1)

The equation of state expresses the pressure, $p$, in terms of the density, $\rho$, the specific internal energy, $e$, and mass fraction, $c$, i.e.:

$$p(\rho, e, c) = (\gamma(c) - 1)\rho e,$$ \hspace{1cm} (2)

where:

$$c = \frac{\rho_l}{\rho}.$$ \hspace{1cm} (3)

In flows with negligible viscous effects, the fluid dynamics of this mixture are described by the Euler equations with an additional equation expressing conservation of mass for the first component, which, in conjunction with the conservation of mass for the mixture, also implies conservation of mass for the second component.

In a generalized curvilinear two-dimensional coordinate system, the governing equations for the mixture are as follows:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial \xi} + \frac{\partial G}{\partial \eta} = 0,$$ \hspace{1cm} (4)

where:

$$U = \begin{pmatrix} E \\ \rho \\ \rho u \\ \rho v \\ \rho e \end{pmatrix}, \quad F = \begin{pmatrix} (E + p)u \\ \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho v \end{pmatrix},$$ \hspace{1cm} (5)

$$G = \begin{pmatrix} (E + p)v \\ \rho v \\ \rho u v \\ \rho v^2 + p \\ \rho v c \end{pmatrix},$$ \hspace{1cm} (6)

where $u$ and $v$ are cartesian velocity and vector components of the mixture, respectively and $E$ is the total energy per unit volume. Also,

$$\mathbf{T} = \frac{1}{J}(G \xi_x + F \xi_y),$$ \hspace{1cm} (7)

$$\mathbf{G} = \frac{1}{J}(G \eta_x + F \eta_y),$$ \hspace{1cm} (8)

where:

$$J = \frac{\partial (\xi, \eta)}{\partial (x, y)} = \xi_x \eta_y - \xi_y \eta_x.$$ \hspace{1cm} (9)

Using the above formulation, a computer code, based on the explicit flux differencing of Roe’s scheme, is developed.

**RESULTS**

**First Shock Tube Problem**

To validate the computer code, the standard shock tube problem for a binary perfect gas mixture is numerically solved. The shock tube problem is defined as follows:

$$p_l = 1, \quad \gamma_l = 1.4, \quad c_{vl} = 1, \quad \rho_l = 1, \quad u_l = 0, \hspace{1cm} (10)$$

$$p_r = 0.1, \quad \gamma_r = 1.2, \quad c_{vr} = 1, \quad \rho_r = 0.125, \quad u_r = 0, \hspace{1cm} (11)$$

where subscripts $l$ and $r$ denote left and right, respectively.

Comparison of the obtained results with those of Marquina and Mulet [10] in Figures 1 to 3, show good agreement. Some differences in the gradient of Mach number near the contact discontinuity can be observed in Figure 3. This is mainly due to the first order scheme.
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and two-dimensional effects of the present method in contrast to the fifth order scheme and one-dimensional model of Marquina and Mulet [10].

The small amount of overheating in the vicinity of the contact surface in Figures 1 and 3, is mainly due to gas mixture effects, which is not present in the conventional single fluid computation.

The prepared algorithm and the computer code are capable of modeling mixture effects in different fluid flows. To present some of these influences, several flow field examples have been computed.

Second Shock Tube Problem

A second shock tube problem, for a binary perfect gas mixture of He-Xe with the following properties, has been considered.

\[ p_l = 1, \quad \gamma_l = 1.66, \quad c_{vl} = 1.0, \quad \rho_l = 1, \quad u_l = 0, \quad (12) \]

\[ p_r = 0.1, \quad \gamma_r = 1.66, \quad c_{vr} = 0.03, \quad \rho_r = 0.125, \quad u_r = 0. \quad (13) \]

Although the specific heat ratios for two gases of this mixture are the same, the specific heat at constant volumes is too different. Therefore, the results for this case should be somehow different from those of the first example, shown in Figures 1 to 3.

Comparison of the results of the first and second shock tube problems is shown in Figures 4 to 6. As can be seen from these figures, overheating in the vicinity of the contact surface has vanished for the He-Xe gas mixture. This is due to the same \( \gamma \) in both components of the mixture. Additionally, Figure 6 shows a small difference in pressure distribution for both cases.

For the next example, wall-cooling of a two-dimensional supersonic converging-diverging nozzle is
considered. The problem properties are Nozzle area ratio:
\[
\frac{A_e}{A_t} = 1.38, \quad p_r = 10^5 \text{ pa}, \quad T_r = 300 \text{ k},
\]
and, at the inlet:
\[
\frac{p_0}{p_r} = 2.4, \quad \frac{T_0}{T_r} = 1.1,
\]
where \(A_e\) and \(A_t\) denote exit and throat areas, respectively, subscript \(r\) denotes reference and subscript \(0\) represents stagnation conditions.

Lighter gas enters from the main entrance at the left and the heavier gas, as the coolant, is blown from lower and upper walls, starting from \(x = 0.87\) afterwards with Cartesian velocity components equal to \((75,10)\) m/s (Figures 7 and 8).

To show the effect of the various properties of different gases, two binary sets of gases (\(N_2-O_2\) and \(He-Xe\)) are selected as the media.

Figure 7 shows the concentration \((\frac{\rho_{N_2}}{\rho_{N_2} + \rho_{O_2}})\) distribution for the mixture of \(N_2-O_2\) and, similarly, Figure 8 shows the concentration \((\frac{\rho_{He}}{\rho_{He} + \rho_{Xe}})\) distribution for the mixture of \(He-Xe\). Comparing these two figures, it is clear that the second type of mixture \(He-Xe\) has a larger zone of mixing than that of the first kind of mixture \(N_2-O_2\). This is due to the effect of the large difference in properties \((m, C_p, \gamma, \cdots)\) of \(He\) and \(Xe\). Note that mass diffusion is not allowed and this mixing is only due to convective terms and different gas properties. Additionally, from Figures 9 and 10, it can be concluded that Mach numbers in the supersonic zone of \(He-Xe\) are smaller than those of \(N_2-O_2\). The case of a mixture of too different gases is more effective in reducing Mach number or eliminating the shock wave. If the aim is just wall-cooling, the case of \(N_2-O_2\)

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure7}
\caption{Concentration contours for \(N_2-O_2\).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure8}
\caption{Concentration contours for \(He-Xe\).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure9}
\caption{Mach number contours for \(N_2-O_2\).}
\end{figure}

is more effective than that of \(He-Xe\), which is due to the almost similar properties of \(N_2-O_2\). By using different gases, a larger mixing zone can be created, which causes a large disturbance in the flow field. These effects are also observed in Mach number contours seen in Figures 9 and 10.

As the next example, the problem of thrust vectoring is presented as follows. The nozzle geometry and binary sets of fluid properties chosen here are the same as those in the previous example. This time, the second gas is blown from the upper wall starting after the throat and extends afterwards (Figures 11 and 12). Concentration contours for the mentioned problems are shown in Figures 11 and 12. A larger mixing region can be observed for the second case. It might be expected that a larger normal force can be extracted from this supersonic nozzle, using binary
The change in direction of the thrust vector was computed for both of these two mixtures, which were held under the same conditions. The results showed that the deviation of thrust vector in the N₂-O₂ mixture is about 27° and about 55° for the He-Xe mixture. In all of the above cases, the rate of blowing was similar.

CONCLUSION

A computer code has been developed for numerical computation of compressible two-dimensional Euler equations in a generalized curvilinear coordinate to
solve binary perfect gas mixture flows. The prepared algorithm and computer code are capable of modeling mixture effects in different fluid flows. It was shown that using gases with large differences in their properties can be more useful in thrust vectoring applications than for nozzle cooling problems, while, for the latter case, it produces more mixing and, hence, more losses. It can also be concluded that, regarding all limitations, the choice of binary fluid in different applications plays an important role in the overall performance of the device.

REFERENCES