Scientia Iranica, Vol. 13, No. 3, pp 217–222

SCIENTIA
IRANICA

Numerical Solution of Compressible Euler Equations for Gas Mixture Applications

R. Kamali[1], M.M. Alishahi[*] and H. Emdad[1]

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 ρ 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}, γ_1 and γ_2 are the specific heat at constant volume, specific

1. *Department of Mechanical Engineering, Shiraz University, Shiraz, I.R. Iran.*
*. *Corresponding Author, Department of Mechanical Engineering, Shiraz University, Shiraz, I.R. Iran.*

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:

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

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

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

where:

$$c = \frac{\rho_1}{\rho}. \tag{3}$$

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:

$$\frac{\partial U}{\partial t} + \frac{\partial \overline{F}}{\partial \xi} + \frac{\partial \overline{G}}{\partial \eta} = 0, \tag{4}$$

where:

$$U = \begin{Bmatrix} E \\ \rho \\ \rho u \\ \rho v \\ \rho c \end{Bmatrix}, \qquad F = \begin{Bmatrix} (E+p)u \\ \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uc \end{Bmatrix}, \tag{5}$$

$$G = \begin{Bmatrix} (E+p)v \\ \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vc \end{Bmatrix}, \tag{6}$$

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

$$\overline{F} = \frac{1}{J}(G\xi_x + F\xi_y), \tag{7}$$

$$\overline{G} = \frac{1}{J}(G\eta_x + F\eta_y), \tag{8}$$

where:

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

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:

$$p_l = 1, \quad \gamma_l = 1.4, \quad c_{v_l} = 1, \quad \rho_l = 1, \quad u_l = 0, \tag{10}$$

$$p_r = 0.1, \quad \gamma_r = 1.2, \quad c_{v_r} = 1, \quad \rho_r = 0.125, \quad u_r = 0, \tag{11}$$

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

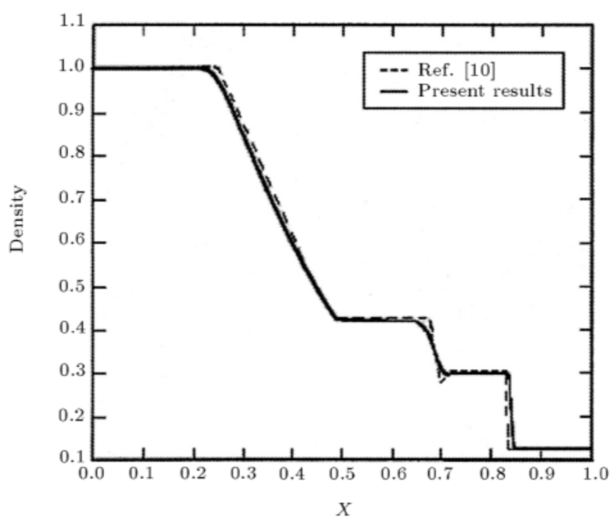

Figure 1. Density distribution.

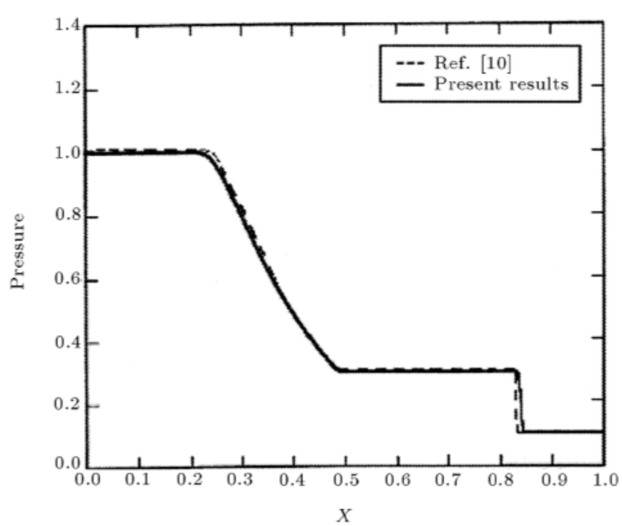

Figure 2. Pressure distribution.

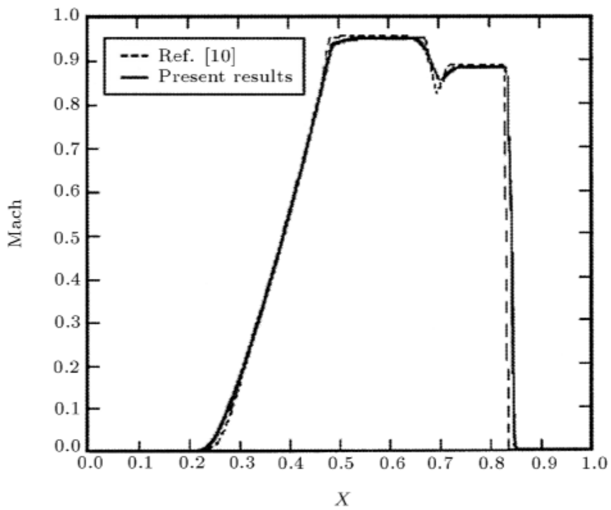

Figure 3. Mach number distribution.

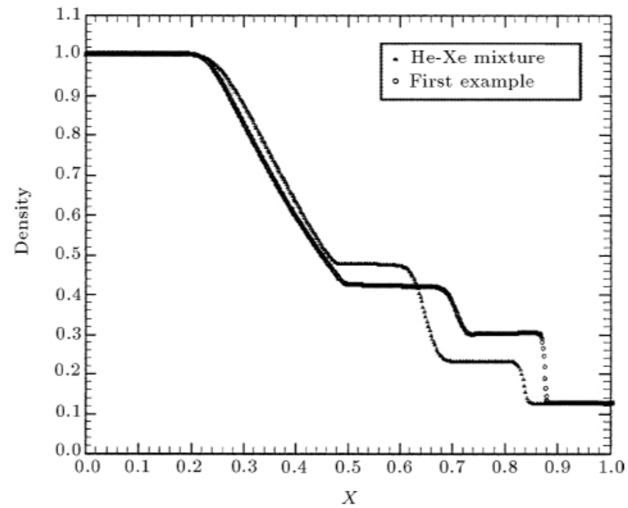

Figure 4. Density distribution for He-Xe and the first example.

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.

$$p_l = 1, \quad \gamma_l = 1.66, \quad c_{v_l} = 1.0, \quad \rho_l = 1, \quad u_l = 0, \qquad (12)$$

$$p_r = 0.1, \quad \gamma_r = 1.66, \quad c_{v_r} = 0.03, \quad \rho_r = 0.125,$$

$$u_r = 0. \qquad (13)$$

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 γ 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

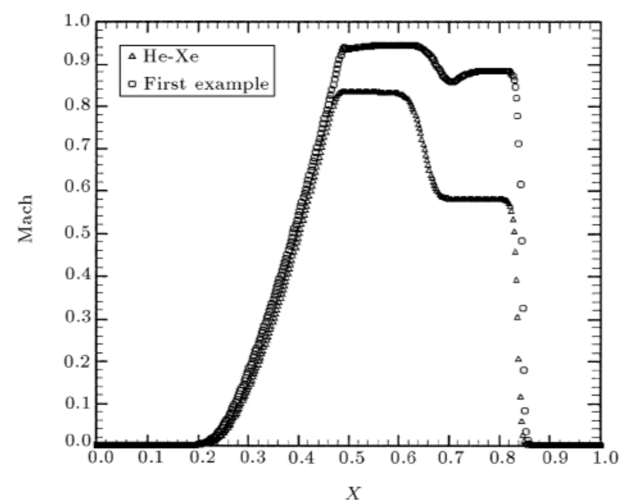

Figure 5. Mach number distribution for He-Xe and the first example.

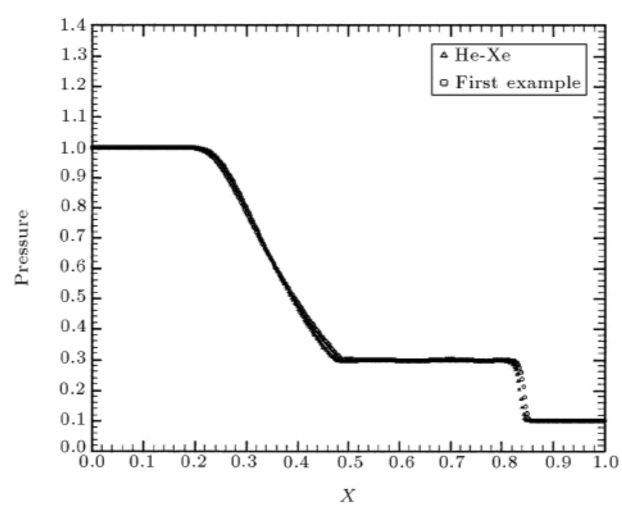

Figure 6. Pressure distribution for He-Xe and the first example.

considered. The problem properties are Nozzle area ratio:

$$\frac{A_e}{A_t} = 1.38, \qquad p_r = 10^5 \text{ pa}, \qquad T_r = 300 \text{ k},$$

and, at the inlet;

$$\frac{p_0}{p_r} = 2.4, \qquad \frac{T_0}{T_r} = 1.1,$$

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 $(m, C_p, R, \cdots)$ 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

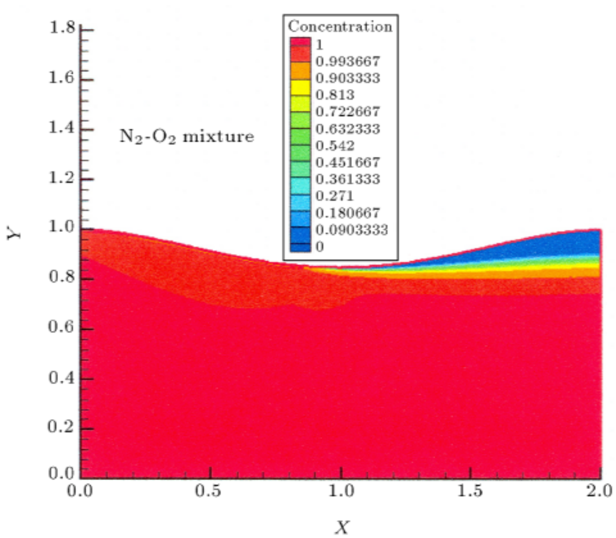

Figure 7. Concentration contours for N_2-O_2.

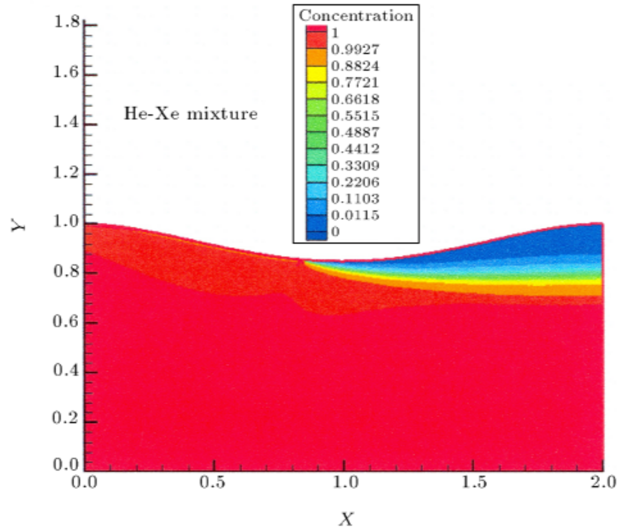

Figure 8. Concentration contours for He-Xe.

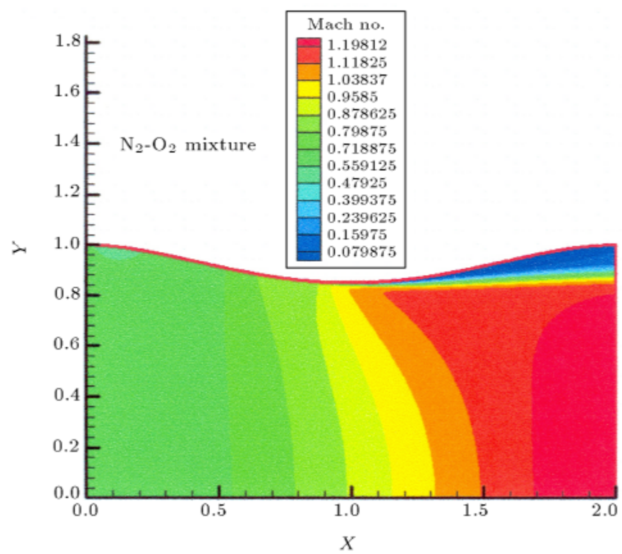

Figure 9. Mach number contours for N_2-O_2.

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

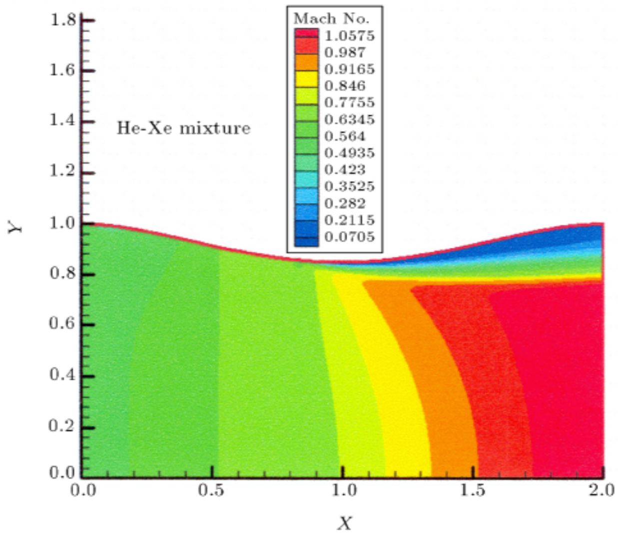

Figure 10. Mach number contours for He-Xe.

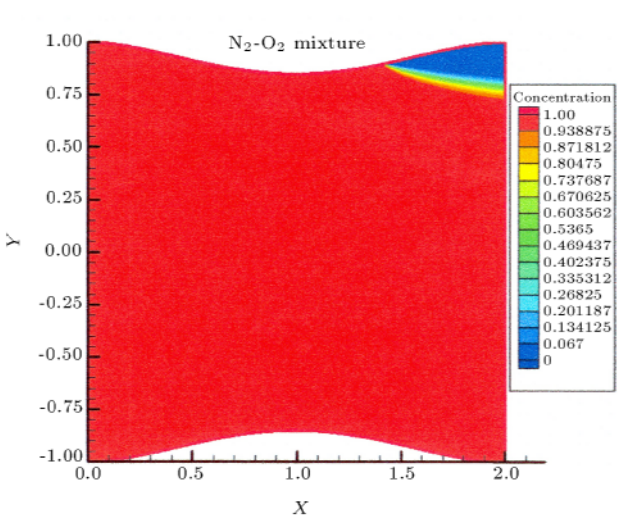

Figure 11. Concentration contours for N_2-O_2 gas flow.

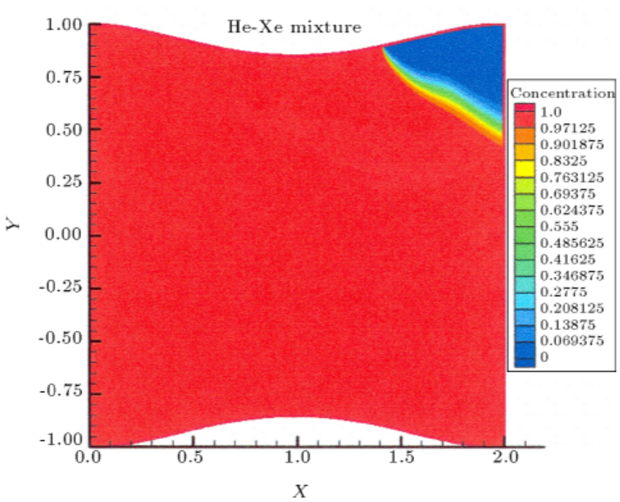

Figure 12. Concentration contours for He-Xe gas flow.

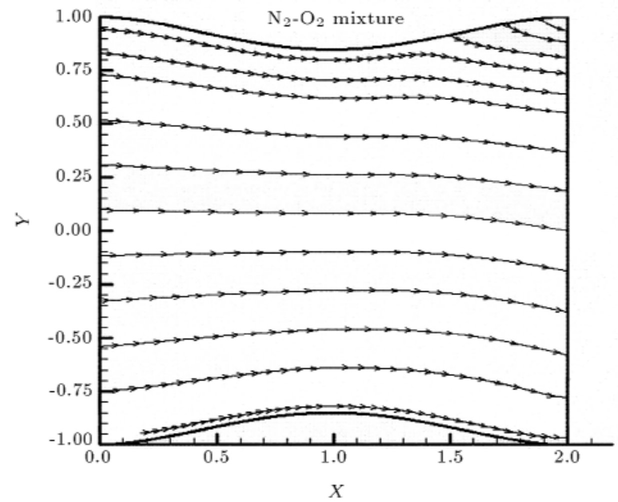

Figure 13. Streamlines for thrust vectoring for N_2-O_2 gas flow.

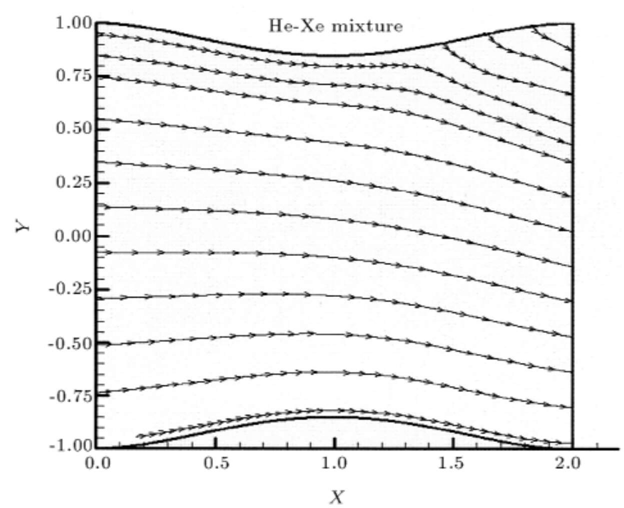

Figure 14. Streamlines for thrust vectoring for He-Xe gas flow.

fluids with too different properties. This is actually the case. Larger deviations in streamline directions for the He-Xe mixture provides more thrust vector capability than that of N_2-O_2 mixture (Figures 13 and 14).

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 N_2-O_2 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

1. Chern, I.L., Glimm, J., McBryan, O., Plohr, B. and Yaniv, S. "Front tracking for gas dynamics", *J. Comput. Phys.*, **62**, p 83 (1986).
2. Karni, S. "A level-set scheme for compressible interfaces", *Numerical Methods for Wave Propagation*, Kluwer Academic Publishers, Dordrecht, pp 253-274 (1988).
3. Larouturou, B. and Fezoui, L., *On the Equations of Multicomponent Perfect or Real Gas Inviscid Flow*, Lecture Notes in Mathematics, Springer-Verlag, Berlin/New York, **1402**, pp 69-97 (1989).
4. Chargy, D., Abgrall, R., Fezoui, L. and Larrouturou, B. "Conservative numerical schemes for multicomponent inviscid flows", *Rech. A'erosp.*, **2**, p 61 (1992).
5. Karni, S. "Multi-component flow calculations by a consistent primitive algorithm", *J. Comput. Phys.*, **112**, p 31 (1994).
6. Abgrall, R. "How to prevent pressure oscillations in multicomponent flows: A quasi conservative approach", *J. Comput. Phys.*, **125**, p 150 (1996).
7. Shyue, K.M. "An efficient shock-capturing algorithm for compressible multicomponent problems", *J. Comput. Phys.*, **1**, pp 208 (1998).
8. Shyue, K.M. "A fluid-mixture type algorithm for compressible multicomponent flow with Van der Waals equation of state", *J. Comput. Phys.*, **1**, p 43 (1999).
9. Abgrall, R. and Karni, S. "Computations of compressible multifluids", *J. Comput. Phys.*, **169**, pp 594-623 (2001).
10. Marquina, A. and Mulet, P. "A flux-split algorithm applied to conservative models for multicomponent compressible flows", *J. Comput. Phys.*, **185**, pp 120-138 (2003).
11. Jenny, P., Mueller, B. and Thomann, H. "Correction of conservative Euler solvers for gas mixtures", *J. Comput. Phys.*, **132**, p 91 (1997).
12. Ivings, M.J., Causon, D.M. and Toro, E.F. "On hybrid high resolution upwind methods for multicomponent flows", *Z. Angew. Math. Mech.*, **77**(9), p 645 (1997).
13. Miller, G.H. and Puckett, E.G. "A high order Godunov method for multiple condensed phases", *J. Comput. Phys.*, **128**, pp 134 (1996).
14. Coquel, F., El-Almine, K., Godlewski, E., Perthame, B. and Rascle, P. "A numerical method using upwind schemes for the resolution of two-phase flows", *J. Comput. Phys.*, **136**, p 272 (1997).
15. Fedkiw, R., Aslam, T., Merriman, B. and Osher, S. "A non-oscillatory Eulerian approach to interfaces in multimaterial flows, the ghost fluid method", *J. Comput. Phys.*, **152**, p 457 (1999).
16. Davis, S.F. "An interface tracking method for hyperbolic systems of conservation laws", *Appl. Numer. Math.*, **10**, p 447 (1992)