

A New Set of Conservation Equations Based on the Kinetic Theory Applied to Gas Mixture Problems

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In this work, the hydrodynamics of multicomponent ideal gas mixtures have been studied. Starting from kinetic equations, the Eulerian approach is used to derive equations of motion for a multicomponent system, where each component may have a different velocity and kinetic temperature. The equations are based on Grad's method of moment derived from the kinetic model, in a Relaxation Time Approximation (RTA). Based on this model, a computer code has been developed for numerical computation of compressible flows of a binary gas mixture in generalized curvilinear boundary conforming coordinates. Since these equations are similar to the Navier-Stokes equations for the single fluid systems, the same numerical methods are applied to these new equations. The Roe's numerical scheme is used to discretize the convective terms of governing fluid flow equations. The prepared algorithm and the computer code are capable of computing and presenting the flow fields of each component of the system separately, as well as the average flow field of the multicomponent gas system as a whole. A comparison between the present code results and those of a more common algorithm based on the mixture theory in a supersonic converging-diverging nozzle provides the validation of the present formulation. Afterwards, a more involved nozzle cooling problem with a binary ideal gas (Helium-Xenon) is chosen to compare the present results with those of the ordinary mixture theory. The present model provides the details of the flow fields of each component separately which is not available otherwise.

INTRODUCTION

Almost all flows encountered in nature and technology are of a gas mixture. The flow of air is the most common example, which is usually disregarded as a multispecies flow of gas. In many practical flows, involving pollutant dispersion, chemical processing and combustor mixing and reaction, mass and momentum transport within multispecies fluids play an important role. Recent years have witnessed a growing interest in developing numerical methods suitable for computing multicomponent flows, as well as their efficient implementation in studying complex flow phenomena [1-13].

Modeling of the multicomponent fluid flows can be separated into two groups. The first one consists of conservation equations, based on the Navier-Stokes

equations [e.g., 14,15]. The second group of models is based on the kinetic theory, i.e., models derived from the Boltzmann equation [e.g., 16].

Based on the first model, the fluid dynamics of a mixture of gases (e.g., a binary gas mixture) is described by the Navier-Stokes equations for the mixture as a whole, with an additional equation expressing conservation of mass for the first component. The last equation, in conjunction with the conservation of mass for the mixture, implies a conservation of mass for the second component as well. This approach is called a Mixture Model. Numerical modeling using the mixture model is traditionally based on Euler solver methods.

Gases can be studied by considering the small scale action of individual molecules or by considering the large scale action of the gas as a whole. Although one can directly measure, or sense, the action of the gas, the action of the molecules can be studied theoretically. This theoretical model, called the kinetic theory of gases, assumes only that the molecules are very small, relative to the distance between molecules.

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The molecules are in constant, random motion and frequently collide with each other and with the walls of any container.

The kinetic theory approach for a multicomponent gas system is based on Boltzmann equations, including collision integrals for each component of the gas mixture. In the case of low Knudsen numbers, defined as the ratio between the mean free path of the molecules and the relevant macroscopic length scale, these equations are solved using the traditional Chapman-Enskog method [17] or Grad's method of moment [18]. This process results in the equations for the conservation (balance) of mass, momentum and energy for a multicomponent gas mixture. Some of the recent works in this area are, as follows.

In 1954, Bhatnagar, Gross and Krook (BGK) [19] presented a model for molecular collisions for single gas. The effect of the molecular collisions in this model is represented by an exponential relaxation toward a Local Thermodynamic Equilibrium (LTE). In 1962, Sirovich [11] gave a generalization of the BGK model for a gas mixture. In 1964, Morse [12] presented free parameters, which were computed, based on conservation relations. In 1971, Wu and Lee [13] studied the one-dimensional binary gas mixture flow in a shock tube, using the kinetic model. In 1989, Garzo, Santos and Bery [14] proposed a kinetic model for a dilute multicomponent gas system, especially when the particle masses of the components are comparable. In 1999, Lian and Xu, Kun [20] defined a gas-kinetic scheme for a mixture of gases. They used a multicomponent gas-kinetic BGK-type scheme. They also studied its application in chemical reactions. In 2003, Luo and Girimanji [21] applied the Lattice Boltzmann Model for the binary mixtures of gases. The model is derived formally from the kinetic theory by discretizing the Boltzmann equation. The proposed model can simulate miscible and immiscible fluids by changing the sign of the mutual-collision term.

The Eulerian multifluid approach for the mixture of gases, based on the kinetic theory without actually determining the form of the distribution function, has not been evaluated yet and has been done in the present work. Contrary to most of the known models, this model consists of separate conservation equation sets for each component of the mixture and which, therefore, is capable of presenting, in detail, the behavior of each component. Using this new formulation, diffusion processes can be automatically modeled without use of any coefficients of an ordinary pressure and thermal diffusion, which are required in the ordinary mixture models.

In this paper, starting from kinetic equations, the Eulerian approach is used to derive hydrodynamic equations of motion for a multicomponent gas system. These equations are based on Grad's method of mo-

ment in a relaxation approximation. Based on this model, an individual set of flow equations is obtained for each species. Since these equations are similar to the Navier-Stokes equations for single fluid systems, the same conventional numerical methods can be applied. A computer code has been developed for numerical computation of these separate sets of equations for compressible flows of a binary gas system in generalized curvilinear coordinates.

MODEL EQUATIONS

In the kinetic theory, the state of a mixture of z ideal gases is characterized by the set of one-particle velocity distribution functions $f_\alpha(\mathbf{x}, \mathbf{c}_\alpha, t)$ ($\alpha = 1, 2, \dots, z$), such that $f_\alpha(\mathbf{x}, \mathbf{c}_\alpha, t) d\mathbf{x} d\mathbf{c}_\alpha$ gives, at time t , the number of particles of constituent α in the volume element between \mathbf{x} and $\mathbf{x} + d\mathbf{x}$, with velocities between \mathbf{c}_α and $\mathbf{c}_\alpha + d\mathbf{c}_\alpha$. In the absence of external forces, the one-particle velocity distribution function of constituent α satisfies the Boltzmann equation [22]:

$$\frac{\partial f_\alpha}{\partial t} + c_i^\alpha \frac{\partial f_\alpha}{\partial x_i} = K_{\alpha\alpha} + \sum_{\beta \neq \alpha}^z K_{\alpha\beta}, \quad (1)$$

where K denotes the non-linear Boltzmann collision operators. This collision term poses the greatest mathematical difficulties. The first term, on the right-hand side of Equation 1, is the standard collision operator for a gas of a single species, while the second term represents the effect of inter-collision between the two different species. While the term "collisions" may stand for various kinds of encounters between two particles, it is used here only for elastic collisions of non-reacting gases. The mathematical complexity of the collision term in gaseous mixtures can be avoided if one replaces the collision operators by simple relaxation-time terms, based on the work of Gross and Krook [23]. Let the mixture consist of two components; gas α and gas β , with number densities, n_α and n_β , and masses of gas molecules, m_α and m_β . Each component has its own temperature, T_α , and its macroscopic or flow velocity, \mathbf{v}_α , with molecular velocity, \mathbf{c}_α , and peculiar velocity, $\mathbf{C}_\alpha = \mathbf{c}_\alpha - \mathbf{v}_\alpha$. According to Wu and Lee [13]:

$$\frac{\partial f_\alpha}{\partial t} + c_i^\alpha \frac{\partial f_\alpha}{\partial x_i} = \nu_{\alpha\alpha}(F_\alpha - f_\alpha) + \nu_{\alpha\beta}(\tilde{F}_\alpha - f_\alpha), \quad (2)$$

$$\frac{\partial f_\beta}{\partial t} + c_i^\beta \frac{\partial f_\beta}{\partial x_i} = \nu_{\beta\beta}(F_\beta - f_\beta) + \nu_{\beta\alpha}(\tilde{F}_\beta - f_\beta), \quad (3)$$

where f_α and f_β are the velocity distribution functions for species α and β , respectively, $\nu_{\alpha\alpha}$ and $\nu_{\beta\beta}$ are the frequencies for self-collisions and $\nu_{\alpha\beta}$ and $\nu_{\beta\alpha}$ are the frequencies for cross-collisions between species α and β .

The total number of collisions between species α and β should be balanced, i.e.,

$$n_\alpha \nu_{\alpha\beta} = n_\beta \nu_{\beta\alpha}. \quad (4)$$

The Maxwellian distribution functions, F_α , F_β , \tilde{F}_α and \tilde{F}_β are defined as follows:

$$F_\alpha = \frac{n_\alpha}{(2\pi R_\alpha T_\alpha)^{\frac{3}{2}}} \exp\left(-\frac{(\mathbf{c}_\alpha - \mathbf{v}_\alpha)^2}{2R_\alpha T_\alpha}\right), \quad (5)$$

$$F_\beta = \frac{n_\beta}{(2\pi R_\beta T_\beta)^{\frac{3}{2}}} \exp\left(-\frac{(\mathbf{c}_\beta - \mathbf{v}_\beta)^2}{2R_\beta T_\beta}\right), \quad (6)$$

$$\tilde{F}_\alpha = \frac{n_\alpha}{(2\pi R_\alpha \tilde{T}_\alpha)^{\frac{3}{2}}} \exp\left(-\frac{(\mathbf{c}_\alpha - \tilde{\mathbf{v}}_\alpha)^2}{2R_\alpha \tilde{T}_\alpha}\right), \quad (7)$$

$$\tilde{F}_\beta = \frac{n_\beta}{(2\pi R_\beta \tilde{T}_\beta)^{\frac{3}{2}}} \exp\left(-\frac{(\mathbf{c}_\beta - \tilde{\mathbf{v}}_\beta)^2}{2R_\beta \tilde{T}_\beta}\right). \quad (8)$$

The collision parameters, \tilde{T}_α , \tilde{T}_β , $\tilde{\mathbf{v}}_\alpha$ and $\tilde{\mathbf{v}}_\beta$, in terms of macroscopic velocities and temperatures are [12], as follows:

$$\tilde{\mathbf{v}}_\alpha = \tilde{\mathbf{v}}_\beta = \frac{m_\alpha \mathbf{v}_\alpha + m_\beta \mathbf{v}_\beta}{m_\alpha + m_\beta}, \quad (9)$$

$$\tilde{T}_\alpha = T_\alpha + \frac{2m_\alpha m_\beta}{(m_\alpha + m_\beta)^2} (T_\beta - T_\alpha + \frac{m_\beta}{6k} (\mathbf{v}_\beta - \mathbf{v}_\alpha)^2), \quad (10)$$

$$\tilde{T}_\beta = T_\beta + \frac{2m_\alpha m_\beta}{(m_\alpha + m_\beta)^2} (T_\alpha - T_\beta + \frac{m_\alpha}{6k} (\mathbf{v}_\beta - \mathbf{v}_\alpha)^2), \quad (11)$$

where k is the Boltzmann constant.

Starting from Equations 2 and 3, the hydrodynamics equations are obtained by taking the different velocity moments of those equations, i.e., the zeroth, the first and the second moments. Namely, multiplying both sides of the kinetic equations by 1, \mathbf{c} and $\mathbf{c}^2/2$, for each component and integrating over the velocity, $\int d^3c$, the equations of mass, momentum and energy conservation will be obtained. This is compatible with the so-called Grad's 5-moment theory. Using this method of moments, it can be easily shown that, for the inviscid binary gas system, the conservation equations of each component will become, as follows:

$$\frac{\partial(n_\alpha m_\alpha)}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot (n_\alpha m_\alpha \mathbf{v}_\alpha) = S_m^{\alpha\beta}, \quad (12)$$

$$\frac{\partial(n_\alpha m_\alpha \mathbf{v}_\alpha)}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot (n_\alpha m_\alpha \mathbf{v}_\alpha \mathbf{v}_\alpha + \mathbf{P}_\alpha) = S_m^{\alpha\beta}, \quad (13)$$

$$\frac{\partial E_\alpha}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot ((E_\alpha + \mathbf{P}_\alpha) \mathbf{v}_\alpha) = S_E^{\alpha\beta}, \quad (14)$$

$$\frac{\partial(n_\beta m_\beta)}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot (n_\beta m_\beta \mathbf{v}_\beta) = S_m^{\beta\alpha}, \quad (15)$$

$$\frac{\partial(n_\beta m_\beta \mathbf{v}_\beta)}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot (n_\beta m_\beta \mathbf{v}_\beta \mathbf{v}_\beta + \mathbf{P}_\beta) = S_v^{\beta\alpha}, \quad (16)$$

$$\frac{\partial E_\beta}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot ((E_\beta + \mathbf{P}_\beta) \mathbf{v}_\beta) = S_E^{\beta\alpha}, \quad (17)$$

where S_m , S_v and S_E refer to mass, momentum and energy exchange terms, respectively and \mathbf{P}_α and \mathbf{P}_β are the partial pressure tensors for the species.

Summing up Equations 12 and 15, the continuity equation for the average flow field of the gas mixture as a whole is obtained, as follows :

$$\frac{\partial(nm)}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot (nm\mathbf{v}) = S_m^{\alpha\beta} + S_m^{\beta\alpha}, \quad (18)$$

where $n = n_\alpha + n_\beta$ and $m = \frac{n_\alpha m_\alpha + n_\beta m_\beta}{n_\alpha + n_\beta}$.

The momentum and the energy equations for the average flow field of the gas mixture as a whole can be obtained in a similar manner, as follows:

$$\frac{\partial(nm\mathbf{v})}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot (nm\mathbf{v}\mathbf{v} + \mathbf{P}) = S_v^{\alpha\beta} + S_v^{\beta\alpha}, \quad (19)$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot ((E + \mathbf{P})\mathbf{v}) = S_E^{\alpha\beta} + S_E^{\beta\alpha}. \quad (20)$$

It will be seen that the right hand sides of Equations 18 to 20 are equal to zero.

COMPUTATION OF EXCHANGE TERMS

The exchange terms can be calculated by direct integration of the zeroth, the first and the second moment of the right hand sides of Equations 2 and 3. From the kinetic theory, the distribution functions have the following relations with macroscopic parameters of the gas:

$$\begin{aligned} \int f_\alpha \mathbf{c}_\alpha \mathbf{d}\mathbf{c}_\alpha &= \int F_\alpha \mathbf{c}_\alpha \mathbf{d}\mathbf{c}_\alpha = \int \tilde{F}_\alpha \mathbf{c}_\alpha \mathbf{d}\mathbf{c}_\alpha = n_\alpha m_\alpha = \rho_\alpha, \\ \int \mathbf{c}_\alpha \tilde{F}_\alpha \mathbf{d}\mathbf{c}_\alpha &= n_\alpha m_\alpha \tilde{\mathbf{v}}_\alpha, \\ \int \mathbf{C}_\alpha f_\alpha \mathbf{d}\mathbf{c}_\alpha &= \int \mathbf{C}_\alpha F_\alpha \mathbf{d}\mathbf{c}_\alpha = \int \mathbf{C}_\alpha \tilde{F}_\alpha \mathbf{d}\mathbf{c}_\alpha = 0, \\ \int \frac{\mathbf{c}_\alpha^2}{2} f_\alpha \mathbf{d}\mathbf{c}_\alpha &= \int \frac{\mathbf{c}_\alpha^2}{2} F_\alpha \mathbf{d}\mathbf{c}_\alpha = E_\alpha, \\ \int \frac{\mathbf{c}_\alpha^2}{2} \tilde{F}_\alpha \mathbf{d}\mathbf{c}_\alpha &= \tilde{E}_\alpha. \end{aligned} \quad (21)$$

It is noted that, since only elastic collisions are considered here, self-collisions conserve mass, momentum and energy in each component and, therefore, the three

moments of the self-collision terms on the right-hand sides of Equations 2 and 3, will vanish [14], as follows:

$$\begin{aligned} \int \nu_{\alpha\alpha}(F_\alpha - f_\alpha) \mathbf{dc}_\alpha &= 0, \\ \int \nu_{\alpha\alpha}(F_\alpha - f_\alpha) \mathbf{c}_\alpha \mathbf{dc}_\alpha &= 0, \\ \int \nu_{\alpha\alpha}(F_\alpha - f_\alpha) \frac{\mathbf{c}_\alpha^2}{2} \mathbf{dc}_\alpha &= 0. \end{aligned} \quad (22)$$

According to Expression 18, integration over the moments of the inter-collision terms on the right-hand sides of Equations 2 and 3 gives:

$$\begin{aligned} \int \nu_{\alpha\beta}(\tilde{F}_\alpha - f_\alpha) \mathbf{dc}_\alpha &= \nu_{\alpha\beta} \left(\int \tilde{F}_\alpha \mathbf{dc}_\alpha - \int f_\alpha \mathbf{dc}_\alpha \right) \\ &= \nu_{\alpha\beta}(n_\alpha m_\alpha - n_\alpha m_\alpha) = 0, \\ \int \nu_{\alpha\beta}(\tilde{F}_\alpha - f_\alpha) \mathbf{c}_\alpha \mathbf{dc}_\alpha &= \nu_{\alpha\beta} \left(\int \tilde{F}_\alpha \mathbf{c}_\alpha \mathbf{dc}_\alpha - \int f_\alpha \mathbf{c}_\alpha \mathbf{dc}_\alpha \right) \\ &= \nu_{\alpha\beta}(n_\alpha m_\alpha \tilde{\mathbf{v}}_\alpha - n_\alpha m_\alpha \mathbf{v}_\alpha) \\ &= S_{\mathbf{v}}^{\alpha\beta}, \\ \int \nu_{\alpha\beta}(\tilde{F}_\alpha - f_\alpha) \frac{\mathbf{c}_\alpha^2}{2} \mathbf{dc}_\alpha &= \nu_{\alpha\beta} \left(\int \tilde{F}_\alpha \frac{\mathbf{c}_\alpha^2}{2} \mathbf{dc}_\alpha - \int f_\alpha \frac{\mathbf{c}_\alpha^2}{2} \mathbf{dc}_\alpha \right) \\ &= \nu_{\alpha\beta}(\tilde{E}_\alpha - E_\alpha) = S_E^{\alpha\beta}, \end{aligned} \quad (23)$$

where,

$$\begin{aligned} \tilde{E}_\alpha &= \frac{n_\alpha m_\alpha \tilde{\mathbf{v}}_\alpha^2}{2} + \frac{\tilde{P}_\alpha}{\gamma_\alpha - 1}, \\ \tilde{P}_\alpha &= n_\alpha m_\alpha R_\alpha \tilde{T}_\alpha. \end{aligned} \quad (24)$$

Therefore, for gases α and β , the exchange terms are of the following forms:

$$S_m^{\alpha\beta} = S_m^{\beta\alpha} = 0, \quad (25)$$

$$S_{\mathbf{v}}^{\alpha\beta} = \nu_{\alpha\beta} n_\alpha m_\alpha (\tilde{\mathbf{v}}_\alpha - \mathbf{v}_\alpha),$$

$$S_{\mathbf{v}}^{\beta\alpha} = \nu_{\beta\alpha} n_\beta m_\beta (\tilde{\mathbf{v}}_\beta - \mathbf{v}_\beta), \quad (26)$$

$$S_E^{\alpha\beta} = \nu_{\alpha\beta} (\tilde{E}_\alpha - E_\alpha),$$

$$S_E^{\beta\alpha} = \nu_{\beta\alpha} (\tilde{E}_\beta - E_\beta). \quad (27)$$

According to Equation 4 ($n_\alpha \nu_{\alpha\beta} = n_\beta \nu_{\beta\alpha} = A$):

$$\begin{aligned} S_{\mathbf{v}}^{\alpha\beta} + S_{\mathbf{v}}^{\beta\alpha} &= \nu_{\alpha\beta} n_\alpha m_\alpha (\tilde{\mathbf{v}}_\alpha - \mathbf{v}_\alpha) \\ &\quad + \nu_{\beta\alpha} n_\beta m_\beta (\tilde{\mathbf{v}}_\beta - \mathbf{v}_\beta) \\ &= A(m_\alpha + m_\beta) \frac{m_\alpha \mathbf{v}_\alpha + m_\beta \mathbf{v}_\beta}{m_\alpha + m_\beta} \\ &\quad - A(m_\alpha \mathbf{v}_\alpha + m_\beta \mathbf{v}_\beta) = 0. \end{aligned} \quad (28)$$

And, in a similar manner:

$$S_E^{\alpha\beta} + S_E^{\beta\alpha} = 0, \quad (29)$$

that coincides with momentum and energy conservation. In conclusion, the present formulation, i.e., Equations 18 to 20, is compatible with ordinary conservation of mass, momentum and energy for the mixtures that were derived in the above equations.

The collision frequency, $\nu_{\alpha\beta}$, which depends on temperature and the law of interaction between the particles, can be calculated from Chapman-Cowling collision integrals, $\Omega_{\alpha\beta}^{(l,r)}$ [24], as follows:

$$\nu_{\alpha\beta} = \frac{16}{3} n_\beta \Omega_{\alpha\beta}^{(1,1)}. \quad (30)$$

Finally, the $\Omega_{\alpha\beta}^{(i,j)}$ are the Chapman-Cowling integrals [16], which, for the rigid sphere interaction, read, as follows:

$$\begin{aligned} \Omega_{\alpha\beta}^{(i,j)} &= \frac{(j+1)!}{2} \left[1 - \frac{1 + \binom{j}{i}}{2(i+1)} \right] \\ &\quad \left(\frac{\pi k T}{2m_{\alpha\beta}} \right)^{\frac{1}{2}} \left(\frac{d_\alpha + d_\beta}{2} \right)^2, \end{aligned} \quad (31)$$

where d_α and d_β are the particle diameters and $m_{\alpha\beta}$ is called reduced mass, i.e.:

$$m_{\alpha\beta} = \frac{m_\alpha m_\beta}{m_\alpha + m_\beta}. \quad (32)$$

The Relaxation Time Approximation (RTA) approach interprets the effect of collisions as a combination of two different relaxation processes, as follows:

- (i) Collisions between the same particles, e.g., of fluid α , which tend to relax this fluid into its own Local Thermodynamic Equilibrium (LTE) state. This is the faster of the two processes;
- (ii) Intercollisions between particles of fluids α and β , which tend to relax each fluid from its own LTE towards a common LTE. In this common LTE, the two fluids have the same flow velocity and kinetic temperature.

NUMERICAL PROCEDURE

To solve Equations 12 to 14 and Equations 18 to 20, an explicit difference scheme was applied, where the steady-state solution was obtained as the limit of a time-evolving process. Roe's numerical scheme is used to discretize the convective terms of the fluid flow equations. The equations in Cartesian coordinates, in the conservative form are, as follows:

$$Q_t^\alpha + (E^\alpha - E_v^\alpha)_x + (F^\alpha - F_v^\alpha)_y = H^\alpha, \quad (33)$$

$$\mathbf{Q}^\alpha = \begin{bmatrix} \mathbf{e}^\alpha \\ \rho^\alpha \\ \rho^\alpha u^\alpha \\ \rho^\alpha v^\alpha \end{bmatrix},$$

$$E^\alpha = \begin{bmatrix} (e^\alpha + p^\alpha)u^\alpha \\ \rho^\alpha u^\alpha \\ \rho^\alpha u^{\alpha 2} + p^\alpha \\ \rho^\alpha u^\alpha v^\alpha \end{bmatrix},$$

$$\mathbf{F}^\alpha = \begin{bmatrix} (e^\alpha + p^\alpha)\mathbf{v}^\alpha \\ \rho^\alpha \mathbf{v}^\alpha \\ \rho^\alpha \mathbf{u}^\alpha \mathbf{v}^\alpha \\ \rho^\alpha \mathbf{v}^{\alpha 2} + p^\alpha \end{bmatrix}, \quad (34)$$

$$E_v^\alpha = \begin{bmatrix} u^\alpha \tau_{xx}^\alpha + v^\alpha \tau_{xy}^\alpha & q_x^\alpha \\ 0 & \\ \tau_{xx}^\alpha & \\ \tau_{xy}^\alpha & \end{bmatrix},$$

$$\mathbf{F}_v^\alpha = \begin{bmatrix} u^\alpha \tau_{yx}^\alpha + v^\alpha \tau_{yy}^\alpha & q_y^\alpha \\ 0 & \\ \tau_{yx}^\alpha & \\ \tau_{yy}^\alpha & \end{bmatrix}, \quad (35)$$

$$H^\alpha = \begin{bmatrix} S_e^\alpha \\ 0 \\ S_u^\alpha \\ S_v^\alpha \end{bmatrix}, \quad (36)$$

in which:

$$e^\alpha = \frac{p^\alpha}{\gamma - 1} + \frac{\rho^\alpha}{2}(u^{\alpha 2} + v^{\alpha 2}), \quad (37)$$

$$\tau_{ij}^\alpha = 2 \sum_{\beta=1}^{\nu} \eta_{\alpha\beta} \frac{\partial v_{<i}^\beta}{\partial x_{j>}}, \quad (38)$$

$$q_i^\alpha = \sum_{\beta=1}^{\nu} \lambda_{\alpha\beta} \frac{\partial T_\beta}{\partial x_i} - \sum_{\beta=1}^1 M_{\alpha\beta} (\mathbf{v}_i^\beta - \mathbf{v}_i^\nu), \quad (39)$$

where,

$$\frac{\partial v_{<i}^\alpha}{\partial x_{j>}} = \frac{1}{2} \left(\frac{\partial v_i^\alpha}{\partial x_j} + \frac{\partial v_j^\alpha}{\partial x_i} \right) - \frac{1}{3} \frac{\partial v_k^\alpha}{\partial x_k} \delta_{ij}, \quad (40)$$

and the quantities $\eta_{\alpha\beta}$, $\lambda_{\alpha\beta}$ and $M_{\alpha\beta}$ are transport coefficients associated with viscous, thermal and thermal-diffusion effects, respectively, which can be calculated using the Chapman-Cowling collision integrals [17].

RESULTS

To validate the formulation and the algorithm, a compressible flow in a two dimensional supersonic converging-diverging nozzle for a binary perfect gas mixture (He-Xe) has been considered. The problem properties are, as follows:

1. Nozzle geometry:

$$\text{area ratio: } \frac{A_e}{A_t} = 1.38,$$

$$\text{length of nozzle} = 2 \text{ cm},$$

$$\text{inlet and exit diameters} = 2 \text{ cm}.$$

2. Reference properties:

$$p_r = 5000 \text{ pa},$$

$$T_r = 700 \text{ k},$$

$$\text{and, at the inlet: } \frac{p_0}{p_r} = 1.4,$$

$$\frac{T_0}{T_r} = 1.1,$$

$$c = 0.85.$$

where, A_e and A_t denote exit and throat areas, respectively, subscript r denotes reference, subscript 0 represents stagnation conditions and c shows the concentration ($\frac{\rho_{\text{He}}}{\rho_{\text{He}} + \rho_{\text{Xe}}}$) distribution for the gas mixture. The problem was solved using 1072(151*71) grids with a stretching ratio of 1.05 in a normal direction, according to the Robertson formula [25] (Figure 1). When refining the grid by a factor of 2, the differences between the computational results were extremely small, which meant that grid independency had been reached. The comparisons of the obtained results at the centerline of the nozzle are given in Figures 2 to 4,

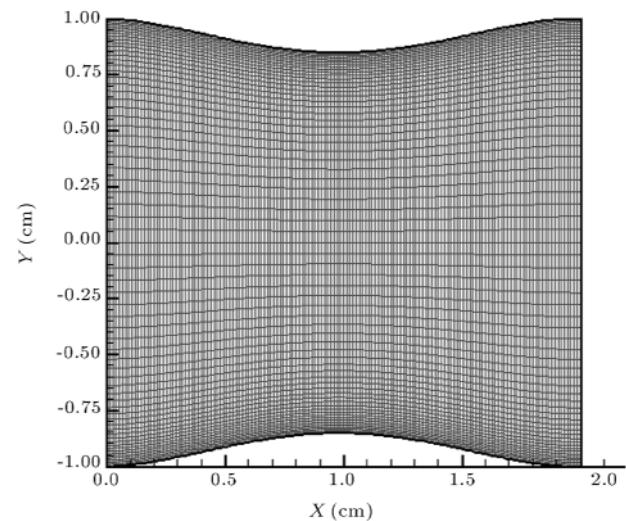


Figure 1. Geometry and grids for the nozzle.

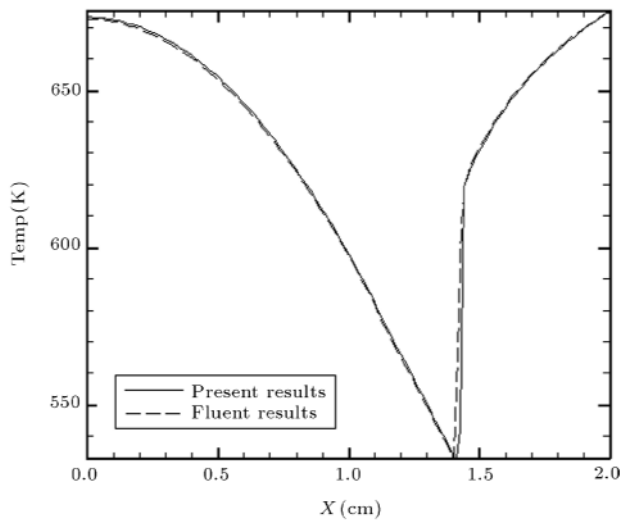


Figure 2. Temperature distribution.

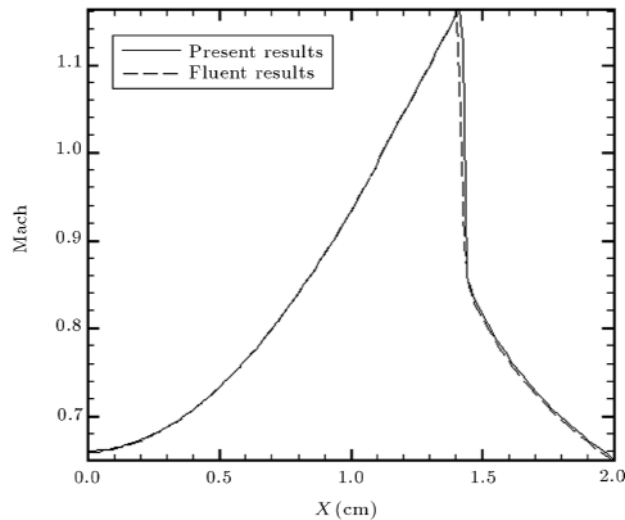


Figure 3. Mach number distribution.

which show good agreement with numerical results obtained by the commercial FLUENT software that uses the mixture model.

The high gradient region caused by the shock wave (Figures 2, 3 and 5), is equally well resolved by both algorithms. Therefore, a new formulation provides the same results for such a nozzle problem.

WALL-COOLING OF THE NOZZLE

As the next example, the wall-cooling of a two dimensional supersonic converging-diverging nozzle has been considered. The same nozzle geometry and the same grids as in the preceding example are chosen here. The problem properties are:

$$p_r = 5 \times 10^3 \text{ pa,}$$

$$T_r = 700 \text{ K,}$$

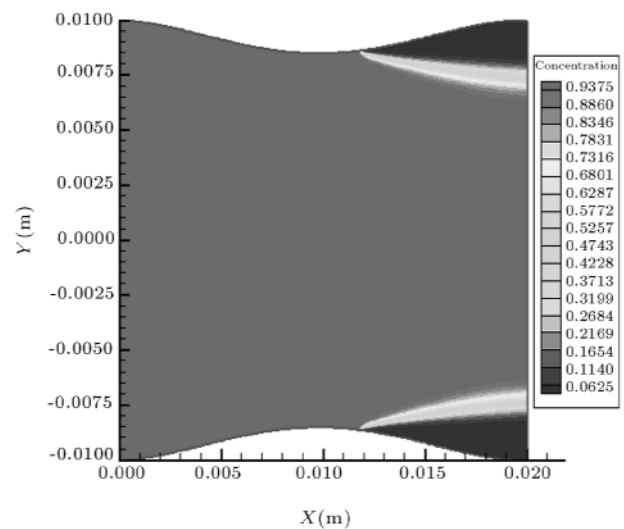
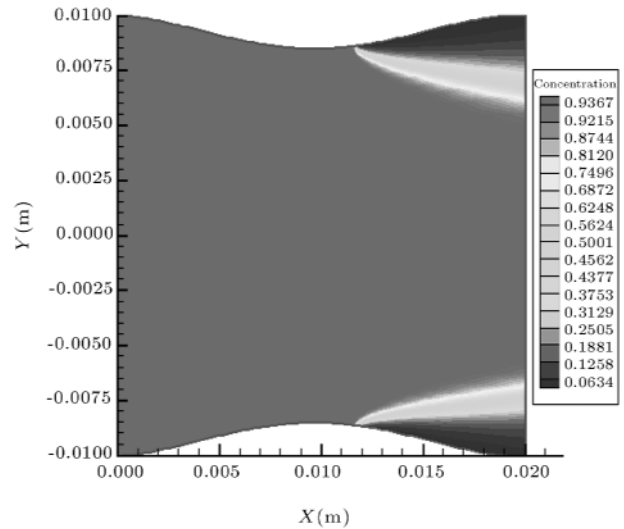


Figure 4. Concentration contours from the present and the mixture models.

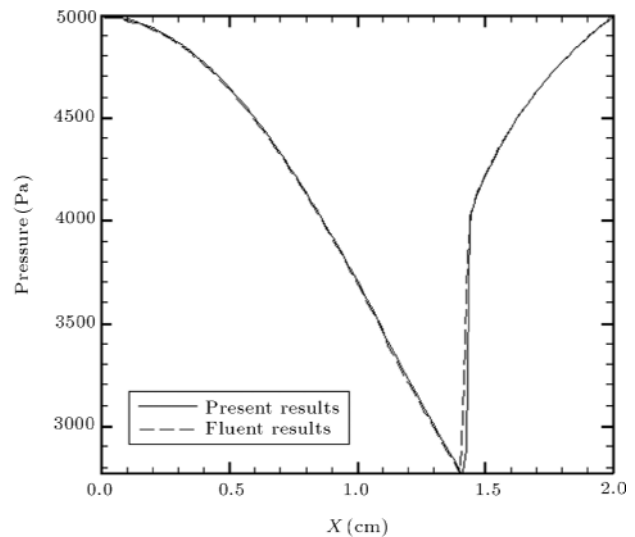


Figure 5. Pressure distribution.

and, at the inlet:

$$\frac{p_0}{p_r} = 1.4, \quad \text{and} \quad \frac{T_0}{T_r} = 1.1.$$

A binary ideal gas system (Helium-Xenon) is chosen as the media. Lighter gas (He) enters from the inlet of the converging part of the nozzle with a temperature of about 740 K and the heavier gas (Xe), as the coolant, is blown from the wall from $x = 1.145$ cm, afterwards, with a temperature of about 300 K and with Cartesian velocity components equal to (100,5) m/s.

Figure 4 shows the concentration distribution for the mixture ($\frac{\rho_{He}}{\rho_{He} + \rho_{Xe}}$) obtained from the present method and the mixture model (FLUENT), respectively. The comparison of the results shows that the present method is more diffusive. This may be due to the diffusive nature of the exchange terms in the conservation equations. This method can provide details of the flow fields of each component of the mixture separately, e.g. the Mach number contours for helium and xenon are shown in Figure 6. It is seen that, although the gas mixture flow is subsonic, Figure 7, the xenon component is supersonic in most of the region. This is due to the large difference in the properties of each component of the mixture. Additionally, the x -velocity and temperature distributions of each component are presented in Figures 8 and 9. As seen, both components have the same temperature and velocity at each location of the nozzle. This means that the components of the mixture have reached the same thermodynamics equilibrium. In fact, although at the interface of the helium and xenon mixing, the particles of the two gases meet each other with two different temperatures, the relaxation time is too small to detect this temperature difference transition zone.

Figure 7 shows the Mach number contours for the whole mixture obtained from the Fluent computer code, based on the mixture model, which is almost identical with the mixture results obtained from the present model. From Figure 7, it is seen that the effective shape of the nozzle would be converging instead of the converging-diverging nozzle, due to xenon blowing from the diverging part downstream. Therefore, the main flow remains subsonic, as can be seen in Figure 7.

CONCLUSION

In this work, starting from kinetic equations, the Eulerian approach was used to derive new hydrodynamic equations of motion for a multicomponent system, where each component may have a different velocity and kinetic temperature. The new equations are based on Grad's method of moment, derived from the kinetic model in a Relaxation Time Approximation (RTA). Based on this binary model, which contains

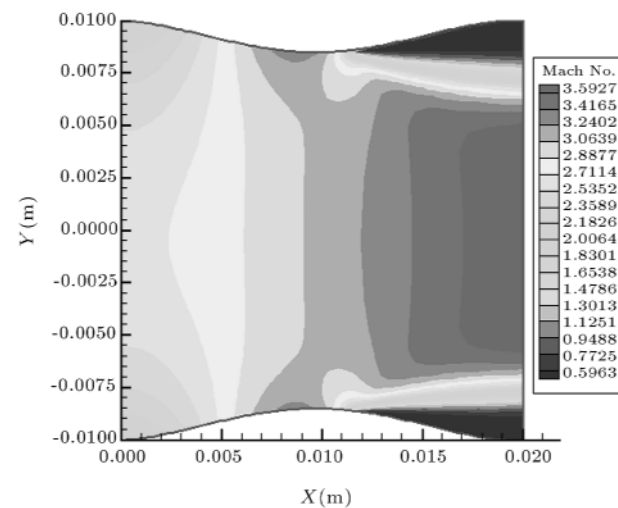
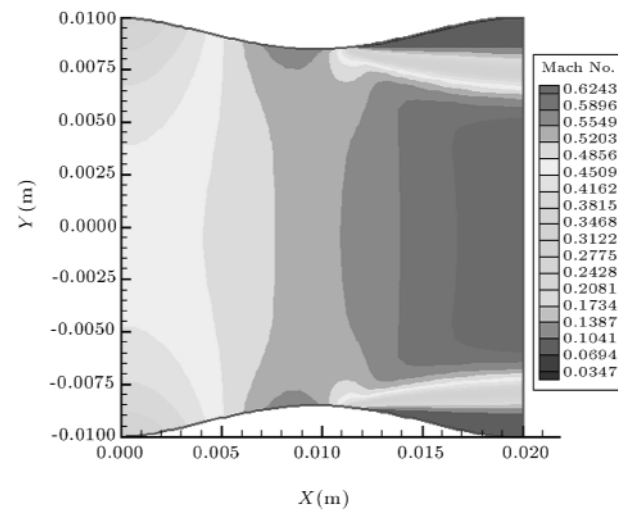


Figure 6. Mach no. contours for the helium and the xenon from the present model.

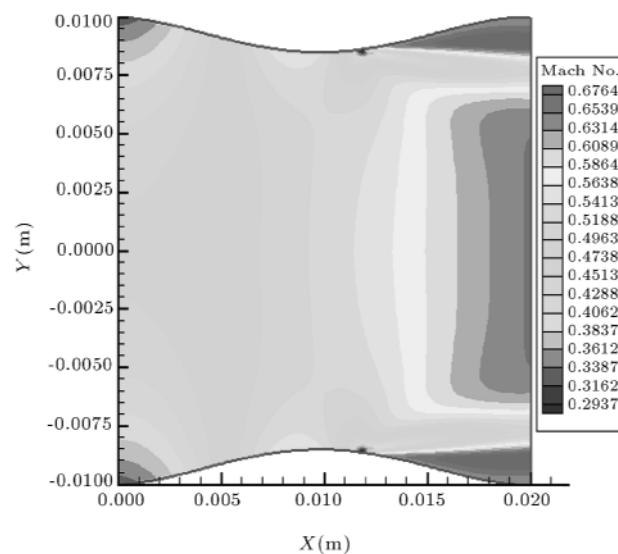


Figure 7. Mach no. contours for the whole mixture from the mixture model.

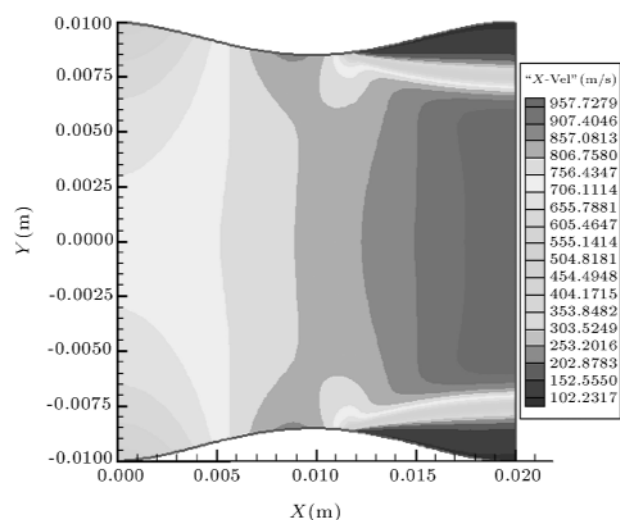
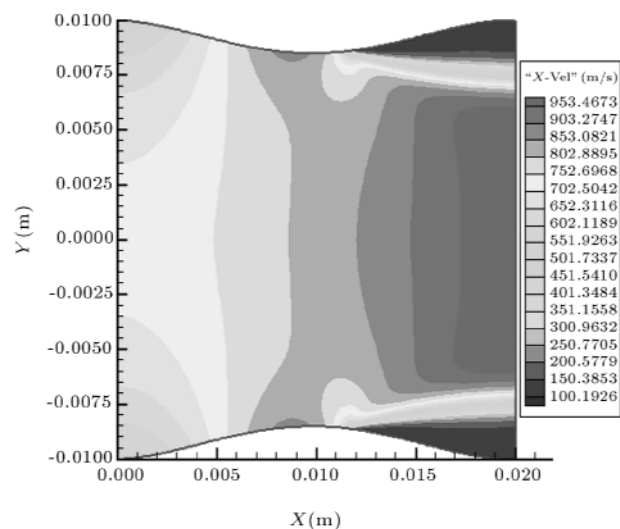


Figure 8. X-velocity distribution for helium and xenon.

a separate equation set for one component of the system and an equation set for average quantities of the mixture, a computer code was developed for numerical computation of compressible flows of binary gas mixtures in generalized curvilinear boundary conforming coordinates. Since these equations are similar to the Navier-Stokes form for the single fluid systems, they can be solved by conventional numerical schemes, which are also used for solving Navier-Stokes equations. The prepared algorithm and the computer code are capable of computing and presenting the flow fields of each component of the system separately, as well as the flow field of the gas mixture as a whole. Some examples were used to evaluate the model and the relevant computer code. It was concluded that, for most ordinary problems, the results of the Eulerian multifluid model and the mixture model are almost identical, mainly due to small relaxation times. It is suggested that the separate fluids treatment is crucial when considering time scales on the order of (or shorter

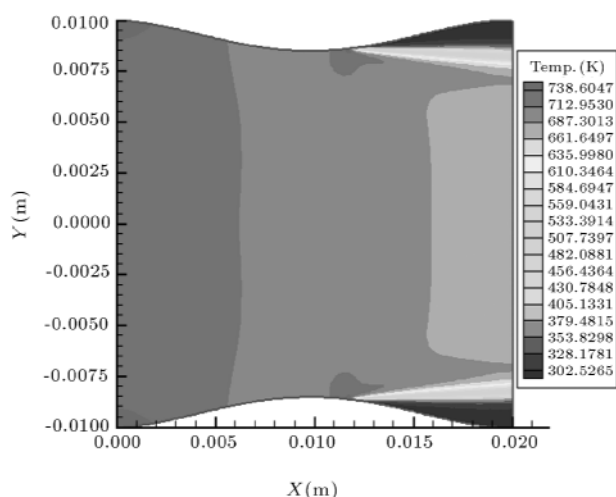
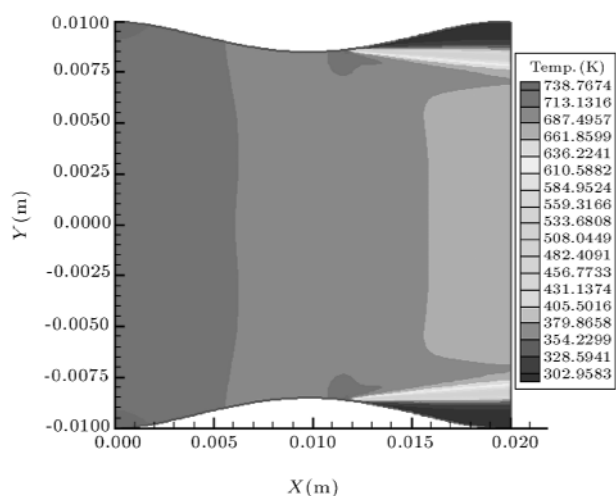


Figure 9. Temperature distribution for helium and xenon.

than) intercollision relaxation times. Therefore, one may find more applications of this new formulation and the algorithm in unsteady problems, including sudden changes in the flow properties or flows of rarefied gases that bring about larger relaxation times.

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