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Navier-Stokes computation of some gas mixture problems in the slip flow regime

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KEYWORDS Gas mixture; Rarefied flow; Slip flow regime; Navier-Stokes equations; Nozzle; Microchannel. **Abstract.** Several kinetic descriptions have already been utilized for the simulation of rarefied gas mixture flows. Although such developments are important, Navier-Stokes computation can find extended use in engineering applications. Recently, the authors have derived new velocity-slip and temperature-jump boundary conditions for slip flows of gas mixtures. Appealing to these new boundary conditions, Navier-Stokes computation of rarefied gas mixture problems has become feasible. In the present contribution, the proposed conditions, in conjunction with the Navier-Stokes equations and an equation for the conservation of species, are solved for some binary gas mixture problems in the slip flow regime. Applications include low pressure flow in a converging-diverging nozzle, wall-cooling of a nozzle under rarefied condition, and parallel mixing in a microchannel. Simulation results are presented in terms of the distributions of overall Knudsen number, Mach number, pressure, temperature, and concentration.

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1. Introduction

The physics of rarefied single-component gas flows has been extensively studied in the past, and a number of interesting phenomena, which vanish at the continuum limit, have been observed. In practice, however, one deals with gas mixtures more often than with single gases and, thereby, attention must be paid to the simulation of such flows. In gas mixture flows, several new phenomena can lead to a somehow surprising behavior, compared with single-component cases. As an example, diffusion can be observed due to imposed pressure, temperature, and concentration gradients. Additionally, concentration gradients may lead to the transfer of heat. Mixture problems also require drastically higher computational effort, as a result of the large number of additional parameters involved in their calculations. Consequently, it is not surprising to see that rarefied gas mixture flows have not been analyzed extensively in the past. Some recent works are as follows.

Yan and Farouk [1] simulated the mixing problem of two parallel gas streams entering a microchannel initially separated by a splitter plate. They used the Direct Simulation Monte Carlo (DSMC) method and concluded that the mixing decreases with increasing the inlet-outlet pressure difference, and that the mixing process for nearly specularly-reflective walls is much slower than for perfectly diffusing walls. Such a problem was further analyzed by Wang and Li [2] that clarified the importance of main flow velocity as well as temperature on the degree of gas mixing. A recent analysis of this flow problem was undertaken by Darbandi and Lakzian [3].

The developed flow of binary mixtures of noble gases between parallel plates driven by small pressure, temperature, and concentration gradients was analyzed by Naris et al. [4]. They utilized the McCormack model

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of the Boltzmann equation [5] and presented some flow features for the whole range of gas rarefaction. Concerning their results, they concluded that the hardsphere molecular interaction model did not provide reliable results when mixture flow problems were studied. This problem was again analyzed by Kosuge and Takata [6]. They constructed a flux database for binary mixtures of noble gases that covers the entire range of Knudsen number and concentration, and a wide range of temperature. Later, Naris et al. [7] extended their previous formulation (i.e. [4]) to developing flows through microchannels.

Sharipov et al. [8] calculated heat flux magnitudes through rarefied binary mixtures of noble gases confined between parallel plates. Their solution was based on the McCormack model [5] and led to the conclusion that using the hard-sphere molecular interaction model, accurate heat fluxes would not be resulted. Recently, DSMC simulation of this problem was undertaken by Strapasson and Sharipov [9]. Comparison of the results of the two approaches demonstrated that, in small temperature differences, the McCormack model provided reliable results with an uncertainty of 2%.

Raines [10] solved the Boltzmann equation for the flow of binary mixtures between parallel plates and presented some flow aspects for a wide range of Knudsen number.

A lattice Boltzmann model was derived for microscale gas flows of binary mixtures by Guo et al. [11]. The proposed model utilizes a collision operator with multiple relaxation times.

Szalmas and Valougeorgis [12] analyzed the flow of gas mixtures through triangular and trapezoidal microchannels. They solved the McCormack kinetic model [5] and presented some flow features for the whole range of gas rarefaction.

Steady, one-dimensional flow of a binary mixture of hard-sphere gases in contact with an absorbing planar wall was studied by Frezzotti et al. [13] through the DSMC method. Recently, they extended their investigation to two-dimensional circumstances [14].

Although such developments are important, the Navier-Stokes description can find extended use in engineering applications due to its (i) simplicity and familiarity, (ii) computational efficiency, (iii) applicability to monatomic, as well as polyatomic, gases, (iv) flexibility for possible extension to multicomponent problems, (v) suitability for simple, as well as complex, geometries.

In spite of that, to the authors' knowledge, Navier-Stokes equations have not been employed for the computation of microscale gas mixture flows, since little have been known about the near wall behavior of the gas mixture. Some models have been proposed for velocity-slip, temperature-jump, and concentrationjump in rarefied mixture flows over catalytic surfaces (e.g. [15,16]). Nevertheless, the inclusion of surface reaction has made them quite complex. Meanwhile, for most gas mixtures, no reaction occurs on the surface, and near wall behavior is not so sensitive to local flow properties.

Recently, Zahmatkesh et al. [17] derived new velocity-slip and temperature-jump boundary conditions for gas mixture flows under rarefied conditions. Appealing to these boundary conditions, the Navier-Stokes computation of gas mixture flows in the slip flow regime has become feasible.

To continue this effort, in the present contribution, the proposed boundary conditions, in conjunction with Navier-Stokes equations and an equation for the conservation of species, are solved for some binary gas mixture problems in the slip flow regime. Applications include low pressure flow in a converging-diverging nozzle, wall-cooling of a nozzle under rarefied condition, and parallel mixing in a microchannel. Since previous investigations in the context of rarefied gas mixtures have been restricted to straight microchannels, the first originality of the current study goes back to the analysis of more complex geometries. This contribution can also be regarded as the first Navier-Stokes computation of gas mixture problems under rarefied conditions.

2. Conservation equations

For simplicity of exposition, binary mixtures in two space dimensions are analyzed in this contribution. Accordingly, fluid dynamics of the binary systems are described by Navier–Stokes equations, with an additional equation, expressing the conservation of mass for the first component. This additional equation, in conjunction with mass conservation for the whole mixture, implies the conservation of mass for the second component as well. In a generalized curvilinear two-dimensional coordinate system, the conservation equations are:

$$\frac{\partial \tilde{\mathbf{Q}}}{\partial t} + \frac{\partial \tilde{\mathbf{F}}}{\partial \xi} + \frac{\partial \tilde{\mathbf{G}}}{\partial \eta} = \frac{\partial \tilde{\mathbf{F}}_{\mathbf{v}}}{\partial \xi} + \frac{\partial \tilde{\mathbf{G}}_{\mathbf{v}}}{\partial \eta},\tag{1}$$

where:

$$\begin{split} \mathbf{Q} &= \begin{cases} E\\ \rho\\ \rho u\\ \rho v\\ \rho c \end{cases}, \qquad \mathbf{F} = \begin{cases} (E+p)u\\ \rho u^2+p\\ \rho uv\\ \rho uc \end{cases}, \\ \mathbf{G} &= \begin{cases} (E+p)v\\ \rho v\\ \rho v\\ \rho vv\\ \rho vz + p\\ \rho vc \end{cases}, \qquad \mathbf{F_v} = \begin{cases} u\tau_{xx} + v\tau_{xy} - q_x\\ 0\\ \tau_{xx}\\ \tau_{yx}\\ j_x \end{cases}\}, \end{split}$$

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$$\mathbf{G}_{\mathbf{v}} = \begin{cases} u\tau_{xy} + v\tau_{yy} - q_y \\ 0 \\ \tau_{xy} \\ \tau_{yy} \\ j_y \end{cases} \right\}.$$
 (2)

Here, ρ is the mass density of the mixture and c is the mass fraction of the constituent, α . Moreover, u, v, q_x , and q_y are the components of velocity and heat flux vector. τ_{ij} is the viscous stress tensor and E is the total energy per unit volume. Meanwhile;

$$\begin{split} \tilde{\mathbf{F}} &= \frac{1}{J} \left(\mathbf{F} \xi_x + \mathbf{G} \xi_y \right), \qquad \tilde{\mathbf{G}} = \frac{1}{J} \left(\mathbf{F} \eta_x + \mathbf{G} \eta_y \right), \\ \tilde{\mathbf{Q}} &= \frac{1}{J} \mathbf{Q}, \qquad \tilde{\mathbf{F}}_{\mathbf{v}} = \frac{1}{J} (\mathbf{F}_{\mathbf{v}} \xi_x + \mathbf{G}_{\mathbf{v}} \xi_y), \\ \tilde{\mathbf{G}}_{\mathbf{v}} &= \frac{1}{J} (\mathbf{F}_{\mathbf{v}} \eta_x + \mathbf{G}_{\mathbf{v}} \eta_y). \end{split}$$
(3)

with:

$$J = \frac{\partial(\xi, \eta)}{\partial(x, y)} = \xi_x \eta_y - \xi_y \eta_x.$$
(4)

In this formulation, j is the molecular mass flux vector, which is defined as [18]:

$$\mathbf{j} = \rho D \lfloor \nabla c + k_T \nabla \ln T + k_p \nabla \ln p \rfloor.$$
(5)

Here, the first term represents diffusion due to concentration gradients, while the contributions associated with temperature gradients and pressure gradients are incorporated in the second and the third terms, respectively. The coefficient, D, is the binary diffusion coefficient. Meanwhile, k_T and k_p can be calculated from the mixture composition as [19]:

$$k_T = 0.0663 \left[\frac{m_{\alpha} m_{\beta}}{\left(cm_{\alpha} + (1-c)m_{\beta} \right)^2} \right],$$
 (6)

$$k_p = (m_\alpha - m_\beta)c(1-c)\left[\frac{c}{m_\alpha} + \frac{1-c}{m_\beta}\right].$$
 (7)

These coefficients become influential in problems with large temperature/pressure gradients. During computations, it must be borne in mind that k_T is not vanishing in the absence of one of the constituents.

The viscous stress tensor and the heat flux vector are obtained from:

$$\tau_{xx} = \mu \left(\frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right),\tag{8}$$

$$\tau_{xy} = \tau_{yx} = \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right), \tag{9}$$

$$\tau_{yy} = \mu \left(\frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} \right), \tag{10}$$

$$q_x = -\kappa \frac{\partial T}{\partial x} + \sum_{i=1}^2 h_i j_{x,i},\tag{11}$$

$$q_y = -\kappa \frac{\partial T}{\partial y} + \sum_{i=1}^2 h_i j_{y,i},\tag{12}$$

with κ and μ being the thermal conductivity and viscosity of the gas mixture, respectively, and h_i being the partial specific enthalpy of the *i*th species. It is noteworthy that the second terms in the right-hand side of Eqs. (11) and (12) represent the contribution of inter-diffusion on the transfer of heat. Here, $j_{x,i}$ and $j_{y,i}$ are the components of the molecular mass flux vector for the *i*'s species. For instance:

$$j_{x,\alpha} = \rho D \left[\frac{\partial D}{\partial x} + \frac{k_T}{T} \frac{\partial T}{\partial x} + \frac{k_p}{T} \frac{\partial p}{\partial x} \right].$$
(13)

The evolution equations are supplemented by the ideal gas equation of state, which expresses pressure, p, in terms of mass density, ρ , specific internal energy, e, mass fraction, c, and the ratio of the specific heats, γ :

$$p(\rho, e, c) = (\gamma(c) - 1)\rho e, \qquad (14)$$

where:

$$\gamma(c) = \frac{c_p}{c_v} = \frac{c_{p,\alpha}c + c_{p,\beta}(1-c)}{c_{v,\alpha}c + c_{v,\beta}(1-c)}.$$
(15)

Here, $c_{v,\alpha}$, $c_{v,\beta}$, $c_{p,\alpha}$ and $c_{p,\beta}$ are the specific heats at constant volume and constant pressure for the component species, respectively.

The conservation equations, in conjunction with the proposed velocity-slip and temperature-jump boundary conditions (that will be described in the forthcoming section), are solved invoking the explicit flux differencing of Roe's scheme [20]. In this method, the inviscid terms are calculated based on the evaluation of eigenvalues and eigenvectors of the Euler equations. The viscous terms are also discretized using a central differencing. Moreover, an upwinding method is applied to the equation of the continuity of the species. During the current computations, transport coefficients of the constituents are taken from Bergman et al. [21], while the Wassiljewa's correlation [22] is adopted for the thermal conductivity of the mixture.

3. The proposed boundary conditions

The proposed velocity-slip and temperature-jump boundary conditions for a binary system take the form

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of [17]:

$$u_s - u_w = \frac{2 - \sigma}{\sigma} \lambda_{\text{overall}} \left. \frac{\partial u}{\partial n} \right|_s + \frac{3}{4} \frac{\mu}{\rho T} \left. \frac{\partial T}{\partial s} \right|_s, \quad (16)$$

$$T_{g} - T_{w} = 2 \frac{2 - \sigma_{T}}{\sigma_{T}}$$

$$\frac{\lfloor c_{s} \kappa_{\alpha} + (1 - c_{s}) \kappa_{\beta} \rfloor}{\rho_{s} \bar{v}_{s} \left[c_{s} \frac{\gamma_{\alpha} + 1}{2} c_{v,\alpha} + (1 - c_{s}) \frac{\gamma_{\beta} + 1}{2} c_{v,\beta} \right]} \left. \frac{\partial T}{\partial n} \right|_{s}, (17)$$

with s and n being the streamwise and normal coordinates, respectively. λ_{overall} is the overall Knudsen number of the gas mixture:

$$\lambda_{\text{overall}} = c_s \lambda_\alpha + (1 - c_s) \lambda_\beta. \tag{18}$$

Moreover, u_s and u_w are the slip and wall velocities, T_g and T_w are the gas and wall temperatures, and γ is the ratio of specific heats. Subscript *s* stands for surface conditions. Coefficients σ and σ_T are the tangential-momentum-accommodation coefficient and the thermal-accommodation coefficient, respectively. \bar{v}_s is the mean molecular speed of the gas mixture:

$$\bar{v}_s = \left(\frac{8}{\pi} \frac{kT_s}{m}\right)^{0.5}.$$
(19)

Meanwhile, μ is the viscosity coefficient of the gas mixture that can be determined in terms of the mixture composition, as:

$$\mu = \mu_{\alpha} \left(1 + G_{\alpha\beta} \frac{\rho_{\beta}}{\rho_{\alpha}} \frac{M_{\alpha}}{M_{\beta}} \right)^{-1} + \mu_{\beta} \left(1 + G_{\beta\alpha} \frac{\rho_{\alpha}}{\rho_{\beta}} \frac{M_{\beta}}{M_{\alpha}} \right)^{-1},$$
(20)

with:

$$G_{\alpha\beta} = \frac{\left(1 + \sqrt{\mu_{\alpha}/\mu_{\beta}\sqrt{M_{\beta}/M_{\alpha}}}\right)^2}{2\sqrt{2(1 + M_{\alpha}/M_{\beta})}},\tag{21}$$

$$G_{\beta\alpha} = \frac{\left(1 + \sqrt{\mu_{\beta}/\mu_{\alpha}\sqrt{M_{\alpha}/M_{\beta}}}\right)^2}{2\sqrt{2(1 + M_{\beta}/M_{\alpha})}}.$$
(22)

Here, M_{α} and M_{β} denote molar masses.

4. Simulation results

In this section, simulation results are presented for three distinct gas mixture problems in the slip flow regime. Nitrogen and oxygen are regarded as the mixtures constituents. The current applications include low pressure flow in a converging-diverging nozzle, wall-cooling of a nozzle under rarefied condition, and parallel mixing in a microchannel. The accuracy of



Figure 1. Simulated velocity profiles at two different sections along the microchannel compared with DSMC results.

the employed Navier-Stokes solver for the description of these flow problems in the continuum flow regime has been established during our previous investigations [23-26]. Now, the validity of this solver in the computation of the slip flow regime is examined. For this purpose, and in the absence of any analytical or experimental data in the current flow problems, a He-Ne flow in a $1 \times 4 \ \mu m$ microchannel is computed, and the corresponding results are compared with those of the DSMC simulation of Wang et al. [27]. Here, the inlet and outlet pressures are taken to be 300 kPa and 100 kPa, respectively. Moreover, a temperature of 300 K and a concentration of 0.2 are assigned to the inflowing gas stream. Under this circumstance, the overall Knudsen number of the mixture is about 0.1 in the outgoing gases, and a slip flow establishes in the microchannel. Figure 1 compares the simulated velocity profiles at two different sections along the microchannel with those of the DSMC method. The centerline distributions of pressure are also indicated in Figure 2. Inspection of the figures demonstrates that the two approaches lead to almost the same simulation results. This provides confidence to the developed Navier-Stokes solver for further studies in rarefied circumstances. Consequently, in the forthcoming sections, it is used to simulate the aforesaid gas mixture problems in the slip flow regime.

4.1. Low pressure flow in a converging-diverging nozzle

As the first example, a low pressure gas mixture flow in a converging-diverging nozzle is regarded. The schematic of the nozzle is depicted in Figure 3. The



Figure 2. Simulated centerline distribution of pressure compared with DSMC results.



Figure 3. Schematic of the first mixture problem.

Table 1. Specifications of the first flow problem in Case I.

Inlet stagnation pressure	$p_{t,i} = 7000$ Pa
Inlet stagnation temperature	$T_{t,i}=750~{\rm K}$
Inlet concentration	$c_i = 0.5$
Exit pressure	$p_e = 5000$ Pa
Length of the nozzle	L = 2 mm
Size of the inlet and exit	2H = 2 mm
Inlet area Throat area	1.18
Thermal condition of the wall	$T_w = 750 \text{ K}$
Wall accommodation coefficients	$\sigma = \sigma_T = 0.85$

computations are undertaken for three distinct cases in the slip flow regime. Specifications of the first case (Case I, henceforth) are illustrated in Table 1. Under this circumstance, the overall Knudsen number of the mixture remains below 0.001 over the entire flow field. Consequently, this case represents the lower limit of the gas rarefaction in the slip flow regime.

In regard to the second case (Case II), the degree of gas rarefaction is increased by assigning $p_{t,i}$ = 700 Pa and $p_e = 500$ Pa at the boundaries. Other specifications are maintained identical to Case I. This makes the maximum value of the overall Knudsen number about 0.01. The last case (Case III), however, corresponds to a flow in the upper limit of the gas rarefaction in the slip flow regime (i.e., with Kn ≈ 0.1). This is attained by prescribing 70 Pa and 50 Pa at the inlet and outlet, respectively.

The flow cases are simulated using $10500 (70 \times 150)$ nodes based on a grid refinement study. In what concerns the centerline distribution of Mach number, simulation results for the three cases of the gas rarefaction are illustrated in Figure 4. Here, results



(c) Case III (Kn ≈ 0.1)

Figure 4. Centerline distribution of Mach number in the first mixture problem.

obtained without the rarefied boundary conditions (i.e., with no-slip/no-temperature jump conditions) are also provided for comparison. Obviously, in all of the current cases, the centerline Mach number increases along the nozzle and a maximum value is attained at the downstream side of the throat. This proceeds with a slight decrease in the diverging part of the nozzle. The behavior is attributed to strong viscous effects in these low Reynolds flow fields. Notice that with an increase in the overall Knudsen number, the centerline Mach numbers diminish. This occurs despite the pressure ratios that are maintained identical here. The physical reasoning for this behavior is the fact that, as the degree of gas rarefaction increases, velocity-slip becomes more pronounced and, thereby, more uniform velocity profiles establish in each section through the nozzle. The aforesaid variations in the Mach number make the centerline distributions of the temperature and pressure as depicted in Figures 5 and 6.

Comparing the results obtained with the proposed boundary conditions and those obtained without such conditions, in the three cases of gas rarefaction, is instructive. Evidently, as the gas becomes more rarefied, the discrepancies that appear between the results of the two approaches enhance, and, thereby, the influence of the implemented rarefied boundary conditions becomes more pronounced.

4.2. Wall-cooling of a nozzle under rarefied condition

As the second example, wall-cooling of a convergingdiverging nozzle under rarefied condition is analyzed here. For this purpose, the same nozzle geometry as in the preceding example is chosen. Figure 7 depicts the schematic of this flow problem. It is assumed that nitrogen enters from the inlet of the nozzle and oxygen, as a coolant, is blown from the walls downstream of the throat. Flow conditions for this case are illustrated in Table 2.

The problem is solved employing a 155×335 grid. Figure 8(a) presents the distribution of overall Knudsen number in the nozzle. Obviously, the lowest values

Table 2. Specifications of the second flow problem.

Inlet stagnation pressure	$p_{t,i} = 460$ Pa
Inlet stagnation temperature	$T_{t,i} = 500 \ \mathrm{K}$
Inlet concentration	$c_i = 1$
Coolant x -velocity	$u_c = 100 \ \mathrm{m/s}$
Coolant y -velocity	$v_c = \pm 5 \text{ m/s}$
Coolant static temperature	$T_c = 300 \text{ K}$
Coolant concentration	$c_{c} = 0$
Exit pressure	$p_{e}=300$ Pa
Thermal condition of the wall	Adiabatic
Wall accommodation coefficients	$\sigma = \sigma_T = 0.85$



Figure 5. Centerline distribution of temperature in the first mixture problem.

of the Knudsen number appear in the vicinity of the oxygen blowing. This occurs since molecular collisions are more frequent between the oxygen molecules that are larger than the nitrogen ones. Notice that the overall Knudsen number lies between 0.0095 and 0.0145, which, again, falls into the slip flow regime.

Simulation results, in terms of the distributions of concentration, Mach number, and temperature, are plotted in Figure 8(b) to (d). Concerning the contour plots of concentration in Figure 8(b), the view of the observer is directed towards the coolant that is blown and convected downstream. Inspection of Figure 8(c) demonstrates that due to oxygen



Figure 6. Centerline distribution of pressure in the first mixture problem.

blowing at the diverging part, the effective shape of the nozzle is converging instead of the convergingdiverging nozzle. Moreover, temperature distribution provided in Figure 8(d) indicates that high temperature gradients appear in the vicinity of the diverging part of the nozzle walls, wherein the coolant is blown.

4.3. Parallel mixing in a microchannel

As the last example problem, simulation results are presented for the mixing flow system depicted in Figure 9. Here, the parallel streams of oxygen and



Figure 7. Schematic of the second mixture problem.



Figure 8. Simulation results for the second mixture problem.

nitrogen, which are initially separated by a splitter plate, enter the mixing chamber. Specifications of this flow problem are illustrated in Table 3.

The problem is solved using 7171 (71×101) nodes based on a grid refinement study. Figure 10(a) presents the distribution of overall Knudsen number in the gas mixture. Evidently, as one proceeds along the microchannel, the gas becomes more rarefied. It is clear that the overall Knudsen number of this mixture problem remains below 0.02 over the entire

Inlet stagnation pressures	$p_{t,i}^{{\rm N}_2}=p_{t,i}^{{\rm O}_2}=15~{\rm kPa}$
Inlet stagnation temperatures	$T_{t,i}^{\mathcal{N}_2} = T_{t,i}^{\mathcal{O}_2} = 300 \ \mathcal{K}$
Exit pressure	$p_e = 7.5 \text{ kPa}$
Thermal condition of the wall	Adiabatic
Wall accommodation coefficients	$\sigma = \sigma_T = 0.85$
Height of the microchannel	$H = 100 \ \mu \mathrm{m}$
Aspect ratio of the microchannel	L/H = 5

Table 3. Specifications of the third flow problem.



Figure 9. Schematic of the third mixture problem.



(a) Distribution of overall Knudsen number



(b) Mach number distribution



(c) Temperature distribution



(d) Concentration distribution

Figure 10. Simulation results for the third mixture problem.

flow field. Consequently, a slip flow establishes inside the microchannel.

In what concerns the distributions of Mach number, temperature, and concentration, simulation results are depicted in Figure 10(b) to (d). Inspection of Figure 10(b) demonstrates that the flow is accelerated in accordance with the density drop brought about by the decrease in pressure, in a way that is consistent with the mass conservation principle. As a consequence of this flow acceleration, a low temperature region gradually forms in the downstream side of the microchannel, which is obvious in Figure 10(c). The mixing pattern of the two parallel gas streams is illustrated in Figure 10(d). Previous observations of Zahmatkesh et al. [23] provide evidence that during the parallel mixing, the heavier species diffuses towards the other gas stream. This is attributed to the higher momentum of the heavier particles during molecular collisions in the mixing layer. In spite of that, molecular masses of nitrogen and oxygen are almost identical, and the current parallel mixing is not so intense.

5. Concluding remarks

In this contribution, recently proposed velocity-slip and temperature-jump boundary conditions were adopted, and several Navier-Stokes computations were undertaken for some gas mixture problems in the slip flow regime. Inspection of the presented results for the low pressure nozzle flow demonstrated that the inclusion of the proposed boundary conditions has prominent consequences on the establishment of the flow fields. The method was also successful in the description of wall-cooling of a nozzle under rarefied condition and parallel mixing in a microchannel

The employed Navier-Stokes description can find extended use in the simulation of gas mixture flows in microelectromechanical systems due to its (i) simplicity and familiarity, (ii) computational efficiency, (iii) applicability to monatomic, as well as polyatomic, gases, (iv) flexibility for possible extension to multicomponent problems, (v) suitability for simple, as well as complex, geometries.

References

- Yan, F. and Farouk, B. "Numerical simulation of gas flow and mixing in a microchannel using the direct simulation Monte Carlo method", *Microscale Thermophys. Eng.*, 6, pp. 235-251 (2002).
- Wang, M. and Li, Z. "Gas mixing in microchannels using the direct simulation Monte Carlo method", Int. J. Heat Mass Transfer, 49, pp. 1696-1702 (2006).
- Darbandi, M. and Lakzian, E. "Mixing enhancement of two gases in a microchannel using DSMC", *Appl. Mech. Mater.*, **307**, pp. 166-169 (2013).
- Naris, S., Valougeorgis, D., Kalempa, D. and Sharipov, F. "Gaseous mixture flow between two parallel plates in the whole range of the gas rarefaction", *Physica A*, **336**, pp. 294-311 (2004).
- McCormack, F.J. "Construction of linearized kinetic models for gaseous mixture and molecular gases", *Phys. Fluids*, 16, pp. 2095-2105 (1973).
- Kosuge, S. and Takata, S. "Database for flows of binary gas mixtures through a plane microchannel", *Eur. J. Mech. B. Fluids*, 27, pp. 444-465 (2008).

- Naris, S., Valougeorgis, D., Kalempa, D. and Sharipov, F. "Flow of gaseous mixtures through rectangular microchannels driven by pressure, temperature, and concentration gradients", *Phys. Fluids*, **17**, pp. 100607.1-12 (2005).
- Sharipov, F., Cumin, L.M.G. and Kalempa, D. "Heat flux between parallel plates through a binary gaseous mixture over the whole range of the Knudsen number", *Physica A*, **378**, pp. 183-193 (2007).
- Strapasson, J.L. and Sharipov, F. "Ab initio simulation of heat transfer through a mixture of rarefied gases", *Int. J. Heat Mass Transfer*, **71**, pp. 91-97 (2014).
- Raines, A.A. "Heat transfer in a gas mixture between parallel plates", Comput. Math. Math. Phys., 48, pp. 306-311 (2008).
- Guo, Z., Asinari, P. and Zheng, C. "Lattice Boltzmann equation for microscale gas flows of binary mixtures", *Phys. Rev. E*, **79**, pp. 026702-9 (2009).
- Szalmas, L. and Valougeorgis, D. "Rarefied gas flow of binary mixtures through long channels with triangular and trapezoidal cross sections", *Microfluid Nanofluid*, 9, pp. 471-487 (2010).
- Frezzotti, A., Ghiroldi, G.P. and Gibelli, L. "Rarefied gas mixtures flows driven by surface absorption", *Vacuum*, 86, pp. 1731-1738 (2012).
- Frezzotti, A., Ghiroldi, G.P., Gibelli, L. and Bonucci, A. "DSMC simulation of rarefied gas mixtures flows driven by arrays of absorbing plates", *Vacuum*, **103**, pp. 57-67 (2014).
- 15. Scott, C.D. "Wall boundary conditions with slip and catalysis for multicomponent nonequilibrium gas flows", NASA TM X-5811 (1973).
- Kiryutin, B.A. and Tirskii, G.A. "Slip boundary conditions on a catalytic surface in a multicomponent gas flow", *Fluid Dyn.*, **31**, pp. 134-143 (1996).
- Zahmatkesh, I., Alishahi, M.M. and Emdad, H. "New velocity-slip and temperature-jump boundary conditions for Navier-Stokes computation of gas mixture flows in microgeometries", *Mech. Res. Commun.*, 38, pp. 417-424 (2011).
- Hirschfelder, J.O., Curtiss, C.F. and Bird, R.B., Molecular Theory of Gases and Liquids, Wiley, New York (1954).
- Landau, L.D. and Lifshitz, E.M., Fluid Mechanics, 6, Pergamon Press (1963).
- Roe, P.L. "Discrete models for numerical analysis of time-dependent multidimensional gas dynamics", J. Comput. Phys., 63, pp. 458-476 (1986).
- Bergman, T.L., Lavine, A.S., Incropera, F.P. and Dewitt, D.P., Fundamentals of Heat and Mass Transfer, 7th Ed., John Wiley & Sons (2011).

- Reid, R.C. and Sherwood, T.K., The Properties of Gases and Liquids, 2nd Ed., McGraw-Hill, New York (1966).
- Zahmatkesh, I., Emdad, H. and Alishahi, M.M. "Effect of temperature level on parallel mixing of two gas streams", *Mech. Res. Commun.*, **38**, pp. 141-145 (2011).
- Zahmatkesh, I., Emdad, H. and Alishahi, M.M. "Viscous and inviscid solutions of some gas mixture problems", *Heat Transfer Res.*, 42, pp. 233-250 (2011).
- Zahmatkesh, I., Emdad, H. and Alishahi, M.M. "Importance of molecular interaction description on the hydrodynamics of gas mixtures", *Scientia Iranica B*, 18, pp. 1287-1296 (2011).
- Zahmatkesh, I., Emdad, H. and Alishahi, M.M. "Twofluid analysis of a gas mixing problem", *Scientia Iranica B*, 20, pp. 162-171 (2013).
- Wang, Q., Yan, X. and He, Q. "Heat-flux-specified boundary treatment for gas flow and heat transfer in microchannel using direct simulation Monte Carlo method", Int. J. Numer. Methods Eng., 74, pp. 1109-1127 (2008).

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