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NUMERICAL INVESTIGATION OF IMPINGING JETS IN RAREFIED CONDITION USING DSMC METHOD*

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Abstract– In this study, the flow field of impinging jets in rarefied condition and high pressure ratios was investigated. Direct Simulation of Monte Carlo (DSMC) method was employed to find the flow field at two different Knudsen numbers (Kn) of 0.1 and 0.01. For each studied Knudsen number the effects of different nozzle-to-plate distances (L) are studied. For all cases a supersonic jet forms downstream of the nozzle. The results show that no shock occurs in the supersonic jet impinging on the plate in contrary to those in the continuum regime. The variations of molecular number density, axial velocity and Mach number on the center line were computed and discussed for two different Knudsen numbers. In general, in these conditions the gas expands from specified upstream condition to a lower background monotonically.

Keywords– DSMC, impinging jet, Knudsen number, rarefied

1. INTRODUCTION

Inertial impactors are simple fluid dynamic devices that consist of one or several jets impinging toward a flat plate normal to the jet axis which is known as an impactor plate. Impactors have been widely used in many important applications such as thin film and pattern deposition of fine particles on surface, optical and electronics fields, cooling or heating the impactor plate and so on. Supersonic impactors working in rarefied condition can be used in separation of nano-particles [1-3].

Rarefied gas flow has been studied theoretically, numerically and with experimental methods so far in the literature. In most studies, rarefied and highly rarefied jets at free molecular flow regime were considered, which can also be modeled as a collision less flow.

Khasawneh et al. [4] presented some analytical solutions for a collisionless two-dimensional plume impinging on a flat plate inclined normal to the plume axis. They also provided several analytical solutions for a collisionless flow resulted by impingement of a circular gas jet on a flat plate [5]. Cai and Boyd [6] proposed two sets of analytical formulas for free molecular flow regime of a free jet exiting the annular and two dimensional slits. They validated their solutions by comparing their results with those from DSMC method . Kanneberg and Boyd [7] presented some results for surface quantities of two plume impingements. A single under-expanded free jet was studied by Wu et al. [8]. They reported the flow field properties for a near continuum regime to transitional regime flow. Legge [9] experimentally measured the surface properties for different angles between the plume axis and impinging plate. He presented some simple correlations for flow properties on the plate.

Mierels and Mullen [10] investigated the unsteady expansion of a free jet in both continuum and free molecular flow regimes. Hyakutake and Nishida [11] numerically studied parallel, oblique and normal

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impingement jets. They compared pressure and shear stress distributions on the adjacent plate with the experimental work of Legge [9] for three different Knudsen numbers in the range of 3.26×10^{-3} to 2.04×10^{-4} based on the upstream stagnation pressure of 1000 to 16000 Pa. Impingement of a round air jet on a circular cylinder has been studied numerically and experimentally by Tahavvor [12] in order to find the optimum distance between the nozzle outlet and the jet stagnation point on a cylinder for cutting procedure.

The flow field of high pressure ratio impinging jets, which involves a wide range of pressure variation from the near continuum regime in the nozzle exit to the high rarefied condition in the nozzle downstream has not been investigated yet. This flow field cannot be simulated by conventional CFD codes that imply Navier-Stokes equations, but DSMC method is an option for simulating this flow regime. Therefore, the goal of this study is to simulate the impinging jets in the slip flow regime for relatively low stagnation pressures (201.65 Pa and 2016.5 Pa) and different nozzle to plate distances (L) by developing a DSMC code.

2. MODEL DESCRIPTION

In the present work, an axisymmetric model for the impinging jet was developed and solved numerically by a developed DSMC code. A schematic of the computational domain is shown in Fig. 1.

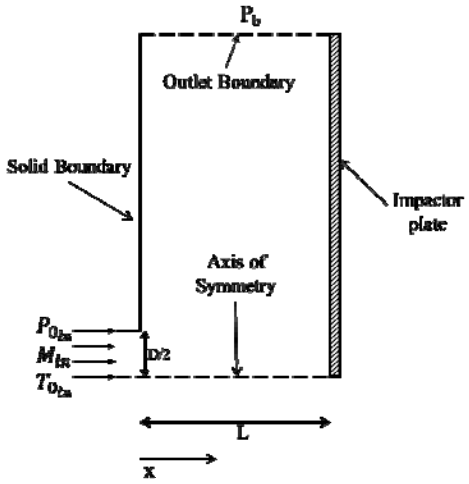


Fig. 1. A schematic of the impactor configuration

The diameter of the circular cross sectional nozzle (D) is 0.27 mm and Knudsen number is computed based on the upstream stagnation pressure and the orifice diameter as the characteristic length. For each studied Knudsen number, flow field properties for different nozzle-to-plate distances are studied. Impactor plate is a flat plate which is directed normal to the jet axis at the distance L from the orifice exit.

The domain under consideration is divided into the structured rectangular cells and each cell is divided to the subcells. Cell size is selected at the order of mean free path for efficient and accurate computation. At least 30 particles are considered in each cell and at least ninety and thirty cells were used for radial and axial directions respectively.

3. BOUNDARY CONDITIONS

The sonic air jet with the stagnation temperature of 300K enters to the domain uniformly in the direction of the jet axis. The carrier gas, air, is a mixture of 0.79 N_2 and 0.21 O_2 by the mole fraction respectively. The upstream stagnation pressure is computed using the assumed Knudsen number. The ratio of the upstream stagnation pressure to background pressure is assumed 400. This pressure ratio is regular in supersonic impactors which are being used in size discrimination of nano-particles [13].

Inlet velocity, temperature and static pressure are set based on an isentropic sonic jet at the orifice exit by the specified stagnation temperature and pressure. The upstream stagnation pressures for Kn = 0.01 and Kn = 0.1 are being set respectively to 2016.5 Pa and 201.65 Pa. Therefore, corresponding values of velocity and temperature at the orifice exit are respectively 316.88 m/s and 250K. The upstream static pressure values of 1065.5 Pa and 106.55 Pa are associated with the studied Knudsen numbers of 0.01 and 0.1 respectively. Consequently, the background pressure for Kn = 0.01 and Kn = 0.1 are 5 Pa and 0.5 Pa respectively.

Mean velocity and temperature of the outgoing molecules in the outflow boundary of the computational domain for subsonic condition were calculated iteratively by using the imposed back pressure. In the case of supersonic flow, all flow properties (such as mean flow velocity, pressure and temperature) were calculated by using upstream flow condition.

When a particle crosses the axis and leaves the flow field, a new particle with the same axial and azimuthal velocities but reversed radial velocity is being substituted. This new particle has the axial and radial position equal to the final position of the exited particle.

4. COMPUTATIONAL MODELING

Molecular mean free path is defined as the average distance traveled by a molecule before collision (λ). The ratio of λ/L is known as the Knudsen number and is generally used to characterize the degree of rarefaction. The overall Knudsen number is based on some overall dimensions of complete flow; but local Knudsen number is defined using macroscopic gradients as a length scale.

Generally, there are no specific limits for different flow regimes; but based on the overall Knudsen number it is accepted that the continuum assumption is valid for the Knudsen number less than 0.01.

In addition, the flow with the Knudsen number between 0.01 and 0.1 is known as the slip flow regime, and the Knudsen number between 0.1 and 10 is considered as the transitional flow regime. Flow with the Knudsen number greater than 10 is known as the free molecular regime.

The DSMC method is an alternative to conventional CFD technique and is often used at high Knudsen numbers. This method is a probabilistic particle based method that employs a large number of simulated particles with the real physical size and property such that each simulated particle represents a large number of physical molecules or atoms.

The number of simulated particles should be large enough to predict the behavior of real gas molecules and at the same time be small in comparison to the number of real molecules such that each simulated particle indicates a large number of the real molecules. The spatial coordinate, velocity components and internal state of each simulated particle are stored in computer's memory and must be updated with time, as molecule is tracked (taking into account intermolecular collisions and surface interactions in physical space).

The physical space is divided to cells and subcells. Collision is always considered as a three-dimensional event and boundary conditions are satisfied through the incoming or outgoing molecules that cross inflow and outflow boundaries. Therefore, the numerical implementation of the boundary condition has an important role in DSMC method.

The DSMC simulation is based on four basic steps: motion of the simulated molecules, indexing and cross-referencing of particles, simulation of collision and sampling the macroscopic properties of the flow field.

Each simulated particle in the physical domain moves through a distance that is proportional to its velocity vector with time step increment. The linear motion of simulated molecules can be represented by the following equation

$$\boldsymbol{R}^{n+1} = \boldsymbol{R}^{n} + \boldsymbol{V}.\,\Delta\boldsymbol{t} \tag{1}$$

where $\boldsymbol{R}$ is the displacement vector, $\boldsymbol{V}$ is the velocity vector and $\Delta\boldsymbol{t}$ represents time interval for particle movement.

As the simulated molecule traverses linearly the physical domain, collision of particle with another particle, surface geometry or domain boundaries can change the orientation of the simulated molecule or force it to leave the computational domain through the outflow boundaries. Therefore, the boundary conditions must be enforced at this level and the macroscopic properties on the surfaces should be sampled [9].

Two simple models (specular reflection and diffusion models) were proposed by Maxwell [14] for modeling the interaction of stationary equilibrium gas with the solid surface under equilibrium condition. The specular reflection was used in the present work.

The specular reflection is a completely elastic model and assumes that the velocity component of the incident molecules that is normal to the surface reverses its direction without any change in the magnitude; but the velocity component of the incident particle that is parallel to the surface remains fixed in magnitude and direction. Consequently, after the specular reflection, the incident and reflection angles relative to the normal to a surface are equal. In specular reflection, the bulk motion of gas stream is parallel to the surface; therefore, specular reflecting surface functionally is identical to a plane of symmetry [15, 16].

On the duration of DSMC computation, the simulation time step represents the real flow time. Simulation time is divided into small time steps, which must be much smaller than the mean collision time. Throughout these time steps, movement and collision phases of DSMC method are happening

The second step is indexing and tracking the simulated molecules. Since, at the first step molecules have moved and their positions have probably been changed (because of moving, colliding with surface or another molecule); it is necessary to re-index and identify the new location of each molecule. In this step the new cell and subcell of each molecule must be identified; then, the index of molecules and the number of molecules in each cell can be found. This step is a prerequisite for the next two steps.

The third step is simulation of collision by probabilistic process. The probabilistic treatments for collision simulation becomes necessary because the molecular movements decouple from intermolecular collision and a simulated particle represents a portion of real molecules. Typical collision pairs are selected through a probabilistic procedure, which is based on the kinetic theory. There are some models for selecting the collision partners. The collision frequency scheme and the 'time-counter' or TC method [17] are two earlier models. The first one is not efficient regarding the computation time and the second one has a problem for extremely non-equilibrium flows.

Bird [18] recommended a scheme which is known as NTC (no time counter) method. This method overcomes the defects of the two previous methods and can also determine the number of collision partners that participate in collision, before computing collision step. The number of the selected collision partners in each cell during time interval $\Delta\boldsymbol{t}$ is computed as

$$\frac{1}{2} N \overline{N} F_N \left(\sigma_T c_r\right)_{\max} \frac{\Delta t}{V_c} \tag{2}$$

N is the instantaneous number of simulated molecules in each cell and $\overline{N}$ is a time or ensemble averaging of it. Then for each candidate collision pair, a molecule is chosen randomly from the list of molecules in the cell. The probability of collision for collision pairs is given by

$$\frac{\sigma_T c_r}{\left(\sigma_T c_r\right)_{\max}} \tag{3}$$

where σ_T , is the total cross section of collision and c_r, is the relative speed between collision partners.

The parameter $(\sigma_T\, c_r)_{\max}$ should be stored for each cell (this parameter is better to be set initially as a small value) and is being automatically updated if a larger value is obtained for it during sampling. The computational time for this method is linearly proportional to the number of molecules.

For computing collision probability, firstly total collision cross section must be computed. In order to compute this total collision cross section it is necessary to use molecular models. There are some molecular models, each of which has some advantages and disadvantages.

From among these models, Variable Hard Sphere model is used. The variable hard sphere (VHS) model suggested by Bird [19] can define finite total collision cross section and the proper relation between viscosity and temperature. In addition to these advantages of the VHS model, collision mechanisms can be easily calculated because of isotropic scattering assumption in the center mass frame reference. In this model, a molecule has an isotropic scatterings probability and has been considered as a hard sphere with diameter (d) that is a function of relative velocity between molecules (c_r). This function generally, but not necessarily, obeys a simple power law

$$\frac{d}{d_{ref}} = \left(\frac{\sigma_T}{\sigma_{T_{ref}}}\right)^{1/2} = \left(\frac{c_{r_{ref}}}{c_r}\right)^{\upsilon} \tag{4}$$

where, subscript *ref* represents reference values. σ_T, is the total collision cross section. The reference diameter (or VHS diameter) for a particular gas can be defined by the effective diameter at particular reference temperature as

$$d_{VHS} = \left(\frac{\frac{15}{8}\left(\frac{m}{\pi}\right)^{1/2}\left(kT_{ref}\right)^{\omega}}{\Gamma(9/2-\omega)\,\mu_{ref}\; E_t^{\omega-1/2}}\right)^{1/2} \tag{5}$$

where ω is defined as

$$\omega = 1/2 + \upsilon \tag{6}$$

and μ_{ref} is the viscosity at reference temperature, T_{ref}, and E_t is relative translational energy $\left(E_t = \frac{1}{2} m_r\, c_r^2\right)$. The viscosity depends on the temperature through the following relation

$$\frac{\mu}{\mu_{ref}} = \left(\frac{T}{T_{ref}}\right)^{\omega} \tag{7}$$

The basic assumption of DSMC method is that the gas must be simple dilute gas. This means that gas must be composed of a single chemical species and all molecules are assumed to have the same structure and satisfy the condition that $\delta \rangle\rangle\, d$. Where δ is the mean molecular spacing that is equal to inverse of the cube root of number density (The number of gas molecules per unit volume).

Molecular collisions in the DSMC method are considered as a binary elastic collision. In the binary collision, linear momentum and energy must be conserved. By implying conservation of linear momentum and energy, the post collision velocities of molecules can be obtained.

After a certain number of time steps, the flow properties are sampled. Finally, the results are printed after enough time steps. The important approximation of the DSMC simulation is that the molecular

motion and the intermolecular collisions are decoupling over the time interval that should be much smaller than the local mean collision time.

In the present work, a computer code was developed based on the DSMC method for solving the impinging jets on the rarefied conditions. The reflection of gas molecules from solid surfaces is simulated by the specular model. Among the methods for selecting collision pairs, in this study the NTC method and VHS model were used for simulating the molecules collision [9].

5. RESULTS AND DISCUSSION

The developed DSMC code is firstly verified for a single under-expanded argon free jet with the data available from Ref. [4] for Kn = 0.1 and pressure ratio (P_R) of 50. Figure 2 shows that the present results are in good agreement with the results presented in [15].

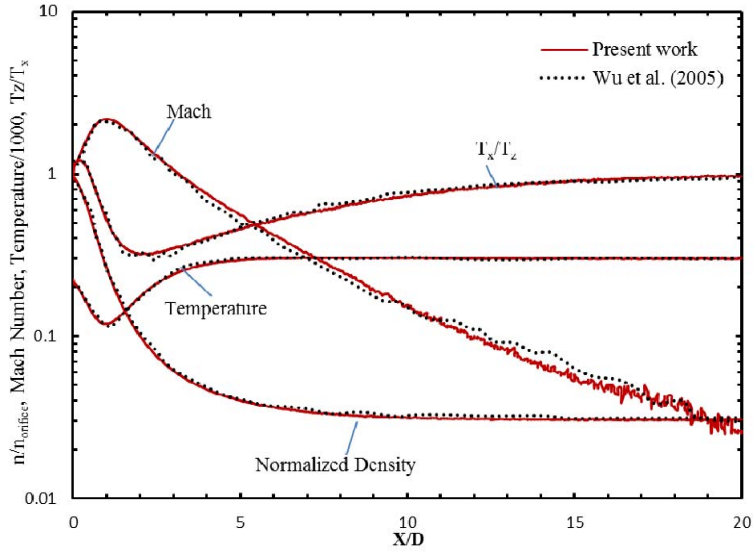


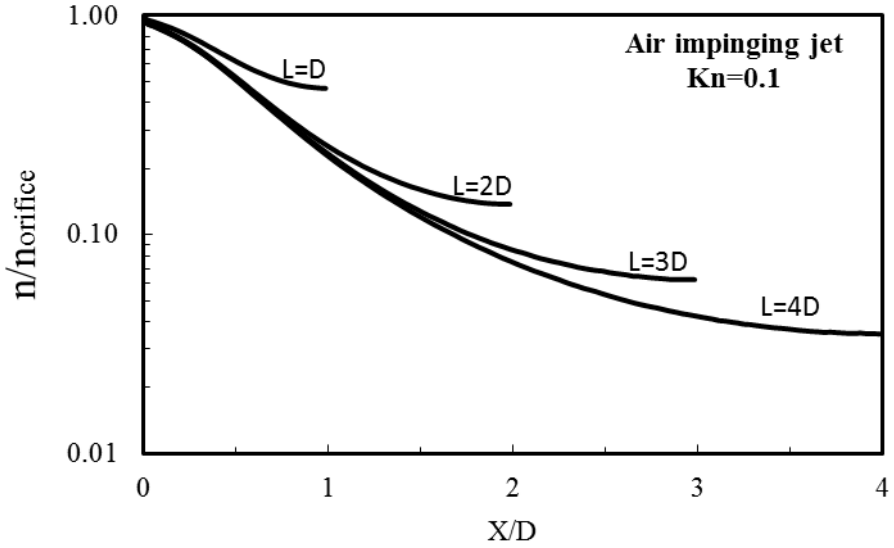
Fig. 2. Centerline properties for Kn=0.1 and P_R=50

The DSMC simulation results of the impinging jet for several L/D ratios and two different values of Knudsen numbers (0.01 and 0.1) are shown in this section.

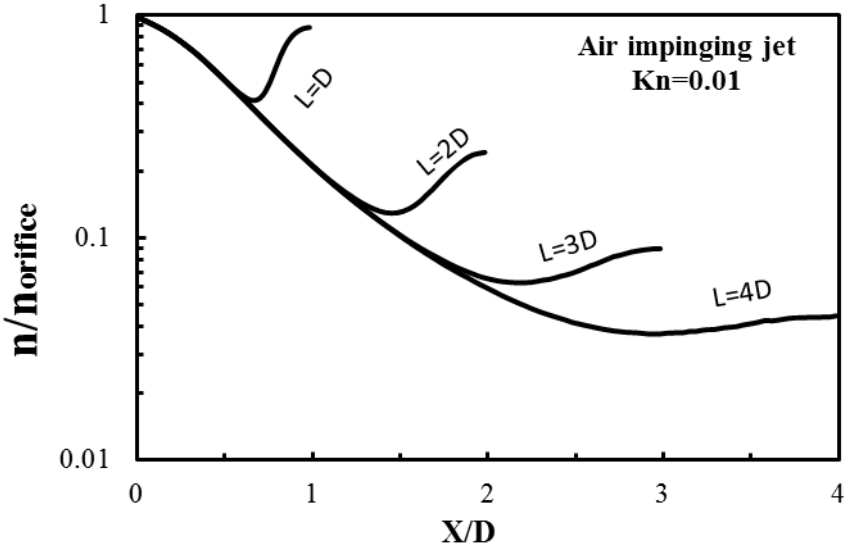
The variation of the ratio of molecular number density to that in the orifice ($n/n_{orifice}$) on the jet centerline is plotted in Fig. 3 for Kn = 0.1 and Kn = 0.01. Results show that for both Knudsen numbers, number density decreases rapidly near the orifice exit due to the rapid expansion of the gas. A slight increase in number density near the impactor plate can be seen due to the deflection of the jet streamlines after impingement on a flat plate.

In addition, for each value of Knudsen numbers a larger nozzle-to-impactor plate distance leads to higher expansion in the jet. The normalized number density at Kn = 0.01 shows a greater decrease compared with that for Kn = 0.1 as a result of rarefaction effect.

Figure 4 shows the effects of the flow regime and L/D ratio on centerline Mach number variation for Kn = 0.1 and Kn = 0.01. These figures illustrate that for both studied Knudson numbers a supersonic jet forms downstream of the nozzle because of the large pressure ratio (P_R) imposed to the jet. Some fluctuations in Mach number distribution are due to the statistical scatter and statistical nature of DSMC method.

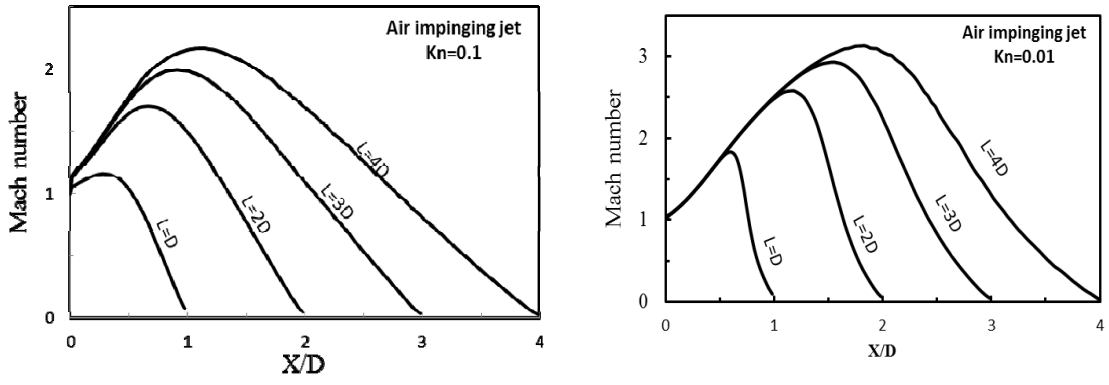


(a)



(b)

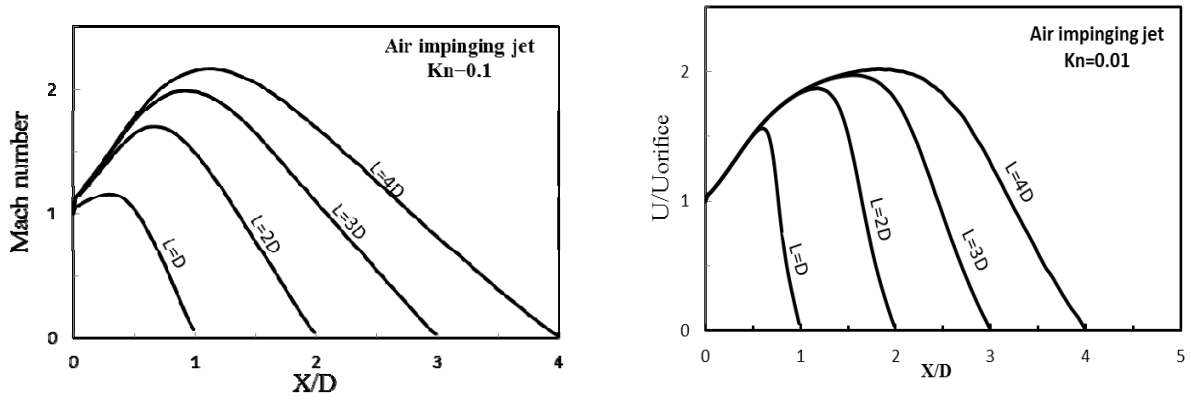
Fig. 3. Variation of number density on the jet centerline with respect to that at the orifice exit for a) Kn = 0.1 and b) Kn = 0.01 at various L/D ratios



(a) (b)

Fig. 4. Variation of Mach number on the jet centerlinefor a) Kn = 0.1 and b) Kn = 0.01 at various L/D ratios

As Fig. 5 shows, the ratio of the centerline axial velocity to that at orifice exit first increases as a result of expansion of the jet and then decreases due to compression of the gas near the impactor plate. Increasing rate of axial velocity is smaller than that of the centerline Mach number because of the dependency of Mach number to temperature.

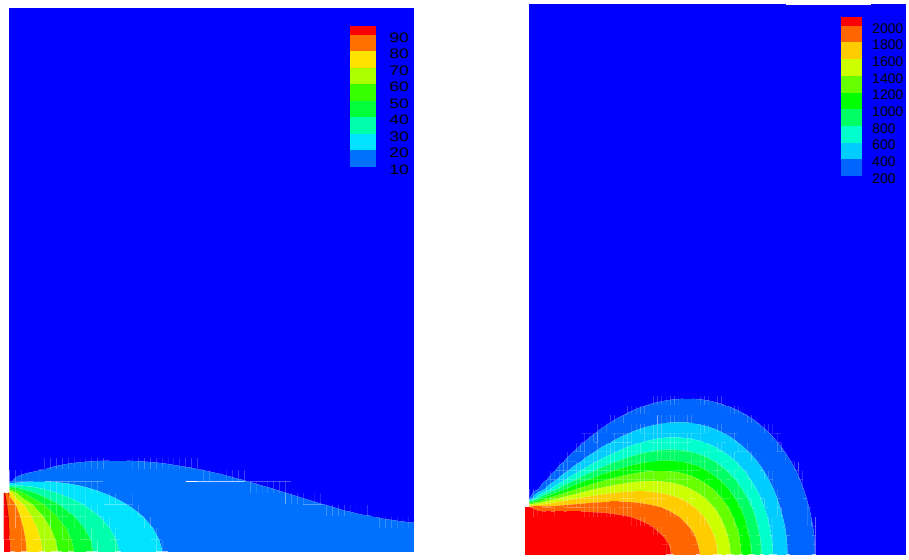


(a) (b)

Fig. 5. Variation of axial velocity on the jet centerline with respect to the inlet axial velocity at the orifice exit for (a) Kn = 0.1 and (b) Kn = 0.01 at various L/D ratios

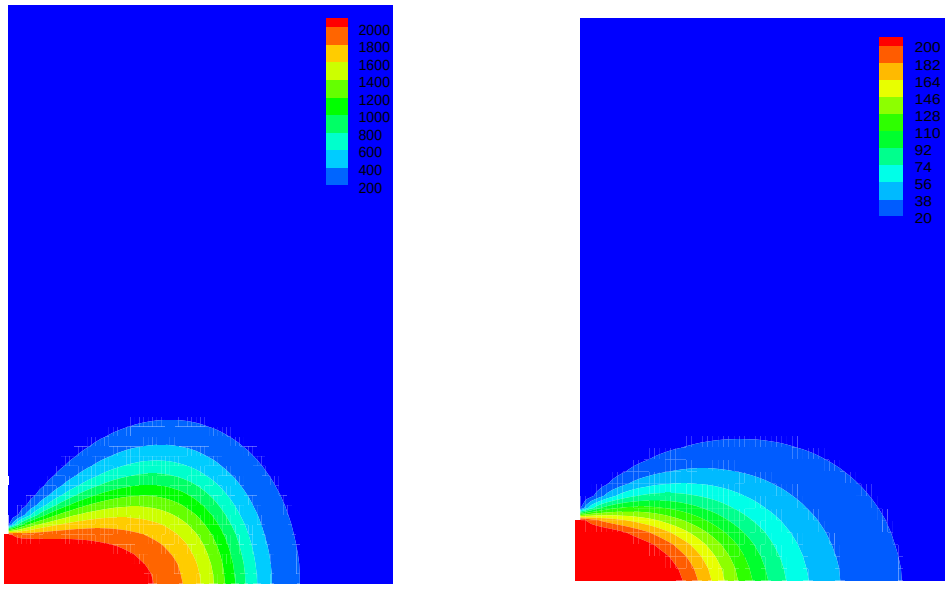
Static pressure contours for Kn = 0.1 and Kn = 0.01 at L/D = 3 are shown in Fig. 6 and total pressure contours of these two cases are presented in Fig. 7. These contours show that pressure decreases slightly without any sudden change. Therefore, there is no shock in the domain.

The supersonic jet expands first near the orifice exit region and then compresses slightly. Therefore, the Mach number increases to a maximum value due to the gas expansion and then smoothly decreases because of the gas compression near the impinging plate. Even though the pressure ratio is the same, the maximum Mach number at Kn = 0.01 is larger than that at Kn = 0.1 for all L/D ratios. In all L/D ratios, the location and the magnitude of the maximum Mach number at the centerline change by the Knudsen number. By increase in the magnitude of the L/D, the maximum Mach number increases due to a higher expansion in the jet.



(a) (b)

Fig. 6. Static pressure (Pa) contour for (a) Kn = 0.1 and (b) Kn = 0.01 at L=3D



(a) (b)

Fig. 7. Total Pressure (Pa) contour for (a) Kn = 0.1 and (b) Kn = 0.01 at L=3D

In general, based on the above results the gas expands shock free in the flow field for both Kn = 0.1 and Kn = 0.01 and all L/D ratios. We expect the shock free flow field in the flow condition with Kn = 0.1 as a result of rarefaction; but no appearance of a bow shock in front of the impactor plate (as is usual for supersonic impactors [1-3,13]) in the flow condition of Kn = 0.01 is noticeable. By increasing the L/D ratio a bow shock may appear as a result of a stronger hypersonic expanded jet downstream of the nozzle which needs further research.

6. CONCLUSION

A DSMC computer code was developed and employed to simulate the axisymmetric flow field of the impinging jets in the slip flow regime. Air continues to expand rapidly in the short axial distance after exiting from the orifice exit and then compressed slowly near the impactor plate except for the case of L = D at the Kn = 0.1 where the gas expansion is slow.

Numerical results of the DSMC code show that there is no shock in this regime for the studied pressure ratio and L/D ratios. This is due to the rarefaction effect and the rather low background pressure for the Kn = 0.1and Kn = 0.01.

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