

DSMC Simulation of Rarefied Gas Flow over a Backward-Facing Step: Effect of Expansion ratio

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ABSTRACT

Numerical simulations have been performed to study the effect of expansion ratio on the hypersonic rarefied flow past a backward-facing step. The Direct Simulation Monte Carlo (DSMC) method is used for the present study. An opensource solver named dsmcFoam has been used for this purpose. The solver has been validated with well-established results from the literature and good agreement is found among them. Simulations have been carried out for expansion ratios (ER) of 2,4,6,8,10 in the transition regime. The different flow field properties such as velocity, pressure and temperature have been studied. The profiles have found to be influenced by the compressibility and rarefaction effects. Limiting case of ER=8 and above has no influence on the flow field properties.

Keywords: *Discrete methods; DSMC; Kinetic Theory; Knudsen number; Rarefied gas flows; Backward-facing step.*

NOMENCLATURE

Kn	Knudsen Number
L	Characteristic length [m]
Ma	Mach Number
R	Gas constant [J/mol. K]
Re	Reynolds Number
X	Mole fraction
c	Molecular velocity [m/s]
d	Particle diameter [m]
f	Velocity distribution function
m	Molecular mass [kg]
n	Number density [m ³]

r	Relative molecular speed [m/s]
σ	Collision cross section [m ²]
Ω	Solid angle [sr]
ω	Viscosity index
ρ_{∞}	Density [kg/m ³]
μ_{∞}	Viscosity [N.s/m ²]
p_{∞}	Pressure [N/m ²]
λ_{∞}	Mean free path [m]
T_{∞}	Temperature [K]
P_0	Reference Pressure [N/m ²]

INTRODUCTION

Development of vehicles for outer space technology involving re-entry type, exploratory type, interplanetary type of vehicles, etc. demands momentous research in gas dynamics in the rarefied regimes. These vehicles operate in the high and sparse atmosphere at very high (often hypersonic) speeds and are quite often designed with contour disruptions, such as steps, gaps or cavities. Although a smooth aerodynamic shape of the surface is preferable, the presence of these discontinuities in advanced aerodynamic configurations might occur as either a desired or undesired design. The Knudsen number (Kn) is used to determine the degree of rarefaction of the gas.

$$Kn = \frac{\lambda}{L} \quad (1)$$

where, λ is the mean free path of the gas molecule, L is the characteristic dimension of the problem under consideration. Based on the Kn , the flows are classified into various regimes as given in the Table 1.

Table.1. Kn number regimes, adapted from Ref.[1].

Kn Range	Type of Flow	Suitable Numerical Approach
$Kn \rightarrow 0$	Inviscid flow	Euler fluid equations
$Kn \leq 0.001$	Continuum regime	Navier–Stokes–Fourier fluid equations
$0.001 \leq Kn \leq 0.1$	Slip regime	Navier–Stokes–Fourier fluid equations with modified boundary conditions
$0.1 \leq Kn \leq 10$	Transition regime	Boltzmann equation or DSMC
$Kn \geq 10$	Free-molecular regime	Boltzmann equation or DSMC

The Backward-facing step (BFS) is a interesting flow configuration due to its separation and reattachment of flow over the step. A varied number of studies have been conducted on the phenomenon of flow separation and reattachment over BFS configuration. The studies regarding the effect of aspect ratio [2], Prandtl Number [3], Reynold's Number [4] and step height [5] have been documented using numerical and analytical methods for 3D and 2D flows to further our understanding of the BFS system. For the purpose of this introduction, it will be sufficient to describe only a few of these studies:

Charawat et al.[6] is a study aimed at finding the distance at which flow impinges after being separated from an isolated backward-facing-step. His study concluded that the flow impinges onto the wall at approximately seven times the step height downstream for a laminar step boundary condition. For a turbulent boundary condition, the distance becomes five times the step height downstream. Rom and Seginer [7] studied rate of heat transfer for a 2D laminar supersonic backward-facing-step flow corresponding to a Reynolds number in the range of 103-105 and a Mach number in the range 1.5-2.5. The results were indicative of the fact that the rates of heat-transfer changed with a change in the distance behind the step. Also, the rate of heat transfer was found to be dependent on the ratio of boundary-layer thickness at the separation to the step height. The computational and experimental results of a high enthalpy flow over a blunted and stepped cone configuration was also studied by Gai and Milthorpe [8]. They used an axisymmetric backward-facing step of 3mm - 6mm in height located 101mm from the nose of the blunted-stepped cone. The results indicated that the heat transfer rate was as expected as in the case of separated flow. A drastic fall in heat transfer near the step and a gradual increase beyond it was observed. The conclusion drawn from the experimental data was that the heat transfer rate decreases after flow reattachment. Laminar flow over forward facing and backward facing step at hypersonic speeds was studied by Grotowsky and Ballmann [9] employing Navier-Stokes Equations. The simulation was done with Mach number (Ma) of 8, Reynolds number (Re) approximately 108 and altitude of 30km under consideration. According to the authors,

the computational results complied with experimental data available in the literature. Significant differences were observed in the wall heat flux, whose probable cause was the inherent difficulty in measuring it accurately. The studies on the flow past BFS have mostly been focused in the continuum regime with very few studies being reported in other regimes. Also, the effect of the Expansion ratio (ER) which is the ratio of the channel height to step height, on the flow properties is very limited. Therefore, the purpose of the present study is to evaluate the effect of expansion ratio on the hypersonic flow past backward-facing step in the transition regime. The study is carried out using the Direct Simulation Monte Carlo method using an opensource solver dsmcFoam [10] under the framework of OpenFOAM.

DSMC METHOD:

The Direct Simulation Monte Carlo (DSMC) method, established by G.A. Bird [11] is one of the most accurate numerical techniques for capturing the flow physics with significant rarefaction effects. This method has been successfully implemented in various flow regimes over the past few decades and has been validated with the experimental results. The DSMC method is based on Boltzmann's Equation employed with certain restrictions. As known, the density of air decreases gradually as altitude increases, and the rarefaction effects become more evident near outer space as the flow changes from near continuum to free molecular regime. As the degree of rarefaction rises, the continuum solvers which use Navier-Stokes equations lose their credibility [12], whereas the Boltzmann equation can aptly describe the behavior of gas flow at every degree of rarefaction [12]. The Boltzmann equation is given as [13], [14]:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{Kn} Q(f, f), \quad x \in \mathbb{R}^{dx}, v \in \mathbb{R}^{dv} \quad (2)$$

where $f(t, x, v)$ denotes the density distribution function of a dilute gas at a position x , velocity v and at time t . Kn represents the Knudsen number of the flow and the collision operator $Q(f, f)$ represents the binary collisions.

The Boltzmann equation can be solved by probabilistic schemes, also known as DSMC. The DSMC method was first proposed by G A Bird[11] and is a microscopic method based on particle collisions that, in the limit of infinite simulated particles, reduces to the Boltzmann equation [13]. The properties of the gas, such as temperature, velocity, shear stress, density, pressure, heat flux, and so on, are obtained by appropriately sampling the microscopic properties of simulated particles. The steps involved in the DSMC method are explained below: (1) Reading the grid data and define the initial and boundary conditions; (2) Calculating the number of DSMC molecules and initializing them in the domain; (3) Modeling the interaction of DSMC molecules with the boundaries; (4)Indexing the simulated DSMC molecules; (5) Using the probabilistic sampling to model the collision of the simulated DSMC molecules (6) Sampling the flow field and repeat the steps 3-6; (7) Output the sampled flow field variables.

COMPUTATIONAL METHODOLOGY

Geometry:

Figure 1 shows a schematic of the computational domain considered for simulating the flow. Here, ‘ h ’ is the step height, and ‘ L ’ is the total length of the flow domain. The step height considered was 3mm. The step is located at a distance of 50λ from the leading edge. The flow domain further extends to 150λ downstream of the step, where λ denotes the mean free path. Owing to computational difficulty, only the 2D flow was considered in the present study.

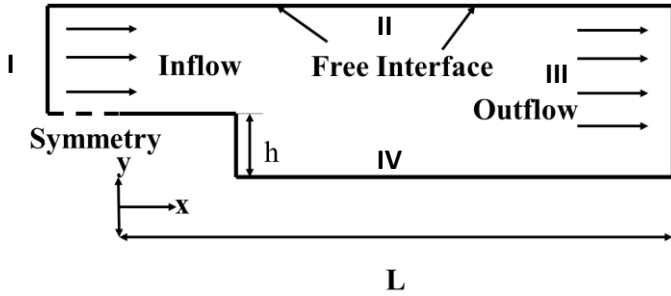


Figure 1. Geometry of the 2D Backward-facing step.

As shown in Figure 1, Side-I represents the Inlet boundary, from where the DSMC molecules can enter, Side-II represents free interface. Side-IV represents BFS with no-slip boundaries, diffuse reflection, and full thermal accommodation. Side-III is the outlet boundary.

Computational grid:

The DSMC method has been used in the present study, which is one of the widely used methods for the simulation of rarefied gas flows. Variable Hard Sphere (VHS) [15] model with No Time Counter (NTC) scheme [16] is used to model the molecular collisions. Larsen-Borgnakke statistical model is used to account for the kinetic and internal modes of energy exchange. The factors mainly affecting the DSMC method are the cell size, time-step and the number of particles per cell. The cell size should be smaller than the mean free path [17], and the time-step should be smaller than mean collision time [18] and in general, there should at least 20-30 particles per cell. Grid independence was tested using three grids viz, coarse, standard and fine in which the coarse grid had 50% fewer cells compared to standard, and fine grid had 50% more cells than the standard grid. The solution obtained (not shown) for all the three grids were nearly identical. Hence a structured grid consisting of around 2,00,000 cells shown in Figure 2 was used.

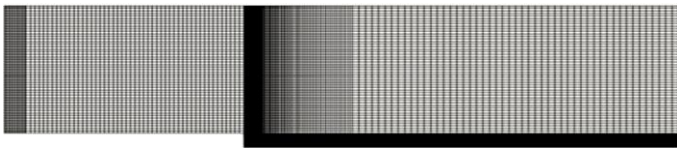


Figure 2. Computational 2D grid used for the present study.

Free stream conditions:

The fluid considered was air which is assumed to be non-reacting and comprised of 76.3% N_2 and 23.7% of O_2 .

Table.2. Free stream Conditions.

T_∞ (K)	p_∞ (N/m ²)	ρ_∞ (kg/m ³)	μ_∞ (Ns/m ²)	λ_∞ (m)	n_∞ (m ³)
219.69	5.582	8.753×10^{-5}	1.455×10^{-5}	9.03×10^{-4}	1.81×10^{21}

Freestream conditions employed are tabulated in Table 2 in which, T_∞ , p_∞ , ρ_∞ , μ_∞ , λ_∞ , n_∞ depict respectively temperature, pressure, density, viscosity, mean free path and number density respectively. The freestream Mach number used for the study was 25 which represents the hypersonic range. The corresponding flow velocities for the above Mach number was 7560 m/s. The wall temperature of the BFS was assumed to be 880K and is considered uniform throughout the wall.

Validation:

The validation dsmcFoam solver is done by comparing results of Leite et al.[19] for flow over BFS. Figure 3 and 4 show the tangential velocity ($\frac{u}{U_\infty}$) distribution along the upper surface of BFS which is normalized by step height at two different positions (a) $X=10$ (b) $X=51$, where X represents the distance x normalized by the freestream mean free path (λ). Our results match well with those of Leite et al.[19]. The close agreement validates the dsmcFoam solver.

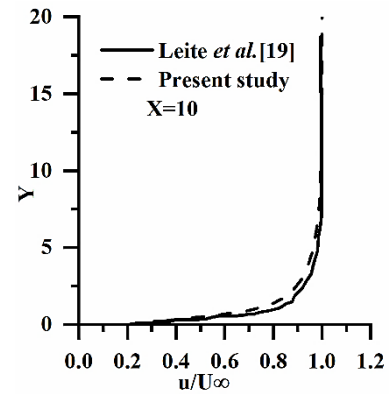


Figure 3. Streamwise velocity ($\frac{u}{U_\infty}$) distribution perpendicular to the surface of BFS for $X=10$.

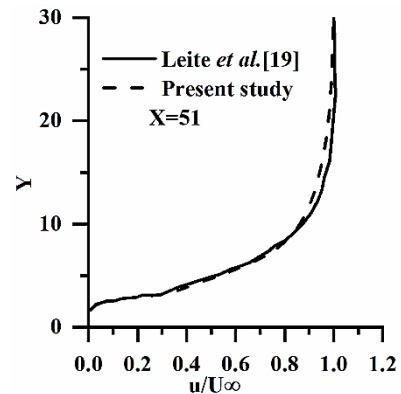


Figure 4. Streamwise velocity ($\frac{u}{U_\infty}$) distribution perpendicular to the surface of BFS for $X=51$.

RESULTS AND DISCUSSIONS

In this section, flow field properties for different expansion ratios (ER=2,4,6,8,10) are compared. The flow field properties such as velocity field, pressure field, and temperature field are also evaluated at different longitudinal locations. (shown in mm).

Velocity Field:

From the velocity contours in figures (5-7) it is observed that the low velocity is found close to the wall, with increasing velocity away from the wall. For ER=2, we see that the flow profile is highly influenced due to the presence of the top boundary. As the expansion ratio increases the development of hydrodynamic boundary layer is less restrained. From the figure (7) it can be observed that for an ER of 10, the presence of the top boundary has no effect on the flow properties.

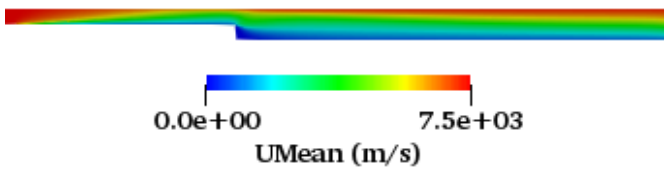


Figure 5. Velocity contour for ER=2.

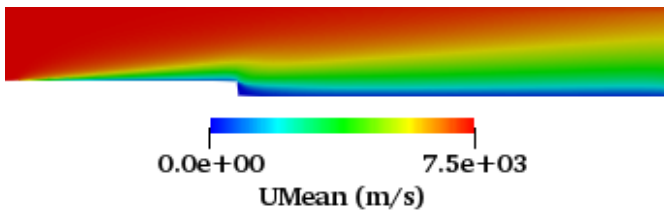


Figure 6. Velocity contour for ER=6.

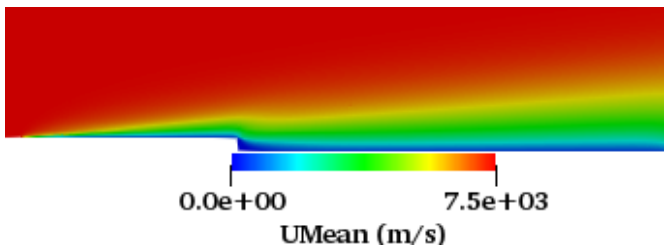


Figure 7. Velocity contour for ER=10.

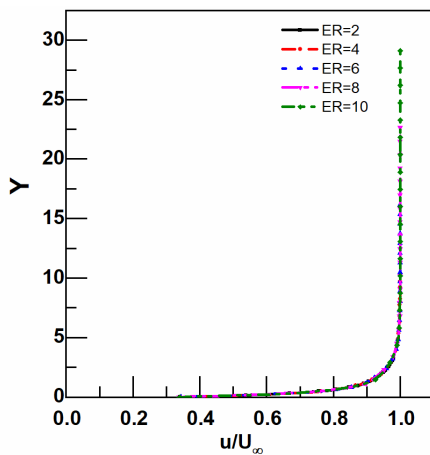


Figure 8. Streamwise velocity ($\frac{u}{U_\infty}$) distribution perpendicular to the surface of BFS for $X=10$.

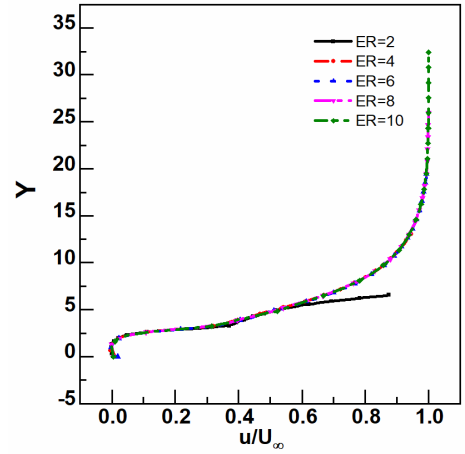


Figure 9. Streamwise velocity ($\frac{u}{U_\infty}$) distribution perpendicular to the surface of BFS for $X=51$.

The distribution of streamwise velocity ($\frac{u}{U_\infty}$) for different ER at two different longitudinal locations $X=10$ and $X=51$ is shown in figures 8 and 9. Here Y represents the distance y normalized by mean free path λ . It can be seen that the profiles overlap for different ER at $X=10$ whereas minor variation can be observed at $X=51$ due to the reduced area available for the flow.

Pressure Field:

From the pressure contours in figures (10-12) variations in pressure along the flow direction is similar for all ER larger than 2. The pressure changes in the transverse direction are more pronounced in the vicinity of the step, with regions of higher pressure near the walls and pressure reducing sharply away from the wall. The sudden increase in the flow cross-section near the step results in the formation of low-pressure region and hence resulting in a recirculation region.

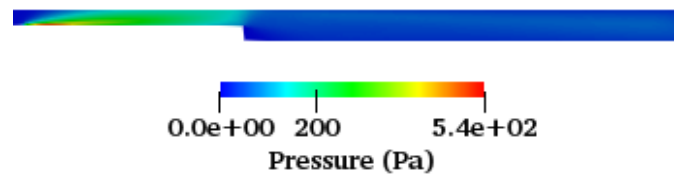


Figure 10. Pressure contour for ER=2.

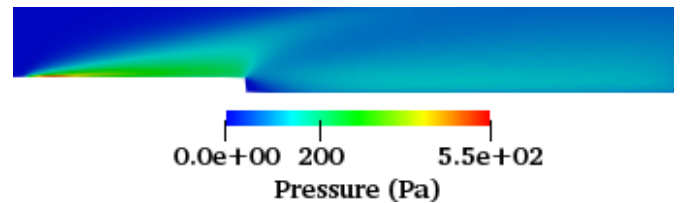


Figure 11. Pressure contour for ER=6.

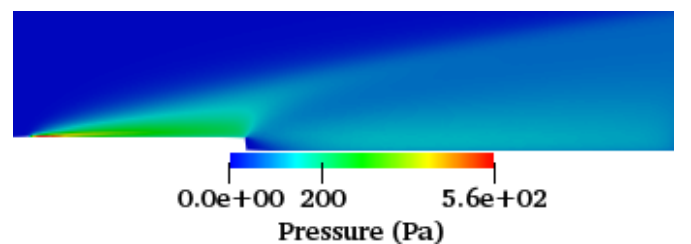


Figure 12. Pressure contour for ER=10.

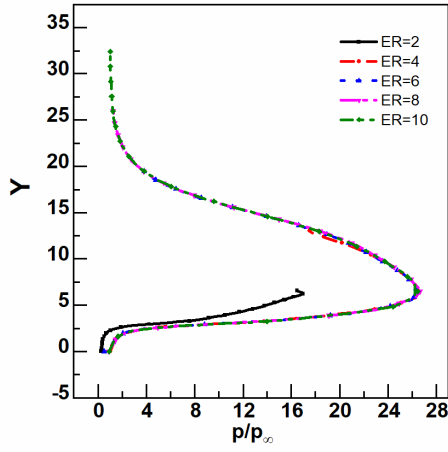


Figure 13. Pressure ratio $\left(\frac{p}{p_\infty}\right)$ distribution perpendicular to the surface of BFS for $X=10$.

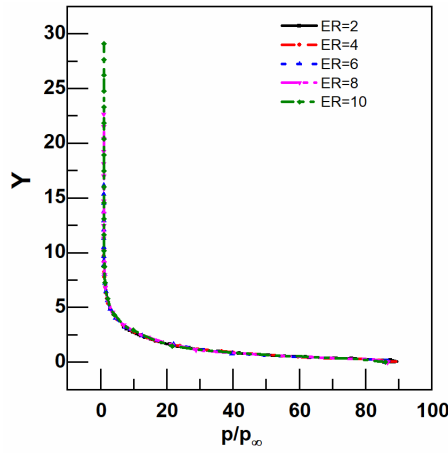


Figure 14. Pressure ratio $\left(\frac{p}{p_\infty}\right)$ distribution perpendicular to the surface of BFS for $X=51$.

The distribution of pressure ratio for different ER at two different longitudinal locations $X=10$ and $X=51$ is shown in figures 13 and 14. Here Y represents the distance y normalized by mean free path λ . At $X=10$, for different ER, $\left(\frac{p}{p_\infty}\right)$ changes by an order of magnitude. At $X=51$, the profiles for different ER overlap and vary by two orders of magnitude.

Temperature Field:

From the temperature contours in figures (15-17) it is observed that wall temperatures are of the order of 10^4 , which is much higher than the imposed wall temperature. The near wall temperatures are of higher magnitude due to the viscous dissipation effects of the hypersonic flow.

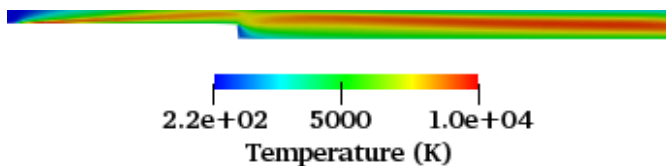


Figure 15. Temperature contour for ER=2.

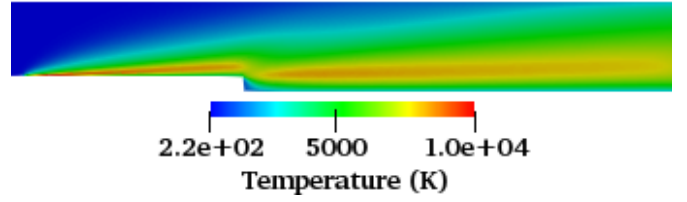


Figure 16. Temperature contour for ER=6.

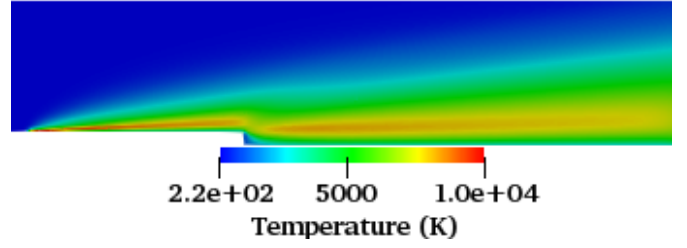


Figure 17. Temperature contour for ER=10.

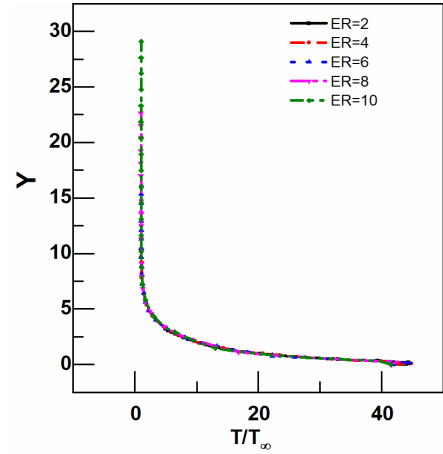


Figure 18. Temperature ratio $\left(\frac{T}{T_\infty}\right)$ distribution perpendicular to the surface of BFS for $X=10$.

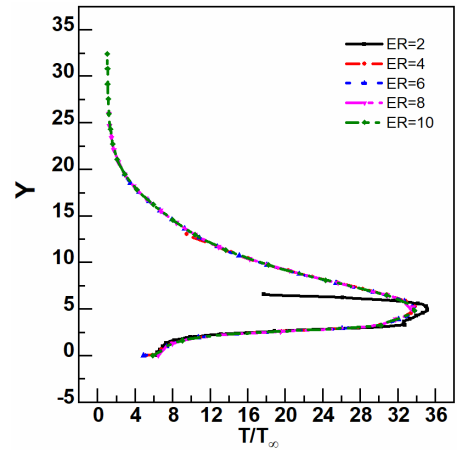


Figure 19. Temperature ratio $\left(\frac{T}{T_\infty}\right)$ distribution perpendicular to the surface of BFS for $X=51$.

The distribution of temperature ratio $\left(\frac{T}{T_\infty}\right)$ for different ER at two different longitudinal locations $X=10$ and $X=51$ is shown in figures 18 and 19. Here Y represents the distance y normalized by mean free path λ . The profiles of different ER overlap at $X=10$ whereas considerable variation is found at $X=51$ due to the higher rate of viscous dissipation.

Conclusions

In the present study, rarefied hypersonic flow over BFS for different expansion ratios was investigated using the DSMC method. Velocity, pressure and temperature profiles were studied. Through simulations, following major findings came out:

- The variation of flow properties for $ER=2$ are very different from those at higher ER as the geometry is very constricted by the presence of top boundary.
- $ER=8$ and above has no influence on the flow field properties for a step height of 3mm even at the outlet.
- The velocity profile resembles the Blasius profile with non-zero velocity at the wall and with the formation of recirculation just after the step.
- The pressure and temperature profiles follow a similar trend with higher magnitude of pressure and temperature near the walls.
- The hydrodynamic and thermal boundary layer development is similar for different expansion ratios.

Findings from present simulations can be used for better understanding of the physics involving rarefied hypersonic flows in the transition and free molecular regimes.

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