Investigation of Subsonic and Hypersonic Rarefied Gas Flow over a Backward Facing Step

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Abstract. In the present study the Direct Simulation Monte Carlo (DSMC) method, which is one of the widely used numerical method to study the rarefied gas flows, is applied to investigate the flow characteristics of a hypersonic and subsonic flow over a backward-facing step. The work is driven by the interest in exploring the effects of the Mach number on the rarefied flow behaviour. The primary objective of this paper is to study the variation of velocity, pressure and temperature with Mach number. The numerical tool is validated with well established results from the literature and a good agreement is found among them. The computational results indicate that the flow downstream of the step is effected by the strong expansion near the step. The compressibility and rarefaction effects also influence the velocity and temperature distributions in the hydrodynamic and thermal boundary layers.

1. Introduction

The flow over a backward-facing step (BFS) is one of the most basic geometrical features which illustrates the effect of sudden expansion resulting in flow separation and reattachment. The flows involving separation and reattachment play a vital role in many engineering applications such as combustors, diffusers, turbine cooling and also in external flows such as flow around buildings, aircrafts [1]. There have been numerous research studies on the separation and reattachment of the flow over BFS using experimental and numerical methods. They have helped in the better understanding of the effect of Reynolds number [2], step height [3], aspect ratio [4], on the flow characteristics of the BFS configuration. The hypersonic flow past a BFS is characterized by a recirculation region in the vicinity of the step, and the low velocity in the recirculation region is expected.

Many experimental and theoretical works have been performed to understand the flow features involving a hypersonic flow past a BFS of which, only a few critical studies have been summarized below.

Experimental investigations on the effect of heat transfer rate on a 2-D backward-facing step in a laminar supersonic flow were conducted by Rom and Seigner [5]. The Reynolds number and the Mach number for the flow were in the range of $10^3$ to $10^5$ and 1.5 to 2.5 respectively. The results indicated that the heat transfer varied with the distance behind the step. Furthermore, it was found that the ratio of boundary layer thickness at separation to the step height influenced the heat transfer rates.

Results obtained by Charawat et al. [6] show that the separated flow past a BFS reattaches on the wall approximately at a distance of seven times the step height for laminar boundary layer and approximately a distance of five times the step height for turbulent boundary layer, downstream of the step.
Experimental and computational results of a high enthalpy flow over a blunted stepped cone were presented by Gai et al. [7]. The geometry was a BFS of height 0.15 to 0.3 times the nose radius of the blunted stepped cone. Their results indicated that the heat transfer rates experienced a fall near the vicinity of the step and then they gradually increased. The experimental results showed a reduction in the heat transfer rates after the flow reattachment, whereas the computational results showed constant heat transfer rates for a significant distance after the reattachment.

Grotowsky and Ballmann [8] studied laminar hypersonic flow over a backward-facing step and forward-facing step in the continuum regime. The flow parameters considered for the study were Reynolds number of the order of $10^6$, altitude of 30 km and the Mach number of the flow of the order of 8. Their computational results were in good agreement with the experimental results available in the literature except the wall heat flux, possibly due to difficulty in accurately measuring the same.

Most of the investigations in the literature have been focused on the study of hypersonic flow past a BFS in the continuum regime and the effects of laminar and turbulent flow on the flow features. There is limited literature with regard to the flow past BFS in other regimes. Therefore, the purpose of the present paper is to investigate the subsonic and hypersonic flow past a backward-facing step in the transitional and free molecular regimes. The Direct Simulation Monte Carlo (DSMC) method is used to understand the flow physics for a two-dimensional flow over a backward-facing step. A C++ code-based solver known as dsmeFoam [9], based on the framework of OpenFOAM will be used to perform the computational analysis.

2. Direct Simulation Monte Carlo (DSMC) Method

The Direct Simulation Monte Carlo (DSMC) method, established by G.A. Bird [10] is one of the most accurate numerical technique for capturing the flow physics where the rarefaction effects are significant. The method has been successfully implemented in various flow regimes over the past few decades, and has been validated well with the experimental results. The DSMC method is based on the Boltzmann’s Equation [11] with certain restrictions.

$$\frac{\partial n_f}{\partial t} + c \cdot \frac{\partial n_f}{\partial r} + F \cdot \frac{\partial n_f}{\partial c} = \int_{-\infty}^{\infty} \int_0^{4\pi} n^2 (f^* f_1^* - f f_1) c_r \sigma d\Omega \, dc_1$$  \hspace{1cm} (1)

Equation 1 is an integrodifferential equation in $n_f$, the product of the number density $n$ and the velocity distribution function $f$. In this equation, $c$ is the molecular velocity, $c_r$ is the relative molecular speed, $F$ is an external force, the superscript $^*$ indicates post-collision values, $f$ and $f_1$ correspond to two different types of molecules, $\sigma$ is the collision cross-section, and $\Omega$ is the solid angle. The right side of the equation is the collision integral, which is the source of problem in finding the solution. In the DSMC method, the flow is modeled as a conglomeration of molecules. Each simulated molecule has a position, velocity and internal energy. The simulated molecules represent a fixed number of actual molecules. The properties of the simulated molecules are stored in the computer memory and are indexed with time as the flow progresses.

The steps involved in the DSMC method are briefly explained below: 1. Read the grid data and define the initial and boundary conditions; 2. Calculate the number of DSMC molecules and initialize them in the domain; 3. Model the interaction of DSMC molecules with the boundaries; 4. Index the simulated DSMC molecules; 5. Use the probabilistic sampling to model the collision of the simulated DSMC molecules by; 6. Sample the flow field and repeat the steps 3-6; 7. Output the sampled flow field variables.

Over the past few years, DSMC method has been used for the simulation of rarefied gas flows. One major drawback of the DSMC method is that it is computationally intensive and was the primary reason for the limited use of the method. The DSMC computations can be made efficient by parallelization, and the same has been implemented in dsmeFoam using OpenMPI.
3. Geometry

Figure 1 shows 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 50\(\lambda\) from the leading edge. The flow domain further extends to 150\(\lambda\) downstream of the step, where \(\lambda\) denotes the mean free path. Owing to computational difficulty only the 2D flow was considered in the present study.

![Figure 1. Schematic diagram of the Backward-facing step](image1)

For the numerical simulation of the problem, the flow field around the BFS is divided into several blocks, which in turn are divided into many cells. The cells provide the reference for selection of collision partners and the sampling of microscopic properties. The computational domain considered is large enough that the boundary effects are not felt in the vicinity of the step.

As shown in the Figure 1, Side-I represents the Inflow boundary, Side-II represents the free stream interface from where the DSMC molecules can enter and exit. Side-IV represents the backward-facing step modelled with no-slip boundaries, diffuse reflection and full thermal accommodation. In the diffuse reflection model, the impinging molecules are equally reflected in all the directions. Side-V is the plane of symmetry, in which the normal flow gradients are zero. Side-III is the outflow boundary from where the DSMC molecules can only exit.

![Figure 2. Computational 2D grid used for the present study](image2)
4. Computational Methodology and Procedure

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) [12] model with No Time Counter (NTC) scheme [13] 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 [14], and the time-step should be smaller than mean collision time [15] and in general, there should at least 20-30 particles per cell. All the above guidelines were accounted for in the present study. 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. Solution obtained for all the three grids were nearly identical. Hence a structured grid consisting of around 200,000 cells was used as shown in figure 2. The grid was refined close to the walls to capture the effects of boundary layer formation.

5. Free Stream Conditions

We consider the flow of air which is assumed to be non-reacting and comprised of 76.3% N₂ and 23.7% of O₂. Freestream conditions employed are tabulated in Table 1.

| T∞(K) | p∞(N/m²) | ρ∞(kg/m³) | μ∞(Ns/m²) | λ∞(m) | n∞(m³) |
|-------|-----------|------------|------------|--------|---------|
| 219.69 | 5.582 | 8.753 x 10⁻⁵ | 1.455 x 10⁻⁵ | 9.03 x 10⁻⁴ | 1.81 x 10²¹ |

In the Table 1, 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 and 0.5 which represents the hypersonic and subsonic range. The corresponding flow velocities for the above Mach numbers were 7456 m/s and 150 m/s respectively. The wall temperature of the BFS was assumed to be 880K and is considered uniform throughout the wall.

The step height was fixed to be 3mm, and the flow was simulated for Knudsen number of Kn=0.3 which represents the transition regime.

6. Validation

The *dsmcFoam* solver is used to compute the flow over a BFS in the transition regime. Well-established results computed by Leite et al.[16] exist for the same problem which is used for validation of the present code. Figure 3 shows the tangential velocity u/ U∞ 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.[16]. The close agreement validates the *dsmcFoam* solver. The velocity streamlines shown in the figure 4 also agree well with the published results.

The near-wall velocity profiles in figure 3 show that u/ U∞ is non zero, which is a peculiarity of rarefied gas flows. Therefore the condition of no-slip velocity which is applicable for the flows in the continuum regime is not applicable in the transition regime.

The streamlines shown in figure 4 depicts the flow separation and recirculation near the step followed by reattachment downstream of the step.
Figure 3. Variation of streamwise velocity ($u/U_\infty$) distribution perpendicular to the surface of BFS for (a) $X=10$ (b) $X=51$. The vertical distance is normalised by the step height ($h$).

Figure 4. Velocity streamlines for a step height ($h$) of 3mm (a) Leite et al (b) Present study.

7. Results and Discussion

7.1. Rarefied Subsonic Flow ($Ma=0.5$)

In the first part of the study, the flow was considered to be subsonic with a Mach number of 0.5 in which the freestream velocity was close to 150m/s. The corresponding velocity, pressure and temperature contours are shown in the figures below.

From the velocity contour in figure 5(a), it can be observed that the velocity is less close to the wall and increases in the y direction due to the development of hydrodynamic boundary layer. This trend is similar to the boundary layer profile observed in the continuum regime, except that the flow velocity is non-zero at the wall. This is one peculiarity found in the transition regime which deviates from zero wall velocity found in the continuum regime.

From the pressure contour in figure 5(b), we see that the pressure distribution is uniform throughout the length of BFS with high pressure at the inlet and gradually reducing towards the outlet. The pressure distribution is unaffected in the y direction and the effect of the step is found to be minimal. This distribution resembles that of a pipe flow where pressure varies only with the downstream location.
From the temperature contour in figure 5(c), it can be noted that the temperature close to the wall is more and it diminishes away from the wall owing to the development of the thermal boundary layer. The presence of step leads to sudden expansion of the flow and the thickness of the thermal boundary layer remains almost uniform thereafter.

7.2. Rarefied Hypersonic Flow (Ma=25)

In the second part of the study, the flow was considered to be hypersonic having a Mach number of 25 in which the freestream velocity was 7456 m/s. The hypersonic flow features were analysed by plotting the velocity, pressure and temperature contours as shown in the figures below.

From the velocity contour in figure 5(d), it can be observed that the velocity profile resembles the laminar boundary layer profile for flow over a flat plate in the continuum regime. Compared to the subsonic flow, the boundary layer thickness in the hypersonic flow is less. This also follows the trend predicted by the boundary layer theory, where the boundary layer thickness is inversely proportional to the square root of the Reynolds number. A recirculation region is also observed near the vicinity of the step due to flow expansion and the flow reattaches downstream of the step.

From the pressure contour in figure 5(e) we see that the pressure distribution is non-uniform with higher pressure near the walls and it gradually reduces towards the outlet. Low pressure is observed near the step due to sudden expansion of the flow owing to the nature of the geometry. It can also be observed that there are pressure changes within the boundary layer which might possibly be due to the compressibility and rarefaction effects. Since the pressure depends strongly on the distance from the obstacle (BFS), these contours resemble those of flow over a flat plate and are in sharp contrast with those of subsonic flow.

Figure 5. (a) Velocity, (b) Pressure, and (c) Temperature contours for Subsonic flow (Ma=0.5) (d) Velocity, (e) Pressure, and (f) Temperature contours for Hypersonic flow (Ma=25)
The temperature distribution in figure 5(f) shows that near wall temperatures are higher by an order of magnitude, of $10^4$, which agree with the estimates of the compressible flows. Shear effects downstream of the step also seem to have an augmenting effect on the magnitude of temperature. The variation of temperature in the vicinity of the recirculation zone is due to competing factors like viscous dissipation and expansion cooling.

Figure 6 shows the distribution of streamwise velocity ($u/U_\infty$) profiles at different locations. Here X represents the distance $x$ normalised by the mean free path. It can be seen that there is a definite amount of slip for both Mach numbers. Thickness of the boundary layer for $Ma=25$ case is smaller compared to the $Ma=0.5$ case at all the locations after $X=10$. This dependence of boundary layer thickness on flow speed is similar to that predicted by the traditional fluid mechanics, where the boundary layer thickness decreases as Reynolds number of the flow increases. From Fig 6 (c) it can be seen that the ratio of streamwise velocity distribution is negative for $Ma=25$, which indicates a recirculation region being generated right after the step. The flow velocity is much smaller for $Ma=0.5$ case in the near wall region, which contributes to a large statistical noise. Also, the sudden change in the flow direction seen from the graph occurs within one grid point. Therefore, the recirculation seen from the graph for this case is not conclusive.

From Fig. 6 (c, d) we also see that the region of influence of the step is much smaller compared to the height of the channel as the velocity profiles look similar at both $X=51$ and 55. From the Fig. 4b, we see that the length of the recirculation region is about the size of the step, 3mm.

![Image](image-url)
8. Conclusion
In the present study, subsonic and hypersonic rarefied gas flow over a BFS is investigated in the transition regime using the DSMC method. The evaluation parameters such as velocity, pressure and temperature were used to investigate the flow characteristics. The following conclusions can be drawn from the present study:

1. The velocity profiles resemble the laminar flow profile over a flat plate in continuum regime for both subsonic and hypersonic flow with the formation of a recirculation region behind the step.
2. The pressure distribution uniform decreases in the flow direction in case of subsonic flow, which is not the case in hypersonic flow.
3. In subsonic flow, the maximum temperature of the fluid is the wall temperature. In the hypersonic flow, the near wall temperature is far greater, owing to the compressibility and shear effects. The above conclusions give insight into the thermal and hydrodynamic boundary layers in the transition regime. This study can be a precursor to the flow behaviour in free molecular regime, which requires further exploration.

9. References
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