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Study of rarefied gas flows in backward facing micro-step using Direct Simulation Monte Carlo

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ABSTRACT

A backward facing micro-step is a building block for many microfluidic devices. Due to micron sized characteristic dimensions, the gas flow in such a geometry is rarefied in nature. Such rarefied gas flows are widely solved using the Direct Simulation Monte Carlo (DSMC) technique. Flow separation, circulation and re-attachment are some of the basic characteristics of step flows. The objective of this study is to analyze the effect of rarefaction on the flow properties and the separation of the flow. The range of selected Knudsen number (Kn) covers the slip and transition regime from a value of 0.0311–13.25. The pressure ratios employed are 3 and 5. It is observed that the slip velocity continuously increases while the centre-line velocity first decreases, then remains constant and finally increases with increase in Kn. At the step, separation of the flow is seen for $Kn < 0.1325$ while no such separation is observed in the range of Kn from 0.198 to 13.25. The corresponding Re for these ranges are 6.43 to 0.67 and 0.392 to 0.012 respectively. The re-attachment length decreases with increase in Kn whereas it increases with increase in Re. A stronger pressure force and a weaker diffusion effect leads to flow separation in the slip regime whereas stronger diffusion and weaker pressure force lead to an absence of flow separation in the transition regime. Finally, this work presents for the first time the existence of the Knudsen minimum for such a backward step geometry.

1. Introduction

The study of flow in a micron sized channel is important to design and develop microfluidics devices. The flow in a microchannel is rarefied on account of small characteristic dimension or low working pressure. The typical Knudsen number (Kn) of the flow is in the slip and transition regime ($0.001 < Kn < 10$). A detailed review of gas flow in microchannels can be found in [1–3].

In the past, rarefied gas flows have been studied experimentally [4–7], analytically [8–12] as well as numerically [13–16]. Experimental techniques have their limitations while conventional Computational Fluid Dynamics (CFD) methods are normally valid up to $Kn < 0.1$ after applying a modified slip boundary condition and are not suitable for rarefied gas flows. The higher order momentum equations are difficult to solve and their applicability is limited to a certain Kn and simple geometry. Among numerical techniques, Molecular Dynamics can be used but is computationally very expensive. The Direct Simulation Monte Carlo (DSMC) technique [17–26] and the Lattice Boltzmann Method (LBM) [27] have been used more extensively to study rarefied flows in a straight microchannel. Even in this case, LBM is not suitable for flows with high Knudsen number. A survey on the deterministic solvers used for rarefied gas flows can be found in [28]. It turns out that DSMC is very well suited to study rarefied gas flows. The DSMC method was devised by Bird [29] in 1960. It is a molecular method which is applicable to both slip and transition regimes.

Most existing numerical studies pertain to straight microchannels. However, the complexity of microfluidics devices is increasing day by day and a typical microfluidics device may include microchannels with different shape and size. Further, it may include bends and change in cross sectional area that may be gradual or sudden. The microchannels with these features have flow characteristics sufficiently different from those of straight microchannels warranting the need for a separate study.

In order to study the complex network of microchannels, individual parts of the network may be analyzed initially which can then help in understanding the flow behavior in the network much better. The sudden expansion kind of arrangement can be found in droplet generators, microchannel cold plates, valves, chemical mixers and injectors [30]. This sudden expansion of the cross-sectional area is often modeled as a backward facing step in micro and mini channels and flows through

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such a geometry have been studied experimentally and numerically for incompressible fluids for a wide range of Re [31–34]. Recirculation regions have been known to form behind the step and the length of the separation region is a strong function of Re. Beskok [35] studied the flow in a backward facing step solving the Navier-Stokes equation with a slip boundary condition and compared the obtained results with DSMC. Xue at al [36]. studied the flow in a backward facing step using the DSMC method. It was stated that the formation of vortex behind the step was affected by Kn, local temperature and pressure ratio. However, an abnormal sudden jump in pressure and velocity was observed at the step. Hsieh [37] studied the flow characteristics of 3-D microchannel backward facing step flow. It was seen that cross aspect ratio greater than 5 approaches the 2-D simplification. The flow separation was shown for only $Kn_o = 0.04$ and compared between 2-D and 3-D microchannels with different cross aspect ratios. Darbandi and Roohi [38] studied subsonic flow through backward facing nano channels using DSMC. It was found that the length of the separation region decreases with an increase in the inlet Kn. Mahadavi and Roohi [39] investigated the effect of Kn, wall temperature and pressure ratio on the flow behavior of a backward facing nano step geometry, for four Kn cases (0.01, 0.1, 1 and 10). It was found that hydrodynamic separation length is 0.18 for Kn equal to 0.01 while it is zero for higher Kn. Agrawal et al. [40] and Liou and Lin [41] studied rarefied gas flow in sudden expansion and contraction cases using LBM and observed recirculation in the corner for low values of Kn. Varade et al. [42] studied the rarefied gas flow in a conventional suddenly expanded tube experimentally. The recirculation zone behind the step was not found in their experiments which was attributed to the finite Kn of the flow. Titarev and Shakhov [43] studied rarefied gas flow into vacuum through a converging and diverging configuration by using the S-model kinetic equation. It was found that the mass flow rate strongly depends on the configuration of the flow.

Another important characteristic of rarefied gas flows is the phenomenon known as the Knudsen minimum, that was first observed by Knudsen [44] experimentally. This phenomenon is the minima shown by a plot of non-dimensional flow rate when plotted as a function of rarefaction (usually the inverse of Kn). This minimum has been observed in experimental and numerical studies for uniform cross section passages [10,45,46]. Hemadri et al. [47] experimentally observed Knudsen minimum in gradually expanded microchannel which is the first such experimental observation for non uniform cross sections channels. Ebrahimi and Roohi [48] observed the Kn minimum for gradually diverging microchannels using DSMC. However, the Kn minimum for a backward facing step flow was not studied previously.

Thus, it can be seen that there are few studies available in the literature for a backward facing step flow using DSMC that have analyzed the effect of rarefaction on the pressure and velocity, and the separation of the flow. Even in these studies, only the effect of rarefaction has been discussed for a limited set of Kn values, while effect of Re has not been discussed at all. The analytical studies are limited to continuum flow regime and incompressible fluid flow wherein the relationship between re-attachment length and Re is discussed. Hence, there is a lack of information regarding the re-attachment length and its variation with Kn and Re, for backward facing micro-step flow in slip and transition regimes. To address this issue, we have used DSMC to study the flow over a backward facing step over a range of Kn and Re. The objectives of this work are: (i) provide one to one comparison of the flow characteristics at various key points in the microchannel between the slip and transition flow regimes, (ii) study the effect of rarefaction (Kn) on the centreline and slip velocities, (iii) compare a backward facing step flow with a corresponding straight microchannel flow and discuss the respective separation, circulation and the re-attachment characteristics and propose a correlation for re-attachment length, and (iv) study the occurrence of Knudsen minimum for backward facing step flow for different expansion ratios.

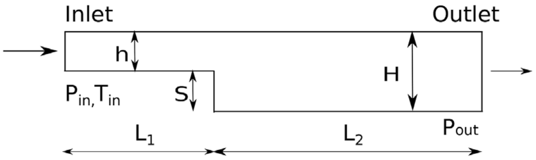

Fig. 1. Geometry of the 2-D backward facing micro-step geometry.

2. Methodology

2.1. Problem statement

Flow over a 2-D backward facing micro-step (see Fig. 1) is studied for different inlet Kn and pressure ratios. The larger height (H) is kept as 1 μm while the smaller height is kept as 0.5 μm to obtain an expansion ratio of two. The step height (S) is the difference between the larger height (H) and smaller height (h). The lengths of smaller (L_1) and larger (L_2) sections are kept as 5 μm and 10 μm such that the aspect ratio for both sections is 10. The total length (L) of the channel is thus 15 μm. For studying the Knudsen minima, expansion ratios of 1.25 and 4 are also simulated. The chosen lengths are sufficient for flow development for the range of Re employed in these simulations.

The inlet Kn is varied from 0.0311 to 13.25. Two different pressure ratios (3 and 5) are used to obtain different values of Re (varying between 0.012 and 6.43). The higher pressure ratio ensures a higher Mach number for the flow, which in turn reduces the statistical scatter. The simulation parameters are listed in Table 1.

2.2. Data reduction

The boundary conditions are inlet pressure (P_{in}) and temperature (T_{in}) and exit pressure (P_{out}). The equivalent mean free path (λ_{eq}) is used to define Kn and is given as

$$\lambda_{eq} = \frac{\mu v_o}{P} \tag{1}$$

where μ is dynamic viscosity ($= 22.669 \times 10^{-6} Pa - s$ [49]), P is pressure and $v_o = \sqrt{2k_B T/m}$ is the most probable molecular speed with k_B, T, and m denoting Boltzmann constant, temperature, and molecular mass respectively. The Kn is defined at the inlet and is calculated as

$$Kn = \frac{\sqrt{\pi}}{2}\frac{\lambda_{eq}}{h} \tag{2}$$

Similarly, Reynolds number is defined at inlet and calculated from the density and velocity averaged over the inlet cross-section and is given as

$$Re = \frac{\rho_{avg} U_{avg} h}{\mu} \tag{3}$$

where ρ_{avg} is the average density and U_{avg} is the average longitudinal velocity. The Mach number is defined locally and plotted along the length. It is given as

$$Ma = \frac{U_x}{\sqrt{\gamma RT}} \tag{4}$$

where U_x is the velocity along the flow direction (x-direction), γ is ratio of specific heats and R is specific gas constant. The shear stress at the wall is calculated as difference in the tangential momentum of incident and reflected molecules from a wall. It is given as

$$\tau = \frac{\sum M_t^i - \sum M_t^r}{A \Delta t^*} \tag{5}$$

where M_t is the tangential momentum, A is the surface area, superscript i is for incident molecules and r is for reflected molecules, and Δt^* is time of interaction. The time of interaction (Δt^*) is calculated as a product of the time step and the total number of samples.