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A study of 'thermophoresis-like' force on a heated trapezoidal nano-object confined between parallel plates

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ABSTRACT

A small scale, trapezoidal rigid nano-body in the gas filled gap between two parallel plates at different temperatures is considered. Direct Simulation Monte Carlo (DSMC) technique is used to determine the 'thermophoresis-like' force on the body in a direction perpendicular to the temperature gradient. The present numerical and analytical results of Hardt et al. (2009) [1] show good agreement, indicating that a temperature gradient orthogonal to the plates can induce a significant force in parallel direction, a phenomenon without analogy in the macro-world. Thereafter, the force external to the object which has more practical applications is studied. The effects of Knudsen number, asymmetry of the nano-object, temperature gradient and pitch on the force are studied. The force is found to increase with the increase in Knudsen number and it is negligible at lower Knudsen numbers ($Kn = 0.1$). Also, the force is found to increase with increase in asymmetry of the nano-object about a direction parallel to the temperature gradient and it vanishes when the object is symmetrical. It can be concluded that the primary factor behind the force inducement is asymmetry in the nano-object while the temperature gradient tends to enhance the magnitude of this force. The force interaction in the presence of two identical objects is studied by varying the distance between them in terms of pitch. As the pitch decreases, the force on the object located towards right end of the channel is decreased and the force on the object located towards left end of the channel is increased by approximately the same amount.

1. Introduction

Internal gas flows at standard conditions exhibit rarefaction effects at micro-scales (scales below 1 μm). These are due to the fact that molecular interactions with the boundary of the flow domain start to play a dominant role as demonstrated by Cerignani [2]. Transport phenomenon that is unknown from or unimportant in macro-scales can appear in such small scale systems as demonstrated by Sharipov [3,4]. Corresponding effects may be exploited to create novel operation while designing nano-machines and devices. An example of such effects is the thermphoretic force on a rigid body immersed in a gas of uniform temperature as demonstrated by Waldmann [5]. In contrast to this effect where a momentum transfer is induced parallel or antiparallel to the temperature gradient, it was shown by Hardt et al. [1] that a motion can be induced to a small rigid body of nano-scale dimension confined between two plates in a direction perpendicular to the temperature gradient. This phenomenon can be used to move DNA molecules by using temperature gradient without any mechanical aid. This can also be used to impart torque to gears of nano-scale dimensions. An analytical expression for the internal force exerted by the molecules on the object valid for a Knudsen number of infinity has been derived by Hardt et al. [1]. This force can be of considerable magnitude for objects of nano-scale dimension (high Kn) and is trivial in macro-scale dimensions. They have attributed the reason for this force to the temperature gradient orthogonal to the induced momentum. However, the effects of varying the Knudsen number (Kn) and temperature difference (ΔT) between the two parallel plates on the magnitude of force were not studied. Also, the interaction of this force on multiple objects was also not studied by them. An attempt has been made in this paper to study all these details.

2. Problem description

2.1. Overview of the problem for validation

The sketch of the geometrical domain for which force calculations have been performed for validation is shown in Fig. 1. The aspect ratio of the object is equal to 10 ($\frac{L_0}{H} = 10$). The situation considered is a trapezoidal nano-object whose bottom and top walls are at constant and different temperatures. The temperatures of the side walls are linearly distributed between the bottom and

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Nomenclature

Kn	Knudsen number $(Kn = \frac{\lambda}{H})$
Pr	pressure (Pa)
F	force (N)
α	angle (°)
L	length of the channel (m)
H	height of the channel (m)
L_o	length of the object (m)
L_c	distance between the two objects (m)
P	pitch, non-dimensional
λ	mean free path (m)
T	temperature (K)
①	object to the left of the channel ($x < 0.5L$)
②	object to the right of the channel ($x > 0.5L$)

Subscripts

x	direction along X axis
y	direction along Y axis
l	orthogonal wall
r	inclined wall
1	bottom wall
3	top wall
0	inclined wall of object ①
2	orthogonal wall of object ①
4	inclined wall of object ②
5	orthogonal wall of object ②
6	boundary at $x = 0$
7	boundary at $x = L$

top wall temperatures. This domain is similar to that considered by Hardt et al. [1] for deriving an analytical expression and is used for validating the present numerical method based on Direct Simulation Monte Carlo (DSMC). In this domain the force due to interaction of gas molecules inside the trapezoidal nano-object is considered.

The analytical expression valid for a Knudsen number of infinity has been derived by Hardt et al. [1]. The dimensionless pressure acting in the x-direction is given by

$$Pr_x = \frac{F_x}{H \cdot Pr_y} = \left(\frac{\alpha_l - \alpha_r}{\pi}\right) \cdot \left(\frac{\sqrt{T_1} - \sqrt{T_3}}{\sqrt{T_1} + \sqrt{T_3}}\right), \tag{2.1}$$

where F_x is the net force acting on the object in the x direction, H is the width of the gap, Pr_y is the total pressure acting perpendicular to the walls and T_1 and T_3 are the temperatures of walls 1 and 3 of Fig. 1 respectively and α_l and α_r are the inclinations of walls 0 and 2 of Fig. 1 respectively.

2.2. Overview of the problem for the study of force external to the object

For practical applications involving momentum transfer to nano-object, the external force due to gas molecules acting upon the object has to be considered. A trapezoidal nano-object in a micro-channel is considered as shown in Fig. 2. The aspect ratio of the object considered is equal to 1 $(\frac{L_o}{H} = 1)$. This is chosen as the physics behind the momentum transfer can be explained clearly with the help of pressure contours as shown in Figs. 6a, b, 7 and 10a, b). The aspect ratio of the channel considered is equal to 5 $(\frac{L}{H} = 5)$. This is chosen so that a sufficient number of molecules are present in the domain to be studied and also interaction between two objects can be studied using the same domain as shown in Fig. 2.

The effects of various parameters on the force external to the object are studied. The parameters and their range of values studied are given in Table 1. The effect of Knudsen number (Kn) on the 'thermphoresis-like' force is studied by varying Kn in the range between 0.1 and 6.25 which span from that of continuum to rarefied

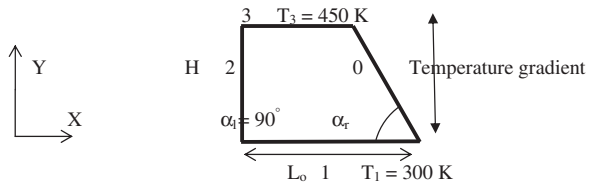

Fig. 1. Sketch of the domain similar to Hardt et al. [1] used for validation.

flow regime at different values of asymmetry of the nano-object measured in terms of $\Delta\alpha$ $(\alpha_l - \alpha_r)$ for a fixed temperature difference (ΔT) as shown in Fig. 2. The effect of temperature gradient (ΔT) as shown in Fig. 2 on the thermphoresis-like' force is studied by varying ΔT from 0 K to 150 K at the Knudsen number of 6.25 and different values of $\Delta\alpha$ from 0° to 45°. The effect of asymmetry of the nano-object is studied by varying the difference in the angles of side walls measured in terms of $\Delta\alpha$ $(\alpha_l - \alpha_r)$ for a fixed temperature difference (ΔT) as shown in Fig. 2. The left wall is always maintained orthogonal while the angle of the right wall is varied relative to it as shown in Fig. 2. The effect of force interaction in the presence of multiple objects is studied by considering two identical trapezoidal nano-objects at two different distances measured in terms of pitch $P = 0.5$ and $P = 0.3$ as shown in Fig. 2. The Knudsen number considered in this case is 6.25 and the temperature gradient is set to 150 K.

3. Numerical procedure

DSMC is a particle simulation method based on kinetic theory proposed by Bird [6]. Direct Simulation Monte Carlo method can be used to model the gas flows at all regimes unlike the continuum based models which are applicable only at low Kn flow regimes. This method is based on employing a number of simulated molecules to mimic the motion of relatively large number of real molecules. The motion of particles and their interactions with boundaries are then used to calculate their new positions and velocities. The intermolecular collisions are then simulated and the post-collision velocities are determined using conservation of mass, momentum and energy. The molecular motions and the intermolecular collisions are uncoupled over small time intervals. The particle motions are modeled deterministically and the collisions are modeled statistically. The core of the DSMC algorithm is made up of four primary processes:

1. Move the particles and enforce boundary conditions.
2. Index and cross reference the particles.
3. Simulate intermolecular collisions.
4. Sample the flow field.

A flow chart outlining the DSMC algorithm used is shown in Fig. 3. These processes are uncoupled during every time step. The selection of the time step is important and it must be less than the mean collision time. Here each process is summarized briefly.

In the first step, the particles are streamed and the boundary conditions are enforced within a single time step. In general, the molecule surface interactions are modeled either using specular