Modeling and Simulation of a Novel Pressure Sensor Based on the Principle of Thermal Transpiration

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Abstract. In this paper we advance novel mechanisms for enhanced functioning of Knudsen micro-cantilevers. Using rarefied gas molecular simulation technique, DSMC, we herein demonstrate the validity of various earlier proposals, made by researchers for the possibility of construction of such devices, for the first time. Further we investigate the onset of thermal transpiration forces, also known as Knudsen forces on the cantilevers, for different pressure and temperature ranges. Our investigation shows that Knudsen cantilevers can be conveniently utilized for the design of sensors for such macroscopic properties as temperature, infrared radiation, etc when the surrounding pressure can be reduced sufficiently, and also for the measurement of ultra-high vacuum pressures, after some initial calibration. Till date measurements of ultra low pressures, have been made using devices such as pirani gauges, cold cathode/ hot cathode ionization gauges etc. However due to many technical complexities, their cost of production, maintenance and usage is very high. On the other hand, this present device presents a novel architecture for use in ultra high vacuum ranges, without inculcating the additional complexities of using the ionization gauges.

1.Introduction
The use of temperature actuated micro-cantilevers has recently gained particular attention of a number of groups through out the research community, for measurement of macroscopic properties such as ambient pressure, temperature, infrared radiation etc in rarefied gases [1-8]. Particularly the measurement and calibration of ultrahigh vacuum has been found to be very comparatively convenient and hence has been the focus of attention. When subjected to ultra-high vacuum and differential heating on the broader sides of a micro-cantilever, it is found that under certain conditions, there is significant deflection of the cantilever. These apparent non-intuitive forces (Knudsen forces) on the two sides of a cantilever which leads to the deflection, are due to thermal transpiration, has been a source of considerable confusion and discussion since the earlier days of discovery.

The phenomenon of thermal transpiration was discovered by Crookes in 1879[9], and subsequently studied in great detail by Knudsen, Maxwell, Einstein and Reynolds. Maxwell’s explanation for the radiometric forces was based on the phenomenon of the thermal creep of the gas molecules arising from the presence of thermal gradients along the solid surface. This thermal gradient facilitates thermal transpiration along a thin film layer adjacent to the solid surface and results in the formation of a pressure gradient. Momentum exchange of such flows gives rise to the rotation of the Crooke’s radiometer and the deflection of the micro-cantilever in our case. The surface heating can take place...
from various sources such as resistive heating by coils placed on the surface of the cantilever, or by optical heating using lasers on the surface itself. In the recent past it has also been recognized that this phenomenon can also be utilized to design miniaturized vacuum pumps [10].

A number of works have appeared earlier which treated a simpler problem of flow between two cylinders connected by a thin pipe using various methodologies. For example, Liang [11] proposed corrections accounting for the difference between gases, and their corresponding molecular diameters, and calculated the value of the thermo-molecular pressure ratio using accurate low pressure measurements, Takashi and Sensui [12] using similar experimental means extended Liang’s empirical formulae for various gases such as hydrogen, neon etc, and showed that the phenomenon can be described by a single formulae for different gases under consideration, and for arbitrary temperature ranges. These curves were recently verified using arrays of parallel silicon capillaries for nitrogen and helium [13,14] by York et al. Using the Hansen Morse polyatomic gas model, and lattice Boltzmann simulation techniques, Loyalka[15] studied the phenomenon of thermal transpiration in various geometries such as plane annular and cylindrical geometries. Using various surface accommodation coefficients (TMAC), their models obtained very closely approximated the experimental results obtained earlier. However their models were very mathematically complicated, even though it had been applied to very simple geometries. Yoki et al. using linearized Boltzmann equations, and the BKW models, numerically simulated the flow of gas molecules, and obtained close agreements with the large theoretical results obtained earlier by Reynolds, Smolderen, and Wendt. Using direct molecular simulation methods Hudson et al. obtained thermal transpiration models for Knudsen pumps [5]. Excellent correlation between the numerical results and the experiments were obtained, which were beyond the capabilities of other analytical or approximation techniques.

Another significant advantage of DSMC simulations over other techniques is the fact that physical surface/boundary conditions and complex geometries can easily be incorporated into the model, thus providing a more realistic picture. Although a few works have appeared for simulations of such devices using stochastic/analytical techniques, the results are at best only approximate. In the following work, we show the influence of various governing parameters on the deflection of the cantilever, for two different gases using DSMC. All simulations are performed for a 2 dimensional geometry, with an outer chamber enclosing the infinitely long cantilever. It is shown that the use of such cantilevers can be used conveniently to detect very small pressures, in the range of .01 Pa, by coupling the device to capacitative devices. Though the Knudsen forces in general are small, it is found that it is large enough to be detected easily by capacitative mechanisms.

2. Numerical Modeling:
Various methods can be utilized to investigate the mechanisms of rarefied gas flows. Of these, it has been emphasized by many authors that molecular simulations can be used conveniently to study the phenomenon [5, 20-21]. Experimental means have been used by many people to investigate the Knudsen forces; however, experimental means are arduous and are not amenable to investigation of all important properties independently [12]. On the other hand molecular simulation can be easily used to relate the macroscopic properties such as pressure, temperature to the deflection of the cantilever without any interference from any other means. Other than molecular simulation, people have also used stochastic modeling using Boltzmann equation; to study the flows Loyalka used linearized Boltzmann equations to explain the phenomenon of thermal transpiration [15]. However an inherent problem with such methods is the inability to model the phenomenon in all ranges of the Knudsen number. DSMC on the other hand can be used to simulate the gas flow in all regions of the Knudsen Number. . In the following sections, we first provided a brief overview of the method, and proceed to describe our comprehensive results. DSMC simulations were performed for two different gases, argon and helium, for different values of pressure and temperature.
2.1 Direct Simulation Monte Carlo:

DSMC is a molecular-based statistical simulation method for rarefied gas flow introduced by Bird[22,23]. The method numerically solves the dynamic equations for gas flow using thousands of simulated molecules. Each simulated molecule represents a large number of real molecules. With the assumption of molecular chaos and a rarefied gas, only the binary collisions are uncoupled if the computational time step is smaller than the physical collision time. The interactions with boundaries and with other molecules conserve both momentum and energy. The macroscopic flow characteristics are obtained statistically by sampling the molecular properties in each cell.

At the beginning of the calculation, the simulated particles are uniformly distributed statistically in the cells. At each time step, all particles move according to their individual velocities, interact with the boundaries, and are then indexed. In each cell, a certain number of collision pairs are selected using the no-time-counter (NTC) method and collisions are calculated. These steps are repeated to increase the sample size until the statistical errors are small enough. The DSMC method can simulate non-equilibrium and unsteady gas flow. A steady-state flow field is obtained with a sufficiently long simulation time. When the perfect gas assumption holds, the hard sphere model without inter-molecular attractive potential is accurate enough for the collisions [24]. However for better accuracy the present simulations use the variable hard sphere (VHS) model for enhanced accuracy [23].

The cell size and time step for DSMC are very important parameters due to their direct effects on the correctness of the results. According to Bird [12], only when the computational time step is less than the mean collision time, could the molecular movements and collisions be decoupled. The cells are made small enough to restrict collisions to nearby particles but should contain a sufficient number of particles so that the method remains statistically accurate. Empirically, it has been found that cells should be no larger than a mean free path and contain at least twenty particles. Recently, the Green-Kubo formalism was used to quantitatively evaluate the dependence of a gas transport properties on the cell size [26, 27] and the time step[28,29]. It has been numerically proved that the sub-cell size, instead of cell size, should be limited to no longer than the smallest mean free path in the domain [30]. In each case of this work, the cell (or sub-cell) size was always smaller than the local gas mean free path. The time step was then chosen as half of the smallest collision time in the channel. Each cell contained about twenty molecules, which ensures the accuracies of the simulations.

2.2 Statistical macroscopic quantities:

Based on kinetic theory [31, 23], the macroscopic velocity is obtained by the statistic laws:

\[ u_j = \frac{1}{N_j} \sum u \]

where \( u_j \) is the macroscopic velocity vector, the subscript \( j \) represents the location index, i.e. the \( j^{th} \) grid; and \( N_j \) is the total number of simulated molecules in the \( j^{th} \) grid during sampling. For a diatomic gas, the Larsen-Borgnakke model with discrete rotational energy is used to model the energy exchange between the translational and internal modes. The vibrational energy is negligible. Therefore, the temperature can be obtained as

\[ T = \frac{T_T + \zeta T_{rot}}{3 + \zeta} \]

where \( T_T \) denotes the translational temperature, \( T_{rot} \) denotes the rotational temperature, and \( \zeta \) is the number of internal degree of freedom. \( T_T \) and \( T_{rot} \) are defined as

\[ T_T = \frac{2}{3k_b} \left( m \vec{v}^2 - \vec{m} \cdot \vec{v}^2 \right) \]

\[ T_{rot} = \frac{2}{k_b} \left( \frac{E_{rot}}{\zeta} \right) \]

respectively, where \( k_b \) is the Boltzmann constant, \( v \) is the velocity vector of molecules, and \( E_{rot} \) is the rotational energy of an individual molecule.

On the surface, the net heat transfer flux \( q \) is the sum of the translational and rotational energies of both the incident and the reflected molecules, i.e.
\[
q = \left[ \left( \sum_{i=1}^{n} E_{tr} + \sum_{i=1}^{n} E_{rot} \right) - \left( \sum_{i=1}^{n} E'_{tr} + \sum_{i=1}^{n} E'_{rot} \right) \right] \frac{\Delta t}{\Delta x}
\]

where the subscripts “inc” and “ref” denote the incident and reflected molecular streams, respectively, \( n \) is the total number of simulated molecules that strike the wall during the sampling, \( N_0 \) is the number of gaseous molecules associated with a computational molecule, \( \Delta t \) is the time period of the sampling.

The code developed was based on the standard code of Bird [23] and has been validated for various micro geometries and different boundary conditions [19, 32]. However in an effort to benchmark our code effectively, additional calculations on a different geometry [21] have also been carried out, though they haven’t been presented here. All calculations in this paper were performed on a Beowulf cluster each CPU of which was 550 Mhz. The sample size in each case was above 5x10^6, with which an acceptable accuracy could be obtained [33] though there are still obvious fluctuations in the results. The CPU time for each typical case was over 150 hrs.

**Figure 1.** Schematic diagram of the volume under consideration

**Figure 2**

a) Variation of deflection of the cantilever vs. Pressure with \( T_{hot}=400^\circ C \)

b) Variation of Deflection vs. Pressure for \( T_{hot}=900^\circ C \), for Argon and Helium.
3. Results:

Figure 1 shows a schematic diagram of the computational domain under consideration. For simplicity an infinitely long cantilever enclosed in an infinitely long rectangular container is assumed. Due to the symmetric nature of the computational domain under examination, a simulation of only one half of the computational domain (shown in gray shade in Fig. 1), along with suitable boundary conditions applied along the line of symmetry gives us an accurate picture of the physics of the problem. A constant temperature boundary condition has been applied at the walls, whereas a spectral boundary condition has been applied at the line of symmetry. This domain decomposition leads to a four fold decrease in the computational time, with no loss in the accuracy of the result.

The system under consideration is a rectangular box of dimension of 160 µm x 100 µm. Computational cell sizes are automatically decided such that there are approximately 100 molecules in each cell. The width of the cantilever has been assumed to be 100 µm, with thickness 1 µm. It must be remembered however that the grid size cannot be made larger than the smallest dimension in the computational domain, here the thickness of the cantilever, hence posing an upper limit on the maximum grid size usable. To circumvent this problem, unstructured grids can be utilized surrounding the smallest domain; however it has not been implemented in our work. To observe the variation in the deflection as a function of the temperature, we performed simulations for two temperature ranges 1) \( T_{hot}=900 \degree C \) and 2) \( T_{hot}=400 \degree C \), where \( T_{hot} \) represents the temperature along the hotter upper surface of the cantilever. Results for the net deflection of the cantilever, as obtained from the differential force acting on the micro-cantilever, from both the simulations are depicted in Fig. 2a and 2b. Simulations were also performed for two different gases, argon and helium. The gases were simulated using the variable soft sphere model [35, 36]. The deflection of the cantilever was obtained using classical beam theories, assuming the Young’s modulus \( E = 170 \text{ Gpa} \) and length of the beam to be 1 mm for all cases. The width and the thickness of the cantilever are 100 µm and 1 µm respectively as mentioned earlier.

As observed from Figure 2a and 2b, when the ambient initial pressure is quite low, the deflection obtained due to the presence of Argon is more compared to that of Helium. However when the pressure is in the comparatively higher i.e. >100 Pa, this trend reverses and we observe a higher deflection and force per unit width in case of Helium as compared to Argon. Qualitative confirmation of the above fact was also obtained by Passian et al in their work [1]. Interestingly the deflection of the cantilever when argon is placed inside the chamber is considerably low as compared to that when Helium is placed with it. This might be attributed to the fact that Helium has a much smaller size as compared to Argon, as a result of which momentum transfer to the cantilever is much more. The result is also in confirmation of the experimental results obtained by Takaishi and Sensui[12], who showed that for gases with lower atomic diameters, a higher pressure difference can be maintained between two cylindrical containers separated by a thin pipe, and maintained at different temperatures. Further examination of the plots shows the fact that the deflection of the tip of the cantilever tends to increase significantly with increase in the hot surface temperature. Here the hotter surface imparts larger energy to the particles which impinge on its surface, hence transferring larger momentum. Since force is basically momentum change per unit time, the net force acting on the cantilever increases considerably. However as obvious from the figures, the pressure tends to equalize out, as the pressure is increased beyond a certain threshold value determined solely by the resident gas and the surface temperatures.

Further examination of the plots show that deflections of the order of \( 10^{-6} \) nm can easily be obtained even at the lowest of pressures. With modern deflection measuring instruments available, a deflection to the tune of even 100 nm can be detected very accurately. Hence a pressure of the order \( 10^{-6} \) bar or around \( 10^{-9} \) Torr can be easily and accurately measured, after an initial calibration, using conventional gauges. Another important point worth noting is the fact that the deflection vs pressure as depicted in Figure 2a and 2b, shows a perfect linear dependence on each other in the low pressure regime. This would significantly augment the design of the pressure sensor. Such a linear dependence of the deflection vs pressure has earlier been shown by Passian et al, using experimental means.
4. Conclusion

A detailed analysis has been made of the Knudsen forces acting on an externally heated micro-cantilever using DSMC techniques. Results obtained earlier by Passian et al. using approximate analytical techniques and experiments has been shown to be qualitatively correct, however exact correlation cannot be obtained at this stage since the macroscopic observables obtained in their case were not the same as used here. The results presented here show the possibility of constructing devices for measuring pressures accurately in the range of .1 Pa without encountering the difficulties associated with ionization gauges, cold/hot cathode gauges etc. Once calibrated this method can be immensely consequential in providing improved methods of obtaining accurate measurements of temperature. However it must be remembered that a large number of assumptions have been made for example the perfectly diffuse surface of the cantilever, the constant surface temperature of the bell jar, etc. These phenomena though not very complex can be accurately modeled using conventional techniques to obtain a very accurate picture of the phenomenon. Another major problem that is encountered is thermal stress generated bending of the cantilever. Novel methods have been devised to eliminate the thermal stress related inaccuracies, and obtain a highly accurate picture. At present extensive numerical and experimental analyses are being carried out on such cantilevers. These and other important results will be communicated soon.

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