What Determines Knudsen Force at the Microscale

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Abstract. Knudsen forces arise in microscale systems when there is a thermal gradient with a characteristic length scale comparable to the molecular mean free path of the ambient gas. These forces are sometimes referred as radiometric or thermo-molecular forces [1] and have been recently measured experimentally in a microscale configuration using heated atomic force microscopy (AFM) probes [2]. The Knudsen force on microstructures with thermal gradients can provide a novel actuation mechanism for mass detection, thermogravimetry, and very high-resolution heat flux measurements. While measuring such forces precisely at microscale can be an arduous task especially since only limited analytical results exist, numerical simulations can provide a basis for understanding the physical mechanisms governing the generation of Knudsen forces. The main goal of this paper is to determine the dependence of the Knudsen force on pressure, geometry and thermal gradients based on rarefied flow simulations and to investigate the effects of the Knudsen force on the dynamics of microbeams.

I. INTRODUCTION

At the microscale, even moderate temperature differences can result in significant Knudsen forces generated by the non-equilibrium energy exchange between gas molecules and solids immersed in a gas. Knudsen forces appear, in principle, in many microsystems when the length scale of temperature gradient - such as the distance between unequally heated structures - is comparable to the molecular mean free path in the ambient gas. Experimental observations of the effect of the Knudsen force have been reported recently[2] for heated atomic force microscopy (AFM) microcantilevers. The computational results reported in the present study provide the first direct comparison with these measurements and indicate that the Knudsen force is highly sensitive to the gas-surface interaction parameters such as the tangential momentum accommodation coefficient.

One configuration frequently encontered in microsystems involves beams - fixed-free and fixed-fixed - suspended over a substrate wall. Such microbeam configurations are used in many devices such as switches, microscopy probes and resonators. Let us consider the mechanism of Knudsen force generation on such a heated microbeam in the vicinity of a colder wall as shown in Fig. 1. Since the beam is closer to the wall than the upper bound of the domain, the gradient of temperature below the beam is greater than the one above. When considering two molecules, one mean free path away from the beam, the molecule above the beam will bounce and give its momentum to the beam in the negative y direction, whereas the one below the beam will give it momentum in the upward direction. According to the difference in gradients of temperature, the molecule below the beam will be in a colder area since the temperature drops substantially faster. Therefore, while moving towards the beam, the molecule will experience a larger gain in momentum than the one coming from above the beam. Consequently, the resulting momentum given to the beam will be in the direction of positive y-axis and the beam will move upward.

The main goal of this paper is to obtain a closed-form model for the Knudsen force on a heated beam near a substrate, describing it's dependence on the gas pressure, temperature difference and geometry. The remainder of the paper is organized as follows. Section II describes the numerical approach for modeling the Knudsen force. Section III contains the compact model for the non-dimensional Knudsen force coefficient based on the numerical results as well as comparison with experiments. Section IV gives an application of the Knudsen force model to calculate the dynamics of microbeam under electrostatic, thermal and gas damping forces. Finally, conclusions are given in Section V.
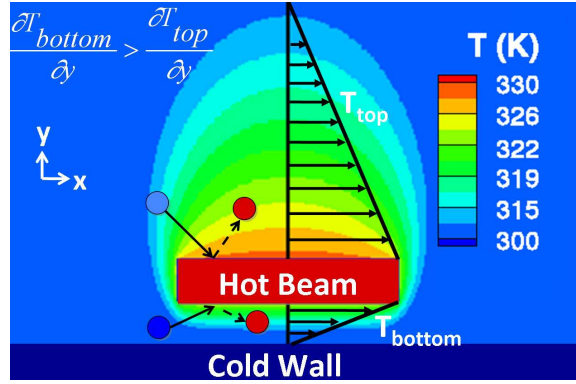
FIGURE 1. Schematic of domain.

II. NUMERICAL MODELING

The Knudsen force on a 2D heated beam is calculated based on numerical solution of Ellipsoidal-Statistical Bhatnagar-Gross-Krook (ESBGK) Boltzmann equations. Details of the formulation and numerical implementation can be found in reference [3, 4]. The solver employs a finite volume method (FVM) with a second order quadrant-splitting scheme applied in the physical space. The velocity space in polar coordinates consisted of 16th-order Gauss-Hermite quadrature in velocity magnitude and 64 uniform velocity angles. In the quasi-steady two-dimensional ESBGK simulations, Knudsen force is obtained by integrating the computed normal pressure component along the width of the cantilever cross section and the shear pressure along the thickness of the beam.

The three-dimensional problem along with the cross section used for the simulations is shown on Fig. 2. The left, top, right and bottom boundaries are symmetry, pressure inlet, pressure inlet and wall boundaries, respectively. The temperature of the boundaries is set to 300 K.
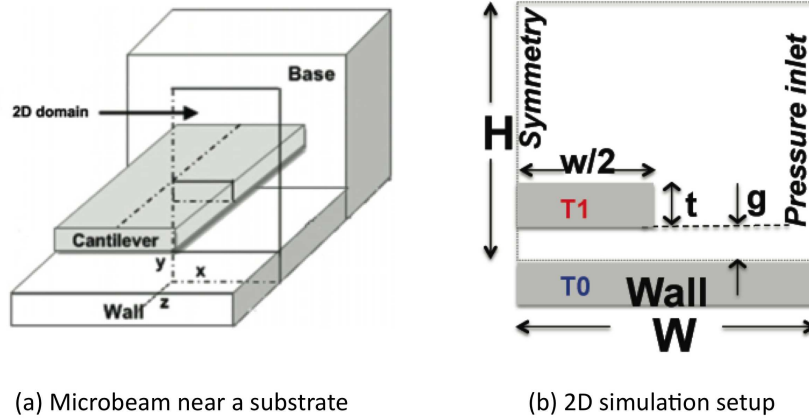

(a) Microbeam near a substrate   (b) 2D simulation setup

FIGURE 2. Schematic of the configuration.

Grid convergence was verified for physical and velocity spaces. The height of the domain has a greater influence than the width for values lower than 20μm. When the height is larger than 20μm, the variations stay within 5% of total force. The velocity grid convergence test showed that the number of velocity angles should be larger than 32. The Richardson Extrapolation [5] was used in order to quantify the accuracy of the code. A numerical error of 6.46% was obtained by combining the results from two proportional meshes.

The simulations have been compared with experimental results from Passian *et. al.* [2]. In these experiments, a surface-micromachined cantilever was heated by focused illumination with a 529nm line of an argon ion laser.

By modulation of the laser frequency, the temperature difference between the cantilever and the substrate remained constant. In order to simulate this three-dimensional configuration with the two-dimensional code, the front-to-side ratio of 0.1 was preserved along with the temperature difference of $\Delta T = 30K$. The simulations agree with the experimental results for both argon and nitrogen (Fig. 3) with a maximum deviation of 3.7% for argon and 9.0% for nitrogen at a working pressure of 6.84 kPa and 6.89 kPa for nitrogen and argon, respectively.
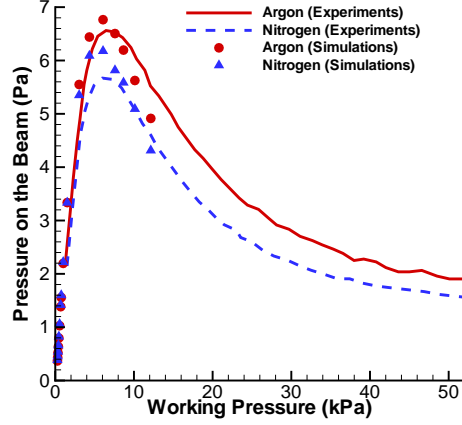

FIGURE 3.   Comparison of Knudsen force simulations with experimental data [2]

III. COMPACT MODEL OF KNUDSEN FORCE

Based on the simulations, a closed-form expression for Knudsen force on a heated beam at a distance g from a substrate at temperature T_0 for a gas with density ρ, ratio of specific heats γ and gas constant R is developed. The dynamic similarity analysis [6], results in the following non-dimensional relation:

$$C_{Kn} = \frac{F'_{Kn}}{\rho R \Delta T w} = f(\frac{T_0}{\Delta T}, Kn, \frac{t}{g}, \frac{w}{g}, \gamma, \alpha_t) \tag{1}$$

where C_{Kn} is the Knudsen force coefficient, F'_{Kn} is the force per unit length on the beam, ΔT is the temperature difference between the beam and the substrate, Kn is the Knudsen number defined as the ratio of the molecular mean free path length to the gap size, t and w are the thickness and width of the beam, respectively, γ is the heat capacity ratio and α_t is the momentum accommodation coefficient for the gas.

Simulations have been performed for both argon and nitrogen with constant $T_0/\Delta T = 10$, $\alpha_t = 1$, W = 50μm, H = 55μm, t = 2μm, w = 20μm, g = 2μm, which gives t/g = 1 and w/g = 10. Figure 4 shows the Knudsen force coefficient obtained from the simulations for both gases. One can see that the specific heat ratio has a low influence since monatomic and diatomic gases follow the same trend, as a result γ can be neglected in Eq. (1). This equation can be further reduced by considering a cantilever with large aspect-ratio and an momentum accommodation coefficient of one.

Hence, equation 1 can be reduced to:

$$C_{Kn} = \frac{F'_{Kn}}{\rho R \Delta T w} = f(\frac{T_0}{\Delta T}, Kn, \frac{w}{g}) \tag{2}$$

By using the least mean square algorithm, the following close-form fit expression for the Knudsen force coefficient based on the Knudsen number is obtained:

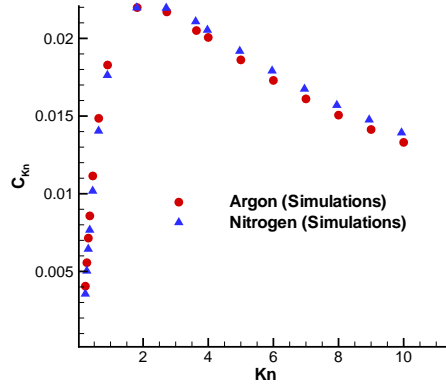$$C_{Kn} = \frac{1}{AKn^\alpha + BKn^\beta + CKn^\gamma} \tag{3}$$

FIGURE 4. Influence of Kn

where $A = 38.0535, B = 5.6832, C = 8.3818, \alpha = -0.3835, \beta = -2.3362$ and $\gamma = 0.8549$.

The effects of $\frac{T}{\Delta T}$ and $\frac{w}{g}$ are taken into account by adding two correction factors based on the simulation results of figure 5. The equation becomes:

$$C_{Kn} = \frac{(1 + D_1(\frac{T}{\Delta T})^{\delta_1} + E_1(\frac{T}{\Delta T})^{\varepsilon_1}) \cdot (1 + D_2(\frac{w}{g})^{\delta_2} + E_2(\frac{w}{g})^{\varepsilon_2})}{AKn^{\alpha} + BKn^{\beta} + CKn^{\gamma}} \tag{4}$$

TABLE 1. Constants for the Compact Model

Constant name	Value	Constant name	Value
A	38.0535	α	-0.3835
B	5.6832	β	-2.3362
C	8.3818	γ	0.8549
D_1	-0.9146	δ_1	-0.4224
E_1	0.6203	ε_1	-0.2602
D_2	-4.0798	δ_2	-0.9019
E_2	0.9511	ε_2	-0.2609
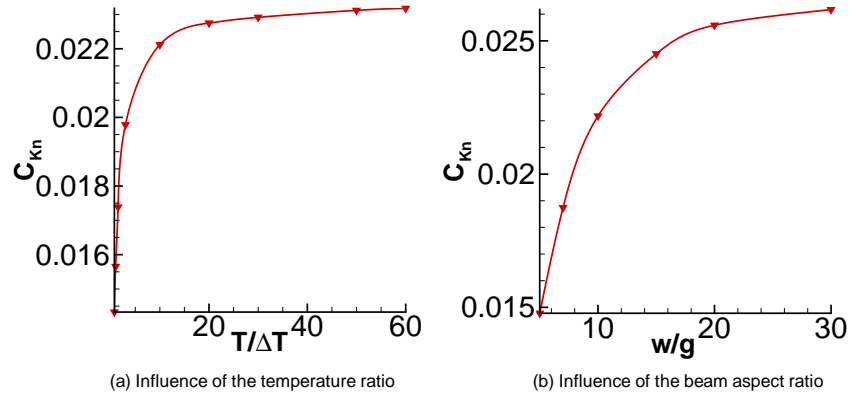
(a) Influence of the temperature ratio

(b) Influence of the beam aspect ratio

FIGURE 5. Force coefficient from simulations and experiments.

IV. APPLICATION: MICROBEAM DYNAMICS

The compact model obtained for the Knudsen force, can be used to predict the deflection of the cantilever. The Euler-Bernoulli beam theory[7] is a simplification of the linear theory of elasticity and provides a good means of calculating the deflection of beams. This model applies with the following assumptions: the beam is long and slender, the beam cross section is constant along its axis, the beam is loaded in its plane of symmetry, deformations remain small compared to the length of the beam, material is isotropic and plane sections of the beam remain plane.

For a constant Young's modulus, E, along the axis, the Euler-Bernoulli beam equation is:

$$\mu \frac{\partial^2 u}{\partial t^2} + EI \frac{\partial^4 u}{\partial z^4} = F'_{Kn} + F'_{damping} + F'_{elec} \tag{5}$$

where, μ is the lineic mass, u is the deflection, z is the coordinate along the length of the beam and I is the moment of inertia defined by $I = \frac{wh^3}{12}$, where w is the width and h the thickness of the beam. $F'_{Kn}, F'_{damping}$ and F'_{elec} are the Knudsen force, damping force and electrostatic force, respectively, per unit length. The damping force is based on the model in reference [8] and the electrostatic force is defined by $F'_{elec} = \frac{1}{2}\varepsilon_0 w \frac{V^2}{g^2}$, where V is the applied voltage and g is the gap size. The finite difference method with implicit scheme has been applied to discretize the differential equation in both time and physical spaces considering a fixed-fixed beam with no initial deflection nor velocity. Detailed micro-cantilever geometry and gas flow conditions are listed in Table 2.

TABLE 2. Microcantilever geometry & flow conditions.

Property	Symbol	Nominal value
Beam length	L	400 μm
Beam width	w	20 μm
Beam thickness	t	2 μm
Gap size	g	1 μm
Beam	Si	Silicon
Young's modulus	E	160 GPa
Beam density	ρ	2,330 kg.m^{-3}
Gas	N_2	Nitrogen
Ambient Pressure	P	0.1 - 1atm
Temperature Difference	ΔT	50-150K

The deflection of the fixed-fixed configuration was simulated and the trajectory of the mid-length point is shown on Fig. 6 for different pressures and temperature gradients. At atmospheric pressure, the Knudsen force doesn't have a large influence on the trajectory and the maximum deflection in steady state slightly reduces by 3.50% and 7.89% at ΔT = 50 K and ΔT = 150 K, respectively. When the pressure drops to a tenth of an atmosphere, the dynamics of the microbeam is highly dependent on the temperature gradient. Increasing the temperature gradients results in a smaller amplitude of the oscillations since the direction of the Knudsen force is opposed to the electrostatic force. The maximum deflection in the steady state drops by 17.5% and 43.8% at ΔT = 50 K and ΔT = 150 K, respectively.
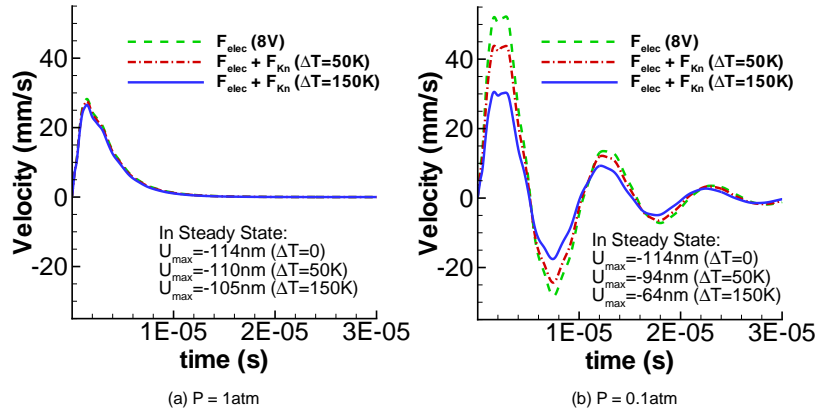

FIGURE 6. Velocity at the Mid-length Point.

V. CONCLUSIONS

In this work, the Knudsen force on a two-dimensional heated microbeam was investigated by using numerical simulations of the Boltzmann model kinetic equation with the ellipsoidal statistical collision model. The simulations were validated with experimental measurements and a closed-form model for the Knudsen force dependence on temperature ratio, Knudsen number and microbeam aspect ratio has been obtained. By simulating the dynamics of a microbeam under Knudsen force, gas damping force and electrostatic force, it has been shown that Knudsen forces are comparable to low-voltage electrostatic forces ($\sim 10\text{V}/\mu\text{m}$) and can therefore be used as a more benign actuation mechanism for microsystems.

ACKNOWLEDGMENTS

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