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Comparison of Kinetic Models for Gas Damping of Moving Microbeams

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Numerical investigations of the gas flow structure and the gas-damping force on moving and heated microbeams are carried out using the Navier-Stokes equations with first-order velocity-slip and temperature-jump boundary conditions (the NSSJ method) and two kinetic numerical techniques: the particle-based direct simulation Monte Carlo (DSMC) method, and a deterministic discrete-ordinate solution of the ellipsoidal statistical (ES) kinetic model equation. The gas-damping coefficients on a moving microbeam for quasi-static isothermal conditions are estimated by the three numerical methods for Kn = 0.1-1.0. The NSSJ simulations tend to overestimate the gas-damping coefficient for Knudsen numbers larger than 0.1, whereas the DSMC and ES kinetic approaches are in good agreement for the slip and transitional flow regimes. The flow structure and the Knudsen force are calculated using the ES kinetic model for a heated microbeam over a wide range of Knudsen numbers. The Knudsen force peaks in the transitional regime (Kn ≈ 2), and the numerically predicted variation of the force with Knudsen number is consistent with experimentally observed displacements of the heated microbeam.

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Nomenclature

$\vec{c}$	=	thermal velocity vector (m/s)
f	=	velocity distribution function
G	=	gap height (m)
g	=	reduced distribution function
h	=	reduced distribution function
i, j	=	indices
Kn	=	Knudsen number
n	=	number density (mol/m^3)
p	=	pressure (Pa)
p_{ij}	=	pressure tensor (Pa)
P	=	quadrature weights
Pr	=	Prandtl number
R	=	gas constant (J/kg·K)
S	=	velocity ordinate (m/s)
T	=	temperature (K)
U	=	beam velocity (m/s)

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u = x-component of velocity (m/s)
v = y-component of velocity (m/s)
w = z-component of velocity (m/s)
W = beam width (m)
x = Cartesian coordinate (m)
y = Cartesian coordinate (m)
z = Cartesian coordinate (m)
Γ = damping coefficient (Pa·s)
δ = Kroneker delta
ϵ_{ij} = ES tensor
Λ = slip length (m)
λ = mean free path (m)
λ_{ij} = ES tensor
μ = viscosity (kg/m·s)
ν = collision frequency (1/s)
ϕ = angular ordinate (radian)
ρ = mass density (kg/m^3)

Subscripts and Superscripts

G = Gaussian
M = Maxwell-Boltzmann
0 = baseline or ambient
δ = discrete velocity
σ = discrete angle

Acronyms

ASCI = advanced simulation and computing initiative
BGK = Bhatnagar-Gross-Krook
CFD = computational fluid dynamics
DSMC = direct simulation Monte Carlo
ES = ellipsoidal statistical
MEMS = micro electro mechanical system
NSSJ = Navier-Stokes slip-jump
TFLOPS = trillion floating-point operations per second

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I. Introduction

The variation in the characteristic length scale from nanometers to millimeters in MEMS devices can lead to the breakdown of the continuum flow assumption underlying the conventional computational fluid dynamics (CFD) approach based on the solution of the Navier-Stokes equations. For example, a MEMS component that has a flow section with a characteristic length of 1 μm has a Knudsen number Kn of 0.06 in air at standard conditions. This means that the flow is in the slip regime, a regime of slight rarefaction where the gas may exhibit some characteristics of its coarse molecular structure near solid boundaries. For Knudsen numbers larger than 0.01, the non-equilibrium rarefaction influences the flow near gas-solid interfaces.

To first order in Knudsen number, these effects can be accounted for in the Navier-Stokes equations by using velocity-slip and temperature-jump boundary conditions: the Navier-Stokes slip-jump (NSSJ) method. For flows with Knudsen numbers larger than 0.1, higher-order kinetic effects become important, and the linear stress-strain relationships in the Navier-Stokes equations become invalid. The Burnett equations, which can be obtained from the Chapman-Enskog expansion of the Boltzmann equation to second order in Knudsen number, can be used as the governing equations in the transitional regime. However, instability problems inherent in the Burnett equations lead to many numerical difficulties and require additional reformulation.[1] Eventually, when the Knudsen number is further increased and the flow deviates significantly from equilibrium, the modeling has to be based on the Boltzmann equation, the principal equation of kinetic theory.

The Boltzmann equation is a non-linear integro-differential equation, and its exact solution is known only for a small number of special cases of collisionless or spatially homogeneous problems. The multi-dimensional Boltzmann collision integral on the right-hand side impedes direct numerical integration of the

Boltzmann equation. The direct simulation Monte Carlo (DSMC) method[2] is based on stochastically solving the Boltzmann equation and has emerged in the last decades as the most powerful numerical approach for rarefied gas flows, especially in the supersonic and hypersonic regimes. Microscale gas flows in MEMS are similar to rarefied low-density flows because they both are characterized by non-negligible Knudsen numbers. However, microscale flows are typically subsonic, low-Reynolds-number flows dominated by surface effects, as opposed to the high-speed aeronautical rarefied flows that have been studied extensively by DSMC. The DSMC method requires large computational resources to simulate low-Mach-number flows because of the inherent statistical scatter, which produces a low signal-to-noise ratio. Moreover, the DSMC method is explicit in time, which imposes additional limits for its application to low-speed microscale flows.

A plausible numerical approach for simulating microscale flows is the deterministic solution of the simplified form of the Boltzmann equation known as the kinetic model equation. The Bhatnagar-Gross-Krook (BGK)[3] and ellipsoidal statistical (ES)[4] kinetic models use a non-linear relaxation term instead of the full Boltzmann collision integral and possess the same collision invariants as the Boltzmann equation. Both the BGK and ES models satisfy Boltzmann's H-theorem, which expresses the increase of entropy in a gas with time. The desired property of kinetic models is to reproduce the Boltzmann-equation transport coefficients: viscosity, thermal conductivity, and species diffusivity.

The main goal of this paper is the detailed comparison of the above three numerical approaches for simulating non-continuum flows. More specifically, the NSSJ method, the DSMC method, and the ES kinetic model are applied to the gas-filled region surrounding a microbeam of rectangular cross section lying parallel to an adjacent substrate. The microbeam is infinitely long in the third dimension, so the situation is mathematically two-dimensional. The microbeam either moves vertically at a constant velocity or is stationary but at an elevated temperature with respect to the substrate. All three methods are applied to model gas damping of a moving microbeam, and additional ES simulations are used to study the effects of the Knudsen force on a heated microbeam over a wide range of Knudsen numbers.

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II. Numerical Methods

A. NSSJ Simulations

The NSSJ method is used to obtain gas-flow solutions around a moving microbeam in the slip and transitional regimes. The microbeam has a rectangular cross section that lies parallel to the adjacent planar substrate. Flow in a two-dimensional slice is considered. The flow is assumed to be isothermal, incompressible, and quasi-static. The quasi-static assumption implies two simplifications. First, the steady Stokes equations are used instead of the full Navier-Stokes equations. Second, the moving microbeam geometry is replaced by a stationary geometry with the microbeam velocity imposed on its surface as a boundary condition. The first-order velocity-slip boundary condition[5] is used.

The computational fluid dynamics code FIDAP[6] is used to simulate the gas flow. Since the governing equations and boundary conditions are linear in the velocity and the pressure, the simulations are performed nondimensionally with the following parameters set equal to 1: the mass density ρ (irrelevant), the viscosity μ, the beam velocity U, and the gap height G. Five values of the slip length Λ are examined: 0, 0.1, 0.2, 0.5, and 1. For each of these values, four values of the beam width W are considered: 10, 20, 40, and 80. The computations use a symmetry boundary condition, so only half of the microbeam is included in the computational domain. Rectangular bi-quadratic elements are employed,[6] and extensive mesh refinement studies are carried out to ensure that the NSSJ numerical solutions are accurate to within 1%.

B. DSMC Simulations

The DSMC method is also used to simulate quasi-static gas flow around a moving microbeam with the same geometry. The DSMC simulations have issues not present in the NSSJ simulations. First, DSMC is a compressible method. Therefore, the microbeam velocity must be small enough to ensure that the pressure drop along the gap is no more than a few percent of the ambient pressure p_0. Second, the smallness of the gas velocity (1 m/s) with respect to molecular speeds (400 m/s) necessitates very long averaging times to reduce statistical noise to acceptable levels. Third, simulations at atmospheric conditions (mean free path λ of 65 nm) require very fine mesh cells with respect to the beam width, with proportionally small time steps. Fourth, a subsonic-inflow boundary condition is required. A boundary condition for subsonic inflow is developed that treats the region behind the boundary as a source of gas at the inflow conditions.[5] Every

exiting computational molecule is reflected, and additional computational molecules are injected to produce the prescribed mass flow. The positions, velocities and internal energies of these computational molecules are selected to reproduce the statistics of a gas of prescribed number density and temperature that enters the domain with the prescribed velocity.

Due to symmetry, only half of the microbeam is included in the computational domain. The following boundary conditions are used: (a) the specular-reflection boundary condition is applied on the symmetry line and on the upper and right sides of the domain; (b) the subsonic inflow and outflow boundary conditions are applied on the top and bottom microbeam surfaces, respectively; (c) the diffuse-reflection boundary condition is used on the substrate and on the microbeam side. An accommodation coefficient of 1 is used for all solid surfaces, so the slip length and the mean free path are equal: $\Lambda = \lambda$.

DSMC simulations are performed for the following conditions. The microbeam thickness and gap height are both 2 μm, and microbeam widths of 10, 20, and 40 μm are considered. The gas is nitrogen at 295 K. Pressures are considered that yield slip lengths of $\Lambda = 0.2$, 0.4, 1, and 2 μm, so the flow Knudsen number has the values 0.1, 0.2, 0.5, and 1. The variable soft sphere (VSS) collision model is used with nitrogen properties.[2] Square mesh cells that are 0.1 μm wide and time steps of 0.02 ns are used. Initially, each cell is populated with 30 computational molecules. The transient phase of a simulation proceeds for 0.02 ms (10^6 time steps), and steady-state averaging is performed for 0.04 ms (2×10^6 time steps). All simulations are performed using the DSMC code Icarus[7] on the TFLOPS-class ASCI Red massively parallel computer at Sandia.

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C. ES Simulations

The ellipsoidal statistical (ES) kinetic equation is also used to simulate quasi-static gas flow around a moving microbeam as discussed above as well as around a heated but stationary microbeam. The motivation for this approach is as follows. The computational cost of DSMC simulations for low-speed flows becomes large because of the low signal-to-noise ratio.[8] The ES kinetic equation is an alternative deterministic computational approach that solves an approximate form of the Boltzmann equation:

$$u\frac{\partial f}{\partial x} + v\frac{\partial f}{\partial y} = \nu(f_0 - f), \tag{1}$$

where $f = f(x, y, u, v, w)$ is the distribution function, x and y are Cartesian coordinates, u, v, and w are velocity components, and ν is the collision frequency. For the conventional Bhatnagar-Gross-Krook (BGK) model,[3] $f_0 = f_M = n(2\pi RT)^{-3/2}\exp(-|\vec{c}|^2/2RT)$ is the local equilibrium Maxwell-Boltzmann distribution function. For the ellipsoidal statistical (ES) model,[9] $f_0 = f_G$ is the local anisotropic three-dimensional Gaussian:

$$f_G = \frac{n}{\sqrt{(2\pi)^3\det[\lambda_{ij}]}}\exp(-\epsilon_{ij}c_ic_j), \qquad \lambda_{ij} = (\frac{1}{\Pr})RT\delta_{ij} + \frac{1-1/\Pr}{\rho}p_{ij}, \tag{2}$$

where $[\epsilon] = [\lambda]^{-1}$, $\vec{c} = \vec{u} - \vec{\bar{u}}$ is the thermal velocity, p_{ij} is the pressure tensor, and Pr is the Prandtl number. If $\Pr = 1$, then $f_G = f_M$, and Eq. (1) gives the original BGK model. Equation (1) is a non-linear integro-differential equation that uses a simplified form of the collision integral compared to the Boltzmann equation and is applicable to model gas flows with arbitrary Knudsen numbers and degree of flow non-equilibrium.

The above BGK-type model, Equation (1), can be solved using a finite-difference method and standard discrete-ordinate method procedures[10,11] for interpolation of the distribution function in velocity space. First, for two-dimensional problems, two reduced distribution functions are introduced:

$$g = \int_{-\infty}^{\infty} f dw, \quad h = \int_{-\infty}^{\infty} f w^2 dw.$$

Polar coordinates in velocity space are introduced as follows:

$$u = S\sin\phi, \qquad v = S\cos\phi.$$

Discrete speeds S_δ and velocity angles ϕ_σ are introduced as the ordinates of the quadratures for integration of the velocity distribution function. The gas flow parameters are then calculated as

$$n = \sum_\delta\sum_\sigma P_\delta P_\sigma g_{\delta\sigma}, \quad n\bar{u} = \sum_\delta\sum_\sigma P_\delta P_\sigma S_\delta \sin\phi_\sigma g_{\delta\sigma},$$

$$n\bar{v} = \sum_{\delta}\sum_{\sigma} P_\delta P_\sigma S_\delta \cos\phi_\sigma g_{\delta\sigma}, \quad \frac{3}{2}nT = \sum_{\delta}\sum_{\sigma} P_\delta P_\sigma (h_{\delta\sigma} + S_\delta^2 g_{\delta\sigma}),$$

where P_δ and P_σ are quadrature weights. Finally, the resulting system of equations

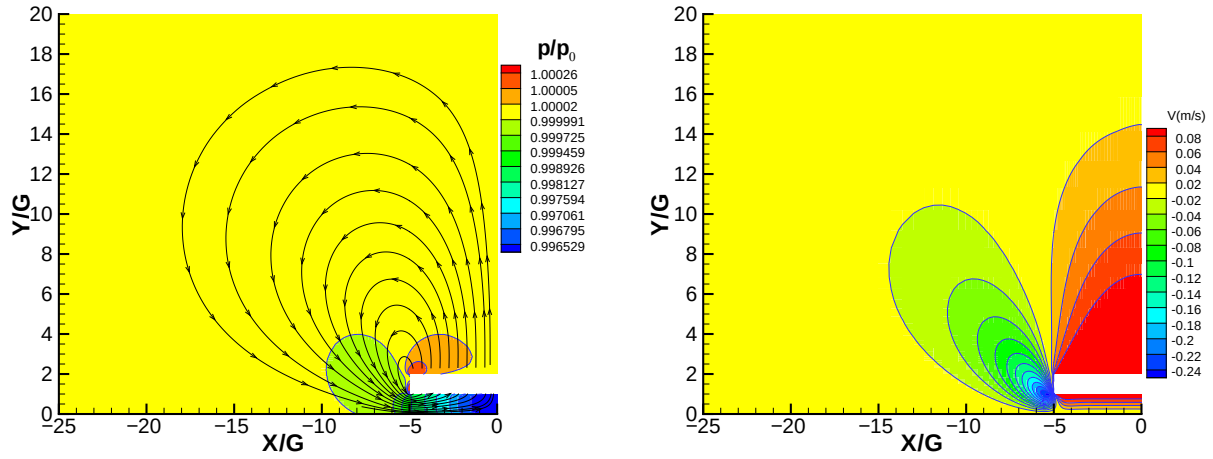
$$S_\delta \sin\phi_\sigma \frac{\partial g_{\delta\sigma}}{\partial x} + S_\delta \cos\phi_\sigma \frac{\partial g_{\delta\sigma}}{\partial y} = \nu(g^0_{\delta\sigma} - g_{\delta\sigma}) \tag{3}$$

$$S_\delta \sin\phi_\sigma \frac{\partial h_{\delta\sigma}}{\partial x} + S_\delta \cos\phi_\sigma \frac{\partial h_{\delta\sigma}}{\partial y} = \nu(h^0_{\delta\sigma} - h_{\delta\sigma}) \tag{4}$$

is solved by the finite-difference method. The Gauss-Hermite half-range quadrature[12] of order 16 and the three-eighths rule with 144 ordinates are used for the integrations over speed and velocity angle, respectively.

III. Gas Damping of a Moving Microbeam

In this section, ES simulations are compared to NSSJ and DSMC simulations for the moving-microbeam geometry described above. In particular, differences are elucidated in the transitional regime, that is, for Kn > 0.1.



(a) (b)

Figure 1. ES flow fields and streamlines for microbeam with W/G = 10, Kn = 0.1, and U = 0.1 m/s: (a) pressure and streamlines; (b) y-component of velocity.

Figure 1 shows the pressure and the y-component of velocity as well as streamlines calculated by the ES model for the case of $W/G = 10$, $U = 0.1$ m/s, and Kn $= 0.1$. The structure of the moving-microbeam flow is qualitatively the same as predicted by NSSJ and DSMC simulations.[5] The streamline plot shows that the gas moves upward from the top surface of the microbeam, around the microbeam edge, into the gap, and toward the bottom surface of the microbeam. The pressure contours extend beyond the gap edge to a distance of several gap heights. The pressure on the upper surface of the microbeam is slightly larger than the ambient pressure because of the upward motion of the microbeam.

Figure 2 shows the ES, DSMC, and NSSJ pressure deviations from ambient normalized by the gas-damping pressure scale, $(p - p_0)/p_s$, where the gas-damping pressure scale is $p_s = 12\mu U/G$. Four different values of the Knudsen number are considered: Kn $= 0.1$, 0.2, 0.5, and 1.0. The numerical predictions of the three methods agree to within 10% for Kn $= 0.1$. For larger Knudsen numbers, the NSSJ simulations overestimate the deviation of the pressure from ambient.

Figure 3 shows a plot of the damping coefficient Γ (force per unit length per unit velocity) versus the ambient pressure p_0 as determined by the NSSJ, DSMC, and ES methods. These values are obtained by integrating the pressure profiles in Fig. 2 over the surface of the microbeam and dividing the force per unit length thus obtained by the velocity of the beam. All three methods are seen to be in agreement at the

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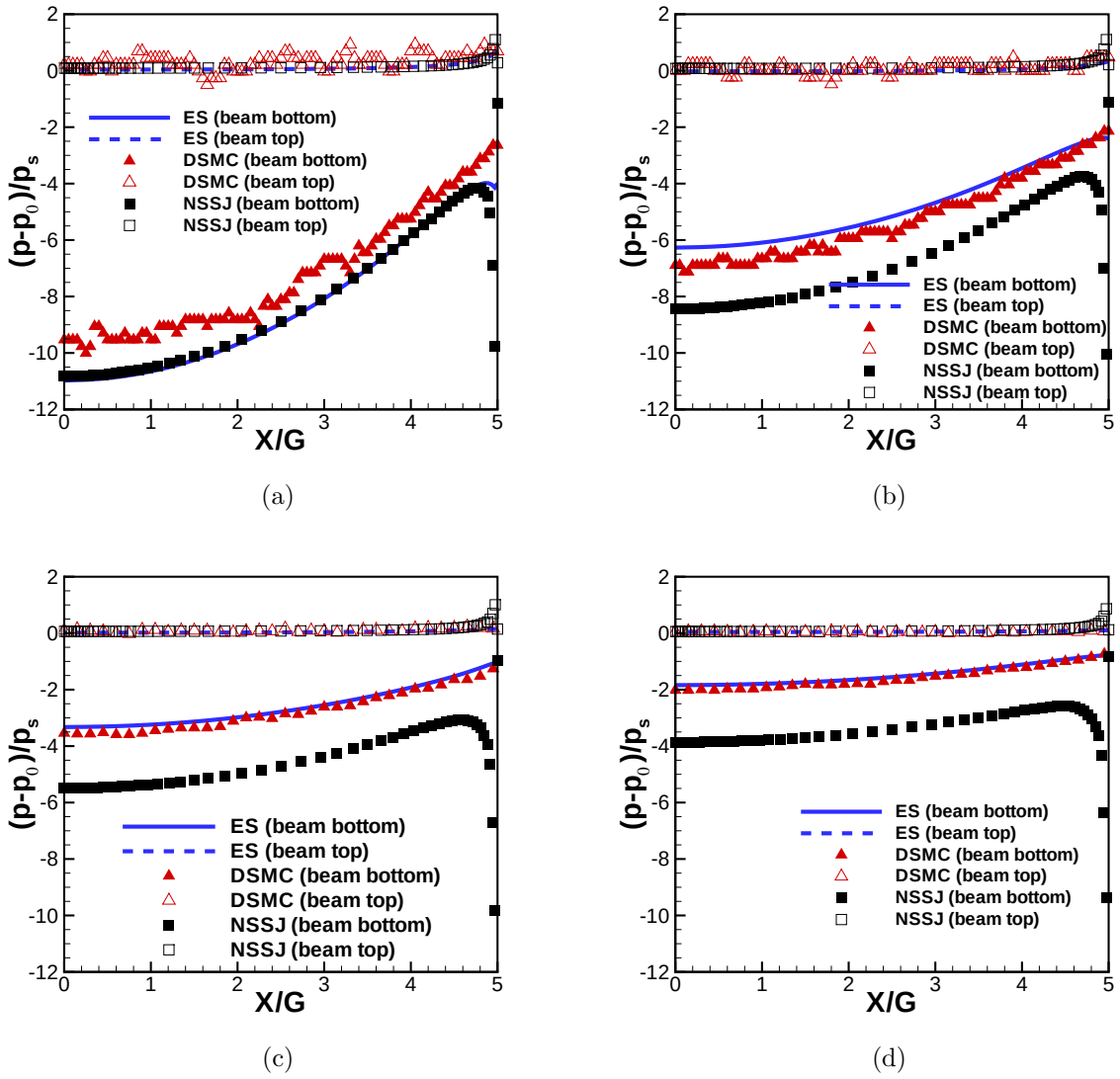

Figure 2. NSSJ, DSMC, and ES pressure distributions along the surface of microbeam with W/G = 10: (a) Kn = 0.1; (b) Kn = 0.2; (c) Kn = 0.5; (d) Kn = 1.

largest pressure investigated (32.5 kPa), which corresponds to a Knudsen number Kn of 0.1. At smaller pressures, which represent larger values of the Knudsen number, the ES values are in good agreement with the DSMC values, whereas the NSSJ values overpredict the DSMC values. Thus, the ES values are able to predict the damping coefficient with reasonable accuracy throughout the transitional regime.

IV. Knudsen Force on a Heated Microbeam

In many applications involving microcantilever beams, there exists a temperature difference between the cantilever and the substrate surface. A piezoresistive cantilever is always at a higher temperature because of resistive heating. Moreover, in the commonly used optical beam deflection technique, the cantilever is at an elevated temperature because of laser heating of the surface.[13] When the mean free path of molecules is comparable to the gap height and a temperature difference exists between the beam and the substrate, Knudsen forces arising from thermal creep and thermal transpiration can significantly affect microbeam displacement. Experimental observations of the effect of this Knudsen force have been reported recently.[13,14]

In this work, two-dimensional ES simulations are applied to numerically investigate the flow generated

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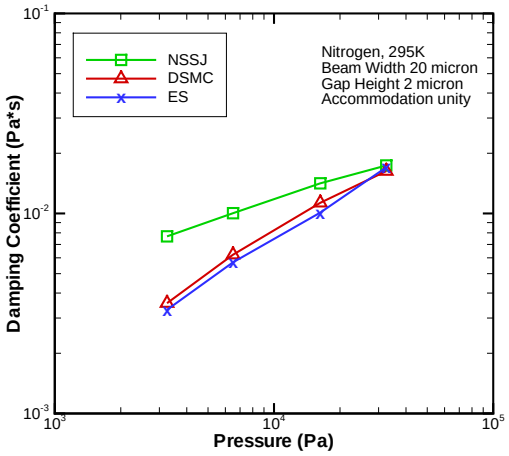

Figure 3. Gas-damping coefficient vs. gap height for the NSSJ, DSMC, and ES methods.

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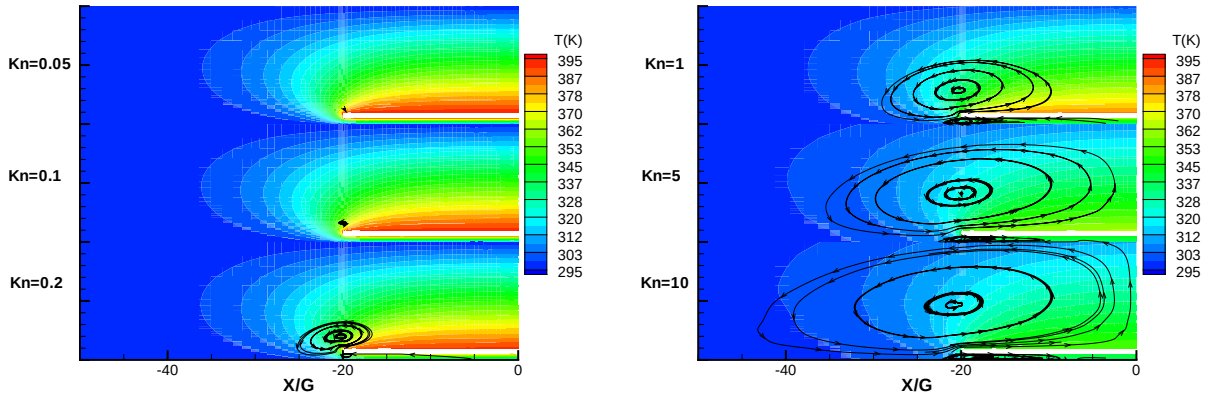
by the Knudsen effect on a heated microbeam. The Knudsen force is calculated for a wide range of Knudsen numbers. In the cases considered, a microbeam with a width-to-height ratio of 80 is maintained at a temperature of 395 K while the substrate and ambient gas away from the beam are at a temperature of 295 K. The Knudsen number based on gap height is varied from 0.05 to 50.

Figure 4 shows the flow structure around the heated microbeam predicted by the ES simulations for different Knudsen numbers. A counter-clockwise vortex develops at the beam tip at Knudsen numbers larger than 0.1. Another important feature of rarefied gas flow driven by temperature gradients is the separation of pressure tensor components. As J. C. Maxwell explains:[15] "When inequalities of temperature exist in a gas, the pressure at a given point is not the same in all directions, and the difference between maximum and minimum pressure at a point may be of considerable magnitude when the density of the gas is small enough." Figure 5 shows the distribution of the principal components of the pressure tensor along the bottom and upper surfaces of the heated microbeam at Kn = 1. The ES simulations show that the separation between the pressure components increases with increasing Knudsen number. This flow effect can be predicted numerically only by kinetic methods such as DSMC and ES models but cannot be reproduced by NSSJ simulations at present.

The ES-calculated Knudsen force on the heated microbeam is plotted in Fig. 6 as a function of the Knudsen number. The Knudsen force has a maximum in the transitional regime around Kn ≈ 2. A similar non-monotonic variation of the displacement of a heated microbeam is observed experimentally by Passian *et al.*[13]

V. Conclusions

Numerical investigations of the gas flow structure and the gas-damping force on moving and heated microbeams are carried out using ES, DSMC, and NSSJ simulations. The gas-damping coefficients on a moving microbeam for quasi-static isothermal conditions are estimated by the three numerical methods for Knudsen numbers from 0.1 to 1.0. NSSJ simulations overestimate the gas-damping force for Knudsen numbers larger than 0.1, while the ES and DSMC methods are in good agreement for the slip and transitional flow regimes. The flow structure and the Knudsen force for a heated microbeam are calculated by the ES model over a wide range of Knudsen numbers. The Knudsen force peaks in the transitional regime at Kn ≈ 2, and the numerically predicted variation of the force is consistent with experimental observations of the displacement of a heated microbeam.



(a) (b)

Figure 4. Temperature field and vortex streamlines for heated microbeam at different Knudsen numbers.

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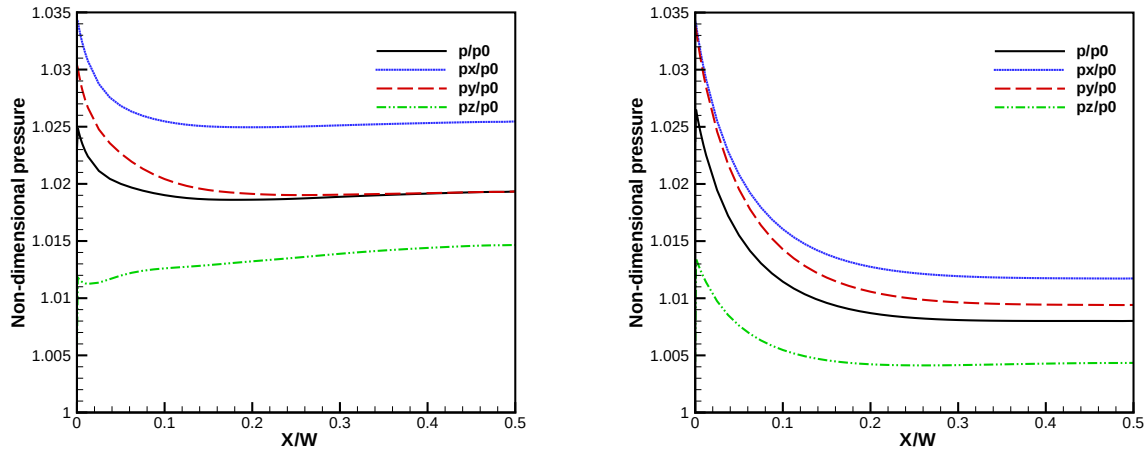

(a) (b)

Figure 5. Pressure tensor components on (a) lower and (b) upper surfaces of heated microbeam: Kn = 1.

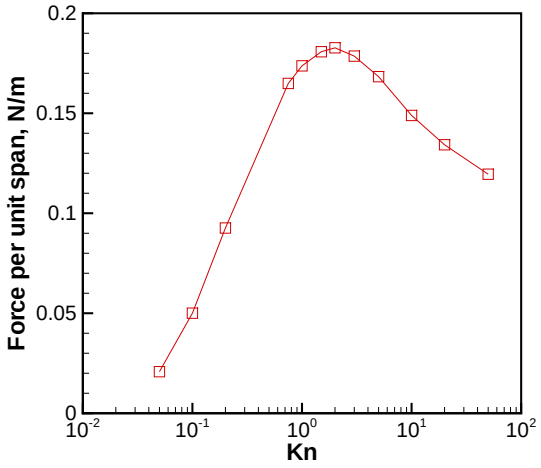

Figure 6. Force per unit span on heated microbeam at different Knudsen numbers.

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