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KINETIC THEORY APPROACH TO THE STUDY OF MEMS

BY

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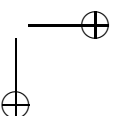
Abstract

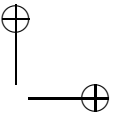
We survey some recent applications of the Boltzmann equation to the study of MEMS.

1. Introduction

I am pleased and honored to contribute to this special issue dedicate to Yoshio Sone, whom I have been knowing for about forty years and whose research has been frequently very close to areas of my interest. In particular, he has been working on rarefied flows at low speed, an area of research that has received a renovated attention in the last few years because of its important role in the study of MEMS. In order to explain these developments, we recall that the presence of a fluid film is known to reduce the sliding friction between solid objects. Although one usually thinks of a liquid (typically, oil), the case of a gas lubricant (typically, air) is also very important in several applications. Sometimes, problems of gas lubrication are not so obvious, because air is so easily available that one tends to disregard its presence. As technology expands and the size of components becomes smaller and smaller, the role of rarefied gases as lubricants becomes increasingly important. We recall that a gas is called rarefied when the mean free path between collisions (of the order of 100 microns at room pressure and temperature) is comparable with the a typical size of the region where it flows. A typical example is provided by modern computers: the read/write head must be as close as possible to a rotating disk, and the air in between has accordingly a thickness of the order of a mean free path.

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In lubrication theory, the thickness of the gas layer is extremely small compared with its lateral dimensions. Properly handled, this observation can be used to eliminate from the equations the dependence upon one of the three space variables. This possibility was exploited since long time by the famous hydrodynamicist Osborne Reynolds [1] to integrate the mass balance equation across the layer and to use the linearized Navier–Stokes equation for momentum balance to evaluate the quantities appearing as integrands. Fortunately, Reynolds’s argument can be extended to rarefied gases; the only difference is that the linearized Boltzmann equation (sect. 3) must now be used to evaluate the averaged velocity components in the mass balance equation.

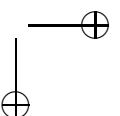
From a very superficial consideration of the matter one might expect that the main problem of lubrication theory is to predict the friction which results from a given configuration of solid objects. However, a little more reflection reveals that the real problem is quite different. Lubricating layers are usually found between two solid bodies which are acted upon by forces (such as gravity) tending to push them together. To carry this load, the gas layer must develop normal stresses, largely dominated by pressure. Thus the first task of lubrication theory is to predict the pressure distribution and from it the load-carrying capacity. Thus we must relate the velocity components to the pressure gradients and to the motion of the solid surfaces bounding the gas layer. Since the variations of thickness are very slow, this result is obtained by solving highly idealized problems between parallel plates, such as plane Couette and Poiseuille flows, which will be considered in Sect. 4. Thus these problems, far from being didactic exercises, play a very important role in applications of enormous practical importance.

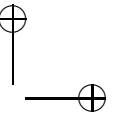
2. The Boltzmann Equation

We briefly recall the basic structure of the Boltzmann equation [2, 3, 4, 5]

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} = Q(f, f) \tag{1}$$

Here $f = f(\mathbf{x}, \mathbf{v}, t)$ is the distribution function, giving the probability density of finding a gas molecule at position \mathbf{x} with velocity $\boldsymbol{\xi}$ at time t . $Q(f, f)$ is the collision term, quadratic in f .





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The solutions describing equilibria of the Boltzmann equation are the so-called Maxwellians, i.e. distributions of the form

$$M = \rho_0(2\pi RT_0)^{-3/2} \exp[-|\boldsymbol{\xi} - \mathbf{v}_0|^2/(2RT_0)] \quad (2)$$

where ρ_0 , \mathbf{v}_0 , T_0 are parameters having the meaning of density, bulk velocity and temperature in an equilibrium state. The vector \mathbf{v}_0 is usually taken to be zero.

We can look for solutions written as

$$f = M(1 + h). \quad (3)$$

Then the Boltzmann equation takes on the form:

$$\frac{\partial h}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial h}{\partial \mathbf{x}} = Lh + \Gamma(h, h) \quad (4)$$

where L is the linearized collision operator:

$$Lh = 2M^{-1}Q(Mh, M) \quad (5)$$

and $\Gamma(h, h)$ the nonlinear part (assumed to be small compared to the linear one):

$$\Gamma(h, h) = M^{-1}Q(Mh, Mh). \quad (6)$$

Here $Q(f, g)$ is the bilinear symmetric operator uniquely associated with $Q(f, f)$. The rigorous theory for solutions of the form (3) was given by S. Ukai (see Ref.[6] for more details).

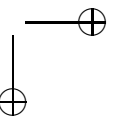
In many applications, the collision term in the Boltzmann equation is replaced by the so-called BGK model (see Refs.[2] and [3] for more details):

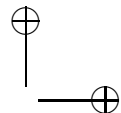
$$J(f) = \nu[\Phi(\boldsymbol{\xi}) - f(\boldsymbol{\xi})] \quad (7)$$

where the collision frequency ν depends on the local density ρ and the local temperature T , whereas Φ is the local Maxwellian:

$$\Phi = \rho(2\pi RT)^{-3/2} \exp[-|\boldsymbol{\xi} - \mathbf{v}|^2/(2RT)] \quad (8)$$

having the same density, temperature and bulk velocity \mathbf{v} as f . Notice that from the viewpoint of nonlinearity the BGK model is worse than the





Boltzmann equation, but offers the advantage that one can derive integral equations for ρ , \mathbf{v} , T . The linearized form reads:

$$L_{BGK} = \nu_0 \left[\int \hat{M}(\boldsymbol{\xi}_*) h(\boldsymbol{\xi}_*) d\boldsymbol{\xi}_* + \frac{\boldsymbol{\xi}}{RT_0} \cdot \int \boldsymbol{\xi}_* \hat{M}(\boldsymbol{\xi}_*) h(\boldsymbol{\xi}_*) d\boldsymbol{\xi}_* + \frac{2}{3} \left(\frac{|\boldsymbol{\xi}|^2}{2RT_0} - \frac{3}{2} \right) \int \left(\frac{|\boldsymbol{\xi}_*|^2}{2RT_0} - \frac{3}{2} \right) \hat{M}(\boldsymbol{\xi}_*) h(\boldsymbol{\xi}_*) d\boldsymbol{\xi}_* - h \right] \quad (9)$$

3. The Modified Reynolds Equation

The starting point to obtain the rarefied version of the Reynolds equation for lubrication is the mass balance equation, Eq. (4.18), which, as we have seen, is a consequence of the Boltzmann equation. This equation is considerably simplified by the fact that the variations of density do not show up for slow motion in the steady case, which is the most important in applications and we shall consider henceforth. Thus

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0, \quad (10)$$

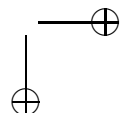
where the three components of the bulk velocity are denoted by u , v , w .

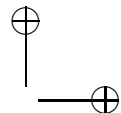
Let us consider a layer of gas between two walls located at $z = 0$ and $z = D(x, y)$; the lower wall moves in its own plane. If we integrate Eq. (10) across the layer, we obtain

$$\frac{\partial}{\partial x} \int_0^D u dz + \frac{\partial}{\partial y} \int_0^D v dz = 0. \quad (11)$$

Since the problem is linear and the pressure gradient is assumed to be constant across the layer, each component u , v is proportional to the sum of the velocities given by a Poiseuille flow with pressure gradient dp/dx , dp/dy respectively and a Couette flow with the lower wall moving with velocity components U and V .

In the case of Couette flow the evaluation of the integral: $F_C^{(1)} = \int_0^D u_C dz$ is easy, if the walls are assumed to be identical. In fact, in this situation the profile is antisymmetric with respect to the midpoint and $F_C^{(1)} = \frac{UD}{2}$. Similarly $F_C^{(2)} = \int_0^D v_C dz = \frac{VD}{2}$. The behavior of the flow





rate for plane Poiseuille flow is much more complicated and is given by

$$F_P^{(1)} = \int_0^D u_P dz = -\frac{1}{\rho_0 \sqrt{2RT_0}} \frac{\partial p}{\partial x} D^2 Q(\delta); \quad (12)$$

$$F_P^{(2)} = \int_0^D v_P dz = -\frac{1}{\rho_0 \sqrt{2RT_0}} \frac{\partial p}{\partial y} D^2 Q(\delta) \quad (13)$$

where δ is the ratio between the distance and the (unperturbed) mean free path:

$$\delta = \frac{pD}{\mu \sqrt{2RT}}$$

and $Q(\delta)$ is the nondimensional flow rate which can be obtained by solving the problem of plane Poiseuille flow. Thus the modified Reynolds equation reads as follows

$$\frac{\partial}{\partial x} \left[\frac{\partial p}{\partial x} D^2 Q(\delta) \right] + \frac{\partial}{\partial y} \left[\frac{\partial p}{\partial y} D^2 Q(\delta) \right] = \rho_0 \sqrt{2RT_0} \left[\frac{U}{2} \frac{\partial D}{\partial x} + \frac{V}{2} \frac{\partial D}{\partial y} \right]. \quad (14)$$

Given $D = D(x, y)$, this is an (elliptic) partial differential equation for p which must be solved for an assigned value of p (usually constant) at the boundary.

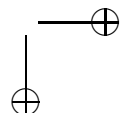
We have assumed so far that the linearization assumption holds everywhere. It may turn out, however, that the pressure undergoes a significant change. In this case, one can still utilize the linearized Boltzmann equation to compute the local flow rate, but one should use the local pressure p throughout, rather than the unperturbed pressure p_0 . The modified Reynolds equation then reads as follows

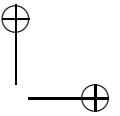
$$\frac{\partial}{\partial x} \left[\frac{D^2 Q(\delta)}{\sqrt{2RT}} \frac{\partial p}{\partial x} \right] + \frac{\partial}{\partial y} \left[\frac{D^2 Q(\delta)}{\sqrt{2RT}} \frac{\partial p}{\partial y} \right] = \frac{1}{2} \left[U \frac{\partial(\rho D)}{\partial x} + V \frac{\partial(\rho D)}{\partial y} \right]. \quad (15)$$

This generalized Reynolds equation was first introduced by Fukui and Kaneko [7, 8].

In the continuum limit we have

$$Q(\delta) = \frac{1}{6} \frac{pD}{\mu \sqrt{2RT}}$$





and Eq. (15) becomes

$$\frac{\partial}{\partial x} \left[\frac{\rho D^3}{\mu} \frac{\partial p}{\partial x} \right] + \frac{\partial}{\partial y} \left[\frac{\rho D^3}{\mu} \frac{\partial p}{\partial y} \right] = 6 \left[U \frac{\partial(\rho D)}{\partial x} + V \frac{\partial(\rho D)}{\partial y} \right] \quad (16)$$

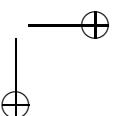
which is essentially the equation originally given by Reynolds [1].

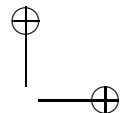
4. The Reynolds Equation and the Poiseuille-Couette Problem

The micromachinery fabrication techniques have become more and more mature in the last ten years. In particular, the micro-electro-mechanical systems (MEMS) developed rapidly and found many applications in micro-electronics, medicine, biology, optics, aerospace and other high technology fields. Both experimental and computational efforts have been undertaken to understand the specific features of the microscale flows. A basic constituent of the MEMS devices is the microchannel, the region between two parallel plates that can reveal many specific features of the low speed internal flows in microdevices. Typically the first devices were integrated microchannel/pressure sensor systems. The Knudsen number at the outlet of the channel at room conditions is 0.05 for nitrogen, and even higher for helium; hence the flow is surely beyond the slip flow regime. The pressure distribution along the channel and the flow rates across these channels are found to deviate from the linear distribution of the Poiseuille flow. Monte Carlo methods were used to simulate microchannel flows but they meet with the excessively high demands to the storage and computation time. The gradual regulation of the inlet and outlet boundary conditions of the channel seems to be tremendously difficult for DSMC in solving the long channel flows. In fact the typical DSMC simulation of the micro channel flow is limited to high speeds. Recently, the so called information preservation (IP) method was proposed[9, 10]; it uses a conservative scheme and a super-relaxation technique, with results in excellent agreement with experimental data.

However, the kinetic theory of MEMS does not require heavy computational tools. The generalized Reynolds equation can be used to calculate the gas film lubrication problem provided that the flow rate of Poiseuille flow is calculated from the linearized Boltzmann equation. The case of a microchannel with parallel plates was treated by C. Shen [11].

Following Refs.[12] and [13], let us consider again two plates separated by a distance D and a gas flowing parallel to them, in the x direction, due





to a pressure gradient. The lower boundary ($z = -D/2$) moves to the right with velocity U , while the upper boundary ($z = D/2$) is fixed. Both boundaries are held at a constant temperature T_o . However, at variance with our previous discussions, we assume the gas-surface interaction to be different at the wall.

As usual, if the pressure gradient and the velocity U are taken to be small, it can be assumed that the Boltzmann equation can be linearized about a Maxwellian. If we assume the linearized BGK model for the collision operator, the Boltzmann equation reads:

$$\frac{1}{2}k + c_z \frac{\partial Z}{\partial z} = \frac{1}{\ell} \left[\pi^{-\frac{1}{2}} \int_{-\infty}^{+\infty} e^{-c_{z1}^2} Z(z, c_{z1}) dc_{z1} - Z(z, c_z) \right] \quad (17)$$

where by definition

$$Z(z, c_z) = \pi^{-1} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} e^{-c_x^2 - c_y^2} c_x h(z, \mathbf{c}) dc_x dc_y \quad (18)$$

$$k = \frac{1}{p} \frac{\partial p}{\partial x} = \frac{1}{\rho} \frac{\partial \rho}{\partial x}$$

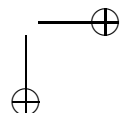
with p and ρ being the gas pressure and density, respectively, and ℓ is the mean free path. Consequently, the bulk velocity of the gas is given by:

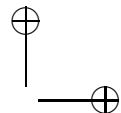
$$q(z) = \pi^{-\frac{1}{2}} \int_{-\infty}^{+\infty} e^{-c_{z1}^2} Z(z, c_{z1}) dc_{z1} \quad (19)$$

From Eq. (17) we obtain the integral relation:

$$Z(z, c_z) = \exp\left(-\left(z + \frac{D}{2} \text{sgn} c_z\right)/(c_z \ell)\right) Z\left(-\frac{D}{2} \text{sgn} c_z, c_z\right) + \int_{-\frac{D}{2} \text{sgn} c_z}^z \exp\left(\frac{-|z-t|}{|c_z| \ell}\right) [q(t) - k\ell/2]/(c_z \ell) dt \quad (20)$$

with the values at the boundary, $Z(-\frac{D}{2} \text{sgn} \zeta, \zeta)$, depending on the model of boundary condition chosen. This problem was first treated by Cercignani and Daneri [12] for completely diffusing walls. In the following, we will consider the Maxwell boundary conditions as in Ref. [13] and consider two walls having different physical properties, i.e. with two accommodation coefficients (α_1, α_2). In this case, the boundary conditions can be written





as:

$$\begin{aligned} Z^+(D/2, \zeta) &= (1 - \alpha_1)Z^-(D/2, -\zeta) \\ Z^+(-D/2, \zeta) &= \alpha_2 U + (1 - \alpha_2)Z^-(-D/2, -\zeta) \end{aligned}$$

where U is expressed in units of $(2RT_o)^{1/2}$; $Z^-(-D/2, \zeta)$, $Z^-(D/2, \zeta)$ are the distribution functions of the molecules impinging upon the walls; similarly, $Z^+(-D/2, \zeta)$, $Z^+(D/2, \zeta)$ are the distribution functions of the molecules reemerging from the same walls.

Once the function at the boundary, $Z(-\frac{D}{2}\text{sgn}\zeta, \zeta)$, has been evaluated following the analytical procedure reported in [13, 14], the substitution of the integral formula (20) in the definition (19) of $q(z)$ gives the following expression for the bulk velocity of the gas:

$$q(z) = \frac{1}{2}kl[1 - \psi_p(u)] + U\psi_c(u) \quad (21)$$

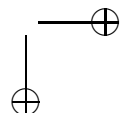
Eq. (21) shows that the gas velocity is induced by the superposition of two distinct effects. The gas moves by an imposed pressure gradient (Poiseuille flow) and by the shear driven flow due to the motion of the bottom surface (Couette flow). The non-dimensional functions $\psi_p(u)$ and $\psi_c(u)$, giving the Poiseuille and Couette contributions, respectively, satisfy the following integral equations:

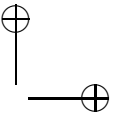
$$\begin{aligned} \psi_p(u) = 1 + \frac{1}{\sqrt{\pi}} \int_{-\frac{\delta}{2}}^{\frac{\delta}{2}} dw \psi_p(w) \left\{ (1 - \alpha_1)S_{-1}(\delta - u - w) + (1 - \alpha_2)S_{-1}(\delta + u + w) \right. \\ \left. + (1 - \alpha_1)(1 - \alpha_2)[S_{-1}(2\delta - u + w) + S_{-1}(2\delta + u - w)] \right. \\ \left. + T_{-1}(|u - w|) \right\} \quad (22) \end{aligned}$$

$$\begin{aligned} \psi_c(u) = \frac{\alpha_2}{\sqrt{\pi}} \left[T_o \left(\frac{\delta}{2} + u \right) + (1 - \alpha_1)S_o \left(\frac{3}{2}\delta - u \right) + (1 - \alpha_1)(1 - \alpha_2)S_o \left(\frac{5}{2}\delta + u \right) \right] \\ + \frac{1}{\sqrt{\pi}} \int_{-\frac{\delta}{2}}^{\frac{\delta}{2}} dw \psi_c(w) \left\{ (1 - \alpha_1)S_{-1}(\delta - u - w) + (1 - \alpha_2)S_{-1}(\delta + u + w) \right. \\ \left. + (1 - \alpha_1)(1 - \alpha_2)[S_{-1}(2\delta - u + w) + S_{-1}(2\delta + u - w)] \right. \\ \left. + T_{-1}(|u - w|) \right\} \quad (23) \end{aligned}$$

where $T_n(x)$ is the Abramowitz function defined by

$$T_n(x) = \int_0^{+\infty} t^n \exp(-t^2 - x/t) dt$$





$S_n(x)$ is a generalized Abramowitz function defined by

$$S_n(x, \delta, \alpha_1, \alpha_2) = \int_0^{+\infty} \frac{t^n \exp(-t^2 - x/t)}{1 - (1 - \alpha_1)(1 - \alpha_2) \exp(-2\delta/t)} dt$$

and the following non-dimensional variables have been introduced:

$$\delta = D/\ell, \quad w = t/\ell, \quad u = z/\ell.$$

Using Eq. (21), the flow rate (per unit time through unit thickness) defined by:

$$F = \rho \int_{-D/2}^{D/2} q(z) dz \quad (24)$$

can be expressed as the sum of the Poiseuille flow (F_p) and the Couette flow (F_c) as follows:

$$F = F_p + F_c = -\frac{\partial p}{\partial x} D^2 Q_p(\delta, \alpha_1, \alpha_2) + \frac{\rho U D}{2} Q_c(\delta, \alpha_1, \alpha_2) \quad (25)$$

where

$$Q_p(\delta, \alpha_1, \alpha_2) = -\frac{1}{\delta} + \frac{1}{\delta^2} \int_{-\delta/2}^{\delta/2} \psi_p(u) du$$

$$Q_c(\delta, \alpha_1, \alpha_2) = \frac{2}{\delta} \int_{-\delta/2}^{\delta/2} \psi_c(u) du$$

are the non-dimensional volume flow rates.

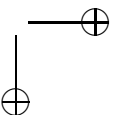
5. The Generalized Reynolds Equation for Unequal Walls

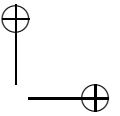
One can easily extend the generalized Reynolds equation to the case of unequal walls:

$$\frac{d}{dx} \left(\frac{dp}{dx} D^2 Q_p(\delta, \alpha_1, \alpha_2) - \frac{\rho U D}{2} Q_c(\delta, \alpha_1, \alpha_2) \right) = 0 \quad (26)$$

For the purpose of a direct comparison with the classical Reynolds equation (16), let us introduce the Poiseuille relative flow rate:

$$\tilde{Q}_p(\delta, \alpha_1, \alpha_2) = \frac{Q_p(\delta, \alpha_1, \alpha_2)}{Q_{con}} \quad (27)$$





where $Q_{con} = \delta/6$. If one introduces the following dimensionless quantities

$$X = x/l, \quad P = p/p_o, \quad H = D/D_o,$$

the rarefaction parameter δ can be expressed as: $\delta = \delta_o PH$, where δ_o is the characteristic inverse Knudsen number defined by the minimum film thickness, D_o , and the ambient pressure p_o as:

$$\delta_o = \frac{p_o D_o}{\mu \sqrt{2RT_o}}.$$

Finally, assuming that the heat generation in the gas is very small, so that an isothermal process can be considered, the non-dimensional generalized Reynolds equation reads:

$$\frac{d}{dX} \left(\tilde{Q}_p(\delta_o PH, \alpha_1, \alpha_2) PH^3 \frac{dP}{dX} - Q_c(\delta_o PH, \alpha_1, \alpha_2) \Lambda PH \right) = 0. \quad (28)$$

The bearing number Λ in Eq. (28) is defined as

$$\Lambda = \frac{6\mu Ul}{p_o D_o^2} \quad (29)$$

where μ is the viscosity coefficient. If the two walls are identical ($\alpha_1 = \alpha_2 = \alpha$), the Couette flow rate is independent of the Knudsen number regardless of the value of the accommodation coefficient α and Eq. (28) reduces to the generalized Reynolds equation introduced by Fukui and Kaneko [7, 8].

Writing the non-dimensional film thickness H in terms of the longitudinal coordinate X ,

$$H = \frac{D_1}{D_o} - \frac{l}{L} \left(\frac{D_1}{D_o} - 1 \right) X \quad (30)$$

such that

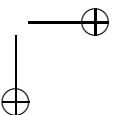
$$\frac{dP}{dX} = -\frac{l}{L} \left(\frac{D_1}{D_o} - 1 \right) \frac{dP}{dH}$$

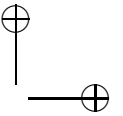
Eq. (28) can be immediately integrated to give:

$$\frac{l}{L} \left(\frac{D_1}{D_o} - 1 \right) \tilde{Q}_p(\delta_o PH, \alpha_1, \alpha_2) PH^3 \frac{dP}{dH} + Q_c(\delta_o PH, \alpha_1, \alpha_2) \Lambda PH = K_1 \quad (31)$$

where K_1 is a constant of integration. The substitution of

$$PH = \zeta \quad (32)$$





in Eq. (31) gives:

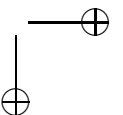
$$\frac{d\zeta}{dH} = \frac{\zeta}{H} - \frac{[Q_c(\delta_o\zeta, \alpha_1, \alpha_2)\Lambda\zeta - K_1]}{l/L(D_1/D_o - 1)\tilde{Q}_p(\delta_o\zeta, \alpha_1, \alpha_2)H\zeta} \quad (33)$$

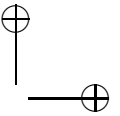
Eq. (33) can be solved numerically using relaxation methods. To apply this numerical scheme, the differential equations have to be replaced by finite-difference equations on a point mesh. The solution of the resulting set of equations is determined by starting with a guess and improving it iteratively using Newton’s method. The Poiseuille flow rate coefficient $Q_p(\delta, \alpha_1, \alpha_2)$ has been evaluated by means of the numerical method described in [14] and the variational technique for the integral form of the Boltzmann equation based on the BGK model. In order to compute the Couette flow rate $Q_c(\delta, \alpha_1, \alpha_2)$ one can solve numerically Eq. (23), extending a finite difference technique first introduced by Cercignani and Daneri [12].

Once $\zeta(H)$ has been numerically evaluated on a grid that spans the domain of interest, Eqs. (30) and (32) give the pressure field in the gas film as a function of X . Furthermore, a prediction of the vertical force acting on the upper surface of the slider bearing, crucial for practical design, may be obtained from the load carrying capacity W , defined as

$$W = \frac{l}{L} \int_0^{L/l} (P - 1)dX \quad (34)$$

One finds that the pressure distribution in the gas film increases with increasing Λ . Furthermore, at fixed bearing number, the pressure field reduces by increasing the fraction of gas molecules specularly reflected by the walls. It is worth noting that, when Λ increases, the Couette contribution to the lubrication flow rate becomes dominant compared with the Poiseuille flow. Therefore, if the two walls are identical, the influence of the Knudsen number on the load carrying capacity decreases as Λ increases, since Q_c is independent of δ and α . On the contrary, if the two walls have a different physical structure the load carrying capacity shows a dependence on both the Knudsen number and the accommodation coefficients α_1, α_2 . For the validation of the code, the results obtained with the modified Reynolds equation have been compared with the results from DSMC (Direct Simulation Monte Carlo) simulations published by Alexander et al. [15] in the case





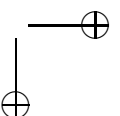
of Maxwell’s boundary conditions on two physically identical walls. The agreement is exceptionally good.

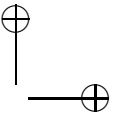
6. A Kinetic Approach for the Evaluation of Damping in MEMS

Beyond the lubrication problems, shear-and pressure-driven gas flows are encountered in several MEMS applications like surface-micromachined inertial sensors, resonating filter structures for signal processing and micromachined capacitive accelerometers, where the distance between the capacitor plates is minimized in order to increase the efficiency of actuation and improve the sensitivity of detection. The damping, due to the internal friction of the flowing gas, in the small gaps between these oscillating microstructures, is an important design parameter since it determines, e.g., the frequency-domain behavior of the sensor or the quality factor of the vibrating filter structure. At low pressures or in ultra thin films, the gas rarefaction effects and the molecular interaction with the surfaces effectively change the viscosity. In this flow regime, the continuum equations are no longer valid and the Boltzmann equation must be considered to understand and compute the rarefied flows related with these devices. In spite of its apparently complex structure, a real micromechanical accelerometer usually has a highly repetitive layout whose basic units consist of two or three-dimensional microchannels where different sets of bounding walls move in the direction perpendicular or parallel to their surfaces.

Let us consider a two-dimensional microchannel where the plates parallel to the x direction generate a Poiseuille-like flow, while those parallel to the y direction induce a Couette-like flux. Since the gaps between the moving elements and the fixed boundaries are only a few micrometres wide, the mean free path of the gas molecules is not negligible compared to the gap width and the gas cannot be treated as a continuous medium. Therefore, the behavior of a gas as it moves along the tube must be studied through the Boltzmann equation. Since the various types of motions experienced by the accelerometer components are typically at very low Mach number, it can be assumed that the velocity distribution of the gas flow only slightly deviates from that occurring at an equilibrium state. Moreover, if one assumes that the flow field can be described quasi-statically, it is convenient to linearize the Boltzmann equation about a Maxwellian M by setting:

$$f = M(1 + h) \tag{35}$$





where $h(\tilde{\mathbf{x}}, \boldsymbol{\xi})$ is the small perturbation of the basic equilibrium state, with $\tilde{\mathbf{x}}$ being the coordinate vector and $\boldsymbol{\xi}$ the molecular velocity. The above mentioned absolute Maxwellian M is given by:

$$M(\boldsymbol{\xi}) = \frac{\rho_0}{(2\pi RT_0)^{3/2}} \exp \left\{ -\frac{(\xi_x^2 + \xi_y^2 + \xi_z^2)}{2RT_0} \right\} \quad (36)$$

where ρ_0 and T_0 are the equilibrium density and temperature, respectively, and R is the gas constant. If one assumes the linearized Bhatnagar, Gross and Krook (BGK) model for the collision operator, which describes the effect of molecular interactions, the steady state Boltzmann equation reads:

$$c_x \frac{\partial h}{\partial \tilde{x}} + c_y \frac{\partial h}{\partial \tilde{y}} = \frac{\pi^{-3/2}}{\ell} \left[\int e^{-c'^2} h(\tilde{x}, \tilde{y}, \mathbf{c}') d\mathbf{c}' + 2c_x \int c'_x e^{-c'^2} h(\tilde{x}, \tilde{y}, \mathbf{c}') d\mathbf{c}' + 2c_y \int c'_y e^{-c'^2} h(\tilde{x}, \tilde{y}, \mathbf{c}') d\mathbf{c}' \right] - \mathbf{h}(\tilde{\mathbf{x}}, \tilde{\mathbf{y}}, \mathbf{c})/\ell \quad (37)$$

where ℓ is the mean free path and the following non-dimensional velocity variable has been introduced:

$$\mathbf{c} = \frac{\boldsymbol{\xi}}{\sqrt{2RT_0}} \quad (38)$$

In Eq. (37) integrations are extended to the whole velocity space. Since the microchannel walls are maintained at the same constant temperature, the thermal perturbation, which would have to appear in Eq. (37), has been dropped out.

Multiplying Eq. (37) by $(1/\sqrt{\pi}) \exp(-c_z^2)$ and integrating with respect to c_z , we obtain the following equation

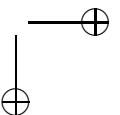
$$c_x \frac{\partial}{\partial x} \mathcal{G}(x, y, c_x, c_y) + c_y \frac{\partial}{\partial y} \mathcal{G}(x, y, c_x, c_y) = -\mathcal{G}(x, y, c_x, c_y) + \rho(x, y) + 2c_x v_x(x, y) + 2c_y v_y(x, y) \quad (39)$$

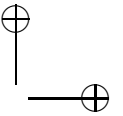
for the reduced distribution function $\mathcal{G}(x, y, c_x, c_y)$ defined by

$$\mathcal{G}(x, y, c_x, c_y) = \pi^{-1/2} \int_{-\infty}^{+\infty} e^{-c_z^2} h(x, y, \mathbf{c}) dc_z \quad (40)$$

where the spatial variables have been rescaled as follows

$$x = \tilde{x}/\ell; \quad y = \tilde{y}/\ell.$$





In Eq. (39), the macroscopic fields associated to the perturbation are defined as

$$\rho(x, y) = \pi^{-1} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} e^{-(c_x^2+c_y^2)} \mathcal{G}(x, y, c_x, c_y) dc_x dc_y \quad (41)$$

$$v_x(x, y) = \pi^{-1} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} c_x e^{-(c_x^2+c_y^2)} \mathcal{G}(x, y, c_x, c_y) dc_x dc_y \quad (42)$$

$$v_y(x, y) = \pi^{-1} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} c_y e^{-(c_x^2+c_y^2)} \mathcal{G}(x, y, c_x, c_y) dc_x dc_y \quad (43)$$

with $\rho(x, y)$ being the perturbation part of the density of molecules, $v_x(x, y)$ and $v_y(x, y)$ the x and y components of the bulk velocity of the gas, respectively. This transformation permits to greatly simplify the numerical solution of the Boltzmann equation since it reduces the three-dimensional molecular velocity field to two-dimensional.

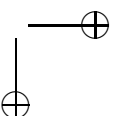
Appropriate boundary conditions on the plates, describing the gas-wall interactions, must be supplied for the equation (39) to be solved. We assume the diffuse-specular reflection condition of Maxwell’s type, according to which the reemitted molecules are partly reflected by the wall in a specular fashion and partly diffused with a Maxwellian distribution described by the wall properties (i.e. its temperature and velocity).

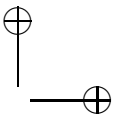
The solution of the problem described by Eq. (39) can be determined by pursuing the long-time behavior of the solution of the initial and boundary-value problem. That is, we consider Eq. (39) with the additional $\partial \mathcal{G} / \partial t$ term on the left-hand side and an initial condition (e.g., $\mathcal{G} = 0$) beyond the boundary conditions of Maxwell’s type. The time-dependent problem can then be solved numerically by a deterministic finite-difference method [16].

The most apparent features of the results are the v_x parabolic profiles in the cross-stream directions of the longest branches of the channel where a Poiseuille-like flow is induced and similar parabolic profiles of the y component of the gas velocity in the stream-wise direction of the transversal section of the channel where a coupled Poiseuille-Couette flow develops.

In order to model the damping forces occurring as a result of the internal friction of the flowing gas underneath the plates, the following elements of the stress tensor have been evaluated:

$$P_{xx}(x, y) = \frac{\rho_0}{2} + \frac{\rho_0}{\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dc_x dc_y c_x^2 e^{-(c_x^2+c_y^2)} \mathcal{G}(x, y, c_x, c_y) \quad (44)$$





$$P_{yy}(x, y) = \frac{\rho_0}{2} + \frac{\rho_0}{\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dc_x dc_y c_y^2 e^{-(c_x^2 + c_y^2)} \mathcal{G}(x, y, c_x, c_y) \quad (45)$$

$$P_{yx}(x, y) = \frac{\rho_0}{\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dc_x dc_y c_x c_y e^{-(c_x^2 + c_y^2)} \mathcal{G}(x, y, c_x, c_y) \quad (46)$$

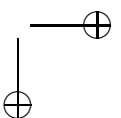
A comparison between the numerical findings and the experimental data collected on a silicon biaxial accelerometer produced by STMicroelectronics show that the agreement is very good in the transitional flow regime as well as in the near-free molecular flow limit.

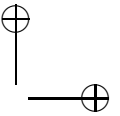
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