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On the application of the BGK kinetic model to the analysis of gas-structure interactions in MEMS

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Abstract

The BGK model of the Boltzmann equation is applied to the analysis of damping in silicon inertial MEMS working at low-moderate frequencies. Assuming small perturbations, the linearized steady-state 2D equation is implemented in a deterministic manner in order to avoid noise intrinsic in statistical approaches. Implementation details are discussed and the comparison with available experimental data in terms of forces exerted on the suspended shuttle is presented.

Keywords: MEMS; BGK model; Boltzmann equation; Damping; Silicon; Gas flow

1. Introduction

MEMS [21] are Micro-Electro-Mechanical-Systems with growing diffusion in several industrial fields. An important class of MEMS is represented by silicon inertial sensors and actuators produced by surface micromachining processes, like accelerometers and gyroscopes. They consist of a collection of suspended and fixed structures coupled into capacitors and vibrating at low/moderate frequencies. MEMS feature electronics typical of complex IC and a mechanical behaviour which is truly multi-physics, stemming from the coupling of (at least) electrostatics, gas flows and structural dynamics. While many features are nowadays fully dominated, the evaluation of fluid damping is still an intriguing and partially unresolved topic and strongly affects the structural response. Damping is due to gas flow in very small gaps between the movable and fixed elements of the MEMS. Since the gaps are typically only a few micrometers wide, the molecular mean free path is not negligible compared to the gap width and the gas cannot be treated as a continuous phase. The parameter employed to estimate the degree of rarefaction in a gas is the Knudsen number $Kn = \lambda/d$, where λ is the mean free molecular path and d is a typical flow dimension, e.g., the gap between electrodes [12,18]. At ambient pressure and for several inertial MEMS like the one analyzed in Section 4, the Knudsen number is of the order of 10^{-2}, which means that the flow mainly develops in the slip flow regime. The evaluation of damping in this regime has been thoroughly investigated in the literature [18,21,22] and more recently in [14,15,33] using the Stokes model and Boundary Element techniques. According to the latter contributions, the use of integral equations and a series of simplifying hypotheses suited for moderate working frequencies permits the full scale 3D simulation of MEMS in the slip regime and guarantees excellent agreement with experimental results.

When environmental pressure or MEMS typical dimensions are further reduced, the flow enters the transition regime in which the regions where kinetic effects are important have the same size of the flowfield. Several authors have proposed to compute via analytical or semi-analytical

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approaches corrected parameters to be employed in classical continuum numerical tools. A correction has been obtained by replacing the static viscosity coefficient with an effective viscosity whose computation is based on the solution of the linearized Boltzmann equation for the one-dimensional Poiseuille and Couette flow problems [28–30]. Alternatively, other authors (e.g., [4]) suggest to employ slip boundary conditions which depend on the Knudsen number and should prove accurate in the whole pressure range. These formulas yield accurate results in specific situations but have been obtained under several simplifying hypotheses which are not always met by real 3D MEMS.

In principle, a correct theoretical description of gas flow in the transition regime can be obtained by solving the Boltzmann Equation (BE) [8,12], a complex non-linear integro-differential equation providing the distribution function of molecular velocities at any flowfield location. Mathematical difficulties prevent from obtaining closed form solutions of BE in cases of practical interest, but efficient Monte Carlo methods have been developed for its numerical treatment [5]. Unfortunately, in most MEMS flows reference Mach numbers and deviations from local equilibrium are small and difficult to capture by traditional statistical Monte Carlo methods. A number of possible modifications to statistical particle schemes have been proposed [7,13] but research in this direction is still very active. Small deviations from equilibrium could be computed more accurately by noise-free deterministic methods. However, their huge memory demand has limited the adoption of such methods to space homogeneous or one-dimensional problems.

A deterministic approach to the numerical solution of kinetic equations becomes viable if the complicated collision integral in the BE is replaced by a simpler expression. As described below, in the BGK model kinetic equation [6] the term giving the collisional rate of change of the distribution function is simply proportional to the departure from local equilibrium. In its simpler and more useful form, the model contains a single disposable function (the collision frequency) which depends on local density and temperature and assigns the same decay rate to all kinetic modes. Hence, the hydrodynamic limit of the model is only partially correct since the collision frequency can be tuned to obtain either the correct fluid viscosity or thermal conductivity, but not both. In spite of its shortcomings, the BGK model is often more accurate than expected, particularly in problems where momentum and heath transport are not equally important and the collision frequency can be adjusted to match the most important transport coefficient. Its applications to rarefied gases date back to the first semi-analytical solutions of [11,27] for Poiseuille and Couette flow. Subsequently, many different numerical applications have been presented in the literature [1,2,19,20,23,32,34] focusing especially on high speed applications. More recently, a number of papers have appeared where low-speed flows of various complexity have been studied by deterministic numerical solutions of the BGK model kinetic equation [25,26]. However,a complete validation of working hypotheses is still lacking since no applications to real MEMS and comparisons with experimental data are presented. Hence, in this paper a simple and straightforward discretization technique is adopted to solve numerically the BGK model equation associated to a rarefied monatomic gas flowing in a two-dimensional domain. The flow geometry is derived from a MEMS for which experimental values of damping forces are available. It is shown that excellent agreement with experimental results can be obtained in a wide range of pressures. The paper content is organized as follows: the theoretical background is presented in Section 2, the numerical method is discussed in Section 3, and an example is finally presented together with the comparison with available experimental results.

2. Formulation

Let $f(\mathbf{x},\boldsymbol{\xi})$ denote the velocity distribution function of molecules, where $\mathbf{x}$ are space coordinates and $\boldsymbol{\xi}$ is molecular velocity. If ∇ denotes the gradient with respect to $\mathbf{x}$, the BGK model of the Boltzmann equation [2,12,32] reads:

$$\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\nabla f=\nu(\rho,T)(f_{\mathrm{M}}-f) \tag{1}$$

where the right hand side relaxation term replaces the collision operator of the Boltzmann equation which accounts for binary collisions between particles; $\nu(\rho,T)$ is the collision frequency which is assumed independent of $\boldsymbol{\xi}$ and f_{M} is the local equilibrium Maxwellian:

$$f_{\mathrm{M}}=\frac{\rho}{(2\pi\mathscr{R}T)^{3/2}}\exp\left(-\frac{|\boldsymbol{\xi}-\mathbf{v}|^2}{2\mathscr{R}T}\right) \tag{2}$$

It can be shown [12] that the correct fluid viscosity $\mu(T)$ in the hydrodynamic limit can be obtained from Eq. (1) by setting

$$\nu(\rho,T)=\frac{\rho\mathscr{R}T}{\mu(T)} \tag{3}$$

Macroscopic velocity $\mathbf{v}$, density ρ and temperature T are moments of f in the velocity space:

$$\rho=\int_{R^3}f\,\mathrm{d}\boldsymbol{\xi},\quad \rho\mathbf{v}=\int_{R^3}f\boldsymbol{\xi}\,\mathrm{d}\boldsymbol{\xi},$$
$$T=\frac{1}{3\mathscr{R}\rho}\int_{R^3}f|\boldsymbol{\xi}-\mathbf{v}|^2\,\mathrm{d}\boldsymbol{\xi}. \tag{4}$$

Finally $\mathscr{R}$ is the specific gas constant (the universal constant divided by the molar mass). The BGK model equation (1) can thus be interpreted as a relaxation towards a local Maxwellian equilibrium state. The gas interacts with both fixed and movable surfaces immersed in a virtually unconfined domain which is often truncated at a sufficient distance from the structures. To simplify the gas–wall interaction, it is assumed that the scattering from the wall is either diffused or specular or a combination of the two.