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IS IT SAFE TO USE NAVIER-STOKES FOR GAS MICROFLOWS?

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Abstract. *Gas phase Micro-Electro-Mechanical-Systems (MEMS) demonstrate that the fluid mechanics at the micron scale can differ significantly from that experienced in the macroscopic world. Effects such as rarefaction and gas-surface interactions need to be taken into account and it is well known that the no-slip boundary condition of the Navier-Stokes equations is no longer valid. Following ideas proposed by Maxwell, it is generally accepted that the Navier-Stokes equations can be extended into the slip-flow regime provided the Knudsen number is less than 0.1. However, improvements in micro-fabrication techniques are enabling systems to be constructed with sub-micron feature dimensions. At this scale, the flow will depart even further from equilibrium conditions and enters the transition flow regime* $(0.1 \le Kn \le 10)$.

In practice, a typical MEMS device will have to operate over a range of Knudsen numbers but of particular interest is the range $0.01 \le Kn \le 1$*, where it is important to understand whether non-equilibrium effects are significant. The results suggest that for non-planar flows, the error associated with the modified Navier-Stokes equations around* $Kn = 0.1$ *may be appreciable. More worryingly, Grad's higher-order Knudsen number approximation also fails to capture the essential physics.*

1 INTRODUCTION

Micro-Electro-Mechanical-Systems (MEMS) have emerged as one of the most exciting and revolutionary new areas of technology. However, one of the most important research issues is the growing realisation that the fluid mechanics in such small-scale devices is not the same as that experienced in the macroscopic world. Inertial forces will be negligible while surface properties and viscous effects will increasingly dominate the fluid motion. In addition, the small length scales may invalidate the continuum hypothesis employed in conventional fluid dynamics. As a consequence, microfluidic systems that are simply scaled down versions of macro-scale devices may not function as intended.

Gas flows, in particular, show a significant departure from the continuum regime. For example, experiments conducted by Pfahler *et al*. [1], Harley *et al*. [2] and Arkilic *et al*. [3] on low Reynolds number gas flows in silicon micro-machined channels have shown that conventional (continuum) analyses are unable to predict the observed flow rates with any degree of accuracy. This has lead to numerous questions regarding the applicability of conventional analysis tools for gas-phase microsystems (Gad-el-Hak [4,5]).

It has long been established that the continuum assumption in the Navier-Stokes equations is only valid when the mean free path of the molecules is smaller than the characteristic dimension of the flow domain. If this condition is violated, the fluid will no longer be in thermodynamic equilibrium and a variety of non-continuum or rarefaction effects will be exhibited, including the breakdown of the conventional no-slip boundary condition. There is also growing experimental evidence to suggest that the gas-surface interactions at the wall are affected by incomplete momentum accommodation (Arkilic *et al*. [6]; Maurer *et al*. [7]).

For an ideal gas modelled as rigid spheres, the mean free path of the molecules, λ, can be related to the temperature, T, and pressure, p, via

$$\lambda = \frac{kT}{\sqrt{2}\pi p \sigma_c^2} \tag{1}$$

where k is Boltzmann's constant and σ_c is the collision diameter of the molecules. An alternative expression for the mean free path is given by

$$\lambda = \frac{\mu}{\phi \rho \overline{c}} \tag{2}$$

where μ is the fluid viscosity, ρ is the density, $\overline{c}$ is the mean velocity of the gas molecules and ϕ is a constant dependent upon the kinetic theory used.

The ratio between the mean free path, λ, and the characteristic dimension of the flow geometry, L_c, is known as the Knudsen number, Kn:

$$Kn = \frac{\lambda}{L_c} \tag{3}$$

The Knudsen number determines the degree of rarefaction of the gas and the validity of the continuum hypothesis in the Navier-Stokes equations. A classification of the various stages of rarefaction has been proposed by Schaaf and Chambré [8], based upon the magnitude of the local Knudsen number:

$$\left.\begin{array}{rl} Kn \le 10^{-2} & \text{Continuum flow} \\ 10^{-2} \le Kn \le 10^{-1} & \text{Slip flow} \\ 10^{-1} \le Kn \le 10 & \text{Transition flow} \\ Kn > O(10) & \text{Free-molecular flow} \end{array}\right\} \qquad (4)$$

For $Kn \le 10^{-2}$, the continuum hypothesis has generally been considered appropriate and the flow can be described by the Navier-Stokes equations using conventional no-slip boundary conditions, although Gad-el-Hak [4] has suggested that the breakdown in the continuum assumption is discernible at Knudsen numbers as low as $Kn = 10^{-3}$. For $Kn > 10$, the continuum approach breaks down completely and the regime can then be described as being a *free-molecular flow*. Under such conditions, the mean free path of the molecules is far greater than the characteristic length scale and consequently molecules reflected from a solid surface travel, on average, many length scales before colliding with other molecules. However, for Knudsen numbers between $Kn = 10^{-2}$ and $Kn = 10$, the gas can neither be considered an absolutely continuous medium nor a free-molecular flow. A further sub-classification is therefore necessary to distinguish between the appropriate methods of analysis.

In the range, $10^{-2} \le Kn \le 10^{-1}$ (commonly referred to as the *slip-flow regime*), the Navier-Stokes equations are considered to offer a reasonable description of the flow provided tangential slip-velocity boundary conditions are implemented between the gas and the substrate. On the other hand, for $10^{-1} \le Kn \le 10$ (*transition flow*), the continuum assumption in the Navier-Stokes equations begins to break down and alternative methods of analysis are required. These methods can be derived from higher-order Knudsen number approaches, such as proposed by Grad or Burnett, particle-based Direct Simulation Monte Carlo (DSMC) approaches (Bird [9]) or solving the gas-kinetic equations derived by Boltzmann [10].

The validity of the Navier-Stokes equations can also be interpreted from the perspective of the *Knudsen layer*. When the Knudsen number is greater than 10^{-2}, the no-slip boundary condition employed in the continuum regime is no longer applicable and a sub-layer of the order of one mean free path starts to affect the fluid interaction between the bulk flow and the boundary wall. The fluid within this so-called Knudsen layer cannot be analysed using the Navier-Stokes equations and, instead, a proper theoretical treatment can only be achieved by solving the Boltzmann transport equation. However, for $Kn \le 10^{-1}$, the dynamics of the Knudsen layer can often be neglected, and the effects of rarefaction can be modelled by the application of a simple first-order slip-velocity boundary condition.

Surprisingly, there has been relatively little work confirming how well the Navier-Stokes equations predict slip flows over non-planar surfaces. In the present paper, we will present results for flow around an unconfined microsphere that raises serious questions on the validity of extending the Navier-Stokes equations into the upper range ($Kn = 10^{-1}$) of the slip-flow regime and, more seriously, questions the benefit of employing certain higher-order schemes.

2 LOW SPEED FLOW PAST A SPHERICAL PARTICLE

Unconfined creeping flow past a sphere was first analysed by Stokes [11] who demonstrated that in the absence of inertia, the total drag force due to the flow of an unbounded incompressible Newtonian fluid, in the continuum regime, could be written as

$$F = 6\pi\mu a U \tag{5}$$

where a is the radius of the sphere and U is the uniform velocity infinitely far from the sphere. Gas microflows are generally associated with low speed flows, often in the Stokes' flow regime. For this particular problem, there are several analytical solutions covering a range of Knudsen numbers that are supported by good experimental data acquired over many years of research.

2.1 Experimental results for flow around spherical particles

One of the first experiments to examine the applicability of equation (5) for increasing Knudsen numbers was performed by Millikan [12] as part of his landmark oil drop experiment. To determine the charge of an electron, he measured the drag force on oil droplets as they settled through air over a range of Knudsen numbers from 0.36 to 96. Millikan realised that Stokes' drag equation (5) had to be modified at higher Knudsen numbers and proposed an empirical formula of the form:

$$F = \frac{6\pi\mu a U}{1 + Kn\left(\alpha + \beta e^{-\gamma/Kn}\right)} \tag{6}$$

where α, β and γ are experimentally determined constants and Kn is the Knudsen number based on the radius of the sphere. Allen and Raabe [13] reviewed Millikan's experimental data using modern, more accurate physical constants and non-linear least-squares fitting techniques. The values obtained by re-analysing Millikan's data are

$$\alpha = 1.155 \pm 0.008 \qquad \beta = 0.471 \pm 0.011 \qquad \gamma = 0.596 \pm 0.050 \tag{7}$$

2.2 Analytical solution derived from the Navier-Stokes equations

For Knudsen numbers in the slip-flow regime, the velocity at the wall can be related to the shear stress, $\vec{\tau}$ by

$$\vec{u}_{slip} = \frac{2-\sigma}{\sigma}\frac{\lambda}{\mu}\vec{\tau} \tag{8}$$

where σ is the <u>T</u>angential <u>M</u>omentum <u>A</u>ccommodation <u>C</u>oefficient which accounts for gas-surface interactions at the wall. The TMAC can vary from zero (for specular reflection) up to unity (for complete or diffuse reflection). The boundary condition at the surface of the sphere ($r = a$) can therefore be rewritten in polar co-ordinates as

$$u_\theta = \frac{2-\sigma}{\sigma}\lambda\left[\frac{\partial u_\theta}{\partial r} + \frac{1}{r}\frac{\partial u_r}{\partial \theta} - \frac{u_\theta}{r}\right] \tag{9}$$

Following Basset [14], the analytical solution for the drag in the slip-flow regime can be shown [15,16] to be given by

$$F = 6\pi\mu a U\left[\frac{1+2\dfrac{2-\sigma}{\sigma}Kn}{1+3\dfrac{2-\sigma}{\sigma}Kn}\right] \tag{10}$$

which for $Kn \to 0$, recovers Stokes' original drag formula.

2.3 Analytical solution derived from Grad's thirteen moment equations

A solution that is second-order accurate in Knudsen number has been derived by Goldberg [17]. In this analysis, Goldberg solved Grad's thirteen moment equations to analyse the flow around a sphere. The thirteen moment equations, which are derived from statistical mechanics considerations, look similar to the Navier-Stokes equations, but the stress tensor is different. The solution obtained takes into account the local velocity, stress, pressure and temperature of the fluid. The drag force calculated using Grads' thirteen moment equation approach is

$$F = 6\pi\mu a U\left[\frac{\left(1+\dfrac{15}{2}\dfrac{2-\alpha}{\alpha}Kn\right)\left(1+2\dfrac{2-\sigma}{\sigma}Kn\right)+\dfrac{6}{\pi}Kn^2}{\left(1+\dfrac{15}{2}\dfrac{2-\alpha}{\alpha}Kn\right)\left(1+3\dfrac{2-\sigma}{\sigma}Kn\right)+\dfrac{9}{5\pi}\left(4+9\dfrac{2-\sigma}{\sigma}Kn\right)Kn^2}\right] \tag{11}$$

where α describes the interchange of energy between the sphere and fluid. For the problem under consideration, it is assumed that the temperature of the sphere and fluid are in equilibrium and α is taken as unity.

2.4 Analytical solutions derived from kinetic theory

Epstein [18] showed that in the free-molecular regime ($Kn \to \infty$), the drag force on a sphere for diffuse reflection is given by

$$F_{\text{diff}} = \left(\frac{4}{3}+\frac{\pi}{6}\right)\pi\rho a^2 \bar{c} U \tag{12}$$

whereas for specular reflection, the free-molecular drag is given by

$$F_{\text{spec}} = \frac{4}{3}\pi\rho a^2 \bar{c} U \tag{13}$$

The total drag force acting on a sphere in the free-molecular regime when a fraction, σ, of molecules reflect diffusely can therefore be written as

$$F = \sigma F_{\mathrm{diff}} + (1-\sigma) F_{\mathrm{spec}} = \left(\frac{8+\pi\sigma}{6}\right)\pi\rho a^2 \bar{c} U \tag{14}$$

Beresnev *et al*. [19] subsequently modified equation (12) to obtain an approximate expression for the drag force over the entire Knudsen number regime $(0 \le Kn \le \infty)$:

$$F = 6\pi\mu a U \left(\frac{8+\pi}{18}\right)\frac{1}{Kn+0.619}\left[1+\frac{0.310Kn}{Kn^2+1.152Kn+0.785}\right] \tag{15}$$

In the continuum limit $(Kn \to 0)$, it can readily be shown that equation (15) tends to Stokes' drag formula (5).

Sone and Aoki [20] have developed an alternative analytical solution that takes into account the Knudsen layer and additional effects, such as thermal stress, which are neglected in classical slip-flow analyses. The drag force was determined to be

$$F = 6\pi\mu a U\left[1 - 1.01619\frac{2}{\sqrt{\pi}}Kn + \left(0.6366 + 0.2991\frac{K}{2K+1}\right)Kn^2\right] \tag{16}$$

where $K = k_{\mathrm{g}} / k_{\mathrm{s}}$ is the ratio of thermal conductivities of the gas and the particle, respectively. Sone and Aoki [20] considered two specific cases, namely $K = 0$ and $K = 1$.

3 RESULTS AND DISCUSSION

Figure 1 presents the non-dimensionalised drag force $(F / 6\pi\mu a U)$, as a function of the Knudsen number, for creeping flow past an unconfined sphere. A comparison is made between Millikan's re-analysed experimental data [13] and various hydrodynamic and kinetic approaches. For consistency with kinetic models, the tangential momentum accommodation coefficient, σ, has been taken as unity, i.e. the molecular interactions at the surface of the sphere are assumed to be fully diffusive. As shown in figure 1, the analytical models derived from kinetic theory [19,20] agree very well with the experimental data. In contrast, it can be seen that the models derived from both Navier-Stokes and Grad's thirteen moment equations quickly deviate from the experimental results. For the case of no-slip, the Navier-Stokes equations predict a constant drag force ($F / 6\pi\mu a U = 1$) irrespective of the Knudsen number. However, taking the hydrodynamic solution to first-order slip provides a dramatic improvement over the no-slip condition at very low Knudsen number, although extending to second-order in Knudsen number does not significantly improve the predictions.

The percentage error in the predicted drag force associated with the analytical models is presented in figure 2. The errors are shown relative to Millikan's re-analysed experimental data [13]. It has been commonly assumed that the modified Navier-Stokes equations provide a reasonable description of the fluid mechanics up to $Kn = 10^{-1}$. From figure 2 the error at this limit is approximately 3%. However, if the characteristic length scale for the Knudsen number is defined to be the diameter of the sphere (more practical from an engineering perspective and more relevant to most flow situations), it would correspond to Kn = 0.2 on the graph. The predicted error has now increased to 8%. Figure 2 also illustrates that there appears to be little benefit to be gained by extending to Grad's method for this class of problem. It is therefore likely that other higher-order schemes, such as Burnett, may have similar limitations.

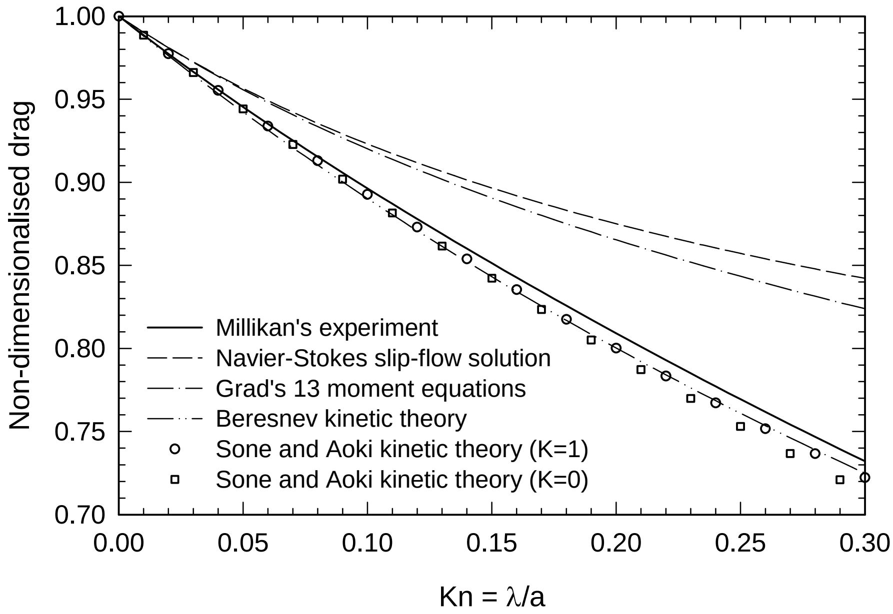

Figure 1. Non-dimensionalised drag as a function of Knudsen number for unconfined flow past a sphere.

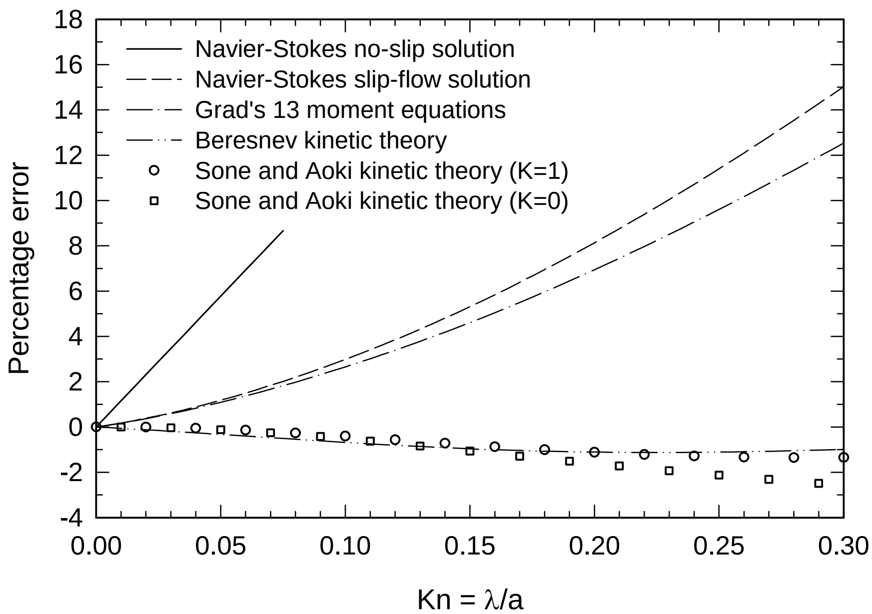

Figure 2. Percentage error in the drag force predicted by various hydrodynamic and kinetic models.

4 CONCLUDING REMARKS

This paper has investigated rarefied, creeping flow past an unconfined microsphere at low Knudsen numbers in order to study the behaviour of slip flow around a non-planar surface. For this particular problem, there are several analytical solutions covering a range of Knudsen numbers that can be compared against good experimental data. The results indicate that analytical models derived from kinetic theory agree well with experimental observations. Extending the Navier-Stokes equations into the slip-flow regime provides a significant improvement to the continuum (no-slip) approach but it is shown that the results quickly deviate from the experimental data. If the Knudsen number is based on the diameter of the sphere, the error approaches 8% at the upper end of the slip-flow regime. Of significant concern, however, is that the solution derived from Grad's method only provides a slight improvement to the predicted drag force and does not allow any extension into the transition flow regime. Other higher-order schemes, such as the Burnett equations, may have similar problems extending beyond the slip-flow regime.

The sphere represents a relatively simple non-planar geometry and any real device would probably involve more significant geometric variations e.g. serpentine bends. The errors involved in simulating practical microsystems, where the Knudsen number could vary throughout the device, are likely to be greater than those reported in this paper.

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