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Calculation of Knudsen layers and jump conditions using the linearised G13 and R13 moment methods

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ABSTRACT

For gas flows in micro-channels the molecular mean free path is often comparable to the channel dimensions and the flow must be modelled using one of the methods of non-continuum gas dynamics. For slip-flow or lower transition regime calculations the Grad 13-moment (G13) method or its extension the Regularised 13-moment (R13) method has been proposed. The R13 method is assumed to be an improvement over the G13 because it can capture, at least to some extent, Knudsen layers close to solid surfaces. This paper investigates the capabilities of the two methods by using them to address the classical problems of viscous slip, temperature jump and thermal creep. For the linearised equations it is possible to obtain analytical solutions and these provide physical insight as well as numerical values. The analysis shows that the Knudsen layer associated with temperature and normal stress decouples from the layer associated with velocity and heat flux. Comparison with more accurate solutions of the kinetic equation shows that the LR13 method underpredicts the velocity slip and temperature jump coefficients by about 10% and only provides a slight improvement over the much simpler LG13 method. Furthermore, the Knudsen layer velocity and temperature profiles bear only a superficial resemblance to more accurate solutions. For reasons that are unclear, the calculation of the thermal creep flow is very much more successful. It is concluded that considerable improvements need to be made before the LR13 method becomes a reliable technique for solving non-continuum flow problems.

1. Introduction

In recent years there has been much interest in calculation methods for low-speed non-continuum gas flows (*i.e.*, gas flows where the continuum hypothesis cannot be justified) [1,2]. Such flows occur, for example, in micro-electro-mechanical systems (MEMS) where the dimensions of the flow passages are comparable to the mean free path of a gas molecule [3]. Non-continuum flows are characterised by the Knudsen number, *Kn*, defined as the ratio of the molecular mean free path to a flow length scale (*e.g.*, a channel width). Traditionally, gas flows are divided into four regimes; continuum flow ($Kn \ll 1$), slip flow ($Kn \sim 0.1$), transition flow ($Kn \sim 1$) and free-molecule flow ($Kn \gg 1$). Continuum flows are well-described by the Navier–Stokes–Fourier (NSF) equations with no-slip boundary conditions and there are now a large number of computational solution methods available. However, in MEM devices the flow conditions are often in the slip and lower transition regimes. In such cases ($Kn < 0.5$) calculations are sometimes performed using the Grad 13-moment (G13) system of equations.

The G13 method was first proposed by Grad [4] who suggested that weakly non-continuum flows could be described by including higher moments of the Boltzmann equation in the equation set to be solved. The lower moments give rise to the equations of mass, momentum and energy conservation as in the NSF system. Closure in this system is achieved using the empirical expressions for viscous stress and heat flux proposed by Stokes and Fourier. In the G13 method, higher moments (specifically the transport equations for viscous stress and heat flux) are added to the conservation equations and closure is applied at this level. Using the original closure conditions suggested by Grad [5], it has been found that the non-equilibrium Knudsen layers adjacent to solid surfaces cannot be captured and these layers are compressed to discontinuous jumps in velocity and temperature at the surface [6]. Such behaviour is non-physical and gives rise to increasing error as the Knudsen number, and hence the thickness of the Knudsen layers, increases. Recently, however, Struchtrup has improved the G13 method by ‘regularising’ the closure conditions [1,7]. For some problems involving *unbounded* gas flows, Lockerby and Reese [8] have shown that the Regularised 13-moment (R13) equations perform much better than any of (i) the NSF equations, (ii) the G13 equations, (iii) the second-order Burnett equations [9] and, (iv) the third-order super-Burnett equations [1]. The relationship

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Nomenclature

Vectors are denoted by upright, bold-face type

A_η A_ξ	constants in Eqs. (7) depending on production term model
$\mathbf{C}$ C_i	peculiar molecular velocity
$\mathbf{c}$ c_i	absolute molecular velocity
f	molecular velocity distribution function
k	thermal conductivity
l_0	length scale defined by Eq. (1)
m_{ijk}	closure tensor
P_{ij}	pressure tensor
p	pressure
$\bar{p}$	$p - p_0$
Pr	Prandtl number
$\mathbf{q}$ q_i	heat flux
R	gas constant per unit mass
R_{ij}	closure tensor
T	temperature
$T_S - T_W$	surface temperature jump defined in Fig. 1(b)
$\bar{T}$	$T - T_0$
U_S	slip velocity defined in Fig. 1(a)
U_C	thermal creep velocity defined in Fig. 1(c)
$\mathbf{u}$ u_i	velocity
x, y, z	Cartesian co-ordinate system

Greek symbols

α	accommodation coefficient
β	$(\alpha - 2)/\alpha$
μ	dynamic viscosity
η	$y(A_\eta l_0)^{-1/2}$
ρ	density
σ_{ij}	stress tensor
σ_{VS}	velocity slip coefficient
σ_{TC}	thermal creep coefficient
θ	RT
ξ	$y(A_\xi l_0)^{-1/2}$
ζ_{TJ}	temperature jump coefficient

Subscripts

G	LG13 solution
K	Knudsen layer correction
0	undisturbed gas
$\sim$	actual gas condition at the wall

between the R13 system and the Burnett and super-Burnett equations is explored in [10] where it is also shown that the latter systems exhibit unstable behaviour in certain regimes whereas the R13 system does not.

For flows bounded by solid surfaces, Struchtrup and Torillhon [11,12] have developed a consistent set of boundary conditions to supplement the R13 equations. It is then found that the R13 method can capture, at least partially, Knudsen layers adjacent to solid surfaces [12,13]. All these advantages indicate that the R13 method may be well-suited for calculating the low-speed flowfields in MEM and other micro-scale devices.

One of the problems in using the R13 method is that the equation set is more complicated than the NSF formulation and the specialist literature tends to concentrate on the mathematics at the expense of physical interpretation. Also, it is difficult to judge the accuracy of the method because there are no absolute benchmarks for comparison. A complete analysis of a gas flow problem would involve solving the non-linear Boltzmann equation with an accurate molecular collision model and an exact specification of the molecular interaction with the solid boundaries. All reported calculations, however, are based on simplified Boltzmann equations and there are no measurements of Knudsen layer structure in the literature.

In this paper we concentrate on the linearised G13 and R13 methods (LG13 and LR13) and address the classical problems of the surface velocity slip due to a shear stress (Kramer's problem), the surface temperature jump due to a normal heat flux and the surface thermal creep velocity due to a tangential temperature gradient. These are the simplest examples of non-equilibrium, non-continuum flows and if the R13 method cannot provide good results for these problems, then it is unlikely that it will perform accurately for more complex flows.

The first objective is to find analytical solutions for the three problems. The solutions depend on the molecular collision model which enters into the moment equations for the stress tensor and heat flux vector. We consider the original BGK model [14], the Ellipsoidal-Statistical BGK (ES-BGK) model [15] and the Maxwell molecule model [1]. The simplicity of the BGK model has made it very popular but it gives a Prandtl number of unity for a monatomic gas rather than the correct value of 2/3. The ES-BGK and Maxwell molecule models both give the correct Prandtl number and represent improvements in this respect. Other authors have used the LR13 equations to address Kramer's problem but either the physics was concealed by the mathematics [13] or few details of the calculations were given [6]. We shall show that the solutions for all three problems can be presented in concise analytical forms.

The second objective is to compare the calculations with other published values of the slip, jump and creep coefficients. Many methods for calculating these coefficients can be found in the literature ranging from the simple kinetic models of Maxwell's time to elaborate solutions of various model kinetic equations. An assessment of the current situation is given by Sharipov [16] who provides a long list of references which the reader can access if interested. Many of these references describe direct solutions of kinetic equations which should give superior values of the slip, creep and jump coefficients compared with those obtained from the moment methods. This is not the point, of course. Moment methods potentially have a wider applicability to practical problems and it is important for engineers to be able to assess the likely accuracy of the methods in more complex flow problems.

The third objective is to compare the structure of the LR13 Knudsen layers with other, more accurate calculations. Although the published database here is much smaller, some information is available which allows useful conclusions to be drawn.

2. Velocity slip, temperature jump and thermal creep

We consider a perfect gas in contact with a flat plate. The co-ordinate x is measured along the plate in the flow direction (assuming a flow exists) and the co-ordinate y is measured normal to the plate with $y = 0$ at the plate surface. In the absence of velocity and temperature gradients, the pressure, temperature, density, dynamic viscosity and thermal conductivity of the gas are p_0, T_0, ρ_0, μ_0 and k_0, respectively. The most probable peculiar speed of the molecules is $C_0 = \sqrt{2RT_0}$ where R is the gas constant per unit mass. Throughout the paper we use a length scale l_0 (which is of the order of a molecular mean free path) defined by