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Near-wall effects in rarefied gas micro-flows: some modern hydrodynamic approaches

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Abstract

Methods for simulating the critical near-wall region in hydrodynamic models of gas micro-flows are discussed. Two important non-equilibrium flow features – velocity slip at solid walls, and the Knudsen layer (which extends one or two molecular mean free paths into the gas from a surface) – are investigated using different modelling approaches. In addition to a discussion of Maxwell's slip boundary condition, a newly implemented 'wall-function' model that has been developed to improve hydrodynamic simulations of the Knudsen layer is described. Phenomenological methods are compared to physical modelling and it is shown that, while both simulation types have merit, and both can quantitatively improve results in most cases, there are drawbacks associated with each approach. Phenomenological techniques, for example, may not be sufficiently general, whilst issues with applicability and stability are known to exist in some physical models.

It is concluded that, at present, neither approach is unambiguously preferable to the other, and that both physical and phenomenological modelling should be the subject of future work.

Keywords: Microfluidics; Rarefied gas dynamics; Velocity slip; Knudsen layer; Wall-function; Gas microsystems

1. Introduction

Gas microsystems present a unique engineering challenge in that, even when operating at atmospheric pressures, they display important physical phenomena attributable to rarefaction of the flow. The physical effects of gas rarefaction can be particularly significant close to solid surfaces, and so they have important implications for system performance at the microscale in that they can directly affect quantities of interest, such as drag force and mass flowrate (Gad-el-Hak, 1999). Numerical simulations of such flows, therefore, need to be able to capture observed non-equilibrium characteristics.

In this paper we focus on the near-wall region, in particular on the occurrence of velocity slip and the presence of the Knudsen layer in some fundamental low speed gas flows. Specifically, we examine how these phenomena may be captured numerically in hydrodynamic models of the flow, i.e., computational fluid dynamics (CFD). The application of the velocity slip boundary condition proposed by Maxwell (1879) is discussed, and two methods for the simulation of the Knudsen layer in gas microsystems are described. We compare and contrast the underlying assumptions of each method and show some key numerical results, before proposing and discussing some alternate modelling techniques.

2. Gas velocity slip at solid surfaces

Perhaps the most widely known aspect of non-equilibrium gas flows is the fact that the velocity of a gas close to a surface is not always the same as the velocity of that surface. Describing this velocity slip accurately, however,

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is still an active area of research. A simple planar Poiseuille micro-flow case illustrates the importance of the phenomenon: for a Knudsen number, *Kn*, of 0.05 (where *Kn* is the ratio of the molecular mean free path of the gas to the channel height), the mass flow rate is typically around 15% greater than would be expected from conventional no-slip fluid dynamic models, with some 70% of this increase arising from the effect of slip at the channel walls (Lockerby et al., 2005a).

The classical description of the velocity slip in rarefied gases flowing over a solid surface is the *Maxwell slip condition*, and this is widely implemented in current rarefied gas flow solvers. Maxwell's original expression for the slip, applicable to any geometry, relates the tangential slip velocity of gas at a solid surface, $\vec{u}_{\text{slip}}$, to the tangential shear stress, $\vec{\tau}$, and heat flux, $\vec{q}$ (Maxwell, 1879). Written in vector form for application to flows over three-dimensional surfaces, the Maxwell slip condition is:

$$\vec{u}_{\text{slip}} = -\frac{(2-\sigma)}{\sigma\mu}\lambda\vec{\tau} - \frac{3}{4}\frac{N_{Pr}(\gamma-1)}{\gamma p}\vec{q}, \tag{1}$$

where $\vec{\tau} = (\vec{i}_n \cdot \Pi)\cdot(1-\vec{i}_n\vec{i}_n)$ and $\vec{q} = \overline{Q}\cdot(1-\vec{i}_n\vec{i}_n)$, with an arrow denoting a vector quantity. The tangential momentum accommodation coefficient is σ, μ is the gas viscosity at the wall, λ the molecular mean free path at the wall, N_{Pr} the Prandtl number, γ the specific heat ratio, and p the gas pressure at the wall. A unit vector normal to, and away from, the wall is $\vec{i}_n$, with Π the stress tensor at the wall, **1** the identity tensor, and $\overline{Q}$ the heat flux vector at the wall. Here, and throughout this paper, the molecular mean free path is defined as follows:

$$\lambda = \mu\sqrt{\frac{\pi}{2\rho p}}, \tag{2}$$

where ρ is the gas density.

It should be noted that, in his original paper, Maxwell used a phenomenological argument to derive his boundary condition, so his original expression, Eq. (1), does not directly model the physical process that generates slip, i.e., intermolecular interaction (Maxwell, 1879). This is evident in the fact that Eq. (1) requires a 'momentum accommodation coefficient' for each particular gas/surface combination. Typically, accommodation coefficients may only be inferred from experimental results, rather than directly measured.

Maxwell's phenomenological slip condition can, however, provide useful predictions of certain gas micro-flows if it is correctly implemented for the geometry of interest. If we assume no streamwise variation in wall-normal velocity (i.e., the solid bounding surfaces of the flow are non-rotating and planar) and the Navier–Stokes–Fourier constitutive expressions are used for the viscous stress and heat flux terms in Eq. (1), the conventional expression of Maxwell slip is:

$$u_{\text{s}} = \frac{(2-\sigma)}{\sigma}\lambda\frac{\mathrm{d}u_x}{\mathrm{d}n} + \frac{3}{4}\frac{\mu}{\rho T}\frac{\mathrm{d}T}{\mathrm{d}x}, \tag{3}$$

where n is the co-ordinate normal to the wall, x is the co-ordinate tangential to the wall, u_x is the x component of the gas velocity, u_{s} is the x component of the slip velocity, and ρ and T are the density and temperature of the gas at the wall, respectively. Eq. (3) has been clearly shown to improve predictions for flow in gas microsystems where, as we would expect, the no-slip condition becomes increasingly inadequate as the Knudsen number increases (Lockerby and Reese, 2003).

While Eq. (3) is the form of the Maxwell slip condition conventionally implemented in numerical solutions, it is important to note that it is not applicable to surfaces with curvature. For example, for a surface in two dimensions (and again using the Navier–Stokes–Fourier constitutive relations), Eq. (1) becomes

$$u_{\text{s}} = \frac{(2-\sigma)}{\sigma}\lambda\left(\frac{\mathrm{d}u_x}{\mathrm{d}n} + \frac{\mathrm{d}u_n}{\mathrm{d}x}\right) + \frac{3}{4}\frac{\mu}{\rho T}\frac{\mathrm{d}T}{\mathrm{d}x}, \tag{4}$$

where u_{n} is the gas velocity normal to the wall (Lockerby et al., 2004).

The additional term featuring in Eq. (4) but not in Eq. (3) can have a significant influence on the velocity slip, and the overall accuracy of the numerical simulation of the flow field. For example, we have recently shown that accurate CFD predictions of both velocity profile inversion in cylindrical micro-Couette flow, and the skin friction drag on a microsphere, are only achieved when using Eq. (1) (or using Eq. (4) for two-dimensional cases) (Lockerby et al., 2004).

3. The Knudsen layer

In addition to velocity slip at bounding surfaces, the so-called Knudsen layer extends one or two molecular mean free paths from the surface into a gas flow. This region is characterised by strong departures from linearity of the stress/strain-rate relationship and, as such, cannot be captured by the Navier–Stokes–Fourier constitutive relations.

The Knudsen layer is, however, an important component of the flow in many microsystem configurations, and should therefore be incorporated within any comprehensive numerical simulation technique. For example, in the planar Poiseuille micro-flow case discussed above, where the mass flowrate is 15% greater than expected, 30% of this increase can be attributed to the non-linear structure of the Knudsen layer (Lockerby et al., 2005a).

The most common approach is to account for (rather than model) the Knudsen layer by employing *fictitious* slip boundary conditions at the bounding surface (u^*_{slip} in Fig. 1). Higher order slip conditions are also fictitious, or *macro*, slip conditions which do not directly capture the Knudsen layer, only prescribing a different value of slip velocity at the wall (Lockerby et al., 2004). This slip does, at least, provide an accurate solution outside the Knudsen layer (the dashed line in Fig. 1) if the Navier–Stokes equations are used as the hydrodynamic model. If the *actual*, or *micro*, velocity slip (u_{slip}) is applied at the boundary, the

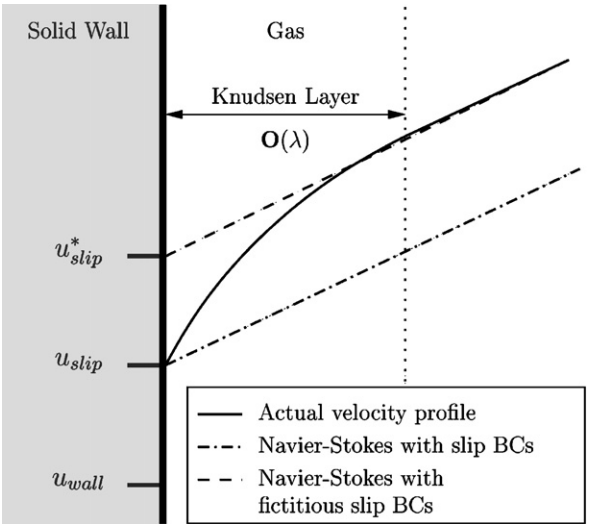

Fig. 1. Schematic of the velocity structure of the Knudsen layer near a wall in a shear flow, with a comparison of two types of slip boundary condition.

prediction of the velocity both inside and outside the Knudsen layer is poor (the dash-dot line in Fig. 1).

Note that either type of velocity slip condition can be implemented for planar surfaces simply by using the Maxwell slip condition with a factor in front of the first term on the right hand side of Eq. (3): Maxwell assumed this factor to be 1.0 (Maxwell, 1879); in the case of macro slip, kinetic theory predicts this factor as 1.146 (Cercignani, 1990); for actual slip, this factor should be 0.8 (Lockerby et al., 2005b).

The major drawback to the macro slip approach is that some part of the flow field is then by definition fictitious. For high Knudsen number micro-flows, this can be a significant proportion of the entire flow. An alternative approach is to apply the Navier–Stokes equations with macro slip boundary conditions to the entire flow field, but then to make a kinetic theory-based correction to either the velocity field, or to an averaged property of interest, such as the mass flowrate. This approach, however, cannot be applied to micro-flow geometries of any complexity.

In the following sections we describe two possible approaches to simulating the Knudsen layer: one newly-implemented phenomenological model, and one physical approach. We compare their effectiveness on simple, incompressible flow cases.

3.1. A wall-function description of the Knudsen layer

A numerically economical approach to incorporating the Knudsen layer in simulations of gas micro-flows is to use a *wall-function* to describe the relationship between viscous stress and strain-rate in the near-wall region. This approach is akin to that used in conventional macro-scale turbulence modelling. Whilst it is a phenomenological approach, like that of Maxwell's to slip, the wall-function method may be able to capture some of the essential features of micro-flows. It also may have a more general applicability across a range of rarefied flow systems than would at first be suggested by the assumptions of flow and geometry, outlined below, on which it is based.

Linearised kinetic theory indicates that the velocity profile through a Knudsen layer close to a planar wall in a monatomic gas flow subject to a uniform shear stress is

$$u = -\frac{\tau}{\mu}(n + \zeta - \lambda I(n/\lambda)), \tag{5}$$

where n is the normal distance from the planar wall, τ is the uniform shear stress, μ is the gas viscosity, λ is the mean free path, and ζ is a constant (Cercignani, 1990). The velocity correction function $I(n/\lambda)$ can be curve-fit from kinetic theory data (Lockerby et al., 2005b) to be:

$$I(n/\lambda) \approx \frac{7}{20}\left(1 + \frac{n}{\lambda}\right)^{-2}. \tag{6}$$

Differentiating Eq. (5) then produces an expression relating stress to the strain-rate that is appropriate throughout the Knudsen layer:

$$\frac{\mathrm{d}u}{\mathrm{d}n} = -\frac{\tau}{\mu}\Psi(n/\lambda), \tag{7}$$

which can be used in place of the Navier–Stokes relation. The wall-function, $\Psi(n/\lambda)$, in Eq. (7) is given by

$$\Psi(n/\lambda) = 1 - \lambda\frac{\mathrm{d}}{\mathrm{d}n}I(n/\lambda) \approx 1 + \frac{7}{10}\left(1 + \frac{n}{\lambda}\right)^{-3}. \tag{8}$$

The limitations of this model are evident in its basic assumptions: low Mach number flow; relatively low Knudsen number; planar surfaces with diffuse molecular reflection. This model does, however, also improve, both qualitatively and quantitatively, predictions of flow over non-planar surfaces (Lockerby et al., 2005b). It is accurate in planar cases for Knudsen numbers as high as $Kn = 0.1$, and the approach remains valid as $Kn \to 0$: as Kn decreases, the wall-function $\Psi(n/\lambda) \to 1$, and the linear relationship between stress and strain-rate (assumed in the Navier–Stokes equations) is restored. As an example, we show a comparison of the performance of this model with direct simulation Monte-Carlo (DSMC) data on a benchmark case in Fig. 2.

It should be noted that the wall-function approach will only give improved results (as compared to using macro slip boundary conditions) within the Knudsen layer itself. Moreover, the stress variation throughout the Knudsen layer from the wall-function method is *identical* to that calculated using fictitious slip boundary conditions. For example, in planar micro-Couette flow, the wall shear stress predicted by the Navier–Stokes equations with a wall-function is the same as the wall shear stress predicted by the Navier–Stokes equations with an equivalent macro slip boundary condition (here, an 'equivalent' slip condition refers to one that predicts the same velocity profile outside of the Knudsen layer). In this case, the improvement that is provided by the wall-function is limited to

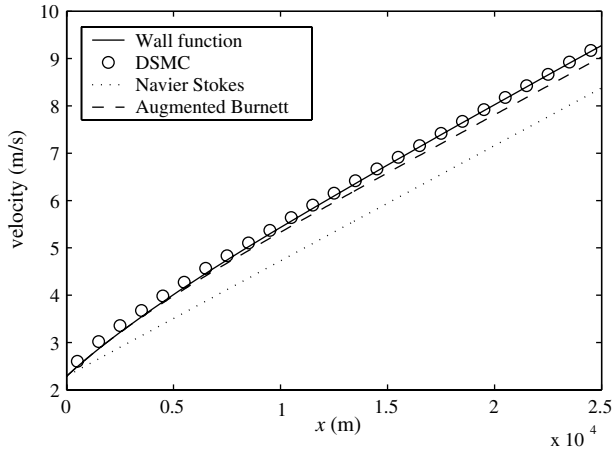

Fig. 2. Comparison of the velocity profile through the Knudsen layer in Kramer's micro-flow problem (planar wall at $x = 0$); DSMC results for argon (○), wall-function within CFD (—), Augmented Burnett equations solution (- -), and conventional CFD (i.e., the Navier–Stokes equations with micro slip) (···) [3].

the Knudsen-layer velocity profile. The non-linearity in the stress/strain-rate relationship that is introduced through the wall-function in Eq. (7) maintains the correct constant shear stress of the Couette flow case.

This wall-function method has the strong advantage of being very easy to implement in a Navier–Stokes flow solver simply by substituting the real gas viscosity, μ, with the scaled quantity, $\mu\Psi^{-1}$ (which tends to the actual gas viscosity in the flow outside the Knudsen layer).

The effective scaling of the gas viscosity in this way will, however, impact other areas of the flow calculation. Although this is a phenomenological approach, and not one developed to model the physical process directly, it is still important that any such additional effects resulting from the chosen method of implementation are both reasonable and physically consistent.

One consequence of the effective gas viscosity scaling is that the normal strain-rate is affected similarly to the shear strain-rate. This non-linear coupling of normal-to-tangential quantities implies that there is an equivalent Knudsen layer in the wall-normal velocity component. This type of Knudsen layer has been predicted by Sone (1990), who also proposed wall-normal macro slip conditions (a slip *into* a non-permeable wall) in order to accommodate this phenomenon within a Navier–Stokes solution.

Effective gas viscosity scaling also impacts the calculation of the mean free path, as required for the micro slip boundary condition Eq. (3). The definition for the mean free path used in Maxwell's boundary condition is given in Eq. (2). This definition is based on *equilibrium* gas properties and shows the mean free path to be proportional to the viscosity. The fact that this definition is affected by the scaling could be considered as a correction to account for departures from equilibrium near the wall, rather than an alteration to the actual mean-free-path itself. At first glance, the reduction in the *effective* mean free path might appear to reduce the slip predicted by Maxwell's boundary condition, but this is balanced by an exactly equal increase in strain-rate at the wall, resulting in the same slip prediction as would be obtained without the wall-function – the velocity micro slip condition is *independent* of the wall-function, and this is consistent with the wall-function's derivation.

Through the constant Prandtl number, our effective gas viscosity scaling will also alter thermal conductivity within the Knudsen layer. This implies the existence of a thermal Knudsen layer, which is well documented. Fig. 3 shows a thermal Knudsen layer within a half space predicted by the current wall-function, compared with a result from kinetic theory (Loyalka, 1989) and a result with no wall-function. The wall-layer result has been obtained by an analytical solution of the one-dimensional steady energy equation – the agreement with the kinetic theory solution is reasonable. Note, each result in Fig. 3 has been obtained with the same boundary conditions and the same prescribed and uniform heat-flux in the gas.

One further noteworthy practical implication of the wall-function technique is that it cannot be implemented in conjunction with governing hydrodynamic equations that have been derived assuming constant viscosity. To illustrate this point we consider the momentum equations, in tensor form:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_k u_i)}{\partial x_k} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ik}}{\partial x_k}, \tag{9}$$

with u_i the velocity in the ith direction and τ_{ik} the second order stress tensor. The divergence of the Navier-Stokes stress tensor is the second term on the right hand side of Eq. (9), and can be expanded as follows:

$$\frac{\partial \tau_{ik}}{\partial x_i} = \frac{\partial(\mu \epsilon_{ik})}{\partial x_i} = \mu \frac{\partial \epsilon_{ik}}{\partial x_i} + \frac{\partial \mu}{\partial x_i}\epsilon_{ik}, \tag{10}$$

where ϵ_{ik} is the strain-rate tensor. In calculations where the viscosity is assumed to be constant (as in isothermal conditions, for example), the second term on the right hand-side of Eq. (10) is zero, and is often removed from numerical

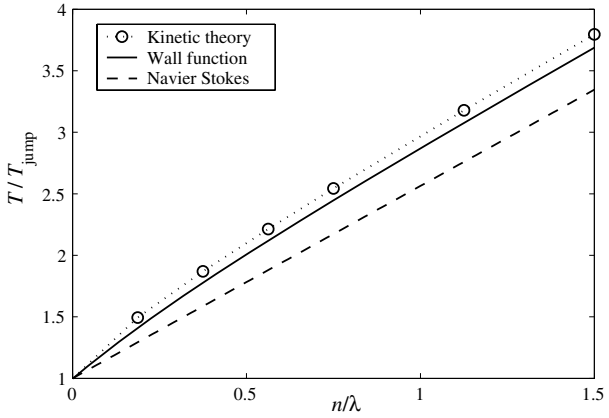

Fig. 3. Wall-function results for a thermal Knudsen layer within a half-space. Comparison of Navier–Stokes solution (- -), wall-function results (—) and kinetic theory (··○··).

solvers. Any implementation of the wall-function technique, however, implies spatial variation in effective viscosity in a direction normal to the wall. Thus, this term coupling the variation of effective viscosity to the strain-rate *cannot* be omitted – even in the isothermal case.

Isothermal Couette flow between rotating cylinders, for example, is a case in which no reasonable solution may be obtained using the wall-function technique unless the coupled velocity–viscosity terms from Eq. (10) are retained in the momentum equations. In the case of a rotating inner cylinder and a stationary outer cylinder, direct simulation Monte Carlo (DSMC) molecular dynamics simulations predict an inverted tangential velocity profile, that is to say, the gas velocity *increases* with radial distance from the moving cylinder (Tibbs et al., 1997). This case has been investigated previously in order to compare results obtained using Eq. (4) in place of Eq. (3) (Lockerby et al., 2004; Barber et al., 2004), however the wall-function approach has not previously been applied to this problem.

Fig. 4 illustrates our results for tangential velocity in the rotating Couette flow problem. The inner and outer cylinders are concentric, with respective radii of 3λ and 5λ, and the gas flowing between the cylinders is argon at standard temperature and pressure (STP). The tangential momentum accommodation coefficient, σ, is 0.1. The figure compares the velocity profile predictions of several numerical models with DSMC data. Both no-slip and conventional slip (Eq. (3)) simulations fail to predict inversion of the velocity profile. Maxwell's original slip equation, in this case Eq. (4), is seen to predict an inverted velocity profile, although it cannot capture the form of the DSMC results. When the wall-function method (shown as the solid line) is applied, not only is good general agreement with Maxwell's original slip condition observed, but the shape of the velocity profile is seen to approach that of the DSMC data. The slight dip in the profile near the inner wall and the reduction in gradient towards the outer cylinder can clearly be seen. Quantitative agreement with the DSMC remains poor, but it should be noted that for this high Knudsen number case ($Kn = 0.5$), we are operating at the very edge of applicability for continuum models, and close numerical agreement is not expected.

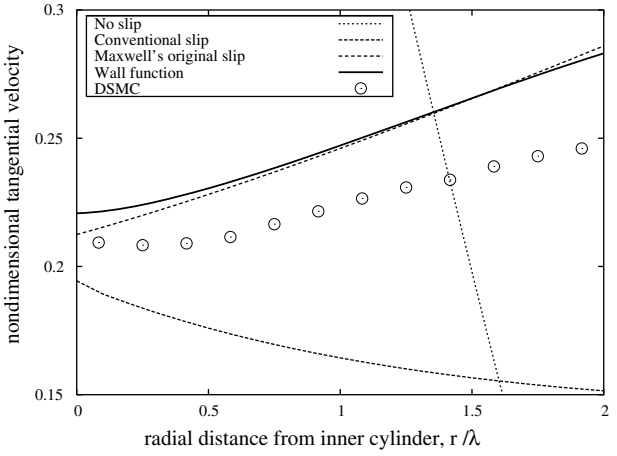

Fig. 4. Velocity profiles in cylindrical Couette flow nondimensionalised by the tangential velocity of the inner cylinder. Comparison of no slip (···), conventional slip (- -), Maxwell's original slip (- · -), wall-function in CFD (—) and DSMC data (○).

Although the wall-function method has been shown to be effective in many applications, it is still the case that the model is phenomenological and, as such, not perfectly general. It has been shown in other work, for example, that the choice of accommodation coefficient in Maxwell's slip equation, Eq. (1), can have a notable impact on flowfield results (Myong et al., 2005). In the current wall function model, the form of the Knudsen layer is independent of the accommodation coefficient. Recent work by Zheng et al. addresses this issue with the formulation of a wall-function that incorporates the accommodation coefficient (Zheng et al., 2006). This recent research will be included in future numerical models with the aim of increasing the generality of the wall-function approach. Further work will also include more detailed verification of the wall-function method with available experimental results for a range of micro-flow cases.

3.2. Higher-order continuum equations

While the Knudsen layer wall-function technique is one way of extending hydrodynamic models into the rarefied regime, the potential of higher-order continuum equations (derived from kinetic theory to be appropriate for high Knudsen number flows) is presently being explored. These have shown promise in the field of hypersonic aerodynamics, in particular, shock wave structure, and may also be a suitable model for rarefied flows in microsystems.

It is well-known that continuum expressions for the viscous stress and heat flux in gases may be derived from the Boltzmann equation via either a *Kn*-series solution (known as the Chapman–Enskog approach) or by an expansion of the distribution function as a series of Hermite tensor polynomials. To first order (i.e., for near-equilibrium flows) both approaches yield the Navier–Stokes–Fourier equations. However, the solution methods can be continued to second and higher orders, incorporating more and more of the salient characteristics of a rarefied flow. The classical second-order stress and heat flux expressions are the *Burnett* equations (from the Chapman–Enskog approach), and the *Grad 13 moment* equations (from the Hermite polynomial method). These can be seen as corrections to the Navier–Stokes constitutive relations to make them appropriate to flows which are more non-equilibrium in nature.

However, differing physical interpretations of the solution methods at second and higher orders, have recently led to a variety of different, competing equation sets. Space considerations preclude listing these complicated and lengthy sets of equations here, but the reader is referred to previous literature that details the derivation of the main sets: the *BGK-Burnett* (Balakrishnan, 2004), *Augmented Burnett* (Zhong et al., 1993), *Regularized Burnett* (Jin and

Slemrod, 2001) and *R13* (Struchtrup and Torrilhon, 2003) equations.

While each purports to be the proper high-order correction to the stress and heat flux (there is no disagreement about the form of the Navier–Stokes–Fourier equations at first-order), no single equation set has demonstrated universal superiority in the prediction of rarefied gas flows – it is an active research question as to which is the 'best' set of equations. All of the higher-order equation sets have disadvantages, which can include:

- high nonlinearity, often requiring exotic and complicated numerical solution methods;
- pathological instability in their numerical solution;
- dependence on the (moving) frame of the observer;
- thermodynamic inconsistency (which may be the cause of the numerical instability noted above), although this issue has been claimed to be resolved (Myong, 1999);
- a critical Mach number beyond which solutions are intractable;
- an inability to predict important non-equilibrium effects, such as the Knudsen layer;
- unknown additional boundary conditions at solid walls and freestream to ensure unique solutions.

A key potential benefit, however, if a physically correct and stable set of governing high-order equations with proper boundary conditions can be identified, is that the equations reduce to the Navier–Stokes equations as Kn tends to zero, so no coupling of solutions within the same simulation is needed for mixed-density and transonic flow fields. Additionally, and importantly, their computational cost would be comparable to traditional CFD.

The model problem we have chosen to examine here in order to compare the effectiveness of the wall-function technique and certain high-order equations in capturing the Knudsen layer, is Kramer's problem: gas flow generated by a uniformly-applied shear stress and bounded by one parallel plane surface. This allows us to study the one-dimensional isothermal Knudsen layer in isolation. DSMC data is available for comparison with our CFD solutions; in this case of Mach 0.05, Couette flow of argon gas, where the channel height is amply sufficient to accommodate the Knudsen layers on both walls without interference with each other (Lockerby et al., 2005a).

Details of the application of the high-order equation sets to Kramer's problem are given in (Lockerby et al., 2005a). We take the extra boundary conditions required from published kinetic theory solutions to Kramer's problem (which closely agree, incidentally, with the DSMC data).

After the linearisation and one-dimensionalisation appropriate for analysing Kramer's problem, the classical Burnett and Grad equation sets both reduce to the Navier–Stokes equations which, as noted above, do not capture any of the non-linearity in the Knudsen layer. However, the other high-order equation sets we examined (Balakrishnan, 2004; Zhong et al., 1993; Jin and Slemrod, 2001; Struchtrup and Torrilhon, 2003) do produce Knudsen-layer-like solutions.

The DSMC data indicates a Knudsen layer 1.4 mean free paths thick; while the Augmented Burnett equations produce a layer 0.9 mean free paths thick; BGK-Burnett equations, 2.1; R13 equations, 2.8; and the Regularized Burnett equations, 4.9 mean free paths thick (Lockerby et al., 2005a). Taking the Augmented Burnett equations, therefore, as the closest to reproducing the DSMC data, we can then compare the predictions of this equation set, with those of the wall-function of Section 3.1. This comparison is shown in Fig. 2. As can be seen, the wall-function technique gives very good agreement with the DSMC data, marginally better than the Augmented Burnett solution. As discussed above, the Navier–Stokes solution from conventional CFD does not display a Knudsen layer structure at all.

It is important to note, however, that this is only one benchmark test case, and neither the wall-function approach nor the Augmented Burnett equations can be said to have proven their general usefulness; in particular, there has been so far little or no investigation into their ability to predict high-speed or non-isothermal flows, nor flows in complex geometries.

4. Conclusions

In this paper some of the key aspects required in simulating gas micro-flows have been investigated; specifically, slip velocities and the Knudsen layer. The application of Maxwell's slip condition has been discussed, along with two methods for incorporating the Knudsen layer into hydrodynamic simulations at the microscale: a wall-function model that scales the viscosity of a gas to capture the Knudsen layer, and the use of higher-order equation sets.

While the higher-order approach offers the promise of a new fluid dynamics that could capture the flow features more generally (particularly in complex geometries), in practice, empirical input is still required. The phenomenological wall-function approach may be straightforward and easy to implement, but it could lack generality based on the tight assumptions on which it is based.

Both approaches have distinct benefits and drawbacks, but it is not the intention of this paper to identify which is the better or most promising of the two. Intuitive phenomenological methods can inform and inspire physical modelling techniques, in the same way that accurately modelling the physics of a system informs the development of 'broad-brush' phenomenological techniques. In some cases, it is also possible to directly relate the physical to the phenomenological. An alternative to Maxwell's slip boundary condition, for example, would be to use the Langmuir slip model, where velocity slip may be directly related to the measureable potential energy of gas-surface adsorption (Myong et al., 2005).

Consequently, it would seem that the development of both physical modelling and phenomenological methods

to capture non-equilibrium gas behaviour should be pursued in parallel; we are investigating both approaches as part of a funded collaborative research programme between Strathclyde University and Daresbury Laboratory in the UK.

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References

Balakrishnan, R., 2004. An approach to entropy consistency in second-order hydrodynamic equations. J. Fluid Mech. 503, 201–245.

Barber, R.W., Sun, Y., Gu, X.J., Emerson, D.R., 2004. Isothermal slip flow over curved surfaces. Vacuum 76, 73–81.

Cercignani, C., 1990. Mathematical Methods in Kinetic Theory. Plenum Press, New York.

Gad-el-Hak, M., 1999. The fluid mechanics of microdevices – the Freeman Scholar Lecture. J. Fluids Eng. (Trans. ASME) 121, 5–33.

Jin, S., Slemrod, M., 2001. Regularization of the Burnett equations via relaxation. J. Stat. Phys. 103, 1009–1033.

Lockerby, D.A., Reese, J.M., 2003. High-resolution Burnett simulations of micro Couette flow and heat transfer. J. Comput. Phys. 188, 333–347.

Lockerby, D.A., Reese, J.M., Emerson, D.R., Barber, R.W. 2004. Velocity boundary condition at solid walls in rarefied gas calculations. Phys. Rev. E 70 art. no. 017303.

Lockerby, D.A., Reese, J.M., Gallis, M.A. 2005a. The usefulness of higher-order constitutive relations for describing the Knudsen layer. Phys. Fluids 17 art. no. 100609.

Lockerby, D.A., Reese, J.M., Gallis, M.A., 2005b. Capturing the Knudsen layer in continuum-fluid models of non-equilibrium gas flows. Aiaa J. 43, 1391–1393.

Loyalka, S.K., 1989. Temperature jump and thermal creep slip: rigid sphere gas. Phys. Fluids A 1, 403–408.

Maxwell, J.C., 1879. On stresses in rarified gases arising from inequalities of temperature. Phil. Trans. Roy. Soc. 170, 231–256.

Myong, R.S., 1999. Thermodynamically consistent hydrodynamic computational models for high Knudsen number gas flows. Phys. Fluids 11-9, 2788–2802.

Myong, R.S., Reese, J.M., Barber, R.W., Emerson, D.R., 2005. Velocity slip in microscale cylindrical Couette flow: the Langmuir model. Phys. Fluids 17, 087105.

Sone, Y., 1990. Kinetic Theory and Fluid Dynamics. Birkhauser, Boston.

Struchtrup, H., Torrilhon, M., 2003. Regularization of Grad's 13 moment equations: derivation and linear analysis. Phys. Fluids 15, 2668–2680.

Tibbs, K.W., Baras, F., Garcia, A.L., 1997. Anomalous flow profile due to the curvature effect on slip length. Phys. Rev. E 56, 2282–2283.

Zheng, Y., Reese, J.M., Scanlon, T.J., Lockerby, D.A. 2006. Scaled Navier–Stokes–Fourier equations for gas flow and heat transfer phenomena in micro- and nanosystems. In: Proceedings of ASME ICNMM2006, June 19–21, Limerick, Ireland 96066.

Zhong, X., MacCormack, R.W., Chapman, D.R., 1993. Stabilization of the Burnett equations and application to hypersonic flows. Aiaa J. 31, 1036–1043.