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Macroscopic description of arbitrary Knudsen number flow using Boltzmann–BGK kinetic theory

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We derive, without approximation, a closed-form macroscopic equation for finite Knudsen number flow using the Boltzmann–BGK kinetic theory with constant relaxation time. This general closed-form equation is specialized into a compact integro-differential equation for time-dependent isothermal unidirectional flows and results are presented for channel flow. This equation provides a clear demonstration of the effects of finite Knudsen number, and it also illustrates the limitations of the Boltzmann–BGK theory with constant relaxation time and bounce-back boundary conditions.

1. Introduction

It is well-accepted that fluid flows at infinitesimal Knudsen number (Kn) are described by the Navier–Stokes equations. Here the non-dimensional number Kn is the ratio of a microscopic length or time scale to macroscopic ones (see below). The Navier–Stokes equations are not applicable in flow regimes at sufficiently small macroscopic spatial and/or time scales, i.e. at finite Kn, because kinetic effects are then important.

In order to obtain a fluid dynamical equation valid at all Kn, one can start from a kinetic model of the flow, namely the Boltzmann equation (Cercignani 1975) with the Bhatnagar–Gross–Krook (1954) (BGK) collision model

$$\partial_t f + \boldsymbol{v} \cdot \nabla f = C, \tag{1}$$

where C is the collision operator with a relaxation time τ,

$$C = -\frac{f - f^{eq}}{\tau}, \tag{2}$$

$f = f(\boldsymbol{x}, \boldsymbol{v}, t)$ is the single-particle distribution function which represents the density of kinetic particles in the phase space $(\boldsymbol{x}, \boldsymbol{v})$ at time t, and the *local* kinetic equilibrium distribution function f^{eq} is the Maxwell–Boltzmann distribution,

$$f^{eq}(\boldsymbol{x}, \boldsymbol{v}, t) = \frac{\rho(\boldsymbol{x}, t)}{(2\pi\theta(\boldsymbol{x}, t))^{D/2}} \exp\left[-\frac{(\boldsymbol{v} - \boldsymbol{u}(\boldsymbol{x}, t))^2}{2\theta(\boldsymbol{x}, t)}\right]. \tag{3}$$

Macroscopic flow variables, like the fluid velocity, are moments of f. For example,

$$\left.\begin{aligned}\rho(\boldsymbol{x},t)&=\int \mathrm{d}\boldsymbol{v}\, f(\boldsymbol{x},\boldsymbol{v},t)=\int \mathrm{d}\boldsymbol{v}\, f^{eq}(\boldsymbol{x},\boldsymbol{v},t),\\ \rho\boldsymbol{u}(\boldsymbol{x},t)&=\int \mathrm{d}\boldsymbol{v}\boldsymbol{v} f(\boldsymbol{x},\boldsymbol{v},t)=\int \mathrm{d}\boldsymbol{v}\,\boldsymbol{v} f^{eq}(\boldsymbol{x},\boldsymbol{v},t),\\ \rho(\boldsymbol{u}^2(\boldsymbol{x},t)+D\theta(\boldsymbol{x},t))&=\int \mathrm{d}\boldsymbol{v}\,\boldsymbol{v}^2 f(\boldsymbol{x},\boldsymbol{v},t)=\int \mathrm{d}\boldsymbol{v}\,\boldsymbol{v}^2 f^{eq}(\boldsymbol{x},\boldsymbol{v},t),\end{aligned}\right\} \tag{4}$$

where ρ, $\boldsymbol{u}$, θ denote, respectively, density, fluid velocity, and temperature, and D is the spatial dimensionality of phase space. Notwithstanding some well-known limitations such as unity Prandtl number, the Boltzmann–BGK kinetic model has been used widely to study high Kn as well as high Mach number flow problems (cf. Xu, Martinelli & Jameson 1994).

In the limit of vanishing Kn, the Navier–Stokes equations with kinematic viscosity $\nu=\tau\theta$ may be derived from (1)–(4) using Chapman–Enskog (see Chapman & Cowling 1970) techniques. In particular, when $Kn\equiv\tau/T_h\rightarrow 0$, where T_h is the characteristic hydrodynamic scale, classical Newtonian hydrodynamics results. Finite-Kn corrections to the Navier–Stokes equations have long been sought in terms of expansions in powers of Kn (cf. Chen *et al.* 2004). There are many problems with these expansions as well as with the resulting models (cf. Cercignani 1975).

In this paper, we pursue a macroscopic description of arbitrary Knudsen number flow. There is a wealth of published work extending over several decades on closed-form macrodynamic descriptions based on Boltzmann–BGK kinetics at arbitrary Kn, including equations for the flow velocity. These works are usually based on the inversion of the simple BGK collisional operator. However, many of these results are obtained using solutions that are ‘linearized’ around a homogeneous absolute equilibrium distribution (Cercignani 1969, and references therein).

There are several reasons then why we believe that is useful to present the macro-dynamic description of BGK kinetics in a general form without imposing constraints like linearization (although our equations for unidirectional flow are, as for unidirectional Navier–Stokes flow, those for linearized flow). First, while the resulting equations are complicated integro-differential equations for which the formulation of easy-to-implement boundary conditions may be difficult (see § 5), these equations do open the opportunity for interesting mathematical analyses. Second, once the dynamical equations for flow velocity are obtained under the assumptions of constant-relaxation-time BGK dynamics, they may be easily generalized and/or modelled to avoid such assumptions (e.g. by simply allowing τ to vary according to local flow properties and near walls) and, hence, may find wider and perhaps more realistic application, e.g. in the numerical analysis of finite-Kn flows. Also, the existence of these equations allows the study of hitherto intractable problems, such as the effect of finite Kn on turbulence transport (cf. Chen *et al.* 2004).

2. General formulation of hydrodynamics for any Kn

By integrating along the microscopic characteristic lines, the Boltzmann–BGK kinetics (1)–(4) at constant τ admits the solution

$$f(\boldsymbol{x},\boldsymbol{v},t)=\int_{-\infty}^{t}\frac{\mathrm{d}t'}{\tau}\mathrm{e}^{-(t-t')/\tau} f^{eq}(\boldsymbol{x}-\boldsymbol{v}(t-t'),\boldsymbol{v},t'), \tag{5}$$

or equivalently,

$$f(\boldsymbol{x}, \boldsymbol{v}, t) = \int_0^\infty e^{-s} f^{eq}(\boldsymbol{x} - \boldsymbol{v}\tau s, \boldsymbol{v}, t - \tau s)\, ds. \tag{6}$$

A constant relaxation time τ is assumed throughout our derivation of the dynamics. This solution, based on the method of characteristics, is unique in free space. For finite domains, there are additional boundary terms which must be included. If the distance from the wall is large compared to the mean free path, the free-space solution is a good approximation.

When combined with (3), (6) reveals the existence of closed-form macroscopic equations for ρ, $\boldsymbol{u}$, and θ for all Kn in a general D-dimensional flow situation. That is, moments of f yield ρ, $\boldsymbol{u}$, and θ via (4), while the right-hand side of (6) is already given by the macro-dynamic variables via (3). Therefore, (6) represents a closed, self-contained projection, and both the equilibrium and non-equilibrium parts of $f(\boldsymbol{x}, \boldsymbol{v}, t)$ are entirely determined (non-locally in time and space) by the inhomogeneity in the macroscopic variables, ρ, $\boldsymbol{u}$, and θ. This fundamental description can be argued to be generally applicable to all flow situations. Furthermore, it should be distinguished from that of the linearized analysis based on a homogeneous absolute equilibrium (cf. Cercignani 1969).

These points can be made clearer by presenting a conventional hydrodynamic equation representation. By taking moments (4) of (1), we obtain

$$\partial_t \rho u_\alpha + \partial_\beta \sigma_{\alpha\beta} = 0, \tag{7}$$

$$\partial_t [\rho(\boldsymbol{u}^2 + D\theta)] + \partial_\beta q_\beta = 0, \tag{8}$$

where the subscripts α and β denote Cartesian components, $\partial_\beta \equiv \partial/\partial x_\beta$, and the fluxes are defined as

$$\sigma_{\alpha\beta} \equiv \int d\boldsymbol{v}\, v_\alpha v_\beta f, \tag{9}$$

$$q_\alpha \equiv \int d\boldsymbol{v}\, v^2 v_\alpha f. \tag{10}$$

Using (3) and (6), it is apparent that a closed-form macroscopic description is established. Indeed, combining (7)–(10) with (6), results in

$$\partial_t \rho(\boldsymbol{x}, t) u_\alpha(\boldsymbol{x}, t) = -\partial_\beta \int_0^\infty ds\, e^{-s} \int d\boldsymbol{v}\, v_\alpha v_\beta \frac{\rho(\boldsymbol{x} - \boldsymbol{v}\tau s, t - \tau s)}{(2\pi\theta(\boldsymbol{x} - \boldsymbol{v}\tau s, t - \tau s))^{D/2}} \times \exp\left[-\frac{(\boldsymbol{v} - \boldsymbol{u}(\boldsymbol{x} - \boldsymbol{v}\tau s, t - \tau s))^2}{2\theta(\boldsymbol{x} - \boldsymbol{v}\tau s, t - \tau s)}\right], \tag{11}$$

$$\partial_t [\rho(\boldsymbol{x}, t)(\boldsymbol{u}^2(\boldsymbol{x}, t) + D\theta(\boldsymbol{x}, t))] = -\partial_\alpha \int_0^\infty ds\, e^{-s} \int d\boldsymbol{v} v^2 v_\alpha \frac{\rho(\boldsymbol{x} - \boldsymbol{v}\tau s, t - \tau s)}{(2\pi\theta(\boldsymbol{x} - \boldsymbol{v}\tau s, t - \tau s))^{D/2}} \times \exp\left[-\frac{(\boldsymbol{v} - \boldsymbol{u}(\boldsymbol{x} - \boldsymbol{v}\tau s, t - \tau s))^2}{2\theta(\boldsymbol{x} - \boldsymbol{v}\tau s, t - \tau s)}\right]. \tag{12}$$

Of course, this system should be augmented by mass conservation, which has the same form as for $Kn = 0$:

$$\partial_t \rho(\boldsymbol{x}, t) = -\partial_\beta \int d\boldsymbol{v}\, v_\beta f = -\partial_\beta \int d\boldsymbol{v}\, v_\beta f^{eq} = -\partial_\beta(\rho(\boldsymbol{x}, t) u_\beta(\boldsymbol{x}, t)). \tag{13}$$

Equations (11)–(13) are a self-contained set of integro-differential equations for the macroscopic fields ρ, $\boldsymbol{u}$ and θ that are valid for all Kn.

A few elementary transformations are useful in order to establish the analogy between the functional equations (11) and (12), whose spatial arguments on the right-hand side are shifted by $\boldsymbol{v}\tau s$, and traditional macroscopic descriptions in physical space. When the dummy integration variable $\boldsymbol{v}$ is shifted by $(\boldsymbol{x}-\boldsymbol{y})/\tau s$, (11)–(12) can be rewritten in terms of integration over the spatial domain R:

$$\partial_t(\rho(\boldsymbol{x},t)u_\alpha(\boldsymbol{x},t)) = -\partial_\beta \int_0^\infty \mathrm{d}s\, \mathrm{e}^{-s} \int_R \frac{\mathrm{d}^D y}{(\tau s)^D} \frac{\rho(\boldsymbol{y},t-\tau s)}{(2\pi\theta(\boldsymbol{y},t-\tau s))^{D/2}} \times \frac{(x_\alpha - y_\alpha)(x_\beta - y_\beta)}{\tau^2 s^2} \exp\left[-\frac{(\boldsymbol{x}-\boldsymbol{y}-\tau s\boldsymbol{u}(\boldsymbol{y},t-\tau s))^2}{2\theta(\boldsymbol{y},t-\tau s)(\tau s)^2}\right], \tag{14}$$

$$\partial_t[\rho(\boldsymbol{x},t)(\boldsymbol{u}^2(\boldsymbol{x},t)+D\theta(\boldsymbol{x},t))] = -\partial_\alpha \int_0^\infty \mathrm{d}s\, \mathrm{e}^{-s} \int_R \frac{\mathrm{d}^D y}{(\tau s)^D} \frac{\rho(\boldsymbol{y},t-\tau s)}{(2\pi\theta(\boldsymbol{y},t-\tau s))^{D/2}} \times \frac{(\boldsymbol{x}-\boldsymbol{y})^2(x_\alpha - y_\alpha)}{\tau^3 s^3} \exp\left[-\frac{(\boldsymbol{x}-\boldsymbol{y}-\tau s\boldsymbol{u}(\boldsymbol{y},t-\tau s))^2}{2\theta(\boldsymbol{y},t-\tau s)(\tau s)^2}\right]. \tag{15}$$

The macroscopic equations (13)–(15) define the dynamics of the hydrodynamic variables ρ, $\boldsymbol{u}$, and θ in a D-dimensional BGK system for finite Knudsen number.

The fact that (14)–(15) are a generalization of Newtonian (infinitesimally small Kn) hydrodynamics is seen by recasting (14) in a form that reflects better the structure of Newtonian hydrodynamics:

$$\begin{aligned}\partial_t(\rho(\boldsymbol{x},t)u_\alpha(\boldsymbol{x},t)) = -\partial_\beta \int_0^\infty \mathrm{d}s\, \mathrm{e}^{-s} \int_R & \mathrm{d}^D y[\rho(\boldsymbol{y},t-\tau s)\theta(\boldsymbol{y},t-\tau s)\delta_{\alpha\beta} \\ & + \rho(\boldsymbol{y},t-\tau s)u_\alpha(\boldsymbol{y},t-\tau s)u_\beta(\boldsymbol{y},t-\tau s) \\ & - \rho(\boldsymbol{y},t-\tau s)\theta(\boldsymbol{y},t-\tau s)\tau s(u_\alpha(\boldsymbol{y},t-\tau s)\partial_\beta \\ & + u_\beta(\boldsymbol{y},t-\tau s)\partial_\alpha) + \rho(\boldsymbol{y},t-\tau s)\theta^2(\boldsymbol{y},t-\tau s)\tau^2 s^2 \partial_\alpha\partial_\beta] \\ & \times \left\{\frac{1}{(2\pi\theta(\boldsymbol{y},t-\tau s))^{D/2}(\tau s)^D} \exp\left[-\frac{(\boldsymbol{x}-\boldsymbol{y}-\tau s\boldsymbol{u}(\boldsymbol{y},t-\tau s))^2}{2\theta(\boldsymbol{y},t-\tau s)(\tau s)^2}\right]\right\}.\end{aligned} \tag{16}$$

Equation (16) is easily derived using the identity

$$\begin{aligned}&[x_\alpha - y_\alpha]\exp\left[-\frac{(\boldsymbol{x}-\boldsymbol{y}-\tau s\boldsymbol{u}(\boldsymbol{y},t-\tau s))^2}{2\theta(\boldsymbol{y},t-\tau s)\tau^2 s^2}\right] \\ &\quad \equiv \left[u_\alpha(\boldsymbol{y},t-\tau s)\tau s - \theta(\boldsymbol{y},t-\tau s)\tau^2 s^2 \frac{\partial}{\partial x_\alpha}\right]\exp\left[-\frac{(\boldsymbol{x}-\boldsymbol{y}-\tau s\boldsymbol{u}(\boldsymbol{y},t-\tau s))^2}{2\theta(\boldsymbol{y},t-\tau s)\tau^2 s^2}\right].\end{aligned}$$

Examining (16) term by term, it seems that, apart from its non-local nature, it is quite similar to the Navier–Stokes equation, while reflecting its kinetic origin more than similar equations based on finite-order perturbative corrections in Kn. Indeed, when $\tau \to 0$, the { } term on the right-hand side of (16) yields a delta function of $\boldsymbol{x}-\boldsymbol{y}$, reducing (16) to the Navier–Stokes equation for an ideal gas. Equation (16) also provides a basis to evaluate finite-Kn effects, using expansion in τ to yield higher-Kn corrections in a systematic way, as an alternative to traditional approaches based on Chapman–Enskog methods. Since the derivation above involves no approximation aside from the BGK approximation and constant τ and is valid for any Kn, (16) may provide consistency checks for approximations and models that are based on expansions in Kn.

3. Unidirectional isothermal flow

As a simple application, we apply the general formulation of § 2 to a special class of flows, namely unidirectional flows in $D=3$ dimensions. In this case, the spatial variation of all macroscopic variables A is perpendicular to the direction of fluid flow, i.e. $\boldsymbol{u}\cdot\nabla A\equiv 0$. We choose the unit vector $\hat{\boldsymbol{z}}$ to be in the flow direction, so that any quantity A has spatial dependence only in x and y. Let us further assume that the flow is isothermal as would occur if the system were in contact with a heat bath, i.e. we assume now that $\theta(\boldsymbol{x},t)=\theta=\text{const}$. We note that isothermal flows exist in nature in various situations, including, but not limited to, incompressible flows. Since for unidirectional flows the continuity equation (13) indicates that mass density is independent of time, it can be shown from (11) (or (16)) that constant density leads to $u_x(\boldsymbol{x},t)=u_y(\boldsymbol{x},t)=0$ for isothermal situations. Hence the only remaining relevant macroscopic variable is the z-component of the flow velocity. Setting $\boldsymbol{u}(\boldsymbol{x},t)=U(x,y,t)\hat{\boldsymbol{z}}$, we can integrate (16) over $\mathrm{d}z'$, resulting in the following compact formulation:

$$\partial_t U(x,y,t)=\nabla\cdot\left[\frac{\sqrt{\theta}}{2\pi\lambda}\nabla\int_0^\infty\frac{\mathrm{d}s}{s}\,\mathrm{e}^{-s}\int_R \mathrm{d}x'\,\mathrm{d}y'\,U(x',y',t-\tau s)\times\exp\left[-\frac{(x-x')^2+(y-y')^2}{2s^2\lambda^2}\right]\right],\tag{17}$$

where $\lambda\equiv\tau\sqrt{\theta}$ is the 'mean free path'. In (17), we have set $\rho=1$ without loss of generality. Various forms of (17), and especially its steady-state variants for classical flows, have been analysed long ago (Cercignani 1969).

Now notice that the non-local component of (17),

$$Q=\int_R \mathrm{d}x'\,\mathrm{d}y'\,U(x',y',t-\tau s)\exp\left[-\frac{(x-x')^2+(y-y')^2}{2s^2\lambda^2}\right],$$

begs to be represented as a solution to a $2D$ heat equation, with the $(t-\tau s)$ argument treated as a parameter while the dummy 'evolution time' r is defined as $r=(1/2)s^2\lambda^2$. Indeed,

$$V(x,y,t-\tau s;r)=\frac{1}{2\pi s^2\lambda^2}\int_R \mathrm{d}x'\,\mathrm{d}y'\,U(x',y',t-\tau s)\exp\left[-\frac{(x-x')^2+(y-y')^2}{2s^2\lambda^2}\right]$$

is the solution of the $2D$ equation

$$\partial_r V(x,y,t,r)=\lambda^2\nabla^2 V(x,y,t,r)\tag{18}$$

with $V(x,y,t,0)=U(x,y,t)$. (Here $\nabla^2\equiv\partial^2/\partial x^2+\partial^2/\partial y^2$ is the two-dimensional Laplacian). On the other hand, the solution to (18) is (formally)

$$V(x,y,t,r)\equiv\exp(r\lambda^2\nabla^2)U(x,y,t).$$

In this way, we obtain the more compact spatial formulation:

$$\partial_t U(x,y,t)=\nabla\cdot\left[\nu\int_0^\infty \mathrm{d}s\,s\,\mathrm{e}^{-s}\exp\left(\tfrac{1}{2}s^2\lambda^2\nabla^2\right)\nabla U(x,y,t-\tau s)\right],\tag{19}$$

where $\nu\equiv\tau\theta$ is the kinematic viscosity given the Boltzmann–BGK model. This equation is valid for any isothermal unidirectional flow (steady or unsteady).

Equation (19) can be also derived using a direct procedure. Indeed, for unidirectional flows, (6) reduces to

$$f(x, y, \boldsymbol{v}, t) = \int_0^\infty \mathrm{e}^{-s} f^{eq}(x - v_x\tau s, y - v_y\tau s, \boldsymbol{v}, t - \tau s)\,\mathrm{d}s.$$

Furthermore, (7) simplifies to

$$\partial_t U + \partial_\beta \sigma_{\beta z} = 0,$$

where $\beta = x, y$, and the momentum flux (9) becomes

$$\sigma_{\beta z} = \int \mathrm{d}\boldsymbol{v}\, v_\beta v_z f. \tag{20}$$

Observing that a spatial shift can be represented as an operator: $F(x + a) = \exp(a\partial_x)F(x)$, allows (20) to be expressed as

$$\sigma_{\beta z}(\boldsymbol{x}, t) = \int_0^\infty \mathrm{d}s\, \mathrm{e}^{-s} \int \mathrm{d}\boldsymbol{v}\, v_\beta v_z \exp[-\tau s \boldsymbol{v}\nabla] \frac{1}{(2\pi\theta)^{D/2}} \exp\left[\frac{(\boldsymbol{v} - \boldsymbol{u}(\boldsymbol{x}, t - \tau s))^2}{2\theta}\right]. \tag{21}$$

Since for unidirectional flow $\partial_z \equiv 0$, Gaussian integration in the z-direction can be separated from integrals in the x- and y-directions so that (21) becomes

$$\begin{aligned}
\sigma_{\beta z} &= \int_0^\infty \mathrm{d}s\, \mathrm{e}^{-s} \int \frac{\mathrm{d}\boldsymbol{v}_\perp}{2\pi\theta} v_\beta \exp\left[-\tau s \boldsymbol{v}_\perp \cdot \nabla - \frac{\boldsymbol{v}_\perp^2}{2\theta}\right] \\
&\quad \times \int_{-\infty}^\infty \frac{\mathrm{d}v_z}{(2\pi\theta)^{1/2}} v_z \exp\left[-\frac{(v_z - U(x, y, t - \tau s))^2}{2\theta}\right] \\
&= \int_0^\infty \mathrm{d}s\, \mathrm{e}^{-s} \int \frac{\mathrm{d}\boldsymbol{v}_\perp}{2\pi\theta} v_\beta \exp\left[-\tau s \boldsymbol{v}_\perp \cdot \nabla - \frac{\boldsymbol{v}_\perp^2}{2\theta}\right] U(x, y, t - \tau s),
\end{aligned}$$

where $\boldsymbol{v}_\perp \equiv (v_x, v_y)$. It is straightforward to show that the operator

$$\int \frac{\mathrm{d}\boldsymbol{v}_\perp}{2\pi\theta} v_\beta \exp\left[-\tau s \boldsymbol{v}_\perp \cdot \nabla - \frac{\boldsymbol{v}_\perp^2}{2\theta}\right] = -\exp\left[\frac{\theta\tau^2 s^2 \nabla^2}{2}\right] \theta\tau s \partial_\beta,$$

leads to

$$\sigma_{\beta z} = -\int_0^\infty \mathrm{d}s\, \mathrm{e}^{-s} \exp\left[\frac{\theta\tau^2 s^2 \nabla^2}{2}\right] \theta\tau s \partial_\beta U(x, y, t - \tau s), \tag{22}$$

which immediately yields (19).

4. Some properties of particular solutions

An important special case of (19) is for flow driven by a constant pressure gradient or body force g. In this case, the right-hand side of (19) is modified by the addition of g. Thus, for steady channel or pipe flow driven by g:

$$\nabla \cdot \left[\nu \int_0^\infty \mathrm{d}s \exp\left(-s - \tfrac{1}{2}s^2\lambda^2\nabla^2\right) \nabla U(x, y)\right] = -g. \tag{23}$$

For small $Kn \equiv \lambda/L$ or λ, (23) becomes the elliptic equation $\nabla \cdot \nu\nabla U = -g$ which together with the boundary condition $U = 0$ yields the well-known Poiseuille flows. On the other hand, at large Kn, one can informally argue that the $\lambda^2\nabla^2$-term dominates the exponent, allowing evaluation of the integral asymptotically as $1/(-\lambda^2\nabla^2)$ yielding

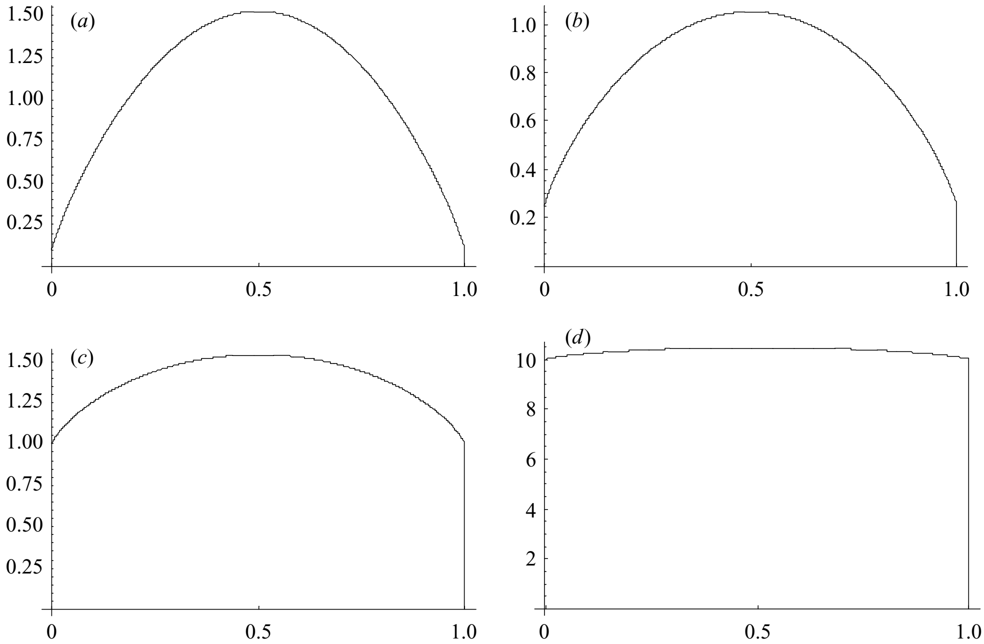

FIGURE 1. Velocity profiles for (*a*) $Kn = 0.1$, (*b*) 0.25 (at the minimum Q_+), (*c*) 1, and (*d*) 10.

the 'plug flow' solution $U = g\tau$ at all points not on the walls. Note that this latter solution is independent of the choice of boundary conditions, (i.e. the details of collision processes at the boundary) and holds for arbitrary cross-sectional channel geometry.

This analysis is made precise by assuming bounce-back boundary conditions applied to the distribution function for $2D$ channel flows; on the macroscopic level, this corresponds to imposing $U(-y) = -U(y)$, for all $y > 0$ where the boundary is located at $y = 0$. Solutions to (23) can be obtained using Fourier sine series in odd harmonics. For planar channel flow in the region $0 \leqslant y \leqslant L$, the solution is

$$U(y) = \sum_{n=0}^{\infty} \frac{4g\tau}{\pi(2n+1)} \left[1 - \frac{1}{\sqrt{2\pi}(2n+1)Kn} \exp\left(\left(\frac{1}{\sqrt{2}(2n+1)\pi Kn} \right)^2 \right) \times \operatorname{erfc}\left(\frac{1}{\sqrt{2}(2n+1)\pi Kn} \right) \right]^{-1} \sin\left(\frac{\pi(2n+1)y}{L} \right). \quad (24)$$

In figure 1, this flow is plotted as a function of y for various Kn using $g = 1$, $L = 1$, and $\tau = Kn$.

These velocity profiles exhibit a slip velocity equal to Kn (or $g\tau$ in dimensional form) at the wall. This slip velocity is an immediate consequence of (24), since the Fourier coefficient of $\sin[\pi(2n+1)y/L]$ in (24) behaves as $4g\tau/\pi(2n+1)$ as $n \rightarrow \infty$ and thus reflects the Gibbs phenomenon satisfied by the Fourier series (24). This slip velocity is consistent with many results for the Maxwell slip velocity, which is proportional to the mean free path; however, the result that the slip equals Kn may overstate the slip velocity owing to the assumptions of constant τ and the bounce-back boundary conditions.

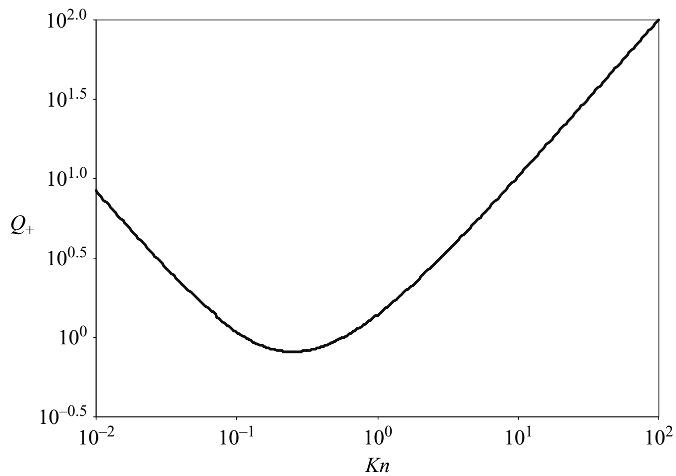

FIGURE 2. Non-dimensional mass flux Q_+ as a function of Kn.

Furthermore, for a channel of a width L, we obtain the well-known Knudsen Minimum phenomenon (Cercignani 1975), namely the non-monotonic behaviour of the dimensionless mass flux $Q_+ \equiv \int_0^L \mathrm{d}y U(y)/(gL^2/\sqrt{\theta})$ exhibiting a minimum at finite Kn (see figure 2). In fact, the minimum mass flux of 0.813 is obtained at $Kn = 0.250$. Also, (24) can be shown to lead to two asymptotic solutions:

$$Q_+ = \frac{1}{12Kn}, \quad Kn \to 0,$$
$$Q_+ = Kn, \quad Kn \to \infty.$$

The $Kn \to 0$ limit is that of Newtonian flow (i.e. the Navier–Stokes equations), while the $Kn \to \infty$ limit is that of plug flow. Notice that the sum of these two asymptotes $Kn + 1/(12\,Kn)$ has a minimum of 0.577 at $Kn = 0.289$, not far from the true minimum. These mass flux results compare well at low-to-moderate Kn with lattice-Boltzmann numerical solutions with the BGK collision term (cf. Toschi & Succi 2005; Zhou *et al.* 2006, and references therein). At high Kn, the actual mass flux is proportional to $\log Kn$ not Kn; this $\log Kn$ behaviour reflects more realistic interaction with the boundaries than is provided by the Boltzmann–BGK approximation with constant relaxation time and bounce-back boundary conditions.

It can be also demonstrated that the plug flow regime can be derived from (24) in the asymptotic limit $Kn \to \infty$:

$$U(y) \sim g\tau \int_0^\infty \mathrm{d}v \frac{\left[v \sin(\pi y/L) + (v^2 \sin^2(\pi y/L) + 1)^{1/2}\right]^{1/(\sqrt{2\pi}\,Kn)}}{1+v^2}$$
$$\to U(y) = g\tau = \text{const}; \quad Kn \to \infty.$$

Let us also briefly comment on the well-posedness of the Cauchy initial-value problem for (19). This problem can be treated in much the same way as that for similar equations based on distribution functions that are analysed in depth by Cercignani (1969). To do this, we consider a single Fourier mode in x, y with wavenumber k so that $\nabla^2 \to -k^2$, and Laplace-transform in time. The resulting single-Fourier-mode solution $F(t)$, obtained by inverse Laplace transform, is

$$F(t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} F(0)\exp(-pt/\tau)G(p)\,dp, \tag{25}$$

where the Green's function $G(p)$ is

$$G^{-1}(p) = p - W\int_0^\infty ds\, s\exp[(p-1)s - Ws^2/2]$$

and $W \equiv k^2\lambda^2 > 0$. Showing that the real parts of all singularities of $G(p)$ are positive suffices to show the well-posedness of (19). Indeed, in this case the integration contour in (25) can be chosen along the imaginary axis, $c=0$, for any W, and the solution $F(t)$ will remain bounded, implying that the norm of the solution is bounded by a multiple of its initial value.

Let us now show that, for any complex $p=a+ib$, such that

$$p = W\int_0^\infty ds\, s\exp[(p-1)s - Ws^2/2] \equiv L(p, W) \tag{26}$$

it follows that $a>0$. Observe first that, in the deep hydrodynamic limit $W\to 0+$, $a\sim W>0$ is the diffusion pole corresponding to classical fluid dynamics. In this limit, we can assume that $a<1$ as that must hold if $a\leqslant 0$. Then, as $W\to 0$, (26) gives $p\sim W/(1-p)^2$, whose solutions are either $p\sim W$ or p is close to 1. Therefore, by continuity of a as a function of W, it is sufficient to show that (26) has no solutions with $a=0$ for any finite W. Let us assume there is a solution with $a=0$ for some W. Then we observe that

$$L(p, W) = W\frac{\partial}{\partial p}\int_0^\infty ds\exp[(p-1)s - Ws^2/2] = W\frac{\partial}{\partial p}(\sqrt{\pi/2W}[\exp(z^2)\mathrm{erfc}(z)]),$$

where $z\equiv(1-p)/\sqrt{2W}$, is well-defined for all complex p. Therefore,

$$L(p, W) = 1 - \sqrt{\frac{\pi}{2W}}(1-p)\left[\exp\left(\left(\frac{1-p}{\sqrt{2W}}\right)^2\right)\mathrm{erfc}\left(\frac{1-p}{\sqrt{2W}}\right)\right]$$

so that (26) gives $p=1$ or

$$\sqrt{\frac{\pi}{2W}}\exp(z^2)\,\mathrm{erfc}(z) = 1.$$

This function has no solutions for $a<0$, i.e. $Re\, z > 1/\sqrt{2W}$.

A straightforward observation here is the recovery of the standard Navier–Stokes results. Indeed, in the limit of $\tau\to 0$ and $\lambda\to 0$, (19) clearly reduces to the Navier–Stokes equation for unidirectional flows, i.e. a standard diffusion equation

$$\partial_t U(x, y, t) = \nabla\cdot[\nu\nabla U(x, y, t)].$$

Other (more interesting) limits may be taken that have either $\tau\to 0$ or $\lambda\to 0$ separately. Equation (19) is restricted in that it is only valid for unidirectional flows, albeit steady or unsteady. Hence, it automatically precludes any so-called secondary flow phenomena (Chen *et al.* 2004).

Equation (19) provides a general description for unidirectional flows that are beyond the applicability of the classical Navier–Stokes equations, either involving very small spatial lengths or very fast time variations, or both. Because it is an exact consequence of the Boltzmann–BGK kinetics, (19) may be used to study various unidirectional flow calculations, approximations and models.

5. Discussion

In this paper, we have presented a finite closed-form formulation of BGK kinetics in terms of the basic hydrodynamic variables. This is derived from the Boltzmann–BGK kinetic model without approximation beyond τ constant. Therefore, it is applicable to general flow situations with arbitrary Knudsen number (and Mach number) assuming validity in the original Boltzmann–BGK kinetics. The key starting point is given by (5), while the general formulation is represented by (13)–(15). Unlike the original kinetic description, the hydrodynamical expressions reveal more direct insights in terms of physical effects. For instance, (14) manifests both memory and non-local spatial effects in flows at finite Knudsen number originating from the finite mean free path. In addition, the general formulation reveals a clear tensorial structure strikingly similar to that of the Navier–Stokes equation. On the other hand, unlike the Navier–Stokes equation or its higher-order (Burnett) approximations, the new formulation does not rely on a small-Knudsen-number approximation, so its range of applicability extends at least to moderate Knudsen number values. (At high Knudsen number, the limitations observed in the channel flow results presented above show the limitations of the Boltzmann–BGK kinetics with constant relaxation time and bounce-back boundary conditions.) This general formulation may also serve as a new foundation for studying various flow situations and limits such as unidirectional flows, or be used to compare results that are obtained from different theoretical procedures or analytical or numerical approximations.

Observe that the existence of a non-local time and space formulation justifies the $U|_{\partial V} = 0$ boundary condition (for a non-moving wall), no matter what interaction of particles with the boundary is specified for the underlying BGK-equation. This is not in contradiction with the fact that in the kinetic regime, for example, (19) yields a variety of solutions with a finite slip velocity (U being finite even infinitely close to the wall), when the solution U is understood in a generalized function sense. To that end, note that derivation of the general macro-dynamic representation presented here is based on the assumption that the microscopic characteristic lines are straight. Strictly speaking, this implies that it holds for unbounded free space, so that all the wall boundaries are sufficiently distant and do not alter (reflect) the particle trajectories. Nonetheless, this formulation can still be used to study flow problems in finite domains. One way to accomplish this is by forming an infinite domain via symmetric or periodic distributions of the velocity field. After all, boundary conditions can be interpreted in terms of flows coming from imaginary domains residing on the other sides of boundaries.

Another possibility is to extend the present theoretical formulation by observing that the boundaries give effective collisional effects so that τ should be a function of the distance d to the wall. Simple intuition suggests that the mean-free-path $\lambda \leqslant d$ and $\tau \leqslant d/\sqrt{\theta}$. This suggests a boundary layer region added to the current description, perhaps by just allowing τ to be *modelled* in (19) as location dependent and not constant. Nevertheless, the non-local nature of finite-Kn flow exposed in the present formulation requires rethinking boundary condition issues. The analogy with the Navier–Stokes vs Euler equation-based descriptions of shock fronts is suggestive that including local variation of τ may lead to extended validity of the present Boltzmann–BGK model.

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