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Dynamics of Small-Scale Devices in Gas

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1 Introduction

The problem tackled in this project is the study of how a heat gradient across a particle affects its flow. This phenomenon is one which only at occurs exclusively in scenarios when gases are rarefied, as although temperature is just particle motion at the atomic/molecular scale, these atomic scale motions cancel out when we zoom out and look at the average motion of a large number of particles. This means we have to adopt a statistically grounded approach to study the flow of rarefied gases, which shall be described in section 2. We provide a framework for calculating the temperature induced flow effects at low levels of rarefaction.

2 Mathematical formulation

When studying rarefied gases, approximating the gases as a continuous objects is an approach that fails to capture important features of the dynamics. This failure calls for utilising a statistical foundation, where only probable locations and velocities can be assigned to particles of the gas. This means that any bulk flow parameters we calculate are only averages, which many particles in our flow will deviate from.

2.1 The Distribution Function

The function at the core of our analysis is the distribution function, F, which describes where our particles are likely to be, and at what velocities they are likely to be travelling at. The fundamental property of the Distribution equation is that if we integrate F over a region in position/velocity space, we obtain the total mass of the particles in that region.

$$m_\Omega = \int_\Omega F(\boldsymbol{x}, \boldsymbol{c})\, \mathrm{d}^3\boldsymbol{c}\mathrm{d}^3\boldsymbol{x}$$

This suggests to us the first way that physical bulk properties of the gas can be calculated from moments of the distribution function, in that if we only integrate over the entire velocity space at a fixed position value, we obtain the mass density of the fluid:

$$\rho(\boldsymbol{x}) = \int_{\mathbb{R}^3} F(\boldsymbol{x}, \boldsymbol{c})\, \mathrm{d}^3\boldsymbol{c}$$

In a similar vein, we can also calculate bulk velocity, temperature and pressure fields from our distribution function:

$$\overline{\boldsymbol{v}}(\boldsymbol{x}) = \frac{1}{\rho(\boldsymbol{x})}\int_{\mathbb{R}^3} \boldsymbol{c}F(\boldsymbol{x},\boldsymbol{c})\,\mathrm{d}^3\boldsymbol{c}$$
$$\frac{3k_BT(\boldsymbol{x})}{m} = \frac{1}{\rho(\boldsymbol{x})}\int_{\mathbb{R}^3} F(\boldsymbol{x},\boldsymbol{c})\left(||\boldsymbol{c}||^2 - \frac{3}{2}\right)\mathrm{d}^3\boldsymbol{c}$$
$$\frac{P(\boldsymbol{x})}{\rho(\boldsymbol{x})} = \frac{k_BT(\boldsymbol{x})}{m}$$

2.2 The Boltzmann equation

The Boltzmann equation is the governing equation for rarefied gas dynamics. In the absence of any external forces on the gas, it has the form:

$$\frac{\partial F}{\partial t} + \boldsymbol{c}\cdot\frac{\partial F}{\partial \boldsymbol{x}} = Q\left[F\right]$$

This equation corresponds to conservation of the number of particles. The derivatives on the left side of the equation is the change of particle number for a specified position and velocity, and the right hand side is the collision operator, which describes how particle collisions effect the system. Collisions always push the distribution function to it's equilibrium distribution;

$$F_{eq}(\boldsymbol{x},\boldsymbol{c}) = \rho(\boldsymbol{x})\left(\frac{m}{2\pi k_bT}\right)^{\frac{3}{2}}\exp\left(-\frac{m}{2k_bT}||\boldsymbol{c}-\overline{\boldsymbol{v}}||^2\right)$$

For our analysis, we will use the steady state Boltzmann equation and apply the BGK approximation,where the collision operator is linearised:

$$\frac{\partial F}{\partial t} + \boldsymbol{c}\cdot\frac{\partial F}{\partial \boldsymbol{x}} = Q[F] = \nu(F_{eq} - F)$$

Where $\frac{\partial F}{\partial \boldsymbol{x}}$ is the gradient of F with respect to position space. It is also advantageous to replace variables with their deviations from the equilibrium:

$$F = F_0\rho_0(1+\phi)$$
$$\rho = \rho_0(1+\omega)$$
$$T = T_0(1+\tau)$$
$$P = P_0(1+p)$$
$$\boldsymbol{v} = \frac{\boldsymbol{c}}{\sqrt{\frac{m}{2k_BT}}}$$
$$\overline{\boldsymbol{v}} = \frac{\boldsymbol{u}}{\sqrt{\frac{m}{2k_BT}}}$$

Where $F_0(\boldsymbol{v}) = \pi^{-\frac{3}{2}} \exp\left(-||\boldsymbol{v}||^2\right)$, and all other properties with 0 subscripts are equilibrium values of the appropriate quantities. As the physical parameters can be calculated as moments of F, their deviations can be calculated as moments of ϕ, but the $\frac{1}{\rho}$ term in some of our previous relations means these relations are nonlinear, so we re-linearise:

$$\omega = \int_{\mathbb{R}^3} \phi F_0 \,\mathrm{d}^3\boldsymbol{v} \tag{1}$$

$$\boldsymbol{u} = \int_{\mathbb{R}^3} \boldsymbol{c}\phi F_0 \mathrm{d}^3\boldsymbol{v} \tag{2}$$

$$\frac{3\tau}{2} = \int_{\mathbb{R}^3} \left(||\boldsymbol{v}||^2 - \frac{3}{2}\right) \phi F_0 \,\mathrm{d}^3\boldsymbol{v} \tag{3}$$

$$p = \omega + \tau \tag{4}$$

The Boltzmann equation is also not linear in ϕ when these substitutions have been made, (consider that $\overline{\boldsymbol{v}}$ is a function of ϕ), so we must again, linearise the equation:

$$\boldsymbol{v} \cdot \frac{\partial \phi}{\partial \boldsymbol{x}} = \frac{1}{k}\left[-\phi + \omega + 2\boldsymbol{v} \cdot \boldsymbol{u} + (||\boldsymbol{v}||^2 - \frac{3}{2})\tau\right] \tag{5}$$

For details about the linearisation process, see [1].

2.3 The Knudsen Number

A Key parameter of the re-scaled governing equation is k, which is a re-scaling of the Knudsen number: $k = \frac{\sqrt{\pi}}{2}\mathrm{Kn}$. The Knudsen number is a key parameter that characterizes our gas flow, It is defined:

$$\mathrm{Kn} = \frac{\lambda}{\mathrm{L_c}}$$

Where λ is the mean free path of the gas, and $\mathrm{L_c}$ is characteristic length scale of the problem. For example, in our sphere problem, it is the radius of the sphere. The Knudsen number controls the degree of rarefaction of the gas. It determines how far gas particles will travel before interacting with other particles, relative to the solid geometry the gas is surrounding. In our analysis we will look at limiting behaviour as the Knudsen number tends to zero or infinity.

2.4 Boundary conditions

We apply a linearised diffuse boundary condition, based on particles adhering to the wall and being re-admitted.

$$\phi_W = \omega + 2\boldsymbol{u}_W \cdot \boldsymbol{v} + (||\boldsymbol{v}||^2 - \frac{3}{2})\tau_W \tag{6}$$

This boundary condition corresponds to particles adhering to the sphere and then being re-emitted. This implies that $\omega, \boldsymbol{u}$ and τ all match their values at the wall. And require that our distribution function tends back to equilibrium infinitely far from the sphere, which implies that $\omega, \boldsymbol{u}$ and τ also tend to 0 infinitely far from the sphere.

3 Near Continuum - $\mathrm{Kn} \to 0$

The equation (5) is an integro-differential equation, so it cannot be directly solved, so we must use perturbation theory.(I.e; expand ϕ in powers of Kn). Substituting this expansion directly into (5) leads to equations unable to satisfy our boundary conditions at the sphere and the far field simultaneously (The details of this will be shown in section 3.2). This issue is caused by a mismatch of dominant effect at different distance to the sphere. Close to the surface, the dominant effects are particle-surface interactions, but far from the sphere particle-particle effects dominate. We have to break our solutions into an inner and outer solution to proceed.

3.1 Asymptotic expansion

When the outer solution is expanded in powers of k, as in [3],

$$\phi = \sum_{n=0}^{\infty} k^n \phi^{(n)}$$

This leads to expansions of our bulk quantities in k, for example, the density perturbation can be expanded:

$$\begin{aligned}
\omega &= \int_{\mathbb{R}^3} F_0 \sum_{n=0}^{\infty} k^n \phi^{(n)} \, \mathrm{d}^3\boldsymbol{v} \\
&= \sum_{n=0}^{\infty} k^n \int_{\mathbb{R}^3} \phi^{(n)} F_0 \mathrm{d}^3\boldsymbol{v} \\
\implies \quad \text{if } \omega^{(n)} &= \int_{\mathbb{R}^3} \phi^{(n)} F_0 \, \mathrm{d}^3\boldsymbol{v} \qquad (7) \\
\omega &= \sum_{n-0}^{\infty} k^n \omega^{(n)} \qquad (8)
\end{aligned}$$

Using (2), (3) and (4)in similar manner, we obtain:

$$\boldsymbol{u} = \sum_{n=0}^{\infty} k^n \boldsymbol{u}^{(n)} \tag{9}$$

$$\tau = \sum_{n=0}^{\infty} k^n \tau^{(n)} \tag{10}$$

$$p = \sum_{n=0}^{\infty} k^n p^{(n)} \tag{11}$$

where

$$\boldsymbol{u}^{(n)} = \int_{\mathbb{R}^3} \phi^{(n)} \boldsymbol{v} F_0 \mathrm{d}^3\boldsymbol{v} \tag{12}$$

$$\frac{3}{2}\tau^{(n)} = \int_{\mathbb{R}^3} \phi^{(n)} \left(||\boldsymbol{v}||^2 - \frac{3}{2} \right) F_0 \mathrm{d}^3\boldsymbol{v} \tag{13}$$

$$p^{(n)} = \omega^{(n)} + \tau^{(n)} \tag{14}$$

This holds for our inner and outer layers. In our asymptotic expansion, we split our solution up into inner (Knudsen) and outer (Hilbert) parts, i.e; $\phi = \phi_H + \phi_K$. The two layers must asymptotically match another. The formula for the bulk quantities of each part are the same as those derived in this section, with appropriate subscripts added.

3.2 Outer layer

Substituting the expansion of ϕ into (5), and collecting powers of k, we get the following equations :

$$0 = -\phi_H^{(0)} + \omega_H^{(0)} + 2\boldsymbol{v} \cdot \boldsymbol{u}_H^{(0)} + (||\boldsymbol{v}||^2 - \frac{3}{2})\tau_H^{(0)} \tag{15}$$

$$\boldsymbol{v} \cdot \frac{\partial \phi_H^{(n)}}{\partial \boldsymbol{x}} = -\phi_H^{(n+1)} + \omega_H^{(n+1)} + 2\boldsymbol{v} \cdot \boldsymbol{u}_H^{(n+1)} + (||\boldsymbol{v}||^2 - \frac{3}{2})\tau_H^{(n+1)} \tag{16}$$

The latter holds for all $n \in \{0, 1, 2, \dots\}$. Considering (7), (12) and (13), it becomes apparent that we are left with a separable integral equation at each order, Define the operator H:

$$\begin{aligned} H\phi_H^{(n)} &= \omega_H^{(n)} + 2\boldsymbol{v} \cdot \boldsymbol{u}_H^{(n)} + (||\boldsymbol{v}||^2 - \frac{3}{2})\tau_H^{(n)} \\ &= \int_{\mathbb{R}^3} \phi_H^{(n)} \left(1 + 2\boldsymbol{v} \cdot \boldsymbol{v}' + \left(\frac{2}{3}||\boldsymbol{v}||^2 - 1 \right) \left(||\boldsymbol{v}'||^2 - \frac{3}{2} \right) \right) F_0 \, \mathrm{d}^3\boldsymbol{v}' \end{aligned}$$

Due to convervation of mass, momentum and energy , (see ([2])), or alternatively by the requirements induced by theory of inhomogenous integral equations (see [3]) we require:

$$\int_{\mathbb{R}^3} \boldsymbol{v} \cdot \frac{\partial \phi_H^{(n)}}{\partial \boldsymbol{x}} F_0 \, \mathrm{d}^3 \boldsymbol{v} = 0 \tag{17}$$

$$\int_{\mathbb{R}^3} \boldsymbol{v} \cdot \frac{\partial \phi_H^{(n)}}{\partial \boldsymbol{x}} \boldsymbol{v} \, F_0 \, \mathrm{d}^3 \boldsymbol{v} = 0 \tag{18}$$

$$\int_{\mathbb{R}^3} \boldsymbol{v} \cdot \frac{\partial \phi_H^{(n)}}{\partial \boldsymbol{x}} ||\boldsymbol{v}||^2 \, F_0 \, \mathrm{d}^3 \boldsymbol{v} = 0 \tag{19}$$

From the above equations, we can derive the following partial differential equations:

$$\nabla p_H^{(0)} = 0 \tag{20}$$

$$\nabla \cdot \boldsymbol{u}_H^{(n)} = 0 \tag{21}$$

$$\nabla p_H^{(n+1)} = \nabla^2 \boldsymbol{u}_H^{(n)} \tag{22}$$

$$\nabla \tau_H^{(n)} = 0 \tag{23}$$

The full derivation of the above equations is omitted, but can be found in ([1]). This gives us stokes flow at every order, and temperature obeys the Laplace equation, in line with classical steady state creeping flow, but these equations cannot satisfy all of our boundary conditions. (20) contradicts having a pressure deviation at the surface of the sphere and the pressure deviation tending to 0 in the far field, so it becomes clear that the outer solution cannot fully solve (5), So we must apply boundary layer theory.

3.3 Inner layer corrections

The behaviour near the surface we desire to model is characterised by particle surface collisions dominating. This occurs where particles have yet to travel a mean free path from the surface, and are not yet colliding with other particles. It is therefore appropriate to re-scale the normal component of the surface to analyze the inner layer solutions:

$$\eta = \frac{x_n}{k}$$

We will expand our inner layer solution, ϕ_K in powers of k, as we did before, but the re-scaling will alter our equations:

$$\boldsymbol{v}_t \cdot \frac{\partial \phi_K}{\partial \boldsymbol{x}_t} + v_n \frac{\partial \phi_K}{\partial x_n} = \boldsymbol{v}_t \cdot \frac{\partial \phi_K}{\partial \boldsymbol{x}_t} + \frac{1}{k} v_n \frac{\partial \phi_K}{\partial \eta} = \frac{1}{k} \left[H - I\right] \phi_K$$

$$\boldsymbol{v}_t \cdot \frac{\partial \phi_K^{(0)}}{\partial \boldsymbol{x}_t} + \frac{v_n}{k} \frac{\partial \phi_K^{(0)}}{\partial \eta} + k \left(\boldsymbol{v}_t \cdot \frac{\partial \phi_K^{(1)}}{\partial \boldsymbol{x}_t} + \frac{v_n}{k} \frac{\partial \phi_K^{(1)}}{\partial \eta} \right) + \dots$$

$$= \frac{1}{k} \left[H - I\right] \phi_K^{(0)} + \left[H - I\right] \phi_K^{(1)} + kk \left[H - I\right] \phi_K^{(2)} + \dots$$

Equating by order in k ...

$$v_n \frac{\partial \phi_K^{(0)}}{\partial \eta} = [H - I]\phi_K^{(0)} \tag{24}$$

$$v_n \frac{\partial \phi_K^{(n+1)}}{\partial \eta} + \boldsymbol{v}_t \cdot \frac{\partial \phi_K^{(n)}}{\partial \boldsymbol{x}_t} = [H - I]\phi_K^{(n+1)} \tag{25}$$

Where the latter holds for all $n \in \{0, 1, 2, \dots\}$. These equations are more complicated than those of the outer layer, and solutions can be described in [3] and [2]. We do not need directly to work with the inner layer to solve for flow velocity, It suffices to use the limit at the surface of the sphere of the outer solution. The boundary conditions on the outer layer that must be imposed for our two layers to match are described for the more general oscillatory problem in [2], our steady case can be recovered by setting oscillation frequency to 0.

3.4 Calculating the induced flow

In this section we will use the theory developed above to outline the framework for calculating the flow velocity induced by the temperature field. It is sufficient to use the outer layer when dealing with calculations of force's on the sphere, as the inner layer is naturally of small length. We apply the boundary conditions imposed by the inner layer to $\boldsymbol{u}_K^{(0)}$ and $\boldsymbol{u}_K^{(1)}$, which are:

$$(\boldsymbol{u}_H^{(0)} - \boldsymbol{V}_{sphere}^{(0)}) = 0 \tag{26}$$

$$(\boldsymbol{u}_H^{(1)} - \boldsymbol{V}_{sphere}^{(1)}) \cdot \boldsymbol{n} = 0 \tag{27}$$

$$(\boldsymbol{u}_H^{(1)} - \boldsymbol{V}_{sphere}^{(1)}) \cdot \boldsymbol{t}_i = -k_0 \boldsymbol{n} \cdot (\nabla \boldsymbol{u}_H^{(0)} + (\nabla \boldsymbol{u}_H^{(0)})^\top) \cdot \boldsymbol{t}_i - K_1 \nabla \tau_H^{(0)} \cdot \boldsymbol{t}_i \tag{28}$$

Note that as the temperature and velocity fields are coupled in the inner layer, in our boundary condition they are coupled. Where $\boldsymbol{t}_i$ are unit basis vectors for the tangent space, and K_1 is a negative constant, (see [2]) . (21),(22) and (26) imply that we have classical stokes flow with no slip boundary conditions, so if we have no sphere motion to leading order, $U_H^{(0)} = 0$. We use the basis $\boldsymbol{t}_1 = \hat{\boldsymbol{\theta}}$, $\boldsymbol{t}_2 = \hat{\boldsymbol{\theta}}$. We impose axisymmetry of $\tau_H^{(0)}$, and that $U_{sphere}^{(1)} = U_p \boldsymbol{k}$, i.e, that the sphere will move rigidly as a response to the temperature gradient, with a velocity deviation at the order of the Knudsen number. With these facts, the boundary conditions (27) and (28) become:

$$u_{H,r}^{(1)} = U_p \cos(\theta) \tag{29}$$

$$u_{H,\theta}^{(1)} = U_p \sin(\theta) - K_1 \frac{\partial \tau_H^{(0)}}{\partial \theta} \tag{30}$$

$$u_{H,\phi}^{(1)} = 0 \tag{31}$$

If we expand the axisymetric first order temperature deviation in Legendre polynomials:

$$\tau_H^{(1)} = \sum_{n=0}^{\infty} a_n P_n(\cos\theta)$$

We can use a stokes stream-function method to find the following velocity field:

$$u_{H,\theta}^{(1)}(r,\theta) = \frac{-K_1 \sin\theta}{2} \sum_{n=1}^{\infty} a_n\, P_n'(\cos\theta)\left((2-n)r^{-n} + nr^{-2-n}\right) \tag{32}$$

$$u_{H,r}^{(1)}(r,\theta) = \frac{K_1}{2} \sum_{n=1}^{\infty} a_n\, n(n+1) P_n(\cos\theta)\left(r^{-n} - r^{-2-n}\right) \tag{33}$$

$$u_{H,\phi}^{(1)} = 0 \tag{34}$$

4 Conclusions

In conclusion, we have explored the framework for calculating the flow around a sphere generated by a temperature gradient. Unlike the continuum analogue, this theory shows that temperature gradient can induce a flow without the need for nonlinear convection. This is a strictly non-continuum phenomenon that can be tackled using the matched asymptotic expansion method, transport equations and boundary conditions studied here. This framework also enable us to explore a general geometry which would require continuum solutions to the standard Navier Stokes equations. These would provide the zeroth order flow.

References

[1] Jason Nassios. Kinetic theory and the bgk equation: Gas dynamics for the nanoscale (honours thesis), 2008.

[2] Jason Nassios and John Sader. Asymptotic analysis of the boltzmannbgk equation for oscillatory flows, 2012.

[3] Yoshio Sone and Yoshimoto Onishi. Kinetic theory of evaporation and condensation* - hydrodynamic equation and slip boundary condition-, 1978.