Accounting for rotational non-equilibrium effects in subsonic DSMC boundary conditions

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Abstract. From study of the kinetic theory of dilute gases, it becomes clear that the subsonic, implicit boundary conditions which are commonly used in direct simulation Monte Carlo simulations of micro-scale channel flows do not take any form of rotational non-equilibrium into account. The consequences of not considering non-equilibration of the rotational mode are discussed and a new form of the boundary conditions which attempt to take this effect into account are proposed. It is shown that for a highly compressible test case involving these implicit boundaries in the literature that a degree of rotational non-equilibrium is present. The changes in the recovered macroscopic properties when the new boundary is applied in the same case include an improved rotational temperature distribution and a slightly lower velocity at the channel exit. A further test case exhibiting no rotational non-equilibrium was performed and it is shown that the macroscopic properties which are recovered are essentially the same for both boundaries. The results indicate that the newly proposed outlet boundary condition increases the range of applicability of these types of boundary conditions, without adding any significant computational expense.

1. Introduction
Gaseous flows in micro-scale geometries are an increasingly important area of research in the design of micro-electro-mechanical system (MEMS) technologies such as micro-pumps, micro-turbines and micro-fuel cells. The operation of MEMS devices can differ greatly to that of their macro-scale companions because the fluid flow characteristics can be vastly different. The micro-metre length scales involved can invalidate the continuum assumption altogether and rarefaction effects such as velocity slip, temperature jump and thermal transpiration may have to be accounted for [1]. The degree of gas rarefaction is normally defined through the Knudsen number

$$Kn = \frac{\lambda}{L}$$

(1)

where $\lambda$ is the mean free path of the gas molecules or atoms and $L$ is a characteristic length scale.

It is the transition Knudsen number regime ($10^{-1} \leq Kn \leq 10$) which presents the greatest difficulty to model numerically. In this regime, the mean free path is becoming significant compared to the characteristic length scale, but molecular collisions are still important. MEMS
devices involving gas flows tend to operate in the slip ($10^{-3} \leq Kn \leq 10^{-1}$) and transition regimes, even at relatively high pressures (i.e. around atmospheric). The direct simulation Monte Carlo (DSMC) method [2], based on the kinetic theory of dilute gases, has emerged as the dominant numerical technique for solving gaseous flows in the transition regime.

A variety of non-intuitive physics in high Knudsen number flows have been observed experimentally and been predicted both analytically and numerically. For example, non-linear pressure gradients have been observed for micro-channel flows [3], along with large velocity slip and temperature jump values. The movement of radiometer vanes when exposed to sunlight is caused by rarefied gas flow effects, i.e. uneven gas heating over an area bounded by one mean free path length from the edges of the vanes and gas creeping from a colder region towards a hotter region [4].

The set of pressure driven, implicit boundary conditions for subsonic flows are well known for use in conjunction with DSMC and have been used to successfully simulate a variety of rarefied gas flows in micro-scale geometries. Several different forms of these boundary conditions have been proposed; particle flux conservation was initially popular [5], but suffered from a high degree of statistical noise. Theory of characteristics based forms of the boundary conditions, using time averaged macroscopic properties obtained from the boundary cells, have emerged as the most efficient and widely used versions. However, these are essentially continuum computational fluid dynamics (CFD) boundary conditions that have been adapted for use with the DSMC algorithm. As such, they do not take into account some of the possible phenomena which may be present in rarefied gas flows, but are not observed in the continuum regime. In the current work the effect of non-equilibration of the rotational energy mode with the translational energy mode, in the context of these subsonic boundary conditions, is investigated. As such, the current work deals with diatomic or polyatomic gases in which the rotational mode is active, but the vibrational mode is not considered as the working temperatures are low enough that the vibrational mode is not likely to be active. It is always considered that the translational mode is in equilibrium, in order to keep the analysis focused on only one form of non-equilibrium for now.

2. Boundary conditions

Gaseous flows in MEMS flows are often characterised as being of low speed and being driven by a pressure gradient. Unlike more traditional hypersonic DSMC boundaries, it is likely that particles will have thermal velocities that will be orders of magnitude larger than the stream velocity. This makes it likely that particles will be able to enter from the outlet or leave the system at the inlet. The velocities at the inlet and outlet are not known due to current experimental limitations at the micro-scale. Pressure and temperature are usually the only known flow conditions at the boundaries.

When using DSMC, it is vital to know the macroscopic velocity, temperature and density in order to obtain the correct number flux at a boundary, since the particle flux $\dot{N}$, at an angle $\theta$ to the surface normal, across a boundary with area $A$, is calculated from the equilibrium Maxwell-Boltzmann distribution

$$\frac{\dot{N}}{A} = \frac{nV_{mp} \{ \exp (-q^2) + \sqrt{\pi}q [1 + \text{erf} (q)] \}}{2\sqrt{\pi}}, \quad (2)$$

where

$$q = \frac{V}{V_{mp}} \cos \theta, \quad (3)$$

$$V_{mp} = \sqrt{\frac{2kT}{m}}, \quad (4)$$
2.1. Upstream boundaries
A theory of characteristic based inlet boundary condition was first proposed by Wang & Li [6]. In this implementation the user defines values of pressure $P_{in}$ and temperature $T_{in}$ for the gas at an inflow boundary and the perfect gas law is used to calculate the inlet number density $n_{in}$

$$n_{in} = \frac{P_{in}}{kT_{in}}. \quad (5)$$

Based on the theory of characteristics, the stream-wise $u_{in}$ and tangential $v_{in}$ velocities at an inlet boundary face $f$ are calculated as

$$(u_{in})_f = u_j + \frac{P_{in} - P_j}{\rho_j a_j} \quad (6)$$

and

$$(v_{in})_f = v_j, \quad (7)$$

where $u_j$ and $v_j$ are first order extrapolations from the cells attached to the relevant boundary face, $\rho$ is mass density and $a$ is the local speed of sound. The subscript $j$ denotes values in the boundary cells.

2.2. Downstream boundaries
At the exit boundaries, only the pressure $P_{out}$ is defined and the boundary conditions as proposed by Nance et al. [7] are:

$$(\rho_{out})_f = \rho_j + \frac{P_{out} - P_j}{(a_j)^2}, \quad (8)$$

$$(u_{out})_f = u_j + \frac{P_j - P_{out}}{\rho_j a_j}, \quad (9)$$

$$(v_{out})_f = v_j, \quad (10)$$

$$(T_{out})_f = \frac{P_{out}}{R(\rho_{out})_f}. \quad (11)$$

Using the implementations of these boundary conditions found in the literature, the values of $P_j$ are calculated using the overall temperature, i.e.

$$P_j = \rho_j R \left[ \frac{\xi_{trans}T_{trans} + \xi_{rot}T_{rot}}{\xi_{trans} + \xi_{rot}} \right]_j, \quad (12)$$

where $R$ is the gas constant and $\xi_{trans}, \xi_{rot}, T_{trans}$ and $T_{rot}$ are the number of translational degrees of freedom, the number of rotational degrees of freedom, the translational temperature and the rotational temperature respectively. When particles are introduced at either the inlet or outlet boundaries, their translational and kinetic energies are also based on the overall temperature.

According the kinetic theory of dilute gases [2, 8, 9], the pressure should be measured using the translational temperature, as it depends only on the translational kinetic motions of the particles. If the gas is in perfect thermodynamic equilibrium, the overall temperature will be equal to both the translational and rotational temperatures and so this is not an issue. However, it is not certain that a gas will be remain in equilibrium along the length of a micro-channel, particularly if the inlet to outlet pressure ratio is high or the aspect ratio of the micro-channel is small.
As a gas travels downstream under the influence of a pressure gradient, the density decreases and the gas expands and cools. This decrease in thermal energy per unit mass initially appears in the translational mode and is redistributed to the rotational mode through inter-molecular collisions, only after a corresponding relaxation time \([10]\). Although the rotational relaxation time is not large, if the gas is sufficiently rarefied, there may not be enough molecular collisions occurring for the translational and rotational energies to equilibrate with one another. If the energy is not being redistributed to the rotational mode effectively enough, there will be a local deficit of energy in the translational mode compared to an equilibrium gas of the same density and total energy. This in turn means that the pressure will be lower than in the corresponding equilibrium gas.

A new form of the characteristics based boundary conditions is proposed here. At the inlet, the boundary conditions remain unchanged from those of Wang and Li \([6]\), which means that it is assumed that the gas is always in rotational equilibrium at the inlet. At the outlet, a state of rotational equilibrium is not assumed and the boundary conditions have been modified as follows to account for a degree of non-equilibrium between the translational and rotational modes. All of the following macroscopic properties are measured after the movement and collision stages and are time averaged for the entire simulation duration. The pressure \(P_j\) in outlet boundary cells is measured as

\[
P_j = \rho_j R (T_{\text{trans}})_j. \tag{13}
\]

The mass density and velocities at the exit boundaries are then calculated as in the Nance \textit{et al.} \([7]\) implementation, but with the new definition of pressure included in the correction terms

\[
(\rho_{\text{out}})_f = \rho_j + \frac{P_{\text{out}} - P_j}{(a_j)^2}, \tag{14}
\]

\[
(u_{\text{out}})_f = u_j + \frac{P_j - P_{\text{out}}}{\rho_j a_j}, \tag{15}
\]

\[
(v_{\text{out}})_f = v_j. \tag{16}
\]

The translational temperature at the exit boundary is calculated using the perfect gas law

\[
[(T_{\text{trans}})_{\text{out}}]_j = \frac{P_{\text{out}}}{R (\rho_{\text{out}})_f}, \tag{17}
\]

and the rotational temperature at the exit boundary is simply taken as a first order extrapolation of the measured rotational temperature from the boundary cell, i.e.

\[
[(T_{\text{rot}})_{\text{out}}]_f = (T_{\text{rot}})_j. \tag{18}
\]

When particles are introduced at the boundaries, they are assigned translational energies based only on the value of \((T_{\text{trans}})_{\text{out}}\) by substituting this term in equation (4) for \(T\). Use of equation (2) to calculate the entering particle flux means that translational equilibrium is being assumed at both the inlet and outlet. Their rotational energies are assigned only from the value of \((T_{\text{rot}})_{\text{out}}\) and the usual rotational energy selection routine. In this way, it is believed that a more realistic representation of gas flows with a degree of rotational non-equilibrium can be obtained.

The boundary conditions of Wang & Li \([6]\) and the new boundaries proposed here have been implemented within the free and open-source DSMC solver, \textit{dsmcFoam}. This solver is released as part of the C++ fluid dynamics toolbox, OpenFOAM, which can be downloaded from \([11]\) and has previously been rigorously validated for a variety of benchmark cases \([12]\).
3. Rotational non-equilibrium

In order to demonstrate that a gas may be out of rotational equilibrium inside a micro-channel geometry, a test case from the literature is chosen and velocity distribution functions at various locations in the channel are measured and compared to the equivalent equilibrium distribution function.

The chosen test case is a micro-Poiseuille flow from Liou & Fang [13]. The channel has a length of 2 µm and a height of 0.4 µm. The inlet gas temperature and the wall temperatures are all constant at 300 K. The inlet pressure is 72640 Pa, with an inlet to outlet pressure ratio of 4.54. The working gas is nitrogen and the Knudsen number based on the channel height and the variable hard sphere (VHS) mean free path ranges from 0.19 at the inlet to 0.72 at the outlet; therefore the problem lies within the transition Knudsen number regime. The boundary conditions used for the current problem are those described in [6].

To remain consistent with the test case in the literature, 100 x 60 regular rectangular computational cells are used to mesh the computational domain and the system has around 180,000 DSMC simulator particles at steady state. Groups of cells were joined together and used as zones in which a variety of macroscopic or microscopic properties can be measured. Figure 1 shows the mesh and measurement zones. The overall temperature and the velocity distribution functions were measured in each of the control zones in order to determine whether the system is in local rotational equilibrium at these points.

![Figure 1: Snapshot of the mesh including measurement zones.](image)
Figure 2: Comparison of measured and equilibrium distribution functions: (a) Entrance measurement zone (b) Exit measurement zone

Around 1 million statistical samples were employed to obtain the following results and the problem was solved in parallel on 2 processors. The total run time was 47 hours. Figure 2 shows the measured velocity distribution functions in the entrance and exit measurement zones and compares them with the equilibrium velocity distributions based on the measured value of overall temperature in the respective measurement zones. If the gas is in rotational equilibrium, the measured distribution should match the theoretical one exactly. In the entrance measurement zone this is the case, as it is in the centre measurement zone (not shown here); however, in the exit measurement zone the measured distribution is shifted slightly to the left of the theoretical one and has a slightly higher peak value. This is consistent with a cooler distribution function and comes about because a degree of rotational non-equilibrium is present in this measurement zone.

As discussed previously, the gas expands and the thermal energy per unit mass decreases as it travels downstream. The translational mode cools first and the rotational mode comes into equilibrium with this only after a certain relaxation time. This relaxation process occurs through inter-molecular collisions, but in this moderately rarefied flow there are not enough collisions occurring for the rotational mode to come into equilibrium with the translational mode. This means that the translational temperature in the exit measurement zone is significantly lower than the rotational temperature. The overall temperature is a weighted average of the translational and rotational temperatures, so this will also be higher than the translational temperature; hence the theoretical distribution function is that of a slightly warmer gas compared to the measured one.

Table 1: Simulation details

| Case | Length (µm) | Height (µm) | P_{in} (Pa) | P_{out} (Pa) | Boundaries        |
|------|-------------|-------------|-------------|--------------|-------------------|
| 1    | 2           | 0.4         | 72,640      | 16,000       | Wang & Li [6]     |
| 2    | 2           | 0.4         | 72,640      | 16,000       | Current work      |
| 3    | 20          | 0.4         | 100,000     | 50,000       | Wang & Li [6]     |
| 4    | 20          | 0.4         | 100,000     | 50,000       | Current work      |

The results in figure 2 show that it can be necessary to account for rotational non-equilibrium
at the exit of a micro-channel and a series of cases are performed in order to compare results obtained using the boundary conditions from [6] and the new boundary conditions described above. The micro-channel dimensions and inlet/outlet pressures used in each case are detailed in table 1. Cases 1 and 2 were meshed with 100 x 60 computational cells, while cases 3 and 4 were meshed using 1000 x 60 computational cells. The working gas is nitrogen in all cases, where the inlet gas temperature is 300 K and all walls are fully diffuse at 300 K. All simulations use the VHS collision model with the phenomenological Larsen-Borgnakke internal energy redistribution technique [14].

4. Results
Cases 1 and 2 were run in parallel on 2 cores each and sampled for 1 million time steps. At steady state, case 1 had roughly 182,000 DSMC simulator particles and case 2 had slightly more at 183,000. The total run time was around 47 hours for each case, with case 2 being around 3% slower than case 1. This indicates that the new outlet boundary condition proposed here does not introduce any significant computational expense with respect to that found in [6].

Figure 3: Centre-line distributions in cases 1 and 2 for (a) Normalised pressure (b) Velocity.
Figure 4: Deviation from a linear pressure profile for cases 1 and 2.

Figure 3a shows the centre-line pressure distributions obtained from cases 1 and 2. In general, the pressure profiles match very well, with the new implementation boundaries resulting in slightly higher pressures towards the channel exit. Figure 3b shows the centre-line velocity profiles from cases 1 and 2. The velocity profiles match well until near the channel exit, where the new boundaries achieve a slightly lower value (around 6 m/s slower). Figure 4 shows how the pressure profile varies from that of a linear pressure drop along the length of the centre-line for both the old and new boundary conditions. There is a difference in the pressure profile towards the exit when using the new boundary conditions, because the measured pressure at the outlet is based on the translational temperature rather than the overall temperature.

The translational, rotational and overall temperature profiles at the channel centre-line in cases 1 and 2 are shown in figure 5. The translational temperature profiles match well for both boundary conditions, however the rotational temperature near the exit is increased slightly when using the newly developed boundary conditions. As a result, the overall temperature profiles match well until near the exit, and because the overall temperature is a weighted average of the three translational modes and the two rotational modes, the magnitude of the difference in overall temperature is smaller than that observed for the rotational temperatures. The temperature profiles from a similar case ran with the pressure difference being generated in a high and low pressure reservoir at either end of the micro-channel are included for reference here.

The temperature profiles highlight the fact that the overall temperature can be significantly higher than the translational temperature at the channel exit (around 15 K in these cases) and demonstrates why it is important to measure pressure using only the translational temperature and introduce new particles based on the respective translational and rotational temperatures at the face they are introduced at, as opposed to a single value of overall temperature.
The translational temperatures achieved when using both types of boundary conditions are lower than that found when using the reservoirs, but the rotational temperature achieved using the new boundary conditions is much closer to that in the reservoir simulation compared to the Wang & Li implementation of the boundaries. It is to be expected that the implicit boundary conditions will be unable to capture the same translational temperature as the reservoir case here because of the rapid expansion which occurs as the gas exits the channel and enters the reservoir. The implicit boundaries are unable to capture this effect as effectively as the reservoir, which is a more realistic representation of the problem, but they do have the advantage of being much more computationally efficient. For example, the reservoir case displayed here required over a week of run time on 64 cores.

Cases 3 and 4 were run in parallel on 8 cores for a total of 2 million time steps. The domain was meshed using 1000 x 60 regular rectangular cells. The expected signal-to-noise ratio was small in these two cases because the channel is much longer and the pressure difference is also reduced with respect to cases 1 and 2. Two million statistical samples were employed to try and reduce the error to an acceptable level. Using equations from [15], the estimated error in the macroscopic velocity at the channel exit centre-line is less than 1%. Both cases contained around 920,000 DSMC simulator particles at steady state.

Figure 5: Centre-line temperature distributions for cases 1 and 2.
Figure 6: Centre-line distributions in cases 3 and 4 for (a) Normalised pressure (b) Velocity.

Figure 7: Deviation from a linear pressure profile for cases 3 and 4.

Figure 6a shows the centre-line pressure distributions obtained from cases 3 and 4. The pressure profiles are in excellent agreement along the whole length of the micro-channel. The
centre-line streamwise velocity profiles for cases 3 and 4 are shown in figure 6b and good agreement is found between the two cases, although the relatively high amount of statistical scatter makes it difficult to see exactly how well these profiles match. Figure 7 shows how the pressure profile varies from that of a linear pressure drop along the length of the centre-line for both the old and new boundary conditions. The magnitude of the deviation from a linear profile is much reduced with respect to the results shown in figure 4 and the results when using the new boundary conditions (case 4) are in much closer agreement with those achieved when using the Wang and Li implementation of the boundary conditions (case 3).

Figure 7: Pressure profile for cases 3 and 4.

Figure 8 shows how the pressure profile varies from that of a linear pressure drop along the length of the centre-line for both the old and new boundary conditions. The magnitude of the deviation from a linear profile is much reduced with respect to the results shown in figure 4 and the results when using the new boundary conditions (case 4) are in much closer agreement with those achieved when using the Wang and Li implementation of the boundary conditions (case 3).

Figure 8: Centre-line temperature distributions for cases 3 and 4.

Figure 8 shows the translational, rotational and overall temperature profiles at the channel centre-line in cases 3 and 4. All of the temperature profiles are in excellent agreement between cases 3 and 4.

The results for cases 3 and 4 are consistent with a gas which is in (or at least very close to) rotational equilibrium. This would be expected because the micro-channel length is longer than in cases 1 and 2 and the pressure difference is also smaller. There will be less compressibility effects and so the gas does not expand and cool, as illustrated by the translational temperature profiles in figure 8. The deviation from a linear pressure profile is also expected to be smaller when compressibility effects are reduced, as was shown in figure 7. The results from cases 3 and 4 show that the new boundary conditions give the same results as the those proposed by Wang & Li [6] when there is no, or very little, rotational non-equilibrium present in a gaseous micro-channel flow.

5. Conclusions

It has been shown, through measurement of velocity distribution functions, that a rarefied gas flow in a micro-channel may not remain in rotational equilibrium along the channel length, especially if compressibility effects are significant. An implicit boundary condition to be applied at the exit of a micro-channel geometry has been proposed which attempts to account for non-equilibration of the rotational energy mode with the translational mode. A comparison, for a highly compressible case, of the new boundary conditions with a previous implementation that does not account for rotational non-equilibrium has shown that the new boundaries lead
to a slightly more non-linear pressure profile than the old boundaries. The velocity near the micro-channel exit is slightly reduced when using the new boundaries.

It is in the rotational temperature profiles where the most significant change can be observed between the two boundaries. The new boundaries result in an improved rotational temperature profile along the micro-channel centre-line, with respect to the old boundaries, compared to the temperature profile from an equivalent micro-channel simulation performed with high and low pressure reservoirs rather than implicit boundary conditions.

When the boundary conditions are compared for a case with significantly less compressibility, and therefore no rotational non-equilibrium effects, the two different boundaries achieve an almost identical solution. The new outlet boundary proposed here provides additional functionality by considering a more complete form of kinetic theory and does so without incurring any significant computational expense, as has been shown in the run times for the simulations performed in the current work.

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