Thermal Creep Flow of Helium Gas at Cryogenic Temperatures

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Abstract. We present a molecular dynamics (MD) simulation of nanoscale gas flow due to thermal creep at cryogenic temperatures. Helium is considered because its low liquefying temperature allows a wide range of cryogenic analysis. The thermal creep flow along a nanochannel is generated by applying temperature differences along the channel. Pressure and density variations are measured at various rarefaction conditions, covering the slip flow to the free molecular regimes. Thermo molecular pressure difference (TMPD) values are also calculated. Our results are compared with those in the literature.

1. Introduction

As is well known, the transport properties of gases at the micro/nanoscale differ from those at the macroscale because of differences in the governing flow characteristics. Nanoscale gas flows are generally analyzed as free molecular flows, and for these kinds of flows between reservoirs at different pressures and temperatures the Knudsen law holds:

\[ \frac{P_h}{\sqrt{T_h}} = \frac{P_c}{\sqrt{T_c}}, \]

where the $h$ and $c$ subscripts indicate quantities at the hot and cold reservoirs. According to the Knudsen law, in a system in the free molecular flow regime, a temperature gradient induces a pressure difference. This is called the “thermo-molecular pressure difference” (TMPD), which enables several effects including thermal creep and the operating principle of the Knudsen pump. The TMPD has been determined in the literature for different gases, system dimensions and temperature gradients [2-4]. For the TMPD at low temperatures, the Weber-Schmidt equation [5-6] represents experimental data over a wide pressure range, utilizing the results obtained by Knudsen.

In this paper, nanochannel gas flows are examined under cryogenic temperature gradients. The pressure and temperature evolutions are analyzed. The TMPD values we obtain are compared with the TMPD generated by the same temperature difference but in a conventional temperature range, and also with the results from the Weber-Schmidt equation. The flow system is simulated using the molecular dynamics (MD) routines in OpenFOAM [7-9], which were developed in the authors’ research group.
2. Molecular Dynamics Simulation

In the current study, monatomic helium gas confined in a rectangular channel is simulated using MD. The channel is thermally in contact with a hot \((T_H)\) and a cold \((T_L)\) reservoir. A schematic of the simulated system is in figure 1, in which all the geometry and gas atoms are coloured depending on the surrounding temperature. The application of a Berendsen thermostat [10] in the reservoir zones ensures that their temperature remains constant around target values.

![Figure 1: Schematic of the simulated flow system. The hot reservoir is at the left, and the cold reservoir at the right.](image)

In the MD simulations, the helium atoms interact with each other through a Lennard-Jones (LJ) potential:

\[
U_{ij} = 4\epsilon \left[ \left( \frac{\sigma}{R_{ij}} \right)^{12} - \left( \frac{\sigma}{R_{ij}} \right)^{6} \right],
\]

where \(R_{ij}\) is the distance between particles \(i\) and \(j\), \(\epsilon\) is the depth of the potential well, and \(\sigma\) is the finite distance at which the inter-particle potential is zero. For helium-helium interactions we set \(\epsilon_{\text{He-He}} = 1.9654 \times 10^{-22} J\) and \(\sigma_{\text{He-He}} = 2.2023 \times 10^{-10} m\) from Ref [11]. The potential is truncated and shifted at a distance \(R_{\text{cut}} = 6.6 \times 10^{-10} m\). Diffusive wall boundary conditions, with a linear temperature gradient, are applied along the system.

3. Results and Discussions

3.1. Thermo-molecular pressure difference

Simulations are run for different temperature gradients and different Knudsen numbers. For the first case, the temperature of the cold reservoir is kept at 100 K and the hot reservoir is at 300 K, and the TMPD is calculated for \(Kn=0.5, 1, 5, \) and 10.

In the second case, the temperature is kept at 10 K and 100 K for the cold and hot reservoirs, respectively. (The liquefaction temperature of He is around 4.3 K and the critical temperature is around 5.2 K. The classical gas limit is also checked for the system and 10 K is chosen as the temperature of cold reservoir, keeping the system within the classical limit so that quantum degeneracy effects are negligible.)
Figure 2: The normalized TMPD values under different temperature gradient

In figure 2, the dashed line represents the system behaviour in the cryogenic range, under a temperature difference of 200 K ($T_L=100$ K and $T_H=300$ K). TMPD values are calculated in this temperature range for the $Kn=0.1, 0.2, 0.5, 0.75, 1, 2, 5, 7.5, \text{and } 10$. The triangular symbols in figure 2 represent the TMPD values at conventional temperatures ($T_L=300$ K and $T_H=500$ K) but also with a 200 K temperature difference. In this case, the simulation were completed for $Kn=0.5, 1, 5, \text{and } 10$.

As is predicted by kinetic theory, normalized TMPD values increase with increasing Knudsen number and converge to 0.5 in free molecular flow. The TMPD values in the cryogenic (100-300 K) and conventional (300-500 K) temperature ranges merge with each other. This is consistent with the results in the literature [3]. We have therefore shown that TMPD values only depend on the temperature difference applied, not the absolute values of the temperature.

For the second case, a lower temperature difference is applied: 90 K ($T_L=10$ K and $T_H=100$ K). The rectangular symbols in figure 2 represent the TMPD values in this case, and it can be seen that a smaller pressure difference is obtained for this smaller temperature gradient. The applied temperature difference is the main determiner of TMPD, rather than the absolute temperature values.

3.2. Weber-Schmidt (WS) Equation

For pressure and temperature evolution in free molecular conditions at cryogenic temperatures, the Weber-Schmidt equation [5-6] represents experimental data over a wide pressure range. The Weber-Schmidt equation is applicable to helium-3 as well as to helium-4, and it is given as follows for helium gases [6]:

\[
\ln \left( \frac{p_h}{p_c} \right) = \frac{1}{2} \ln \left( \frac{T_h}{T_c} \right) + 0.18131 \ln \left( \frac{y_h + 0.1878}{y_c + 0.1878} \right) + 0.41284 \ln \left( \frac{y_h + 1.8311}{y_c + 1.8311} \right) - 0.15823 \ln \left( \frac{y_h + 4.9930}{y_c + 4.9930} \right)
\]  

(3)

In this equation, $y$ is defined as $y = r/\lambda$, where $r$ is the radius of the channel and $\lambda$ is the molecular mean free path. The $y_h$ and $y_c$ values are calculated for the hot and the cold regions. The other constants in equation (3) were obtained by fitting to the experimental data. In our case we have a rectangular domain, so $r$ is chosen as the height of the channel, $r=102.5$ nm, and the mean free path is calculated as $\lambda = k_t T / \sqrt{2 \pi \sigma^2 p}$ for each case, where $k_t$ is the Boltzmann’s constant. The calculated pressure ratio for different Knudsen numbers at cryogenic temperatures is then compared with the Weber-Schmidt results in figure 3 for $Kn=0.5, 1$ and 5.
Figure 3: Pressure ratio calculated by MD (gray lines) and the Weber-Schmidt equation (black lines) versus time (ns). The results for Kn=5, 1 and 0.5 are represented using dotted, dashed and dot-dashed lines, respectively.

The Weber-Schmidt equation represents a system at steady-state; these results are represented as black lines in figure 3, with dotted, dashed and dot-dashed lines for Kn=5, 1 and 10, respectively. Our MD simulation results reach a steady-state after 10 to 15 ns. When the simulations reach steady-state, the MD values are quite closer to the values predicted by the Weber-Schmidt equation. The best comparison between the two is obtained for a $\Delta T=200$ K temperature difference, while the MD values for $\Delta T=90$ K are slightly underpredicted.

4. Conclusion

Monatomic helium gas in a nanochannel under different temperature gradients has been simulated using molecular dynamics. Thermo-molecular pressure differences in the cryogenic ranges have been compared with those in conventional temperature ranges. For the same temperature difference, the TMPD values were very close to each other, so operating the system in cryogenic temperature ranges does not affect the TMPD values. As a secondary case, the system has been analyzed under a smaller temperature difference, with the temperature of the cold reservoir reduced to 10 K. The smaller temperature difference introduces a smaller pressure difference, as is consistent with the literature. The calculated pressure values have been compared with those from the Weber-Schmidt equation, and better agreement was shown for the higher temperature difference case.

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