Monte Carlo analysis of thermal transpiration effects in capacitance diaphragm gauges with helicoidal baffle system

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Abstract. The Capacitance Diaphragm Gauge (CDG) is one of the most widely used vacuum gauges in low and middle vacuum ranges. This device consists basically of a very thin ceramic or metal diaphragm which forms one of the electrodes of a capacitor. The pressure is determined by measuring the variation in the capacitance due to the deflection of the diaphragm caused by the pressure difference established across the membrane. In order to minimize zero drift, some CDGs are operated keeping the sensor at a higher temperature. This difference in the temperature between the sensor and the vacuum chamber makes the behaviour of the gauge non-linear due to thermal transpiration effects. This effect becomes more significant when we move from the transitional flow to the free molecular regime. Besides, CDGs may incorporate different baffle systems to avoid the condensation on the membrane or its contamination. In this work, the thermal transpiration effect on the behaviour of a rarefied gas and on the measurements in a CDG with a helicoidal baffle system is investigated by using the Direct Simulation Monte Carlo method (DSMC). The study covers the behaviour of the system under the whole range of rarefaction, from the continuum up to the free molecular limit and the results are compared with empirical results. Moreover, the influence of the boundary conditions on the thermal transpiration effects is investigated by using Maxwell boundary conditions.

1. Introduction
Capacitance Diaphragm Gauges (CDG) consist basically of a very thin ceramic or metal diaphragm which forms one of the electrodes of a capacitor. The pressure is determined by measuring the variation in the capacitance due to the deflection of the diaphragm caused by the pressure difference established across the membrane. In order to minimize zero drift, some CDGs are operated keeping the sensor at a higher temperature [1]. This difference in the temperature between the sensor and the vacuum chamber makes the behavior of the gauge non-linear due to thermal transpiration effects. Besides, CDGs may incorporate different baffle systems to avoid the condensation on the membrane or its contamination. In figure 1 a schematic representation of a CDG with the helicoidal baffle system is shown.
The thermal transpiration or thermal creep is a rarefaction effect which appears when there is a temperature gradient along the boundaries of a channel, which creates a flow next to the walls from the colder to the hotter side. The tube of the gauge connecting vacuum chamber and membrane is such a channel filled with gas under rarefied gas conditions. The rarefaction of the gas is defined by the Knudsen number ($Kn$) as the ratio of the mean free path and the characteristic size of the channel

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

where the mean free path for a hard sphere gas is defined as $\lambda = \left(\sqrt{2\pi d^2 n}\right)^{-1}$, $d$ is the diameter of the molecules and $n$ is the number density of the gas. The mean free path can be related to the viscosity of the gas $\mu$ by:

$$\lambda = \frac{\sqrt{\frac{\pi \mu v_0}{2P}}}{P}$$  \hspace{1cm} (1)

where $v_0 = \sqrt{2k_BT/m}$ is the most probable velocity and $k_B$ is the Boltzmann constant. In the free molecular limit the pressure ratio created by the temperature gradient along the channel is:

$$\frac{P_H}{P_C} = \left(\frac{T_H}{T_C}\right)^{0.5}$$  \hspace{1cm} (2)

where $T_H$ and $T_C$ are the temperatures of both ends of the channel ($T_H > T_C$).

An excellent explanation of the physical mechanism of the thermal creep flow can be found in Sone’s book [2]. A critical review of the numerical data and analytical results available was made by Sharipov and Seleznev [3]. The thermal creep flow and the thermomolecular pressure difference are described and experimental and analytical solutions are given for different configurations, rarefaction conditions and pressure and temperature drops. Several authors have performed experiments in order to measure the thermal transpiration either in capacitance manometers or in microchannels. Hobson [4] carried out the experiments under very low pressures matching the ideal limiting value in the free molecular regime when using a leached pyrex tube joining the cold and hot regions. However, the results did not match the theoretical value when the tube was smooth due to the fact that the reflection of the molecules in this case in not purely diffusive. Storvick et al. [5] measured the absolute thermal transpiration differential pressure in a capillary tube for different gases and compared their
measurements with their numerical results obtained by solving the BGK kinetic model. Recently experimental measurements of the mass flow rate caused by thermal transpiration due to a temperature gradient along a microchannel have been reported in [6]. The calibration of CDGs with heated heads has been analyzed by Poulter et al. [7], studying the thermal transpiration effect in such devices and comparing their results with some empirical equations proposed by Liang [8] for different pressures and gases. Additional empirical equations relating the pressure measured at the sensor to the actual pressure for various gases can be found in [9]. These results have been widely used for calibrating CDGs for different gases to those employed in the calibration procedure. Complete descriptions on the operation of CDGs and analysis of their deviations and calibration errors have been done by Jousten [10]. Šetina suggested [11] later a universal expression for the thermal transpiration correction in CDGs as a function of normalized pressure using viscosity and molecular mass of the gas to simplify the expression. More recently Nishizawa and Hirata [12] applied the DSMC method to compute numerically the pressure distribution along the connecting tube of the gauge in the whole range of rarefaction and Iwata and Kusumoto [13] analysed by using DSMC the limits of the Takaishi-Sensui formula and suggested a rescaling factor for short pipes.

In the present work, the thermal transpiration effect on the behavior of a rarefied gas and on the measurements in a CDG with a helicoidal baffle system is investigated by using the Direct Simulation Monte Carlo method (DSMC). The study covers the behavior of the system under the whole range of rarefaction, from the continuum up to the free molecular limit for the channel confined in the double helix which acts as a baffle system to protect the diaphragm of the instrument. The results obtained are compared with the empirical Takaishi-Sensui formula and the effect of different accommodation coefficients is studied.

2. Problem formulation and numerical simulation
The traditional Direct Simulation Monte Carlo (DSMC) method proposed by Bird [14] is used for simulation of the gas flow in gauge system. This method combines deterministic aspects for modeling particle motions and statistical aspects for computing collisions between particles. The collision-sample technique that we use is the “No Time Counter” scheme suggested by Bird, except for a slight modification in the calculation of maximum collision number in a cell, as described by Stefanov et al. [15]. The simulation is carried out in three-dimensional computational domain defined by the geometry of the baffle system.

The geometry of the studied baffle system is a double helix as it is shown in figure 2. The inner radius of the helix is \( R_{in} = 1.7 \) mm, its outer radius \( R_{out} = 4.8 \) mm, the vertical distance between the ramps is \( \Delta z = 4.0 \) mm and the thickness \( \varepsilon = 1.0 \) mm. The helix contains two channels with rectangular cross section (width 3.1 mm and height 4.0 mm) and, as each channel corresponds to 1.5 turns, the total length of the channel is 34.1 mm.

Only one of the two channels confined within the helix is taken into consideration in the numerical calculations under the assumption that the behavior of the gas in both channels is the same because of the system symmetry. The calculations are realized in cylindrical coordinates, by using the procedure for axially symmetric flows, and the 3D-space domain is then divided into uniform cells in the radial direction \( r \), in the axial direction \( z \) and in the polar angular direction \( \theta \). The cell size is always kept smaller than the mean free path, the time step smaller than the cell traversal time and the average number of particles in cells was never smaller than 15. The most demanding calculation which has been carried out employed 50x300x50 basic cells with approximately \( 2.1 \cdot 10^7 \) simulators.
The two ramps which form the lower and upper boundaries of the channel are situated at $z_1 = \frac{\Delta z + \varepsilon}{\pi} \theta$ and $z_2 = \Delta z + \frac{\Delta z + \varepsilon}{\pi} \theta$. In general, the boundary conditions are chosen to be purely diffusive at the temperature of the wall and the hard sphere model is used to compute the interaction between molecules. The simulations are carried out in a dimensionless manner and the results expressed in non-dimensional form can be applied for any gas which is simulated as a hard sphere gas. The reference quantities are taken to be $n_0$, $T_0$ and $P_0 = n_0 k_B T_0$, which define the number density, temperature and pressure at the inlet and are kept constant during the calculations. Moreover, we define the reference Knudsen number as:

$$Kn = \frac{\lambda}{R_{out} - R_{in}}$$

For the dimensional results, the gas used for the calculations was nitrogen, with molecular diameter $d = 3.75 \times 10^{-10}$ m and $m = 4.65 \times 10^{-26}$ kg respectively. The slope of the upper and lower boundaries must be taken into account when computing the reflection of the particles, due to the fact that the slope of the ramp varies depending on the radial coordinate, being larger next to the inner cylinder and smaller near the outer cylinder. This slope ($m$) can be determined by $m = \text{arctan} \left( \frac{\Delta z + \varepsilon}{\pi r} \right)$ as a function of the radial coordinate for each molecules hitting any of those two boundaries. Besides, the inlet is defined as an open boundary where particles crossing it are automatically removed, while, at the same time, particles are produced at a given rate and with a certain molecular velocity depending on the pressure and temperature defined at that boundary. For this reason, all mentions to inlet properties in this work are equivalent to the properties at the vacuum chamber in the reality.
3. Steady calculations of thermal transpiration in CDGs with helicoidal baffle system

In this section the effect of the thermal transpiration on the pressure distribution along the channels at equilibrium is investigated in the whole range of rarefaction. The vacuum chamber is maintained at $T_0 = 23^\circ C$, while the diaphragm is kept at a higher temperature of $T_{\text{diaph}} = 82^\circ C$. This temperature difference between the inlet and the diaphragm is large enough to reduce the statistical fluctuations and hence the sample size of the calculations. The temperature is considered to vary linearly along the $z$-axis in a certain region of the helix, as defined in figure 3.

The calculations have been performed for different values of the pressure at the inlet of the helix. In figure 4 the pressure distribution inside the helix is shown for a pressure in the vacuum chamber of $P_0 = 0.01$ Pa. Under these conditions the Knudsen number takes a value of $Kn \approx 200$, which corresponds practically to free molecular regime. As it can be seen, a pressure variation along the helix appears in the steady state as a consequence of the temperature difference between the diaphragm and the vacuum chamber.

![Figure 4. Pressure distribution in the helicoidal baffle system for $T_{\text{diaph}} = 82^\circ C$, $T_0 = 23^\circ C$ and $P_0 = 10^{-2}$ Pa.](image)

In order to obtain a better quantitative representation of the results, the distributions of the macroscopic properties along the central line of the channel, at $r = (R_{\text{in}} + R_{\text{out}})/2$ and $z = \frac{\Delta z}{\pi} + \Delta z + \frac{\epsilon}{\pi} \theta$, are plotted in figure 5 for different values of the reference pressure at the inlet.

The effect of the thermal transpiration can be clearly seen. The ratio between the pressure measured at the diaphragm at equilibrium and the pressure at the vacuum chamber is increased as the reference pressure in the vacuum chamber is decreased (the $Kn$ is increased). It can be seen that for $Kn = 208$, which defines practically free molecular conditions, the numerical results match the theoretical value of this pressure ratio due to thermal transpiration effect in the free molecular limit.
This value tends to unity when the conditions are close to continuum regime. It can be seen that the temperature distributions remain unchanged for the different values of the pressure at the inlet. As for the density distributions, its value at the hotter region is always smaller than at the inlet region. This difference becomes smaller as the flow regime approaches the free molecular regime and it becomes larger in the continuum limit.

\[
\frac{P_{\text{diaph}}}{P_0} = \sqrt{\frac{273 + 82}{273 + 23}} = 1.095
\]  \hspace{1cm} (4)

\[\begin{align*}
\frac{P_{\text{diaph}}}{P_0} - 1 &= \frac{1}{A^*X^2 + B^*X + C^*\sqrt{X} + 1} \\
\sqrt{T_{\text{diaph}}/T_0} - 1 &= \frac{1}{A^*X^2 + B^*X + C^*\sqrt{X} + 1}
\end{align*}\]  \hspace{1cm} (5)

where \( X = P_0 D/\bar{T} \), \( D \) is the hydraulic diameter of the channel (3.49 mm) and \( \bar{T} \) is the mean temperature along the channel. The empirical constants (\( A^*, B^* \) and \( C^* \)) for nitrogen are taken from table 1 of [9]. The two curves are shown in figure 6. Although near the free molecular regime the DSMC results deviate slightly from the TS curves, in general the agreement between the results is good.

In the following part of this section, the effect of the accommodation coefficient (\( \alpha \)) on the pressure difference created by thermal transpiration effects is investigated. The specular-diffuse reflection model is used for this purpose, where \( \alpha \) defines the fraction of particles reflected diffusively and \((1 - \alpha)\) is the fraction of particles which reflect specularly. The results for various values of the accommodation coefficient and different rarefaction conditions are shown in table 1. It can be deduced from the results that, in the free molecular regime, the value of the accommodation coefficient in the range analyzed here has no effect on the induced pressure gradient. However, in the transition and slip flow regimes, the induced pressure gradient depends slightly, but clearly, on the values of the accommodation coefficient included in this work. As shown in table 1, the pressure gradient for the same rarefaction conditions becomes larger as the accommodation coefficient is
increased. It is expected that in the continuum limit the accommodation coefficient has again no effect on the pressure, because the thermal transpiration effect is negligible under those conditions.

![Graph showing the variation of the ratio between the pressure at the diaphragm and at the vacuum chamber as a function of the reference pressure obtained by using DSMC (blue circles) and TS formula (black solid line) for $T_{\text{diaph}} = 82^\circ C$, $T_0 = 23^\circ C$.](image)

**Figure 6.** Variation of the ratio between the pressure at the diaphragm and at the vacuum chamber as a function of the reference pressure obtained by using DSMC (blue circles) and TS formula (black solid line) for $T_{\text{diaph}} = 82^\circ C$, $T_0 = 23^\circ C$.

**Table 1.** Pressure measured at the diaphragm for various accommodation coefficients and rarefaction conditions.

| $\alpha$ | $P_\theta = 0.01$ Pa | $P_\theta = 0.1$ Pa | $P_\theta = 1.0$ Pa | $P_\theta = 10$ Pa |
|----------|----------------------|---------------------|---------------------|-------------------|
|          | ($Kn = 208$)        | ($Kn = 20.8$)       | ($Kn = 2.08$)       | ($Kn = 0.208$)    |
| 0.7      | 1.0958               | 1.0905              | 1.0754              | 1.0217            |
| 0.8      | 1.0963               | 1.0937              | 1.0772              | 1.0277            |
| 0.9      | 1.0959               | 1.0955              | 1.0806              | 1.0294            |
| 1        | 1.0952               | 1.0941              | 1.0812              | 1.0302            |

Finally, it is interesting to have an estimation of the computational cost needed for solving the problem under various conditions. As mentioned above, the minimum number of particles per cell which was used was 15 in order to obtain accurate results. This minimum number of particles occurs in the region near the inner cylinder, while the number of particles per cell becomes larger in cells close to the outer cylinder. The required CPU time needed to obtain a sample size of at least 150000 particles is given in table 2 for two different cases: the first near free molecular conditions and the second close to the continuum regime. The calculations were run in a single core with processor Intel(R) Core(TM) i7 CPU 860 at 2.80 GHz. The time which is shown in table 2 is the time needed to obtain the sample size described above, without taking into account the transient time until the steady state solution is achieved, which is of the same order of magnitude.
Table 2. CPU time for the indicated conditions.

| $P_0$ [Pa] | Cells      | Number of particles | Time steps | CPU time [h] |
|-----------|------------|---------------------|------------|-------------|
| 0.01      | 25x200x25  | 3.45·10^6           | 10000      | 4.52        |
| 100       | 50x300x50  | 21.1·10^6           | 10000      | 47.8        |

4. Conclusions
In order to improve the stability of the CDGs, these devices operate usually keeping the sensor at higher temperature. In this work, the thermal transpiration effect caused by this temperature difference between the sensor and the vacuum chamber on the behavior of a rarefied gas and on the measurements in a CDG with a helicoidal baffle system has been investigated by using the Direct Simulation Monte Carlo method (DSMC). The ratio between the pressure measured at the diaphragm and the pressure at the vacuum chamber has been obtained under the whole range of rarefaction, from the continuum up to the free molecular limit. The results have been compared with those obtained from the empirical Takaishi-Sensui formula showing good agreement. The effect of the accommodation coefficient on the induced pressure gradient was investigated by using the Maxwell boundary conditions model.

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