Limits of one dimensional modeling of rarefied Couette Poiseuille clearance flow in vacuum pumps

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Abstract. Clearance flows are the main loss mechanism in dry running positive displacement vacuum pumps. In order to calculate the operation of those pumps a detailed knowledge of the clearance mass flow rates is crucial. The dimensions of such pumps and the large pressure range of the operating points require a wide range of gas rarefaction to be taken into account. The clearance flow can be described by a combined Couette Poiseuille flow due to the pressure gradient between two chambers and the rotation of the rotary pistons. A clearance of variable cross section is investigated and in order to determine the mass flow rate, the DSMC (direct simulation Monte Carlo) method is used. Results in the slip and transition flow regime are compared to experimental findings and a good agreement can be found. In addition, a one dimensional theory is presented based on a linear superposition of Poiseuille and Couette flow rates. The aim of the present work is to determine the limits of the one dimensional theory concerning the geometry of such clearances. For this, the boundary conditions circumferential speed, inlet and outlet pressure are varied.

1. Introduction
Dry running vacuum pumps have become an important part of vacuum systems due to their oil-free working principle. The need for a clean vacuum, for instance in the semiconductor industry, has pushed the development of dry running positive displacement pumps, such as screw and roots pumps (see Ref. [1]). Due to contactless operation of the pistons, the sealing between the working chambers is realized by small clearances. Regarding Figure 1 a) the effective mass flow rate of a screw machine can be calculated by the delivered mass flow rate $\dot{m}_d$ of a working chamber driven by the rotation of the pistons and reduced by the clearance mass flow rate $\dot{m}_cl$. Clearances typically appear between both, rotary pistons and the housing in such machines. The geometry of the surrounding boundary varies in dependence of the shape of the rotors and the housing. Calculating the thermodynamical operation of such pumps, the knowledge of these clearance mass flow rates is essential, which represent the main loss mechanism.

In the current work a clearance geometry formed by a plane contour on one side and a contour with a radius $R$ on the other side shall be regarded, which is shown in Figure 1 b). The clearance height is defined by $h_{min}$. Due to the rotation of the rotors a moving boundary is present. This is considered by a circumferential speed $U = \omega R$ for the contour of radius $R$. The clearance has a finite width $w$, which is constant in the flow direction $x$. The thermodynamic state of the connected working chambers is defined by the static pressure and static temperature at the inlet ($p_{in}, T_{in}$) and outlet ($p_{out}, T_{out}$).
Figure 1. Screw vacuum pump and investigated clearance geometry.

Screw vacuum pumps are deployed as fore vacuum pumps and the suction pressure ranges from atmospheric state down to only a few Pascal, meaning that the pressure ranges in more than five decades. In addition, the circumferential speed of the tip of the rotary piston can reach up to 80 m/s. In this context two basic flow problems can be identified in order to predict the mass flow rate in such clearances. The Couette flow, which is driven by the movement of the rotary piston and the Poiseuille flow, driven by the pressure gradient between two working chambers. In addition, the prediction of the mass flow rate is complicated by the fact, that rarefaction effects of the clearance flow have to be taken into account, due to the large pressure range. The degree of rarefaction is expressed by the Knudsen number, which can be described by the ratio of the mean free path of the molecules and a characteristic length (the minimal clearance height $h_{\text{min}}$). Typically all flow types appear in these machines, ranging from the continuum flow to the free molecular flow.

The rarefied gas flow in channels, tubes and clearances has been studied extensively in the field of microelectromechanical systems during the past decades. These systems often operate at atmospheric flow conditions with very small length scales (see Ref. [2]). Thus, the range of Knudsen numbers which has to be dealt with is comparable to clearance flows in vacuum pumps. Regarding the literature various approaches modeling rarefied flows are present. While in the continuum flow regime normally the Navier-Stokes equations are used applying a no-slip boundary condition on the walls, this approach fails at higher Knudsen numbers. Therefore in the so called slip flow regime a slip boundary condition at the walls can be introduced to improve the results of the Navier-Stokes equations (Ref. [3]). The application of a first order slip model fails to predict the Knudsen minimum, so that a second order model has to be introduced (see Ref. [2]). If the Navier-Stokes equation fail at moderately high Knudsen numbers, one can calculate the rarefied flow on the basis of the Boltzmann equation, but the solution is complicated because of the collision term (see Refs. [4] and [5]). A widely used method for the solution of the collision term is the Bhatnagar-Gross-Krook model (BGK-model) described in Ref. [6]. The idea of the model is that due to the collision term the distribution function tends to equilibrium state. Often this is combined with a linearization of the Boltzmann equation. Cercignani uses this method to determine the volume flow rate between two parallel plates and compares it with experimental data (see Ref. [7]). The method is suitable to predict the Knudsen minimum (Ref. [8]). Beside the BGK-model different models for the collision term exist, like the S-model (Ref. [9]) in order to represent the correct Prandtl number. Sharipov uses this model to calculate a Poiseuille and thermal creep flow through a long tube (Ref. [10]) and parallel plates (Ref. [11]). A method for solving the Boltzmann equation statistically is provided by the direct simulation.
Monte Carlo (DSMC) method (see Ref. [4]), which considers a discrete set of particles, each owning a position and a velocity. Key feature of the method is the decoupling of molecular movement and intermolecular interactions. The method has been used widely in the context of microdevices, see Refs. [12], [13], [14], [15] and [16].

As described earlier, two basic flow problems have to be handled for calculating the mass flow rate in clearances of vacuum pumps, the Couette flow and the Poiseuille flow. For both flow problems various investigations can be found in the literature and a summary is located in Ref. [17]. The one dimensional approach to calculate a combined Couette Poiseuille flow is described in Ref. [17]. The aim of the current work is to determine the limits of applicability of the one dimensional approach due to assumptions of this flow model. In a first step results of the DSMC method are compared to those obtained by experiment in order to verify the DSMC method. Following this, the radius $R$ is varied for the presented clearance for different Knudsen numbers and boundary velocities using the one dimensional approach. Results are then compared to simulations using the DSMC method in order to evaluate the range of applicability of the one dimensional approach.

2. Theoretical approaches

In order to achieve a universal declaration of applicability, it is useful to describe the flow by dimensionless numbers. Assuming a flow of constant temperature $T(x) = T_{in} = T_{out}$ five dimensionless numbers are needed for the investigated geometry, naming the Knudsen number $Kn$, the pressure ratio $\Pi$, the dimensionless circumferential speed $U/c_m$, the ratio of the radius to the minimal clearance height $R/h_{min}$ and the normalized mass flow rate $C_0$.

The Knudsen number using the model of hard sphere molecules is defined as

$$Kn = \frac{\mu \cdot c_m \cdot \sqrt{\pi}}{2 \cdot h_{min} \cdot p_{in}},$$  

(1)

$\mu$ is the viscosity and

$$c_m = \sqrt{\frac{2 \cdot k \cdot T_{in}}{m}},$$  

(2)

is the most probable molecular speed with the molecular mass $m$ and the Boltzmann constant $k$.

$$\Pi = \frac{p_{in}}{p_{out}},$$  

(3)

is the pressure ratio. The results are given in the dimensionless mass flow rate

$$C_0 = \frac{\dot{m}}{\dot{m}_{mol}} = \frac{\sqrt{\pi} \cdot c_m}{p_{in} \cdot w \cdot h_{min}} \cdot \dot{m},$$  

(4)

with $\dot{m}_{mol}$ being the mass flow rate through an orifice with equal cross sectional area at molecular flow into a perfect vacuum.

2.1. One dimensional approach

The one dimensional approach is described in Ref [17] and a brief summary shall be given in the current work. The aim is to calculate the mass flow rate $\dot{m}$ of a clearance for given boundary velocity $U$, inlet pressure $p_{in}$ and outlet pressure $p_{out}$. The temperature of the gas and the boundaries is assumed to be equal $T_{in} = T_{out} = T$.

According to Refs. [18] and [19] the clearance is assumed to be long (i.e. $max(h) \ll L$) so that the local dimensionless pressure gradient

$$\xi_p = h \cdot \frac{dp}{dx}, \quad |\xi_p| \ll 1,$$  

(5)
is considered to be small in any cross section. Following Refs. [18] and [20] a superposition of the Couette and Poiseuille flow is assumed leading to the mass flow rate in any cross section

\[ \dot{m} = \frac{h \cdot w \cdot p}{c_m} \cdot \left( 2 \cdot G_C \cdot \frac{U_x}{c_m} - G_P \cdot \xi_P \right), \]  

where \( U_x = U_x(x) \) is the local wall velocity of the moving boundary in flow direction. \( G_C \) is the reduced flow rate of the plane Couette flow, which can be calculated to the constant value \( G_C = 1/2 \) due to the symmetry of the Couette flow for a clearance of infinite width \( w \) (see Ref. [20]). The reduced flow rate \( G_P \) of the Poiseuille flow depends on the local Knudsen number and the local aspect ratio \( h/w \). The determination of \( G_P \) is described in Ref. [17] and values are extracted from Ref. [21], [22], [23] and [24]. Eq. 6 then can be solved using a finite difference scheme, also described in Ref. [17].

2.2. DSMC method

The DSMC method provides a statistical tool for determining the solution of the Boltzmann equation. The method, developed by Bird [4], is a particle-based simulation tool, according to the kinetic theory of gases. The key feature of the DSMC method is, that one particle represents a set of molecules and that the movement of particles and intermolecular collisions are decoupled. Figure 2 shows the complete algorithm sequence, as it is implemented in the open source software package OpenFOAM.

The algorithm starts with a grid generation and initialization of particles according to a given uniform number density of the flow field. A velocity and inner energy is assigned to every particle according to a given uniform temperature. The main loop starts with the calculation of the movement of every particle. According to a given time step new positions are calculated and potential collisions with boundaries are handled according to the underlying model. Particles which leave the simulation domain via the inlet or outlet have to be removed. To be able to simulate an inflow and outflow at a given pressure and temperature, new particles have to be inserted at the inlet and outlet. For this, a new boundary condition according Ref. [4] was implemented in the OpenFoam software package. Next, the particles are indexed to every cell, as is necessary to calculate the intermolecular collisions for every cell separately. The collision algorithm itself is based on a non-deterministic approach, using the probability of collisions. The NTC-method (no time counter method), developed by Bird [25], allows the calculation of the correct number of collisions. For every time step the macroscopic flow fields are calculated and are then time-averaged in order to minimize the statistical noise. This procedure is repeated \( N_{av} \) times until the end of the averaging interval is reached. All averaged fields are written and reset and the next averaging interval begins. The procedure is repeated until a flow of steady state is reached, regarding the mass flow at the inlet and outlet. In order to reduce the statistical noise, a subsequent longer averaging run is necessary.

Within this study, the flow of air in the clearance geometry presented in Figure 1 is investigated. In all cases the length \( L \) is chosen such, that the pressure gradient at the inlet and outlet of the clearance is small. The gas model is composed as a mixture of nitrogen and oxygen with the appropriate fraction of number density. The used values for the relaxation collision number, the mass of molecule, the variable hard sphere (VHS) diameter, the number of inner degrees of freedom and the viscosity index for each molecule type is given in Table 1. For the intermolecular collisions the Larsen-Borgnakke-VHS model is used, described in Ref. [4]. Wall collisions are handled according a diffuse reflection of the molecule and in case of a moving boundary, the wall velocity is superposed.
Figure 2. DSMC-Algorithm

Table 1. Model of gas (according Ref. [4]) and boundary conditions used in the DSMC method.

| inflow/ outflow boundary conditions | specifying: $p, T$ |
|------------------------------------|--------------------|
| wall interaction model             | diffuse (Maxwell)  |
| Binary collision model             | Larsen-Borgnakke-VHS |
| relaxation collision number        | $5$                |
| gas                                | $N_2$ $77.7\%$ $O_2$ $22.3\%$ |
| mass of molecule                   | $46.5 \cdot 10^{-27}$ kg $53.12 \cdot 10^{-27}$ kg |
| VHS diameter at 273 K              | $4.17 \cdot 10^{-10}$ m $4.07 \cdot 10^{-10}$ m |
| number of inner degrees of freedom | $2$                |
| viscosity index                    | $0.74$ $0.77$      |

3. Comparing theoretical approaches to Experimental results

In order to validate the simulations of the DSMC method a comparison to experimental results is carried out. For this, an experimental setup is used with a clearance geometry according to Figure 1, where the upper contour is realized by a rotatable shaft. It is possible to adjust the inlet and outlet pressure $p_{in}$ and $p_{out}$ and the circumferential speed $U$. A complete description of the
setup and the method of measurement can be found in Ref. [17]. Figure 3 shows experimental results and simulations of the DSMC method for the dimensionless mass flow rate as a function of the Knudsen number. The dimensionless circumferential speed $U/c_m$ is varied for constant pressure ratio $\Pi = p_{in}/p_{out} = 8$ and geometry $R/h_{min} = 250$. Measurements are conducted in the transition, slip and continuum flow regimes. Simulations are carried out in the transition and slip flow regimes. The smallest Knudsen number calculated by the DSMC method is $Kn = 0.044$ because for smaller values the computational time gets very large.

**Figure 3.** Dimensionless mass flow rate as a function of the Knudsen number. A variation of the dimensionless circumferential speed $U/c_m$ is shown for simulations using the DSMC method and results are compared to experimental findings from Ref. [17].

Regarding the experimental results for a stationary boundary $U/c_m = 0$ a characteristic dimensionless mass flow rate as a function of the Knudsen number can be observed. For small Knudsen numbers $0.004 < Kn < 0.05$ in the continuum and slip flow regime a linear decrease of the dimensionless mass flow rate with increasing Knudsen number can be observed. This is due to a higher influence of the friction in the flow, which is laminar in this regime. For very small Knudsen numbers $Kn < 0.004$ the dimensionless mass flow rate slightly tends to a constant value due to a choked flow in the clearance. For greater Knudsen numbers $Kn > 0.05$ a slip of the gas flow at the wall occurs, so that the effect of increasing friction is reduced. In the transition flow regime rarefaction effects get significant, and the Knudsen minimum can be found for a Knudsen number of $Kn \approx 0.8$. For greater Knudsen numbers the normalized mass flow rate increases again, until it reaches the mass flow rate for a molecular mass flow rate, which is independent of the Knudsen number. Regarding a positive dimensionless circumferential speed $U/c_m = 4.88 \cdot 10^{-2}$ and $U/c_m = 9.75 \cdot 10^{-2}$ the dimensionless mass flow rate is shifted towards higher values due to the Couette flow, which operates in the same direction as the Poiseuille flow. The highest impact can be observed in the transition flow regime and gets very small in...
the continuum flow regime. Here the flow is highly influenced by the Poiseuille flow. A negative circumferential speed \( U/c_m = -4.88 \cdot 10^{-2} \) and \( U/c_m = -9.75 \cdot 10^{-2} \) shifts the normalized mass flow rate towards lower values. Again, the highest impact can be found in the transition flow regime. For a Knudsen number smaller than \( Kn < 0.08 \) and a negative circumferential speed of \( U/c_m = -9.75 \cdot 10^{-2} \) a negative dimensionless mass flow rate can be observed.

Comparing the simulation results of the DSMC method with the experimental results a very good agreement can be found. The DSMC method is able to depict the normalized mass flow rate for the shown Knudsen numbers and circumferential speeds. Regarding a negative circumferential speed, the simulation using the DSMC method is within the confidence interval of the experimental results, except for a Knudsen number \( Kn = 0.044 \). Here, the relative error is within 20%. Regarding the results without circumferential speed and a positive circumferential speed \( U/c_m = 4.88 \cdot 10^{-2} \), the normalized mass flow rate obtained by the DSMC method is smaller than the experimental results for all calculated Knudsen numbers. Here, the relative error is within 13%. For a positive circumferential speed \( U/c_m = 9.75 \cdot 10^{-2} \) the results of the DSMC method are within the confidence interval of the experimental results, again.

4. Variation of geometry

As described in section 1, the aim of the current work is to evaluate the applicability of the one dimensional approach regarding different geometries. Therefore, the geometrical parameter \( R/h_{min} \) is varied and the calculated dimensionless mass flow rates of the one dimensional approach are compared to those, obtained with the DSMC method. Further on, the relative deviation is shown, which is defined as

\[
f = \frac{C_{0,\text{one dim.}} - C_{0,\text{DSMC}}}{C_{0,\text{DSMC}}} \cdot 100\% \tag{7}
\]

Figure 4 shows the dimensionless mass flow rate as a function of \( R/h_{min} \) for three different Knudsen numbers, which are located in the transition and slip flow regimes. No circumferential speed \( U/c_m = 0 \) is present in this case and the pressure ratio is \( \Pi = 10 \). Reducing the geometrical parameter \( R/h_{min} \) a rise of the normalized mass flow rate occurs for all three Knudsen numbers. A smaller radius of the clearance results in a smaller effective clearance length in the flow direction and yields less frictional losses in the flow. This is depicted by the DSMC method and the one dimensional approach as well. It has to be stated, that the normalized mass flow rate using the one dimensional approach offers higher values compared to the DSMC method in all cases and diverges for smaller values of \( R/h_{min} \). Regarding a Knudsen number \( Kn = 4.4 \) the relative deviation is \( f = 7.5\% \) for \( R/h_{min} = 250 \) and rises to \( f = 28\% \) for \( R/h_{min} = 16 \). A similar process can be observed for smaller Knudsen numbers, starting with a relative deviation \( f = 3\% \) for \( R/h_{min} = 250 \) rising to \( f = 10\% \) for \( R/h_{min} = 16 \) for a Knudsen number \( Kn = 0.44 \) and \( f = 3.3\% \) for \( R/h_{min} = 250 \) rising to \( f = 18.5\% \) for a Knudsen number \( Kn = 0.044 \). It can be stated in general, that the deviation of both methods is small in the region of the Knudsen minimum and rises for higher and smaller Knudsen numbers. The diverging results of both methods for smaller values \( R/h_{min} \) can be explained by an increasingly influence of a two dimensional flow. With a smaller radius \( R \), the z-component of the flow has a higher impact, which can not be depicted by the one dimensional approach, but the DSMC method can. It can be stated, that a great increase in the deviation \( f \) can be observed for \( R/h_{min} < 100 \) for all Knudsen numbers and no circumferential speed.

Figure 5 shows the dimensionless mass flow rate as a function of \( R/h_{min} \) for three different Knudsen numbers, a positive circumferential speed \( U/c_m = 9.75 \cdot 10^{-2} \) and a pressure ratio \( \Pi = 10 \). Due to the positive Couette flow, a higher normalized mass flow rate can be observed compared to the results without circumferential speed for all Knudsen numbers. Again, the deviation \( f \) rises for smaller values of the geometrical parameter \( R/h_{min} \), due to a higher
influence of the z-component of the flow. Regarding a Knudsen number \( Kn = 4.4 \), a reduction of the geometrical parameter \( R/h_{\text{min}} \) only has a small impact on the normalized mass flow rate. Results of the DSMC method indicate a constant normalized mass flow rate so that a high influence of the Couette flow can be stated for this Knudsen number. A slight rise in the normalized mass flow rate can be observed for smaller values of \( R/h_{\text{min}} \) using the one dimensional approach. For smaller Knudsen numbers \( Kn = 0.44 \) and \( Kn = 0.044 \) a rise in the normalized mass flow rate can be observed for smaller values of \( R/h_{\text{min}} \). For \( R/h_{\text{min}} > 100 \) the deviation \( f \) is smaller than 4% for all Knudsen numbers.

Figure 6 shows the dimensionless mass flow rate as a function of \( R/h_{\text{min}} \) for three different Knudsen numbers, a negative circumferential speed \( U/c_m = -9.75 \cdot 10^{-2} \) and a pressure ratio \( \Pi = 10 \). Due to a negative Couette flow, lower normalized mass flow rates can be observed compared to the results without circumferential speed. For smaller values of the geometrical parameter \( R/h_{\text{min}} \) an increase of the normalized mass flow rate can be observed for all Knudsen numbers. Again, a smaller radius \( R \) decreases the effective length of the clearance and thus the frictional losses of the Poiseuille flow. For a Knudsen number \( Kn = 0.044 \) an increase of the deviation \( f \) of both methods for smaller values of the geometrical parameter \( R/h_{\text{min}} \) can be observed again. In contrast to this, for higher Knudsen numbers \( Kn = 0.44 \) and \( Kn = 4.4 \) the deviation rises for smaller values \( R/h_{\text{min}} \). Because the absolute values in the normalized mass flow rates tends to zero the deviation \( f \) is large. Here, the Poiseuille and the negative Couette flow nearly compensate. But the absolute deviation is small again for \( R/h_{\text{min}} > 100 \).
Figure 5. Dimensionless mass flow rate as a function of the ratio $R/h_{\text{min}}$ for different Knudsen numbers and a boundary velocity $U/c_m = 9.75 \cdot 10^{-2}$ and a pressure ratio $\Pi = 10$. Results of one dimensional theory are compared with the DSMC method and relative deviation $f$ is given.

5. Conclusion
In the present paper, the combined Couette Poiseuille flow of a rarefied gas is investigated using a one dimensional approach and the DSMC method. A comparison of the normalized mass flow rate obtained by the DSMC method and experimental results show, that the DSMC method is able to depict the combined Couette Poiseuille flow. A variation of the geometrical parameter $R/h_{\text{min}}$, the circumferential speed $U/c_m$ and the Knudsen number is conducted. In summary the one dimensional approach seems to provide reasonable results for geometrical parameters $R/h_{\text{min}} > 100$. 
Figure 6. Dimensionless mass flow rate as a function of the ratio $R/h_{min}$ for different Knudsen numbers and a boundary velocity $U/c_m = -9.75 \cdot 10^{-2}$ and a pressure ratio $\Pi = 10$. Results of one dimensional theory are compared with the DSMC method and relative deviation $f$ is given.
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