Rarefied Gas Flow Through a Thin Orifice

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Abstract. A rarefied gas flow through a thin orifice is studied on the basis of the direct simulation Monte Carlo method. The flow field and the mass flow rate have been calculated over a wide range of the Knudsen number in case of outflow into vacuum. The diffuse gas - surface interaction and the hard sphere molecular model are assumed. A comparison with experimental data available in the open literature has been performed.

I INTRODUCTION

A rarefied gas flow through an orifice is an important applied problem, because such type of the flow takes place in vacuum equipment, it is used to create molecular beams and in many other practical applications. This problem has also a great scientific interest. As is known the mass flow rate through an orifice and slit is very weakly depends on the gas-surface interaction law that was proved experimentally [1,2] and theoretically [3]. Since this type of rarefied gas flow is determined by the intermolecular interactions law only, it can be successfully used as a test for kinetic equations, for numerical methods applying to these equations, and for intermolecular interaction models.

The solution of the problem is determined by the two main parameters: the Knudsen number \( Kn = \lambda_0 / a \) and the pressure ratio \( P_0 / P_1 \). Here, \( a \) is the orifice radius, \( P_0 \) is the upflow pressure, \( P_1 \) is the downflow pressure, and \( \lambda_0 \) is the mean free path at the pressure \( P_0 \). Really, the solution is determined by the temperature ratio \( T_0 / T_1 \) too, but here we assume the temperatures to be the same in the upflow and downflow containers, i.e. \( T_0 / T_1 = 1 \).

In spite of the great practical importance till now this problem has not been investigated profoundly. As was noted in the review [4] a number of papers [5–8] offered asymptotic formulas for the mass flow rate near the free-molecular regime (\( Kn \rightarrow \infty \)) in case of outflow into vacuum (\( P_0 / P_1 = \infty \)). But there is no agreement between them and the range of their validity is very small. Some numerical data for intermediate Knudsen numbers and for the infinite pressure ratio \( P_0 / P_1 \) can be found in the work by Shakhov [9]. But the presentation of the data is very poor. In case of the small pressure difference, i.e. \( |P_0 - P_1| \ll P_0 \), the problem can be solved analytically in the hydrodynamic regime (\( Kn \ll 1 \)). The corresponding results are given in the works by Roscoe [10] and by Hasimoto [11]. Thus, one can see that the theoretical results on the orifice flow is restricted by the small ranges of the Knudsen number \( Kn \) and of the pressure ratio \( P_0 / P_1 \).

Experimental results on the mass flow rate through an orifice in case of outflow into vacuum (\( P_0 / P_1 = \infty \)) are presented in the papers by Liepmann [5], by Fujimoto and Usami [12], and by Barashkin et al. [13,14]. Experimental data for some intermediate values of the pressure ratio \( P_0 / P_1 \) but for a restricted range of the Knudsen number are given in the paper by Sreekanth [15]. The works by Borisov et al. [1] and by Porodnov et al. [2] provide the experimental results for the small pressure difference, i.e. \( |P_0 - P_1| \ll P_0 \), in a wide range of the Knudsen number. So, the experimental material on the orifice flow is also poor.

The aim of the present work is to carry out a numerical simulation of the rarefied gas flow through a thin orifice over a wide range of the Knudsen number in case of outflow into vacuum (\( P_0 / P_1 = \infty \)).
Consider an orifice in an infinitely thin partition that separates two semi-infinite reservoirs. One of them contains a monoatomic gas at a temperature $T_0$ and at a pressure $P_0$. The other container is maintained under a high vacuum so it can be considered that $P_1 = 0$. The schematic diagram of the flow is given in Fig. 1, where $x$ is the axis of the orifice and $r$ is the radial coordinate.

We are going to calculate the mass flow rate and the flow field as a function of the rarefaction parameter $\delta$ defined as

$$\delta = \frac{\sqrt{\pi}}{2} \frac{1}{Kn} = \frac{\sqrt{\pi}}{2} \frac{a}{\lambda_0},$$

where the mean free path $\lambda_0$ is related to the pressure $P_0$ and the temperature $T_0$ as

$$\lambda_0 = \frac{\mu(T_0)}{P_0} \left( \frac{\pi k T_0}{2m} \right)^{1/2}.$$

Here, $\mu(T_0)$ is the viscosity at the temperature $T_0$, $m$ is the mass of a gaseous particle and $k$ is the Boltzmann constant.

The numerical results will be given in terms of the reduced mass flow rate defined as

$$W = \frac{\dot{M}}{\dot{M}_0},$$

where $\dot{M}$ is the dimension mass flow rate and $\dot{M}_0$ is the mass flow rate in the free molecular regime flow, which reads

$$\dot{M}_0 = a^2 P_0 \left( \frac{\pi m}{2 k T_0} \right)^{1/2}.$$

III METHOD OF SOLUTION

The problem was solved by the direct simulation Monte Carlo method [16]. It was assumed the diffuse gas-surface interaction and the hard sphere molecular model. The region for the flow simulation has the form of two cylinders as is shown in Fig. 1. The cylinders have the radii $R_0$ and $R_1$ and the lengths $L_0$ and $L_1$ in
the upflow and downflow containers, respectively. The sizes of the region were as follows: $L_0 = R_0 = 8a$ and $L_1 = R_1 = 4a$. The numerical grid was regular with the cell size equal to $\Delta x = \Delta r = a/8$. The time increment was 0.01 of the mean free time. The number of simulated molecules fluctuate during the calculation. It was maintained about the value $10^6$.

To simulate the collision the so-called NTC method, see Ref. [16], p.219, was used. In every cell the number of selected pairs was calculates as

$$
\frac{1}{2} N_c N_c F_N \sigma c_{r,max} \Delta t V_c,
$$

where $N_c$ is the number of particles in the cell, $N_c$ is the average value of $N_c$, $F_N$ is the number of real molecules that each simulated particle represents, $\sigma$ is the diameter of particle, $c_{r,max}$ is the maximum relative velocity, $\Delta t$ is the time increment, and $V_c$ is the volume of the cell.

In every time step the number of particle passed through the orifice from the upflow container to the downflow one and the number of particles passed the orifice in the opposite direction were counted. The mass flow rate was calculated based on the average numbers of particles passed through the orifice during $10^5$ time steps that correspond to the time interval equal to $10^3$ mean free times.

**IV RESULTS AND DISCUSSIONS**

The calculations were carried out for the rarefaction parameter range $0.05 < \delta < 80$. For the values of $\delta$ smaller than 0.05 the mass flow rate $W$ does not differ from the unity within 1%. In the range $20 \leq \delta \leq 80$ it was observed the variation of the mass flow rate within 0.5%. So, a significant variation of the mass flow rate occurs in the range $0.1 \leq \delta \leq 20$.

The reduced mass flow rate $W$ is presented in Fig. 2 as a function of the rarefaction parameter $\delta$. One can see that the quantity $W$ varies in the range from 1 to 1.5. Then, beginning from $\delta = 20$ the mass flow rate $W$ is practically constant by increasing the rarefaction parameter $\delta$. 

![FIGURE 2. Mass flow rate W vs δ: points - present work, solid line - empirical formulae [12], dashed line - experiment at δ → ∞ [5], dashed-pointed line - experiment at δ → ∞ [13]](image)
Fujimoto and Usami [12] measured the mass flow rate through short tubes. The length-to-radius ratio of the shortest tube was \( l/a = 0.025 \) that can be considered as an orifice. They offered an empirical equation of the mass flow rate based on the experimental data for the interval \( 0.025 \leq l/a \leq 12.7 \) and for the large pressure ratio \( P_0/P_1 > 0.01 \) that can be considered as an outflow into vacuum. If one extrapolates their empirical equation for the orifice \((l/a = 0)\), one obtains

\[
W = 1 + \frac{0.4733 + 0.6005/\sqrt{\delta}}{1 + 4.559/\delta + 3.094/\delta^2}.
\]

This formula is presented by the solid line in Fig. 2. One can see that in the range \( 0 < \delta < 20 \) the empirical formulae and the numerical simulation results are in a good agreement. The systematic understanding of the empirical formulae is explained by the fact that the shortest tube in the experiments [12] was of \( l/a = 0.025 \) that decreases the mass flow for few percents. Moreover, the downflow pressure that always exists in experiment also slightly decreases the mass flow rate.

Because of a large dispersion of the experimental results by Liepmann [5], here we do not present his results for the intermediate Knudsen numbers. But it is worth to give his interesting result in the hydrodynamic regime \( \delta \to \infty \). Considering the orifice as a nozzle, to which one can apply the Euler equation, Liepmann obtained the following expression for the mass flow rate

\[
W = A(\zeta) \sqrt{2\pi \zeta} \left( \frac{2}{\zeta + 1} \right)^{(\zeta+1)/2(\zeta-1)},
\]

where \( \zeta \) is the ratio of the specific heats and \( A \) is a coefficient to be obtained from an experiment. For the argon gas \((\zeta = 1.66)\) the value \( A = 0.812 \) was given by Liepmann [5], i.e. \( W = 1.476 \). This result is presented in Fig. 2 by the dashed line, from which it can be seen that the experimental limit value of \( W \) is smaller than its theoretical value in the range of \( \delta \) from 20 to 80.

Barashkin et al. [13] also measured the mass flow through an orifice. They reported the constant \( A = 0.826 \) for the argon gas that correspond to the mass flow rate \( W = 1.501 \). This result is given in Fig. 2 by the dashed-pointed line. One can see that the numerical results in the range \( 20 \leq \delta \leq 80 \) are in a fine agreement with the experimental data by Barashkin et al. [13].

The small disagreement between the two experimental values of the mass flow rate in the hydrodynamic limit \((\delta \to \infty)\) can be explained by analyzing the results by Fujimoto and Usami [12]. They show that in the interval of the rarefaction parameter \( \delta \) from 50 to 1000 the mass flow rate \( W \) has a small decrease. So, it is possible that the constant \( A \) reported in the paper [5] was measured for very large values of the rarefaction parameter, i.e. about \( \delta \sim 1000 \), while the result obtained in the work [13] are based on moderate values of \( \delta \), i.e. about 50. To obtain theoretically the limit value of the mass flow rate a new simulation should be carried out for larger values of \( \delta \) that will require great computational efforts.

The number density field \( n/n_0 \) is given in Fig. 3 for the three values of the rarefaction parameter \( \delta = 0.1; 1.0 \) and \( 10 \). Here, \( n_0 = P_0/kT_0 \) One can see that near the free molecular regime \((\delta = 0.1)\) the density field is practically symmetric, i.e.

\[
n(x, r) = n_0 - n(-x, r).
\]

It is easy to prove that in the free molecular regime \((\delta = 0)\) the density field satisfies the relation (6) exactly. By increasing the rarefaction parameter \( \delta \) the contour lines dislocate to the downflow container and at \( \delta = 10 \) the density is almost uniform in the upflow container.

The temperature field \( T/T_0 \) is presented in Fig. 4. It can be seen that the temperature is practically constant in the upflow container and has a large gradient in the section of the orifice. The variation of the temperature field by increasing the rarefaction parameter is small. There is also a small dislocation of the contour lines into the downflow container.

The mass flux vector \( \mathbf{J} = nu \) is given in Fig. 5. Here, \( u \) is the bulk velocity. This field changes quantitatively by increasing the rarefaction parameter \( \delta \), i.e. the mass flux increases. But the qualitative variation is small.
FIGURE 3. Density field $n/n_0$: (a) - $\delta = 0.1$; (b) - $\delta = 1.0$; (c) - $\delta = 10$. 
FIGURE 4. Temperature field $T/T_0$: (a) - $\delta = 0.1$; (b) - $\delta = 1.0$; (c) - $\delta = 10$. 
FIGURE 5. Mass flux vector field: (a) - $\delta = 0.1$; (b) - $\delta = 1.0$; (c) - $\delta = 10$. 
V CONCLUSIONS

The mass flow rate of rarefied gas through a thin orifice has been calculated by the direct simulation Monte Carlo method in the range of the rarefaction parameter from 0.005 to 80 under the assumption of a large pressure ratio. It has been found that in this range the reduced flow rate varies from 1 to 1.5. Outside of this range the variation of the mass flow rate is very small, i.e. within 1%. The numerical data are in a good agreement with the experimental data available in open literature.

Other values of the pressure ratio $P_0/P_1$ will be considered in forthcoming papers.

REFERENCES

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