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Rarefied Gas Flow into Vacuum Through Thin Orifice: Influence of Boundary Conditions

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A rarefied gas flow through a thin orifice is studied, based on the direct simulation Monte Carlo method. Mass flow rates have been calculated over the whole range of the Knudsen number in the case of outflow into vacuum. The diffuse-specular interaction between gas and surface was assumed. It has been found that the dependence of the mass flow rate on the gas–surface interaction law is very weak. A comparison with experimental data available in the open literature has been performed.

Nomenclature

a = orifice radius
k = Boltzmann constant
$\dot{M}$ = mass flow rate
m = molecular mass
P = pressure
T = temperature
W = reduced mass flow rate
α = part of diffusely reflected particles
δ = rarefaction parameter
ζ = ratio of the specific heats
λ = mean free path
μ = shear viscosity

Introduction

THE problem of rarefied gas flow through an orifice has many practical applications. However, in spite of the great practical importance, there are very few papers about these flows.

The solution of the problem is determined by two main parameters: the Knudsen number $Kn = \lambda_0/a$ and the pressure ratio P_1/P_0. Here, P_0 is the upflow pressure, P_1 is the downflow pressure, $\lambda_0 = (\mu/P_0)\sqrt{(\pi kT/2m)}$ is the mean free path at the pressure P_0, μ is the shear viscosity of the gas, T is the gas temperature, and m is the mass of gaseous particles.

In the case of the small pressure difference, that is, when $P_1 \approx P_0$, the dependence of the mass flow rate through an orifice and slit on the gas–surface interaction law is very weak. This was proved experimentally[1,2] and theoretically.[3] However, no information is available about such an influence in the case of the large pressure difference, that is, when $P_1 \ll P_0$.

The aim of the present work is to carry out a direct numerical simulation of the rarefied gas flow through a thin orifice over the whole range of Knudsen numbers in the case of outflow into vacuum ($P_1/P_0 = 0$). To study the influence of the boundary condition on the mass flow rate, the diffuse-specular kernel of the gas–surface interaction is assumed. The numerical results will be given in terms of the reduced mass flow rate defined as

$$W = \dot{M}/\dot{M}_0 \tag{1}$$

where $\dot{M}$ is the mass flow rate at any Knudsen number, whereas $\dot{M}_0$ is the mass flow rate in the free molecular regime flow ($Kn = \infty$), which is calculated analytically.[4]

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Consider an orifice in an infinitely thin partition that separates two semi-infinite reservoirs. One of them contains a monatomic gas at a pressure P_0. The other container is maintained under a high vacuum so that it can be considered that $P_1 = 0$. We are going to calculate the reduced mass flow rate W as a function of the rarefaction parameter δ, which is inversely proportional to the Knudsen number:

$$\delta = \sqrt{\pi}\big/2Kn = \sqrt{\pi}a\big/2\lambda_0$$

Short Review

In spite of its great practical importance, this problem has not been investigated in detail. As noted in the Ref. 4 review, a number of papers[5–8] offered asymptotic formulas for the quantity W near the free-molecular regime ($\delta \ll 1$) in the case of outflow into vacuum ($P_1/P_0 = 0$). However, there is no agreement between them, and the range of their validity is very small. Some numerical data for the transition regime ($\delta \approx 1$) at $P_1/P_0 = 0$ can be found in the work by Shakhov.[9] However, the presentation of the data is very poor. For the small pressure difference, that is, when $|P_0 - P_1| \ll P_0$, the problem can be solved analytically in the hydrodynamic regime ($\delta \to \infty$). Corresponding results were obtained by Roscoe[10] and Hasimoto.[11] Thus, theoretical results on the orifice flow are restricted by the small ranges of the rarefaction parameter δ and of the pressure ratio P_1/P_0.

Borisov et al.[1] and Porodnov et al.[2] provide experimental results for the small pressure difference ($|P_0 - P_1| \ll P_0$) in a wide range of rarefaction δ. These data show that the reduced mass flow rate W does not depend on the type of the gas in the whole range of the rarefaction parameter δ.

Some experimental results on the mass flow rate through an orifice in the case of outflow into vacuum ($P_1/P_0 = 0$) are presented by Liepmann.[5] However, in the transition regime of the flow ($\delta \sim 1$), the dispersion of experimental points is rather large, which makes the data unreliable. At the same time, his theoretical result in the hydrodynamic regime ($\delta \to \infty$) is very interesting. When the orifice as a nozzle was considered, to which one can apply the Euler equation, Liepmann obtained the following expression for the mass flow rate:

$$W = A(\zeta)\sqrt{2\pi\zeta}[2/(\zeta + 1)]^{(\zeta+1)/2(\zeta-1)} \tag{2}$$

where A is a coefficient to be obtained from an experiment. For instance, for argon gas ($\zeta = \frac{5}{3}$), the constant A is equal to 0.812, which corresponds to the flow rate $W = 1.476$. The expression given by Eq. (2) shows that in the case of outflow to vacuum ($P_1/P_0 = 0$) the hydrodynamic mass flow rate significantly depends on the molecular structure of the gas, whereas for a small pressure difference, the mass flow rate W does not depend on the gaseous species.[1,2]

Fujimoto and Usami[12] reported experimental results on the mass flow rate through short tubes. The length-to-radius ratio of the shortest tube was $l/a = 0.025$, which can be considered as an orifice. They offered an empirical formula of the mass flow rate based on the experimental data for the interval $0.025 \le l/a \le 12.7$ and for the small pressure ratio $P_1/P_0 < 0.01$, which can be considered as an outflow into vacuum. If one extrapolates their empirical equation for the orifice ($l/a = 0$), one obtains

$$W = 1 + \left(0.4733 + 0.6005/\sqrt{\delta}\right)(1 + 4.559/\delta + 3.094/\delta^2)^{-1} \quad (3)$$

Barashkin et al.[13,14] also reported some experimental data on the outflow into vacuum through an orifice. In the transition regime of flow, their results are in a good agreement with those given by Fujimoto and Usami.[12] In the hydrodynamic regime, ($\delta \to \infty$) Barashkin et al. reported $W = 1.501$, which is slightly larger than the value given by Liepmann.[5] Experimental data for some intermediate values of the pressure ratio P_1/P_0, but for a restricted range of the rarefaction δ, are given by Sreekanth.[15] Thus, the experimental material on the orifice flow is also poor.

Method of Solution

In the present work, the problem was solved by the direct simulation Monte Carlo method.[16] The hard sphere molecular model was assumed. For the gas–surface interaction, the Maxwellian boundary condition was used, that is, an α part of the incident particle is reflected diffusely and remainder $(1 - \alpha)$ is reflected specularly. The region for the flow simulation had the form of two cylinders with radii R_0 and R_1 and 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 cell size equal to $\Delta x = \Delta r = a/16$ in the small region near the orifice and twice as large in the remainder of the region. The time increment was 0.01 of the mean free time. The number of simulated molecules fluctuated during the calculation, but it was maintained at about 10^6. To simulate the collision, the so-called non-time count method (Ref. 16, p. 219) was used.

In every time step, the number of particles passed through the orifice from the upflow container to the downflow one, and the number of particles that passed the orifice in the opposite direction were counted. The mass flow rate was calculated from the number of particles that passed through the orifice in both directions during 10^5 time steps that corresponds to the time interval equal to 10^3 mean free times.

To estimate the numerical error, test calculations were carried out for four values of the rarefaction parameter δ: 0.1, 1, 10, and 100. In these calculations, the number of model particles was increased up to 5×10^6, the cell size was decreased twice, the size of the calculation region was increased as $L_0 = R_0 = 12a$ and $L_1 = R_1 = 6a$, and the time increment was decreased to 0.002. An analysis of the test calculations showed that the variation of the mass flow rate due to these parameter modifications does not exceed 0.5%. This can be considered as numerical error for the data presented here.

Results and Discussion

The calculations were carried out for the rarefaction parameter range $0.05 \le \delta \le 100$. To study the influence of the gas–surface interaction on the mass flow rate, three values of the parameter α were regarded: 1) $\alpha = 1$, which corresponds to completely diffuse scattering, 2) $\alpha = 0.5$, which corresponds to the half diffuse and half specular reflection, and 3) $\alpha = 0$, which describes the totally specular reflection.

The reduced mass flow rate W is presented in Fig. 1 as a function of the rarefaction parameter δ. One can see that for the values of δ smaller than 0.05 the mass flow rate W does not differ from unity within 1% at any value of the parameter α. In the range $30 \le \delta \le 100$, the mass flow rate W is practically constant. Its variation does not exceed 0.5%. At the same time, in this interval of δ the largest influence of the gas–surface interaction on the mass flow rate W is observed. The value of W corresponding to the completely diffuse reflection ($\alpha = 1$) is larger by only 3% than that for the totally specular reflection ($\alpha = 0$). The difference between W for $\alpha = 1$ and for $\alpha = 0.5$ is less than 1%. In reality, it is impossible to reach the totally specular reflection. To the author's knowledge, the smallest value of the parameter $\alpha = 0.65$ was reported in Refs. 17 and 18 for an atomically pure surface and for light noble gases. However,

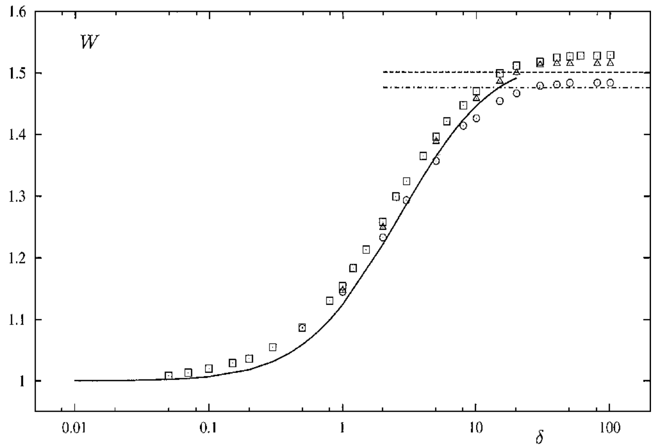

Fig. 1 Mass flow rate W vs rarefaction parameter δ: □, α = 1; △, α = 0.5; ○, α = 0; ——, empirical formulas[12]; - - -, experimental data[5]; and -·-, experimental data.[13]

in practice, one deals with diatomic gases interacting with contaminated surfaces. In such situations, the accommodation coefficient α is close to unity. Therefore, the real influence of the gas–surface interaction on the mass flow rate does not exceed 1%.

The experimental result by Liepmann[5] in the hydrodynamic regime ($\delta \to \infty$) is given in Fig. 1 by the dashed–dotted line. The corresponding result by Barashkin et al.[13] is presented by the dashed line. The small disagreement between experimental and theoretical results could be because in both experiments the partition was not as thin as is assumed in the present theoretical calculation. Moreover, the downflow pressure, which always exists in any experiment, also slightly decreases the mass flow rate.

As Fig. 1 shows, a significant variation of the mass flow rate occurs in the range $0.1 \le \delta \le 20$. In this range, the theoretical results are compared with the empirical formula (3) by Fujimoto and Usami,[12] which is presented by the solid line. Note that the empirical formula and the numerical simulation results are in a good agreement. The systematic understatement of the empirical formulas is explained by the same arguments that were used earlier: The thickness of the partition is not zero, and the pressure in the downflow container is not zero.

The distributions of the number density, temperature, and streamlines for the diffuse reflection ($\alpha = 1$) were presented in a previous paper.[19] An analysis of the data for the other values of the accommodation coefficient ($\alpha = 0$ and 0.5) showed that the flowfield is not affected by the gas–surface interaction law. Therefore, the flowfield is not given here.

Conclusions

The outflow of rarefied gas through a thin orifice into vacuum has been calculated by the direct simulation Monte Carlo method in the range of rarefaction parameter δ from 0.05 to 100 for the diffuse-specular scattering of gaseous particles on the surface. It has been found that in this range of δ the reduced flow rate W varies from 1 to 1.5. Outside of this range, the variation of the mass flow rate is very small, that is, within 1%. The numerical data are in good agreement with the experimental data available in the open literature.

The largest influence of the boundary conditions on the mass flow rate is observed in the hydrodynamic regime. Analyzing the experimental values of the accommodation coefficient α, we concluded that this influence does not exceed 1% in practice. As was noted in Ref. 3, this feature of the orifice flow allows us to test accurately kinetic equations, intermolecular potential models, numerical methods etc., comparing theoretical results based on the diffuse scattering with experimental data for any kind of gases and surfaces, even if the real scattering is not diffuse.

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