Numerical Simulation of the Rarefied Gas Flow through a Short Channel into a Vacuum

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Abstract. The rarefied gas flow through a short channel into a vacuum is studied by the direct simulation Monte Carlo method. The mass flow rate through the channel is calculated over the wide range of gas rarefaction. This study demonstrates that the effects of the gas molecule–molecule interaction and the gas–surface scattering can make a noticeable impact on the mass flow rate. The analysis of the flow field both within the channel as well as in upstream and downstream containers is presented.

Keywords: rarefied gas flow, mass flow rate, gas-surface scattering, molecule-molecule interaction.
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INTRODUCTION

A rarefied gas flow through a short channel into a vacuum presents a complex task due to significant non-equilibrium. Therefore, it is possible to find a good number of empirical formulas in open literature for calculating flow rate in this case. Correct approach to solving this problem should be based on the Boltzmann equation [1]. The difficulties of numerical solutions for this equation, caused by a large number of independent variables and a complex structure of a non-linear collision integral, are well-known. In our opinion, direct simulation Monte Carlo (DSMC) method [2], which is customarily viewed as a stochastic solution for Boltzmann equation, is preferable for use in tasks with strong non-equilibrium. DSMC method is an effective tool to solve problems of rarefied gas dynamics from free molecular to viscous regimes. An approach based on using DSMC method allows to take into account several factors, such as strong non-equilibrium and complex geometrical configuration of the model system, as well as to use various models of the gas-surface scattering, gas molecule-molecule interactions and surface structure. Therefore, it is appropriate to use DSMC method to study the rarefied gas flow through a short channel into a vacuum.

Practical application of the results of such research can be in the development and creation of such devices as micro- and nanoseparators, micropumps, microshutters, microgyroscopes, micro- and nanosatellites, and other micro- and nanoelectromechanical systems (MEMS/NEMS) [3]. The flow of gas in MEMS/NEMS, depending on device size and gas pressure, can be viscous, transitional or free molecular. Incidentally, the free molecular flow in nanodevices can be observed even at normal atmospheric pressure.

In this study, a rarefied gas flow through a short channel into a vacuum is studied by the direct simulation Monte Carlo method. The mass flow rate Q through the channel is calculated over the wide range of gas rarefaction as a function of the length-to-height ratio l/h. Gas rarefaction will be characterized with a parameter $\delta = (h \cdot P_1)/(\mu \cdot v_1)$, where P_1, μ and v_1 are the gas pressure, viscosity and the most probable molecular velocity, respectively, in the upstream container far from channel. Value δ is connected to the Knudsen number as $\delta = 0.5\sqrt{\pi}/Kn$, which (Kn) is defined as a ratio of the mean free path of gas molecules to the channel height.

We chose a two-dimensional statement of the problem, i.e., when the channel width significantly exceeds its height; the mass flow rate Q was calculated per unit width of the channel. Calculated data is expressed in the form of $Q^*=Q/Q_{\text{fm}}$, where Q_{fm} is a value of mass flow rate through a slit (channel with l=0) in the free molecular limit. As previously [4-6], we use two-level regular grid, weight-factor and sub-cell procedures. Simulation parameters used in present work – number of samples, cell size, number of model particles in the cell, time step length, time to reach stationary flow and computational domain size – all guarantee the computation error of no more than 0.5%.

MASS FLOW RATE AND FLOW FIELD

Fig.1 presents calculation results of the dimensionless mass flow rate Q^* as a function of gas rarefaction parameter δ for several values of the length-to-height ratio l/h=0; 0,5; 1; 5 and 10. Results for l/h=0 (slit) are taken from our previous paper [5]. In the figure, the arrows indicate values Q^* in a free molecular limit, resulting from using the formula [7] for calculating transmission probability of a two-dimensional channel. Indeed, in the case of presenting calculated data in the form of $Q^*=Q/Q_{\mathrm{fm}}$ value Q^* in free molecular limit coincides with transmission probability of a channel. Transmission probability of a channel can also be obtained using test particle Monte Carlo method (TPMC). In [8], we have shown excellent agreement between TPMC results and the formula [7].

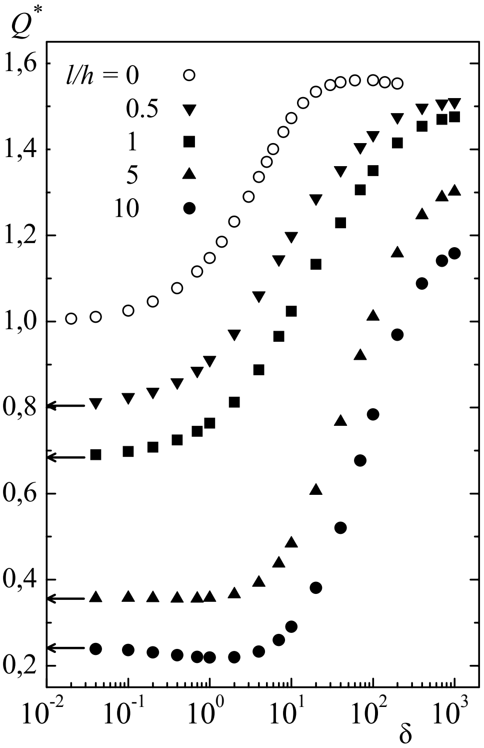

FIGURE 1. The dimensionless mass flow rate Q^* as a function of gas rarefaction parameter δ for various length-to-height ratio l/h.

From Fig.1, it also follows that, in a case of rather long channel with l/h=10 in a transitional regime, a Knudsen minimum is clearly observed. For shorter channels, this minimum is either absent, as it is for l/h=0.5 and 1, or is expressed very weakly, as it is for l/h=5.

Fig. 2 presents the dimensionless macroscopic distributions of density n/n_1 (top), where $n_1 = P_1/kT_1$ and k is Boltzmann constant, temperature T/T_1 (middle) and lateral mass velocity u_Y/v_1 (bottom) in YZ-plane near and within a channel with l/h=0.5 (left) and 5 (right) where rarefaction parameter δ=10 (top of each of the 9 elements in the figure) and 10^3 (bottom). Shaded area in the figure represents the channel wall. As it follows from the figure, macroscopic distributions depend on the rarefaction parameter δ as well as on the length-to-height ratio l/h. The differences in macroscopic distributions with different δ and same l/h is more significant for a longer channel (l/h=5) than for shorter one (l/h=0.5).

IMPACT OF THE GAS-SURFACE SCATTERING

We used models such as Maxwell [9], Cercignani–Lampis [10], and Epstein [11] to study the effect of gas-surface scattering on the rarefied gas flow through a short channel into a vacuum.

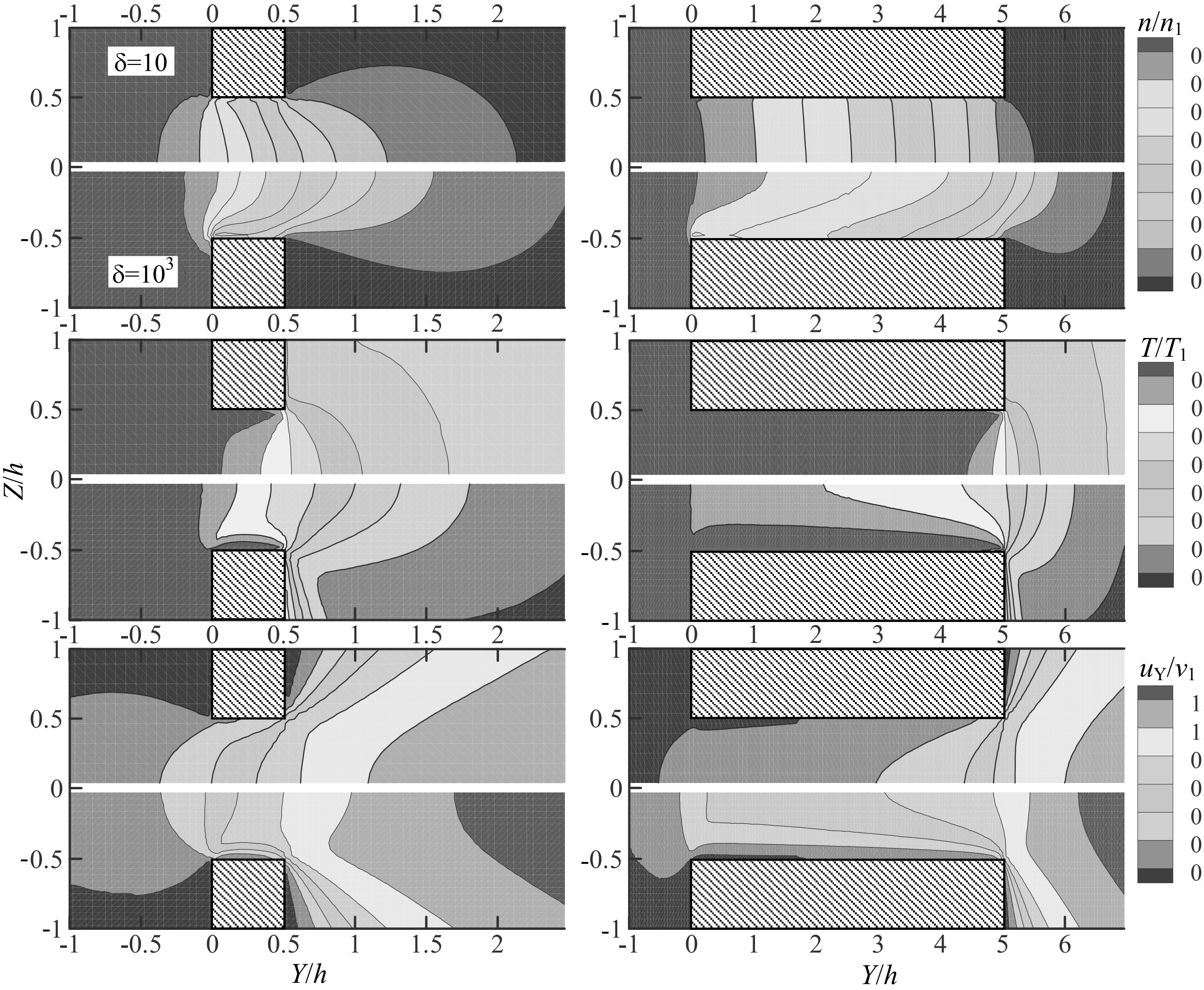

FIGURE 2. The dimensionless macroscopic distributions of density n/n_1 (top), temperature T/T_1 (middle) and lateral mass velocity u_Y/v_1 (bottom) in YZ-plane near and within a channel with l/h=0.5 (left) and 5 (right) where rarefaction parameter δ=10 (top of each of the 9 elements in the figure) and 10^3 (bottom). Shaded area is the channel wall.

Quite recently, we have used the Maxwell model for interpreting results of our experiment in studying a free molecular isothermal gas flow through a tube of finite length (l/r=34.4, l – tube length, r=3.6 mm – its radius) into a vacuum, depending on the chemical composition of tube's surface [12;13]. With this purpose, we calculated of gas flow through a tube using the test particle Monte Carlo method and compared with the experiment results. In particular, by simulating the flow of helium through a tube with atomically clean surface of silver or titanium, we obtained the lowest diffusion coefficient value (ε=0.71) represented in open literature for the rarefied gas flow through a capillary of finite length into a vacuum. Simulation showed that on so-called contaminated (or non-prepped) surfaces; i.e., surfaces that have not undergone special preparation procedures, gas-surface scattering is close to being diffuse. Thus, it is possible to suppose that for rarefied gas flow in capillaries at large pressure difference, such as when gas expands into a vacuum, the range of change parameter ε is between 1 (diffuse scattering) and 0.71 (specular-diffuse). Therefore, to evaluate the impact of gas-surface scattering on rarefied gas flow through a capillary into a vacuum, these two extreme cases need to be studied.

In this paper, we also used the Cercignani–Lampis (CL) and the Epstein models for interpreting the results of our experiment [12;13]. In case of applying CL-model, the mass flow rate practically does not depend on α_n; therefore, its value can be assumed to equal 1. In order to describe the flow of helium through a tube with atomically clean surface made of silver or titanium, it is necessary to specify CL-model parameters as α_n=1 and α_τ=0.63 (α_n is the accommodation coefficient of the kinetic energy corresponding to the normal molecular velocity, and α_τ is tangential momentum accommodation coefficient). If the Epstein model is used for interpreting the same experiment, then the best agreement between the experiment results and simulation are observed at model parameters θ_1/T_S=1, θ_2/T_S=2.28, and C=0.90 (T_S is surface temperature). Thus, as with parameter ε, let us assume that the Cercignani–Lampis and the Epstein model parameters obtained during the interpretation of our experiment are extreme values.

In Table 1, calculation results of dimensionless mass flow rate Q^* through a two-dimensional channel into a vacuum are presented for different values of rarefaction parameter δ and the length-to-height ratios l/h = 0, 1 and 10 in the case of diffuse scattering, as well as scattering according to the Maxwell, Cercignani–Lampis and Epstein kernels, at extreme parameters. Hard sphere model was used as a model for gas molecule-molecule interaction for all computations presented in this section.

TABLE 1. Dimensionless mass flow rate Q^* through a channel into a vacuum for different values of rarefaction parameter δ and the length-to-height ratios l/h in the case of diffuse scattering, as well as scattering according to the Maxwell, Cercignani–Lampis (CL) and Epstein kernels at extreme parameters.

l*/*h	**δ**	**Mass flow rate, *Q****			
		Diffuse	**Maxwell**	**CL**	**Epstein**
0	0.1	1.025	1.024	1.025	1.024
	1	1.147	1.143	1.148	1.143
	10	1.473	1.469	1.473	1.469
	100	1.561	1.557	1.558	1.557
1	0	0.684	0.757	0.768	0.758
	0.1	0,697	0.773	0.784	0.772
	1	0,764	0.841	0.864	0.842
	10	1.024	1.097	1.124	1.096
	100	1.351	1.372	1.379	1.370
10	0	0.241	0.322	0.326	0.322
	0.1	0,237	0.316	0.323	0.317
	1	0,219	0.296	0.319	0.297
	10	0.290	0.367	0.397	0.364
	100	0.784	0.817	0.829	0.814

As seen in the Table 1, if the impact of gas-surface scattering is practically non-existent for a slit (l/h=0), then such impact is observed for the channels. Indeed, for l/h=1, as well as for l/h=10, the results obtained using the Maxwell, Cercignani–Lampis and Epstein models significantly exceed corresponding results in the case of diffuse scattering. Notably, mass flow rate values obtained using the Maxwell and the Epstein models have coincided within the margin of error. In the case of the CL-model, the results were slightly higher for all values δ. As follows from Table, and as was expected, with the increase of gas rarefaction parameter δ, i.e., for the more dense gas, the impact on the gas-surface scattering decreases.

In Figure 3 (a;b), the dimensionless mass flow rate Q^* for channels with l/h =1 (a) and 10 (b) is presented as a function of rarefaction parameter δ as follows: for the diffuse scattering, the Cercignani–Lampis and Epstein scattering kernels at extreme parameters. As seen in the Figure 3 (b), for channel with l/h=10, the Knudsen minimum is observed in the case of diffuse scattering, as well as in scattering according to the Epstein and the Cercignani–Lampis kernels. In the case of simulation using the Cercignani–Lampis model, the Knudsen minimum is less deep than when using both the diffuse scattering and the Epstein models, and is shifted to the more rarefied gas. Indeed, if for the diffuse scattering and the Epstein scattering kernel the minimum is observed at δ=1.5, then in case of the Cercignani–Lampis kernel, it is at δ=0.7.

IMPACT OF THE GAS MOLECULE-MOLECULE INTERACTION

Based on previous results [6], in order to evaluate the impact of gas molecule-molecule interaction on the rarefied gas flow through a short channel into a vacuum, it is appropriate to use the variable soft sphere (VSS) model [14] for light and heavy gases. In this study, the VSS model is used for helium (He) and xenon (Xe), and the results were compared to the data for a more frequently used hard sphere (HS) model, which does not require specifying the kind of gas.

Table 2 presents calculation results for the dimensionless mass flow rate Q^* through a two-dimensional channel into a vacuum. These were obtained using HS and VSS models of the gas molecule-molecule interaction for different rarefaction parameters δ and the length-to-height ratio l/h=0, 1, and 10.

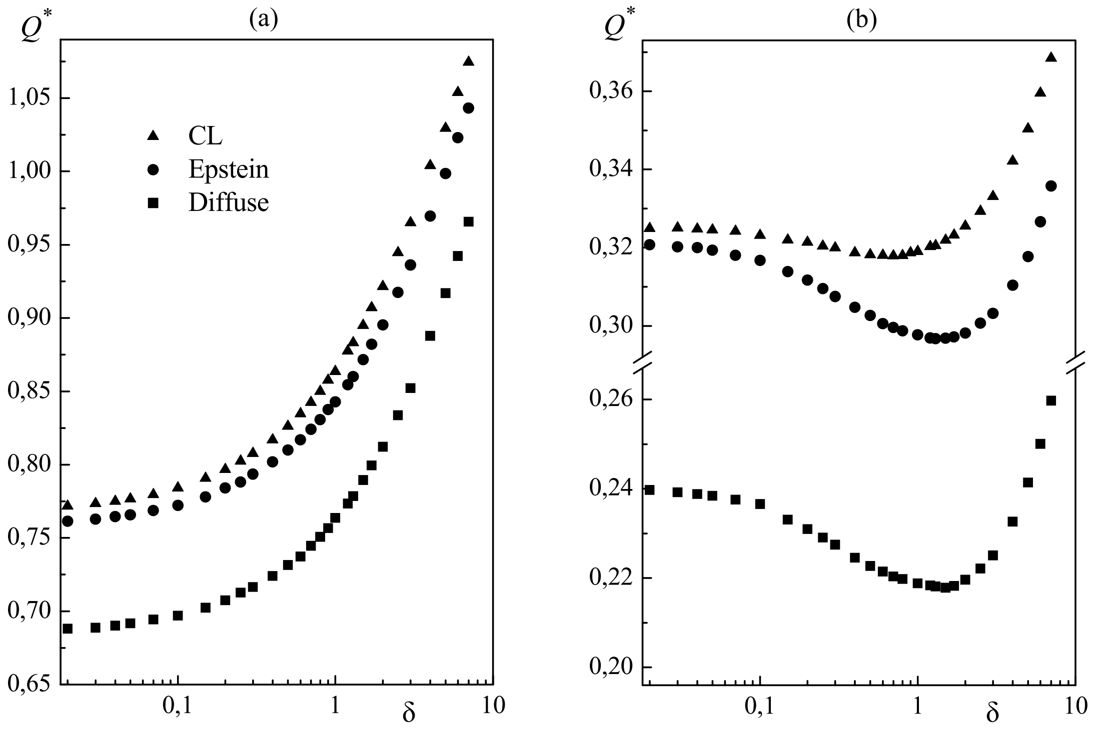

FIGURE 3 (a;b). Dimensionless mass flow rate Q^* for channels with l/h =1 (a) and 10 (b) as a function of rarefaction parameter δ in the case of diffuse scattering, as well as scattering according to the Cercignani–Lampis (CL) and Epstein kernels at extreme parameters.

As follows from the Table 2, as was expected, maximum values Q^* are observed when using the HS model, because this model of the gas molecule–molecule interaction is «too hard».

Table 2 shows that the dimensionless mass flow rate Q^* in the transitional flow regime is noticeably higher for helium then for xenon. For both gases, since gas-surface scattering was simulated as completely diffuse, the difference in the dimensionless mass flow rate can only be caused by the difference in the gas molecule-molecule interaction. Higher values of the dimensionless mass flow rate for light inert gases, such as He and Ne, in comparison with the mass flow rate of heavier inert gases Ar, Kr, and Xe in the transitional flow regime for channels with a non-prepped surface, were also obtained experimentally [15].

TABLE 2. Dimensionless mass flow rate Q^* through a channel into a vacuum obtained using the hard sphere (HS) model and the variable soft sphere (VSS) model for helium (He) and xenon (Xe) in the case of different rarefaction parameters δ and the length-to-height ratio l/h.

l/h	**δ**	**Mass flow rate, *Q****		
		HS	**VSS for He**	**VSS for Xe**
0	0.1	1.025	1.024	1.021
	1	1.147	1.139	1.125
	10	1.473	1.460	1.437
	100	1.561	1.559	1.558
1	0.1	0,697	0.696	0.695
	1	0,764	0.756	0.749
	10	1.024	1.008	0.984
	100	1.351	1.340	1.324
10	0.1	0,237	0.236	0.235
	1	0,219	0.218	0.217
	10	0.290	0.281	0.269
	100	0.784	0.759	0.715

As shown in Table 2, for the VSS model, it follows that for the slit l/h=0 and a short channel l/h=1, the maximum impact of gas molecule-molecule interaction is observed at δ=10. In this case, the dimensionless difference in the mass flow rate values, defined as $\Delta=(Q^*_{He}-Q^*_{Xe})/Q^*_{Xe}$, reaches about 0.02. However, for longer channel with l/h=10, the maximum value Δ equaling 0.06 is already observed at δ=100.

Thus, the impact of the gas molecule-molecule interaction on the dimensionless mass flow rate through a channel strongly depends on the length-to-height ratio. With the increase of the length-to-height ratio, the impact of gas molecule-molecule interaction increases and most of impact shifts to the more dense gas.

SUMMARY

The direct simulation Monte Carlo method has been applied to study the rarefied gas flow through a two-dimensional short channel into a vacuum. The calculation results of the dimensionless mass flow rate for a channel with various length-to-height ratios are presented in gas rarefaction range from a free molecular regime to a viscous one. The range of gas rarefaction, where significant changes of flow rate, as well as value of change in the flow rate, considerably depends on the length-to-height ratio. The longer the channel, the more significant are changes in the flow rate and the specified range of gas rarefaction moves to a more dense gas. In a transitional regime for rather long channels, a Knudsen minimum was discovered.

An analysis of dimensionless macroscopic distributions, both within the channel as well as in upstream and downstream containers, is presented. Significant changes in dimensionless macroscopic distributions are observed when gas rarefaction is in the range of considerable change in the value of flow rate. Differences in macroscopic distributions with dissimilar gas rarefaction and similar length-to-height ratio are more significant for a longer channel than for a shorter one.

The impact of the gas-surface scattering and the gas molecule-molecule interaction on the mass flow rate of the rarefied gas through a short channel into a vacuum has been investigated. Cercignani–Lampis and Epstein scattering kernels at extreme parameters were used to study the impact of gas-surface scattering. The variable soft sphere model for light and heavy gases was used to study the impact of the gas molecule-molecule interaction. It has been demonstrated that the dependency of the results on the gas–surface scattering and the gas molecule–molecule interaction could be significant. The impact of the gas-surface scattering and the gas molecule-molecule interaction strongly depends on the gas rarefaction and the value of the length-to-height ratio. With the increase of the length-to-height ratio, the impact of these effects on the mass flow rate through a channel increases.

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