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RAREFIED GAS FLOW THROUGH A CHANNEL OF FINITE LENGTH INTO A VACUUM

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A rarefied gas flow through a finite-length 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 rarefactions. The analysis of the flow field, both within the channel and in upstream and downstream containers, is presented.

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1. INTRODUCTION

In recent years, the direction in rarefied gas dynamics related to the analysis of micro- and nanofluidic systems is being developed [1]. In contrast to the traditional approach, where gas movement is studied on a macroscopic size, the abovementioned direction is a field of rarefied gas dynamics where gas movement is studied on a micro- and nanoscale. Practical application of the results of this research can be in the development and creation of devices such as micro- and nanoseparators, micropumps, microshutters, microgyroscopes, micro- and nanosatellites, and other micro- and nanoelectromechanical systems (MEMS/NEMS). The flow of gas in MEMS/NEMS, depending on the 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 studying the internal flow of rarefied gas, special attention is paid to the capillaries of various geometric shapes and sizes. A rather large number of theoretical works is dedicated to the rarefied gas flow, caused by a small pressure difference, through straight capillaries of infinite length [2, 3]. In this case, the gas concentration and temperature change linearly along the capillary axis, and hence linearized models of the integral differential Boltzmann equation is successfully used for flow calculation. In particular, in one of the pioneering works [4], the mass flow rate of gas through a straight infinitely long channel (capillary with a rectangular cross section) was calculated in a wide range of gas rarefaction. An important outcome of this study is the discovery of the so-called Knudsen minimum (or Knudsen paradox) — a minimum of the flow rate through a channel in the transitional regime. Subsequently, a minimum of the gas flow rate through a channel was also confirmed experimentally [5].

Rarefied gas flow through finite-length capillaries presents a much more complex task. In the case of a small pressure difference, the gas flow through a channel is calculated in [6] using the BGK model of the Boltzmann equation. From this work, in particular, it follows that the position of the Knudsen minimum depends on the length of the channel.

In the case of a finite-length capillary and a large pressure difference, as in the case of gas flow into a vacuum, the problem becomes even more complex due to essential nonequilibrium. Many empirical formulas for calculating the flow rate in this case can be found in open literature. Most of such formulas are derived by combining flow rates in free molecular and hydrodynamic limits, first introduced by Knudsen [7]. For example, in [8], the Knudsen method was developed for a finite-length channel and large pressure difference. In [9], several then-known empirical formulas were verified and limitations for their practical application were stated. A method of calculating gas flow through capillaries that in author's view overcomes the limitations related to the capillary cross section and length, the value of pressure difference, and the flow regime is pro-

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posed in [10]. However, in our opinion, empirical formulas for the gas flow through a finite-length channel into a vacuum do not presently give reliable results because a formula for the gas flow rate through a channel in the hydrodynamic limit with large pressure difference is still not obtained [11].

On the other hand, the correct approach to solving problems of rarefied gas dynamics should be based on the Boltzmann equation [12]. The difficulties in solving this equation numerically, caused by a large number of independent variables and a complex structure of a nonlinear collision integral, are well known. In our opinion, direct simulation Monte Carlo (DSMC) method [13], which is customarily viewed as a stochastic solution of the Boltzmann equation, is preferable for use in strongly nonequilibrium tasks. The DSMC method is an effective tool in solving problems of rarefied gas dynamics from the free molecular to viscous regimes. An approach based on the DSMC method allows taking several factors into account, such as strong nonequilibrium and complex geometric configuration of the model system, as well as using various models of the gas–surface scattering, gas molecule–molecule interactions, and surface structure. Therefore, it is appropriate to use the DSMC method to study the rarefied gas flow through a finite-length channel into a vacuum.

To our knowledge, a comprehensive theoretical research into the process of gas flow through a finite-length channel at large pressure difference is not available in open literature. In particular, there is no data on gas flow through a finite-length channel into a vacuum in a wide range of rarefaction. For the pressure difference that is not large, analytic and numerical studies of gas flow through a channel can be found, e.g., in [14–20].

Experimental studies of this process touch upon only the cases of a finite ratio of pressures at the ends of the channel. For example, experimental data on the gas outflow through a short channel in the transitional regime with the maximum pressure ratio 15 are given in [21]. In [22], the distribution of macroscopic parameters in a long channel with the maximum pressure ratio 20 is studied experimentally. There are many works devoted to experimental study of the gas flow caused by a small pressure difference, through very long channels (see, e.g., [23–27]).

Recently, with the use of the DSMC method, we studied a rarefied gas flow through a short tube (capillary with a round cross section) into a vacuum in detail [28]. Rectangular geometry of the capillary is also important from the practical standpoint [29]. The aim of the present work is to compute the gas flow through a capillary with a rectangular cross section (or channel) into a vacuum using the DSMC method. We calculate the mass flow rate and the flow field as functions of the gas rarefaction for various channel lengths.

2. STATEMENT OF THE PROBLEM AND THE METHOD OF SOLUTION

We consider a stationary flow of a monatomic gas in the system of two infinitely large containers connected with a channel of length l. In the upstream container, far from the channel, the gas is in equilibrium at a pressure P_1 and temperature T_1. In the downstream container, the pressure P_2 is so small compared with P_1 that it is possible to suppose that $P_2 = 0$. The surface temperature in the entire simulated system is T_1. We suppose that the channel width w is significantly larger than its height h; this allows us to work with a two-dimensional geometry problem.

Figure 1 presents the geometry of the problem and the system of coordinates. As follows from the figure, only half of the problem geometry is studied, because a symmetry in the flow field with respect to the central channel line is assumed. For this, the channel central line, which coincides with the y axis, is fitted with a specular reflector. To simulate the gas molecule–molecule interaction, the model of hard spheres is used; the model of complete diffuse scattering is used to simulate gas–surface scattering.

The gas mass flow rate Q is the main calculated value during the simulation of gas flow in the studied system. The results are presented in terms of the dimensionless flow rate defined as

$$Q^* = Q/Q_0, \tag{1}$$

where Q_0 is the value of the mass flow rate through a two-dimensional slit ($l = 0$) in the free molecular limit. Gas rarefaction is characterized by the parameter $\delta = hP_1/\mu v_1$, where P_1, μ, and v_1 are the gas

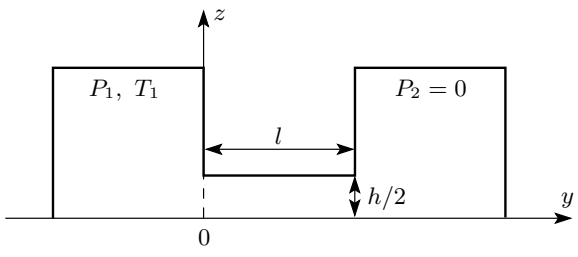

Fig. 1. Simulation geometry and coordinates

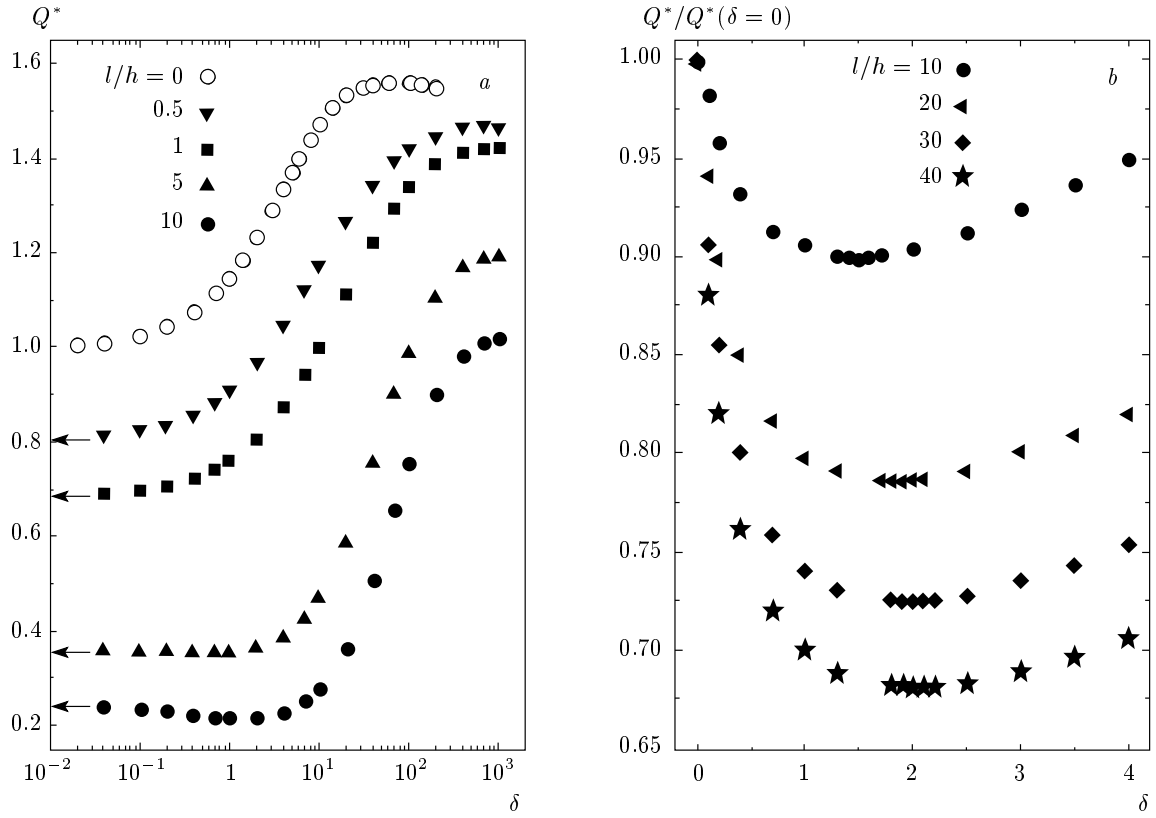

Fig. 2. The dimensionless mass flow rate Q^* (a) and the relative dimensionless mass flow rate $Q^*/Q^*(\delta = 0)$ (b) as functions of the gas rarefaction parameter δ for various reduced channel lengths l/h

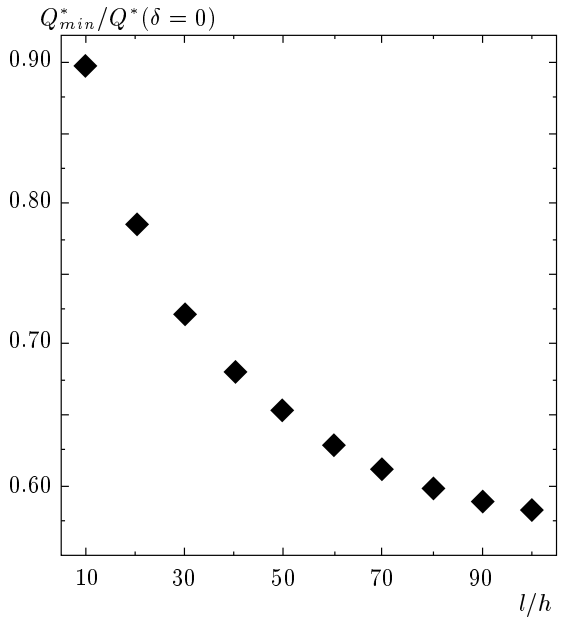

Fig. 3. Relative Knudsen minimum $Q^*_{min}/Q^*(\delta = 0)$ as a function of the reduced channel length l/h

pressure, the viscosity, and the most probable molecular velocity in the upstream container far from the channel. The rarefaction parameter is inversely proportional to the Knudsen number $\mathrm{Kn} = \sqrt{\pi}/2\delta$, which is defined for the channel as $\mathrm{Kn} = \lambda/h$, where λ is the mean free path of gas molecules. In the free molecular limit, when $\delta = 0$, the mass flow rate through a two-dimensional slit can be calculated as $Q_0 = hP_1/\sqrt{\pi}\,v_1$. From the physical standpoint, Q and Q_0 correspond to the values of the mass flow rate through a channel and a slit with $w \gg h$ per unit width.

Very recently, we used the DSMC method based on the majorant frequency technique [30] to compute the mass flow rate and flow field through a two-dimensional slit into a vacuum [31, 32]. In the present work, we further develop the code used previously for simulating rarefied gas flow through a two-dimensional channel. As previously, we use the two-level regular grid, weight-factor, and subcell procedures. Simulation parameters used in this work — the number of samples, the cell size, the number of model particles in the cell, the time step length, time to reach the stationary flow,

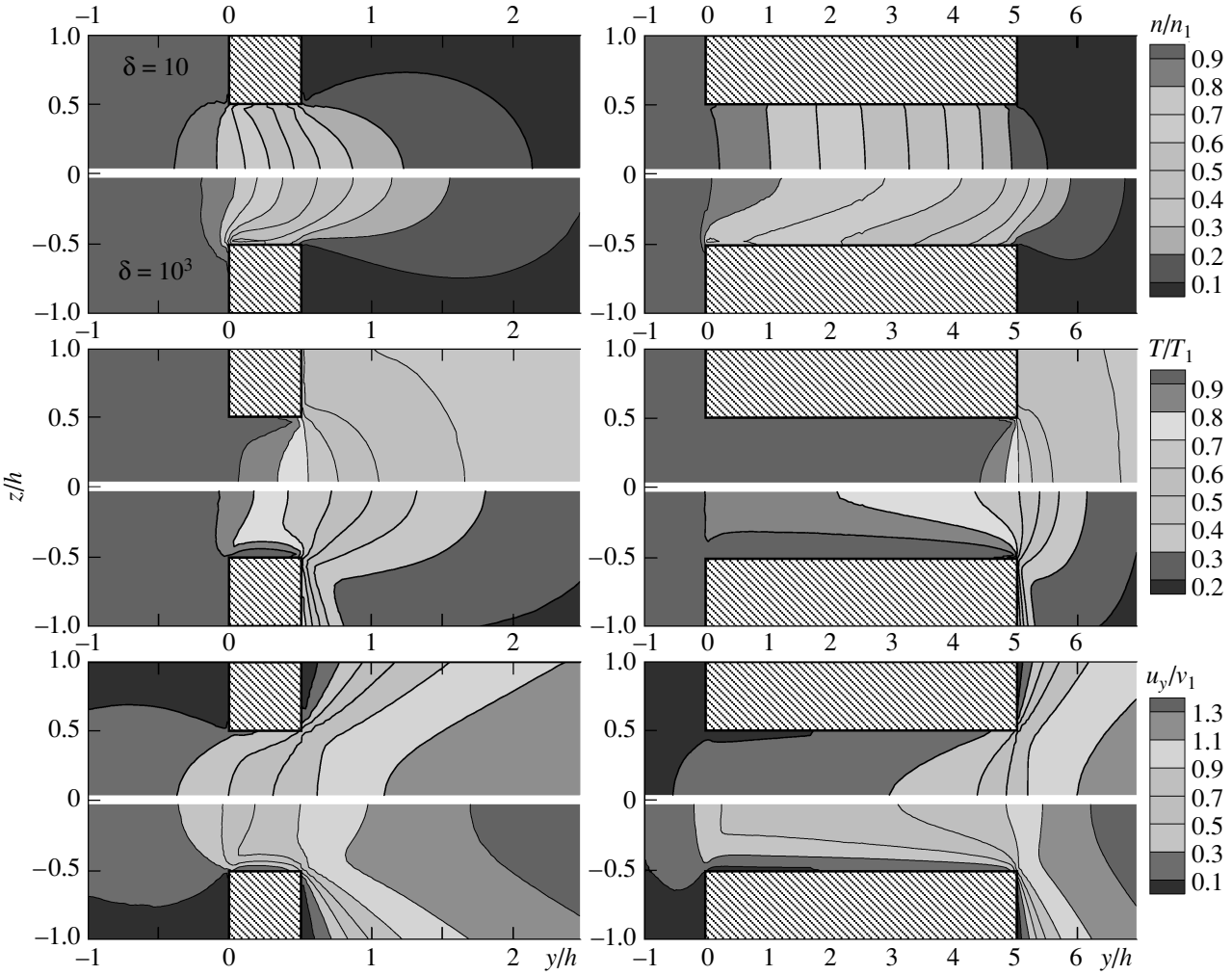

Fig. 4. The dimensionless macroscopic distributions of the density n/n_1 (top), the temperature T/T_1 (middle), and the lateral mass velocity u_y/v_1 (bottom) in the yz plane near and within a channel with $l/h = 0.5$ (left) and 5 (right), where the rarefaction parameter is $\delta = 10$ (top of each of the 9 elements) and 10^3 (bottom). The shaded area is the channel wall

and the computational domain size — all guarantee the computation error of no more than 0.2 %. The choice of simulation parameters that ensure this computation error in calculating the flow rate is discussed in detail in [31].

3. MASS FLOW RATE

Figure 2*a* presents calculation results of the dimensionless mass flow rate Q^* as a function of the gas rarefaction parameter δ for several values of the reduced length channel $l/h = 0$, 0.5, 1, 5, and 10. The results for $l/h = 0$ (slit) are taken from our previous paper [31]. In the figure, the arrows indicate the values of Q^* in the free molecular limit, resulting from using the formula in [33] for calculating the transmission probability of a two-dimensional channel. Indeed, in presenting the calculated data in form (1), the value of Q^* in the free molecular limit coincides with the transmission probability of the channel. The transmission probability of the channel can also be obtained using the test particle Monte Carlo (TPMC) method. In [34], we have shown excellent agreement between the TPMC results and the formula in [33].

As is evident from Fig. 2*a*, in the vicinity of the free molecular regime, the values of Q^* change only slightly and differ little from the corresponding results given by the formula in [33]. Then, as the rarefaction parame-

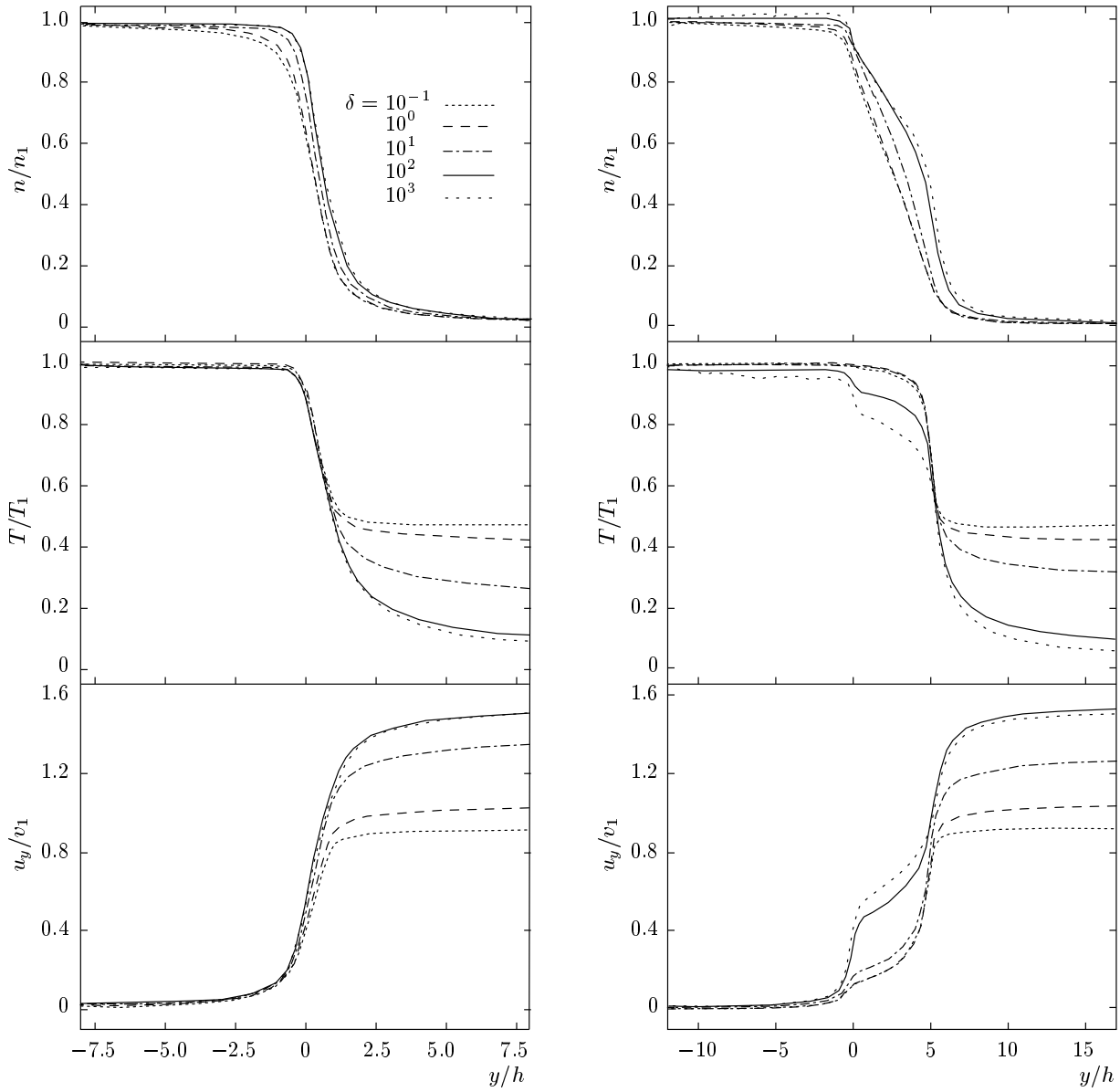

Fig. 5. The dimensionless macroscopic distributions of the density n/n_1 (top), the temperature T/T_1 (middle), and the lateral mass velocity u_y/v_1 (bottom) along the central line ($z = 0$) of a channel with $l/h = 0.5$ (left) and 5 (right) for various rarefaction parameters

ter δ increases, a significant increase in Q^* is observed. This increase is determined by value of l/h. For example, when $l/h = 0.5$, a significant increase in Q^*, by 76 % is observed in the range of δ from 0.2 to 200; when $l/h = 5$, the range is from 4 to 400 and the increase is 220 %. Finally, for larger values of δ, values Q^* vary little with the increase in δ, reaching their hydrodynamic limit as $\delta \to \infty$.

It also follows from Fig. 2*a* that in the case of a rather long channel with $l/h = 10$ in the 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 $l/h = 5$. For a more detailed study of the position and depth of the Knudsen minimum, we have completed calculations of the dimensionless mass flow rate Q^* in the transitional regime for channels with $l/h > 10$.

Figure 2*b* shows calculation results of the dimensionless mass flow rate represented as $Q^*/Q^*(\delta = 0)$ in the transitional regime for channels with $l/h = 10$, 20, 30, and 40. As can be seen from the figure, for

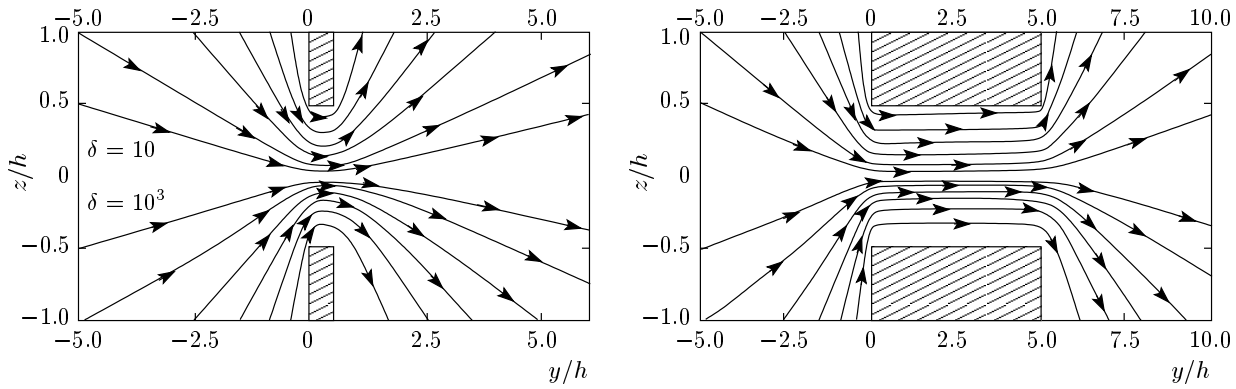

Fig. 6. The streamlines near a channel with $l/h = 0.5$ (left) and 5 (right) for $\delta = 10$ (top) and 10^3 (bottom)

the channel with $l/h = 10$, the Knudsen minimum is observed at $\delta = 1.5$, whereas for longer channels with $l/h = 20$, 30, and 40, it is seen at δ close to 2. The result that the Knudsen minimum position is related to a reduced channel length corresponds with [6]. It is interesting to note that the Knudsen minimum for an infinitely long channel at a small pressure difference is observed both theoretically [4] and experimentally [5] when the gas rarefaction δ is about 1. It also follows from Fig. 2*b* that the depth of the minimum depends on the value of l/h.

Figure 3 presents a relation between the relative Knudsen minimum $Q^*_{min}/Q^*(\delta = 0)$ and the reduced channel length l/h. As follows from Fig. 3, the longer the channel, the deeper the minimum, leading to a certain limit at large values of l/h. Indeed, the difference between Knudsen minima for $l/h = 10$ and 20 comprises 11.3 %, and for values between $l/h = 90$ and 100, it is 0.5 %.

4. FLOW FIELD

Figure 4 shows the dimensionless macroscopic distributions of the density n/n_1 (top), where $n_1 = P_1/kT_1$ and k is the Boltzmann constant, the temperature T/T_1 (middle), and the lateral mass velocity u_y/v_1 (bottom) in the yz plane near and within a channel with $l/h = 0.5$ (left) and 5 (right), where the rarefaction parameter is $\delta = 10$ (top of each of the 9 elements in the figure) and 10^3 (bottom). The shaded area in the figure represents the channel wall. As follows from the figure, macroscopic distributions depend on the rarefaction parameter δ as well as on the reduced channel length l/h. The differences in macroscopic distributions with different δ and the same l/h is more significant for a longer channel ($l/h = 5$) than for a shorter one ($l/h = 0.5$).

Figure 5 shows dimensionless macroscopic distributions of the density n/n_1, the temperature T/T_1, and the lateral mass velocity u_y/v_1 along the central line ($z = 0$) of a channel with $l/h = 0.5$, 5 for various rarefaction parameters. As expected, the qualitative behavior of the lateral velocity is inversely proportional to the density and temperature. When the gas rarefaction parameter δ is the same, the macroscopic distributions along the central line of the simulated system at $l/h = 0.5$ and $l/h = 5$ differ quantitatively. In the case of large δ, a significant qualitative difference in distributions within the channel is also observed. However, downstream, the distributions along the central line are practically the same in the case of large and small δ.

According to Fig. 5, the dimensionless macroscopic distributions for $\delta = 10^2$ and $\delta = 10^3$ differ only little for both $l/h = 0.5$ and $l/h = 5$. The distributions for $\delta = 10^{-1}$ and $\delta = 10^0$ differ only in the downstream container. Taking the rarefaction range of change of the dimensionless mass flow rate Q^* into account (Fig. 2*a*), it is possible to state that significant changes in the dimensionless macroscopic distributions are observed in the rarefaction range where the flow rate value changes considerably.

The streamlines near a channel with $l/h = 0.5$, 5 for $\delta = 10$, 10^3 are presented in Fig. 6. As follows from the figure, with an increase in the rarefaction parameter δ, the streamline symmetry relative to the axis $y = 0.5l/h$ is broken.

5. CONCLUSION

The direct simulation Monte Carlo method has been used to study the rarefied gas flow through a two-dimensional finite-length channel into a vacuum. The calculation results for the dimensionless mass flow rate for a channel of various reduced lengths are presented in the gas rarefaction range from the free molecular

regime to the viscous one. The range of gas rarefactions where significant changes of the flow rate, as well as the value of change in the flow rate, considerably depends on the reduced channel length. The longer the channel, the more significant changes in the flow rate are and the specified range of gas rarefactions moves to a more dense gas.

In the transitional regime for rather long channels, a Knudsen minimum was discovered. The position and the depth of the Knudsen minimum change with an increase in the reduced channel length, reaching its limit values.

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

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