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Numerical investigation of gas–surface scattering dynamics on the rarefied gas flow through a planar channel caused by a tangential temperature gradient

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ABSTRACT

A numerical analysis of the rarefied gas flow caused by a temperature gradient in the direction tangential to a wall through a planar channel of finite length is carried out based on the nonlinear Shakhov model of the Boltzmann kinetic equation. The Maxwell diffuse and Cercignani–Lampis gas–surface interaction models are provided as a boundary condition at solid walls. An implicit scheme for solution of the S-model kinetic equation was applied and the algorithm has been optimized for the use of massive parallellization in both physical and velocities spaces. The competition between rarefaction, gas–surface scattering model and temperature gradient effects on a gas flow is discussed in terms of both mass flow rate and streamwise heat flux. A comparison with available literature results has been carried out and showed a good agreement. It was found that the temperature gradient as well as the gas–surface scattering dynamics play a significant role for the highly rarefied gas flow, beginning from the transition flow regime. At the same time, under certain gas–surface scattering conditions a change of the value of temperature gradient does not affect the heat flux. For the weakly rarefied flow the temperature gradient effect on the mass flow rate is small for any gas–surface scattering condition, while the heat flux does not depend neither on value of temperature gradient nor choice and details of gas–surface scattering dynamics.

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1. Introduction

Flows induced solely by the effect of steady temperature field are peculiar to rarefied gases and are an intriguing research subject in the rarefied gas dynamics see, e.g., [1–3]. One of the most famous is the thermal-creep flow [4,5], where a temperature gradient tangential to a surface induces a flow in the same direction. Hotter particles impart larger tangential momentum to a wall than colder ones; a shear stress is exerted on a wall, and the gas flow creeps from cold to hot direction along the surface due to the reaction force. Thus, the stationary velocity of gas is the "thermal creep" velocity, parallel to the wall. This phenomenon was experimentally investigated by Reynolds [6] and Knudsen [7] and analyticity explained by Maxwell [8].

The numerical investigation of the thermal creep flow is generally based on the Boltzmann kinetic equation and its models considering a flow through planar channels of different length [9–11]. Even this simplified two-dimensional flow configuration

allows to model flow features encountered in actual devices [9,10]. Unfortunately, the direct numerical solution of kinetic equations is computationally expansive due to a high dimensionality of the problem even in a two-dimensional case, large gradients of the velocity distribution function near channel's entrance and exit and an exceedingly small Mach number, especially for the thermal creep flow. Therefore, most part of papers presented in the open literature deals with very long channels and low pressure and/or temperature gradients acting along a channel [9–11]. In this case a problem can be linearized and becomes one-dimensional, hence, less computationally expensive.

However, a linearization procedure should be use with care. For example, as indicated in [11] the linearized solution may not be valid for planar flows since, the planar one-dimensional linearized solution becomes singular when the Knudsen number approaches infinity. Furthermore, in [11] it was shown that a linearization of the kinetic equation may not be applicable to short and medium length channels: the linearized solution provided an accurate approximation of the mass flow rate in the pressure-driven regime, whereas for the temperature driven flow (thermal creep) a direct nonlinear calculation was required. A range of validity of the

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linearized method applied for an investigation of a gas flow through a slit at arbitrary pressure drop was studied in [12]. Moreover, in [9] it was found that an application of the linear theory based on the average rarefaction parameter to a gas flow at the large temperature ratio gave a significant error.

Therefore, for finite-length channels a complete nonlinear formulation of a problem including not only a channel, but surrounding reservoirs should be considered. In this case, arbitrary pressure and/or temperature ratios between inlet and outlet reservoirs are allowed. However, due to a computational complexity of the problem there are only few works available so far in the literature studying a gas flow through short/medium length channels for the complete nonlinear formulation, see, e.g., [11,13].

It is well known that a choice of the gas–surface interaction model has a profound effect on a gas flow [14–19]. The commonly used Maxwell diffuse-specular gas–surface interaction model based on the idea that the part of molecules impinging on a wall reflects from it having the Maxwell velocity distribution function according to the wall temperature and velocity, while the rest part of molecules is reflected specularly. This gas–surface interaction model is easy for a numerical implementation and less computationally expensive. Despite the fact that the Maxwell boundary condition provides reliable results in a variety of physical systems, some discrepancies are found between numerical and experimental data even in standard configurations, such as flows through ducts and tubes [14]. In particular, the mass flow rate in experiments was lower than it was predicted by numerical calculations. Moreover, Refs. [20,21] have reported that the number of diffuse reflected molecules may depend on the gas rarefaction level. Thus, trying to integrate in only one free parameter all types of gas–surface interaction mechanisms may not be always correct and physically justified [19].

As an alternative to the Maxwell gas–surface interaction model, the use of the more realistic Cercignani–Lampis (CL) model [22] has become widely popular in the rarefied gas dynamics community during last decades. The CL model successfully overcomes some drawbacks of the Maxwell model by adjusting two distinct accommodation coefficients, α_t and α_n, defining an accommodation of the tangential momentum and the normal kinetic energy (i.e., the kinetic energy associated with the normal component of molecular velocity), respectively. In particular, the CL model well reproduces actual data for the distribution of scattered molecules obtained in molecular beam scattering experiments [23]. Furthermore, diffuse and specular scattering kernels are easily retrieved by setting two coefficients equal to unity or zero, respectively. The case of backscattering, i.e. a reversal of the velocity vector of molecule after the collision with a wall, is simulated using $\alpha_t = 2$ and $\alpha_n = 0$.

Unfortunately, due to a complexity of experiments nowadays, there is a shortage of reliable experimental data. Therefore, only a few references provide measured data suitable for an estimation of actual values of accommodation coefficients. As an example, comparing numerical results for the CL model with data of molecular beam scattering experiments (conducted for smooth metal surfaces and noble gases) the tangential momentum accommodation coefficient α_t was reported in the range $0.6 \lesssim \alpha_t \lesssim 0.9$ and depending on surface materials, gases and temperature [23,24]. The value of tangential momentum accommodation coefficient α_t in the range from 0.82 to 1 was indicated in [15,16] for several gases (xenon, argon, helium and neon) interacted with a glass surface. A lower value $\alpha_t = 0.63$ was found in [18] for the flow of helium through a tube with an atomically clean surface of silver. In [17] it was demonstrated that heavy noble gases interact diffusely with a technical surface (i.e., $\alpha_t = 1$ and $\alpha_n = 1$). On the other hand, the interaction of noble light gases even with a contaminated surface deviates from the diffuse scattering: $\alpha_t = 0.9$ and $\alpha_n = 0.75$

for neon, while for helium $\alpha_t = 0.9$ and $\alpha_n = 0.1$. Moreover, as stated in [18] an interaction of noble light gases with an atomically clean surface can be significantly different from the diffuse scattering.

Additionally, considering a wide range of α_t from 0 up to 2 and α_n from 0 up to 1 authors of [1] demonstrated that the flow field has changed according to values of accommodation coefficients and suggested that α_t would be less than unity for ordinary smooth surfaces, while on a rough surface it should be possible to obtain $\alpha_t > 1$ (when a backscattering is dominant). A similar flow behaviour was observed in [25] for the highly rarefied gas flow under the same values of accommodation coefficients. In [26] the use of the CL model with $\alpha_t = 1.045$ allowed to simulate a conical rough surface model (with an opening angle β of 66°) close to an experiment. Moreover, it was shown that α_t is a function of cone opening angle β. On the other hand, in [19] setting $\alpha_t = 1.06$ for the smooth channel of rectangular cross section flow demonstrated a better agreement with experimental data in comparison with the Maxwell diffuse boundary condition in a wide range of rarefaction level.

Thus, there are not yet enough experimental data on accommodation coefficients to easily identify correct values of α_t and α_n for particular physical configurations. As a consequence, numerical analysis of flow with the CL boundary condition usually reports results for a wide range of theoretically possible values, see, e.g., Refs. [1,14–17]; this approach is followed in the present paper as well. Furthermore, to the author's knowledge, an investigation of gas–surface scattering dynamics in the presence of an arbitrary temperature ratio has not been extensively studied yet; thus, the present paper is meant to partially fill this gap.

In this work a temperature gradient driven flow through a planar channel of finite length is simulated based on the nonlinear S-model kinetic equation coupled with the Maxwell and CL boundary conditions in the Knudsen number range from free-molecular up to slip regime. A global mass flow rate and a streamwise heat flux are presented as a function of CL accommodation coefficients α_t and α_n, rarefaction parameter and temperature ratio. A comparison with available literature results with the Maxwell and CL boundary conditions is provided. The competing effect of rarefaction, gas–surface scattering dynamics and temperature gradient on a gas flow is discussed.

2. Statement of the problem

The monatomic temperature-driven gas flow through a planar microchannel of finite length l and height H connecting two large reservoirs is examined. Let Ox axis is directed along the channel, Oy is along its height, and Oz is along its infinite width (see Fig. 1). The flow is considered as two-dimensional in xOy surface. The center of the coordinate system is located in the middle of the channel $x = y = 0$. Hence, the bottom wall of the planar channel is placed at $-l/2 \leqslant x \leqslant l/2$ and $y = -H/2$. Due to the spatial
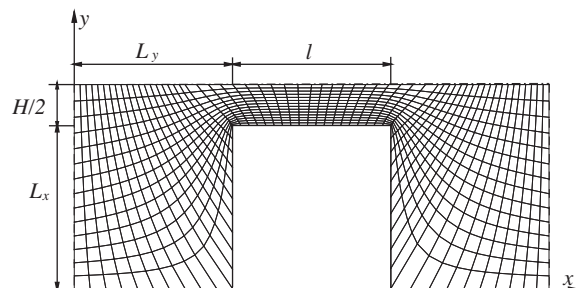

Fig. 1. Sketch of computational domain.