The Monte Carlo and Molecular Dynamics Simulation of Gas-Surface Interaction

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Abstract. A testing procedure and a program product for modeling gas-surface scattering process have been developed. Using the developed product the numerical simulation of the thermal transpiration phenomenon at free molecular conditions of the gas flow in channels with the use of different scattering kernels has been carried out. The surface structure influence on energy and momentum exchange in a gas-surface system has been studied by the use of Molecular Dynamics method.

1 Thermal Transpiration Phenomenon Study by Monte Carlo Method Realized for Different Gas-Surface Scattering Kernels

The most well-known diffuse-specular scheme of the boundary conditions to the heat and mass transfer equations of rarefied gas dynamics developed by Maxwell is successfully used for the majority of practical calculations (see, for instance, [1]). But some experimental data and corresponding theoretical calculations based on this scheme come into conflict with each other. As an example, one of the results of such calculations affirms that the thermal transpiration phenomenon (or "thermo molecular pressure difference effect" as it appears in scientific papers) does not depend on the kind of the gas and the surface state [2]. Such result contradicts the rather reliable experiments, for instance [3]. Apparently, the diffuse-specular scheme is not suitable for the correct description of the gas-surface scattering process at the non-isothermal rarefied gas flow, the striking example of which is the thermal transpiration phenomenon.

The use of the diffuse-specular scheme does not provide the dependence of scattering process on the gas molecule state that leads to contradiction between the theory and the experiment especially for non-isothermal gas flow. To eliminate such contradiction the boundary conditions that include certain data about the state of gas molecules interacting with the surface must be applied.

Nowadays, besides the diffuse-specular scheme other boundary conditions based on scattering kernels developed by Epstein [4] and Cercignani-Lampis [5,6] are widely recognized. The mathematical forms of these kernels contain certain expressions where the velocity of a gas molecules incident on the surface and the surface temperature are included. The Cercignani-Lampis and the Epstein scattering kernels are based on a certain physical ground and they satisfy all the requirements established for a scattering kernel [7].

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To test the correctness of modeling the gas-surface scattering the program product that provides simulating the behavior of non-interacting molecules in finite space while changing the shape of the limited surface as well as the modeling method of the scattering process, the surface temperature distribution and the initial gas state has been developed. The free molecular version of the Monte Carlo direct simulation method [8] has been realized. The efficiency of the program product has been demonstrated on the example of reaching the equilibrium state of the gas in the bulbs of various forms at the temperature perturbation of the surface. On the base of this product the results that do not contradict the principal postulates of the gas kinetic theory have been achieved. This fact has initiated our interest to apply the developed approach for studying the thermal transpiration phenomenon in rarefied gas at non-isothermal conditions that meets the problem in description while using the scheme of boundary conditions based on the Maxwell scattering kernel.

To understand the problem let us consider the free molecular stationary gas flow in cylindrical channel connecting two bulbs where the gas is in the equilibrium with the "hot" and the "cold" bulb at the temperature T_h and T_c accordingly. The main equation for the gas pressure reached in each bulb is

$$\frac{P_h}{P_c} = \left(\frac{T_h}{T_c}\right)^{\gamma}, \tag{1}$$

where P_h – the gas pressure in the hot bulb, P_c – the gas pressure in the cold bulb, γ – a so called thermal transpiration coefficient.

The γ value is observed close to ½ in all simulation procedures that use the Maxwell kernel with any kernel parameter. The simulation of the thermal transpiration phenomenon with the use of Cercignani-Lampis and Epstein kernels demonstrates significant dependence of the thermal transpiration coefficient γ on the kernel parameters.

It has been shown that with the use of both the Cercignani-Lampis and the Epstein kernels the thermal transpiration effect depends on the channel's length/radius ratio, the surface temperature distribution along the channel and does not depend on the bulbs' temperature ratio. The stationary gas temperature distribution inside the channel depends on the channel's length/radius ratio and practically does not depend on the kernel parameters. The stationary gas concentration distribution depends both on the channel's length/radius ratio and the kernel parameters.

The comparison with the most reliable experiments shows that the simulation based on the use of the Cercignani-Lampis scattering kernels provides satisfactory description of the gas-surface scattering at non isothermal rarefied gas flow conditions at all. Due to strong dependence of the thermal transpiration coefficient on kernel parameters one can expect similar result while using the Epstein kernel.

2 Molecular Dynamics Simulation of Energy and Momentum Transfer in a Gas/Solids System

A great number of structural models describing current gas dynamics experiments and forecasting and momentum exchange in a "gas – rough surface" system have been

developed. Every model corresponds to definite material, grain orientation and surface structural phase. An attempt to build an adequate model of surface structure and to describe the real experiment for rarefied gas flow in a rectangular channel with the rough walls has been realized with the use of Monte Carlo Test Particle Simulation Method [9]. Other approach for statistical modeling the roughness proposed in [10] is based on the assumption that the separate elements of the surface microstructure are the cones of the same height and top angle. These approaches for simulation of the surface structure as similar ones are not adequate completely to the real situation because of their "artificial" character based on "imagination" but not on the topography of the real surface.

The methods of scanning probe microscopy, in particular, atomic force microscopy that are developed intensively last years give on opportunity to get an information on specific features of the surface structure and to develop boundary conditions adequate to the real situation. The attempt to simulate the surface structure with the use of such approach has been realized recently [11].

In this study we investigate the topography of platinum plate used in gas dynamics experiments to estimate the roughness of the real surface. The surface structure has been studied with the use of AFM Explorer in a contact regime of scanning. Using the obtained data the main parameters characterizing surface microstructure have been determined.

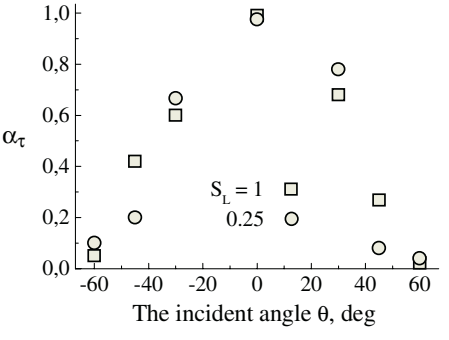

Fig. 1. The tangential momentum accommodation coefficient α_τ for xenon/platinum system

To simulate the gas-solids interaction the classical molecular dynamics method is applied. The Knudsen's accommodation coefficients for tangential and normal momentum, as well as for kinetic energy have been calculated taking into account the gas nature and the surface structure. The results of the tangential momentum accommodation calculation for xenon/platinum system as a function of an incident angle θ for two values of the velocity ratio S_L are presented in figure 1. S_L is introduced as a ratio of the surface movement velocity to the most probable gas molecule velocity.

3 Conclusions

The results of numerical simulation of the thermal transpiration phenomenon at free molecular conditions of the gas flow in channels with the use of the Maxwell, the Cercignani-Lampis and the Epstein scattering kernels are presented. The principal outcome of the study is the statement that in contrast to the Maxwell scheme of boundary conditions the use of the Cercignani-Lampis and the Epstein kernels permits to describe more correctly the non-isothermal internal rarefied gas flow. The obtained results show that there are no principle problems for gas-surface interaction description using numerical simulation procedures, in particular DMCS and molecular dynamics method. Some technical problems could be met under way of the AFM data use in simulations and finding acceptable form of interaction potentials as well as their parameters.

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References

1. Siewert, C. E.: Poiseuille and thermal-creep flow in cylindrical tube. J. Comp. Physics 160 (2000) 470-480.
2. Sharipov F., Seleznev V.: Data on Internal Rarefied Gas Flow. J. Phys. Chem. 27 (3) (1998) 657-706.
3. Edmonds T., Hobson J.P.: A study of thermal transpiration using ultra high vacuum techniques. J. Vac. Sci. Technol. 2 (1965) 182-197.
4. Epstein M.: A model of the wall boundary condition in kinetic theory. J. AIAA 5(10) (1967) 1797-1800.
5. Cercignani C., Lampis M.: Kinetic model for gas-surface interaction. Transp. J. Theory and Stat. Phys. 1 (1971) 101-114.
6. Lord R.G.: Some further extensions of Cercignani-Lampis gas-surface interaction model. J. Phys. Fluids 7 (1995) 1159-1161.
7. Cercignani C.: The Boltzmann Equation and its Application. Springer, New York (1988).
8. Bird G.A.: Molecular Gas Dynamics and Direct Simulation of Gas Flows. Oxford University Press, Oxford (1996).
9. Sazhin O.V., Kulev A.N., Borisov S.F.: The role of the surface structure in formation of an ultra rarefied gas flow in a channel. J. ThermoPhysics & Aeromechanics, 8(3) (2001) 391-399.
10. Sawada T., Horie B.Y., Sugiyama W. J. Vacuum, 47(6-8) (1996) 795-797.
11. Gerasimova O.E., Borisov S.F., Boragno C., Valbusa U.: Modeling of the surface structure in gas dynamic problems with the use of the data of atomic force microscopy. J. Eng. Phys. & Thermophys., 76(2) (2003) 413-416.