Influence of Rarefied Gas-Surface Interaction on Flow Stability in Channels

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Abstract. Small modification of gas-surface interaction parameters at high Knudsen numbers can generate large deviations of the macroscopic parameters of the flow [1], [2]. The reason for this behavior of the flow is that nonlinear iterative equations describing rarefied gas flows in long channels and nozzles have solutions becoming instable for certain values of the parameters of scattering function V of gas atoms on the walls. Calculated by Monte-Carlo simulation distributions of the number of gas atoms and of the angles of inclination of gas atom trajectories along the channel demonstrate that the flow becomes instable if the values of gas-surface interaction parameters are close to the points where analytical limit solution has singularity [1]. Near these points two flows with negligible small difference in corresponding parameters of the gas and of the surface have large difference between calculated characteristics. Ray-diffuse model of scattering function on channel walls is considered, i.e. diffuse scattering is combined with ray model of reflection (velocity of reflected gas particles is unique determined as a function of the velocity of incident gas atoms).

Keywords: Atoms scattering from surface, numerical computation, rarefied gas, flows in channels, stability.
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INTRODUCTION

In previous analytical and numerical investigations we considered the cascade of bifurcations appearing for ray model of scattering function V [2]. This model determines only one velocity of reflected gas atoms which is different from the velocity of specular reflected atoms. Diffuse addition (multiplied by the coefficient σ) to ray model gives us more general ray-diffuse model, which causes randomization and changes fundamentally the limit behavior of studied dynamic system [3].

The main purpose of our new calculations is to detect the regions (and corresponding physical values in the flows) where bifurcations of examined type can be observed in experiments. However the problem of empirical confirmation of obtained numerically effect is still difficult since scattering conditions, as well as the regions of the parameters are quite particular and hardly reproducible experimentally. Considered bifurcations can essentially affect different gas flows applied in practice, such as flows in propulsion systems and in microelectronic vacuum devices.

Scattering function $V(\vec{u}_0, \vec{u})$ of gas atoms on the surface (where $\vec{u}_0$ and $\vec{u}$ are the velocities of incident upon the channel wall and reflected gas atoms) determines entirely the parameters of rarefied gas flow in a channel at high Knudsen number Kn (near free-molecular flow, $\mathrm{Kn}\to\infty$). Previous analytical and numerical investigations have showed that the instability of the flow takes place for some transition parameter values of V under following conditions. First, the channel or the nozzle is long enough. Second, the scattering function V is described by means of ray model. Simulating successive gas atoms reflections from channel walls we obtain nonlinear dynamic system. If the solutions become instable, the system gets many different attractors (limit solutions), so that the cascade of bifurcations appears [1]. Corresponding parameters of scattering function V represent the values of singularity. Close to these values the numerical calculations demonstrate significant changes of the aerodynamic characteristics of the flow.

In the present paper we consider the scattering function V of more general ray-diffuse form [2]

$$V(\vec{u}_0,\vec{u}) = (1-\sigma)\delta(\vec{u}-\vec{u}_*(\vec{u}_0)) + \sigma\frac{2h_d^2}{\pi}u_n e^{-h_d u^2}\ , \tag{1}$$

where σ and h_d are constant parameters, σ changing from 0 to 1. One part of the molecules (σ) follows according to this model diffuse scattering, and another part (1– σ) reflects in compliance with ray model. Second term on the right side is diffuse addition to ray model of scattering, it describes the effects of adsorption and contamination of the surface of channel walls. Generally speaking this term is just basic function which changes fundamentally the limit behavior of the dynamic system because of randomization.

The purpose of present investigation is to study the influence of diffuse addition to scattering function V on the instability of the flow.

STATEMENT OF THE PROBLEM

Simulating the trajectory of gas atoms in different points of the collisions with channel walls (fig.1), we can determine non-linear relationship between the angles θ_m, θ'_m, θ_{m+1} etc. Geometrical shape of the channel and scattering function V are supposed to be given.

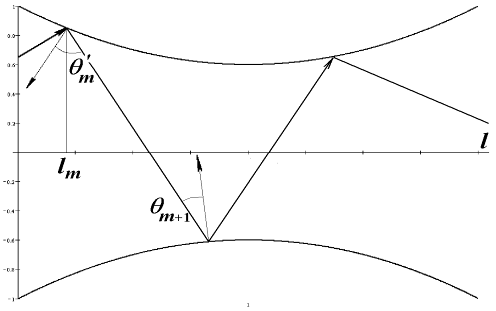

FIGURE 1. Iterative scheme in a channel or nozzle.

The equation proposed in [3] for free-molecular flow in flat or cylindrical channel gives the connection between the angles θ_m and θ_{m+1} in the form

$$x_{m+1} = \frac{x_m}{a\sqrt{1+x_m^2}-b}\ , \tag{2}$$

where $x_m = \tan\theta_m$, $x_{m+1} = \tan\theta_{m+1}$; θ_m and θ_{m+1} are the angles of incidence in m-th and (m+1)-th collisions of gas atom with the surface, and the variables a and b are constant parameters connected with the momentum exchange coefficients p and τ by the equalities

$$p(\theta) = p_1\cos\theta + p_2\cos^2\theta,\quad \tau(\theta) = \tau_0\sin\theta\cos\theta,\quad a = \frac{p_1}{2-\tau_0},\ b = \frac{2-p_2}{2-\tau_0}\ , \tag{3}$$

considered in [4], [5].

The iterative equation (2) has instable solutions for certain values of the parameters a and b [1]. It means that comparative small modification of gas-surface interaction parameters a and b causes significant difference between corresponding limit values $x_m = \tan\theta_m$. The interpretation from aerodynamic point of view is that macroscopic parameters of the flow become vary unsteady while the difference in microscopic values describing gas-surface interaction remains negligible. However the regions in which the flow becomes instable are very narrow, therefore it is difficult to find them numerically or experimentally. To find the values a and b where the instability takes place we apply analytical results [1] concerning analytical limit solution of non-linear iterative equation (2). In the coordinate system (a, b) the regions of instability obtained analytically are concentrated near the line $a = b$.

In the case of complex geometrical shape of a channel or of a nozzle, for instance, similar to the shape outlined above (fig.1), equation (2) could be converted to

$$x_{m+1} = \tan\left[\psi\left(l_m, \arctan\frac{x_m}{a\sqrt{1+x_m^2}-b}\right)\right], \tag{4}$$

where l_m is the coordinate of the point of –th collision of gas atom with the surface and the function transforms the angle θ'_m into the angle θ_{m+1} of incidence in next interaction of gas atom with nozzle walls.

NUMERICAL SIMULATIONS

The length l of the channel relative to its width is assumed in the Monte-Carlo simulations quite large (from 10 to 100). Other parameters (σ, a, b and θ_0) are changed in accordance with known limit analytical solution of equation (2). In the initial section of the channel a uniform flow is set consisting of N gas atoms having identical velocities with the angle of inclination θ_0 (N changes from 10000 to 50000).

To illustrate obtained results comparative graphs of velocity distribution in different directions are presented (fig.2).

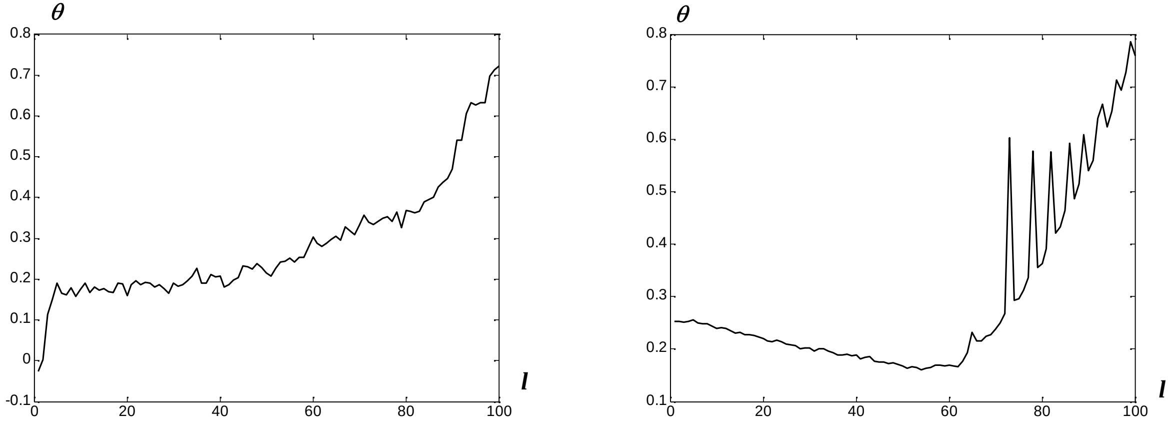

FIGURE 2. The change of average scattering angle θ'_m along the channel by the modification of the parameter from a = 1.47 (left graph) to a = 1.48 (right graph) by constant b = 1.7, σ = 0.05, ray-diffuse scattering function.

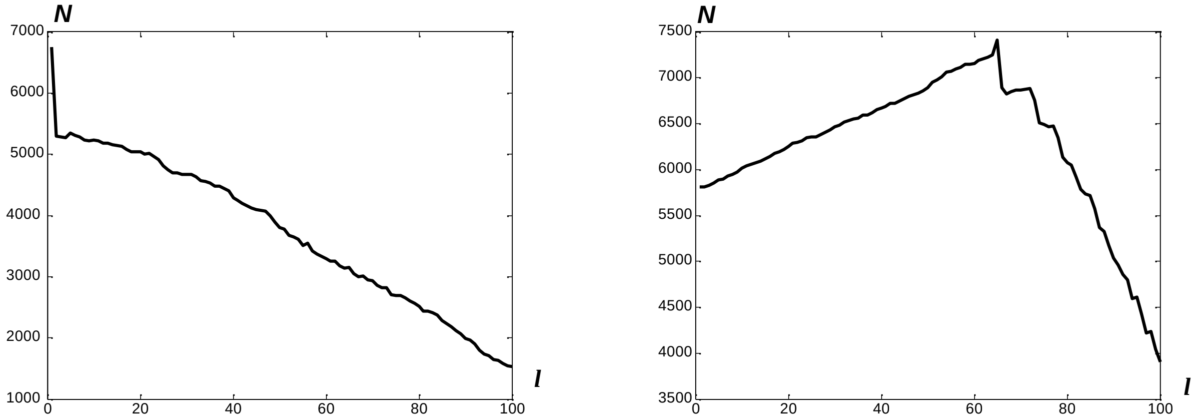

FIGURE 3. The change of the number N of gas atoms along the channel by the modification of the parameter from a = 1.47 (left graph) to a = 1.48 (right graph) by constant b = 1.7, σ = 0.05, ray-diffuse scattering function.

The number of gas atoms in sections of a channel for ray-diffuse model (1) with identical value $\sigma = 0.1$ is shown on fig.3. To demonstrate various points of instability the parameters are changed at different values. For instance, variable a changes near 1.7 (fig. 2) and near 1.2 (fig. 3).

Corresponding bifurcation diagrams are shown in figs. 4, 5 and 6.

The results of numerical calculations show that for relative small values of σ the effect of significant change of flow parameters by small modification of gas-surface interaction coefficients a and b stays qualitative the same as for ray scattering $(\sigma = 0)$ and by the same parameter values of a and b.

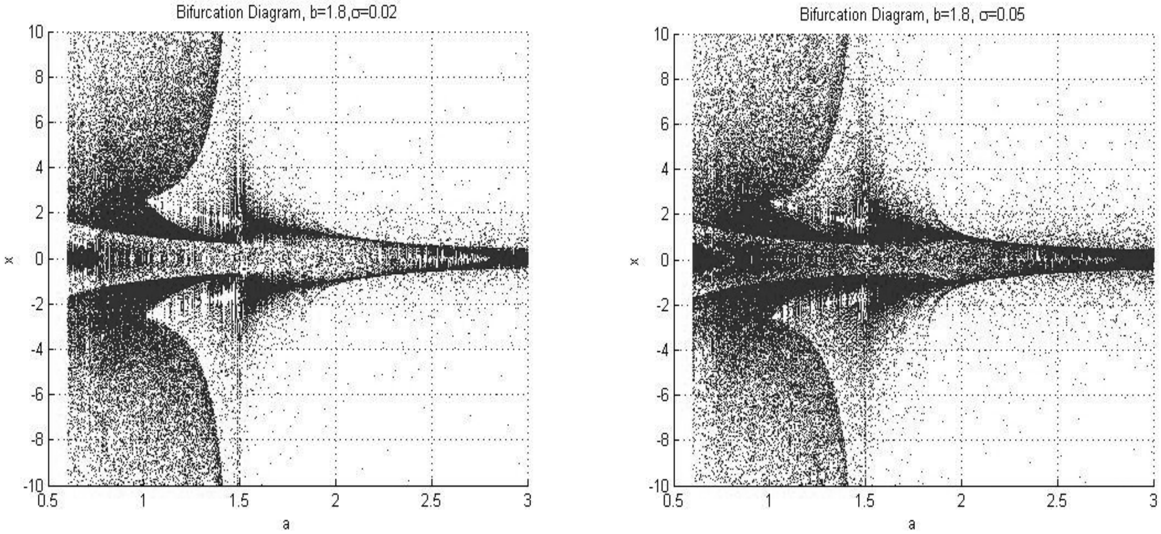

FIGURE 4. Two bifurcation diagrams, representing the influence of scattering parameter σ (the share of diffuse scattered gas atoms) on the flow instability for the same geometrical scattering parameters a (from 0.5 to 3), b =1.8 and initial value $x = \tan(\theta_0)$ from –10 to 10, $\sigma = 0.1$, ray-diffuse scattering function**.**

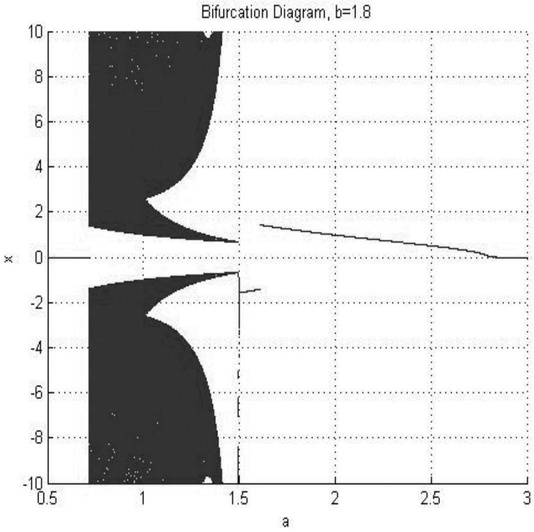

FIGURE 5. The bifurcation diagram by constant parameter $b = 1.8$ and a changing from $a = 0.5$ to $a = 3$, ray-diffuse scattering function, $\sigma = 0.001$, initial value $x = \tan(\theta_0)$ from –10 to 10**.**

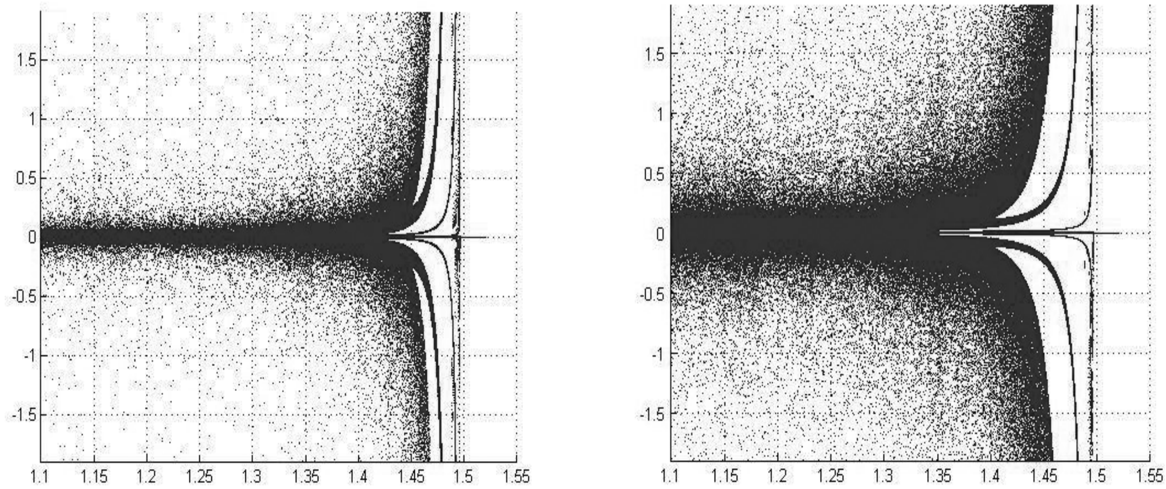

FIGURE 6. Two bifurcation diagrams, representing the influence of scattering parameter σ (the share of diffuse scattered gas atoms, σ=0.02 on the left and σ=0.05 on the right graph) on the flow instability for the same geometrical scattering parameters *a* (from 1.1 to 1.55), *b* =1.8 and $x = \tan(\theta_0)$ (from –2 to 2).

However obtained results of numerical calculations show that relative small deviations of the parameters of scattering function *V* do not affect the considerable change of macroscopic characteristics of the flow. Typical results are presented on the bifurcation diagrams displaying for different values of σ the distribution of gas atoms in the channel for ray-diffuse model of scattering of gas atoms with geometrical parameters of the trajectory of a gas atom in the channel *a* (*x*-axis) and tan(θ) (*y*-axis). Near the point of the bifurcation negligible change of one of the parameters of ray-diffuse model (less than 1%) causes substantial difference in gas flow in the channel (or in the nozzle).

CONCLUSION

Analytical reason for the instability of internal rarefied gas flows at high Knudsen numbers is that nonlinear iterative equation describing these flows in long channels or nozzles have instable solutions for certain values of the parameters of scattering function *V* of gas atoms from the walls [1]. Very small modification of gas-surface interaction parameters of instable flow can generate large deviations of the macroscopic parameters. However this effect obtained in analytical and numerical investigation still could not be observed in experiments.

To verify the bifurcations of this type experimentally all considered physical values in the flows are to be set exactly to the same values as detected in our calculations. Therefore the problem of empirical confirmation of obtained numerically effect is still difficult since the regions of the parameters are quite particular and corresponding scattering conditions are hardly reproducible experimentally.

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