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Simulation of Unstable Rarefied Gas Flows in Channels and Nozzles for Large Knudsen Numbers

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Abstract

Rarefied gas flow in a channel considered as nonlinear dynamic system is described by iterative equations. Under certain conditions the solutions of these equations may be unstable in some regions of the values of gas-surface interaction parameters [1]. In particular, we obtain numerically the substantial difference in gas flow in a channel caused by a negligible change of one of the parameters of scattering function (less than 1%) near the bifurcation point. As well non-random solutions as random solutions can be observed on bifurcation diagrams. As a result, the conductivity of the channel may be reduced significantly, i.e. some of obtained solutions have a physical meaning of locking the channel. The scattering function is supposed to be close to ray-diffuse collision kernel (the mixture of ray reflection and diffuse scattering). The scattering conditions of this type are hardly reproducible experimentally. Therefore, the bifurcations of simulated type may be verified experimentally only if all considered physical values in the flows are set exactly to the same values as detected in our calculations. Adding the extra parameter of scattering function allows us extending the region in the parametric space where considered dynamic system (related to rarefied gas flow) is unstable. Obtained connection between the parameters of nonlinear dynamic system and momentum exchange coefficients (or accommodation coefficients) makes it possible to express analytic evaluations in terms of aerodynamic characteristics including Knudsen and Mach numbers, temperature factor etc.

1. Introduction

Rarefied gas flows in channels are discrete dynamic systems (unlike continuous dynamic systems specified by differential equations), because they are described by the laws of mutual interactions of gas particles and of collisions with the surface. Discrete dynamic systems can produce strange attractors whatever their dimensionality. On the contrary, according to the Poincaré-Bendixson theorem a strange attractor in a continuous dynamical system can arise only if the system has three or more dimensions. The cascade of bifurcations in rarefied gas flow in a channel was studied in [1] for the ray model of scattering function V of gas atoms from channel walls. The ray model, as well as the specular reflection, determines only one velocity of reflected from the surface gas atoms by given incident velocity. However, the angles of incident and of reflected gas atoms for the ray model could be different. So the ray model defined by the expression $V(\vec{u},\vec{u}')=\delta(\vec{u}'-\vec{u}_*(\vec{u}))$ [2] could be regarded as the generalized specular reflection. Here δ is Dirac delta function and $\vec{u}_*$ is some specified velocity of reflected from the surface gas atoms that is in general different from the specular velocity. The function $\vec{u}_*(\vec{u})$ is not arbitrary –some restrictions are required to ensure that $V(\vec{u},\vec{u}')$ satisfies the known criteria on wall collision kernels. For example, if the distribution of the velocities $\vec{u}$ of incoming gas atoms is Maxwellian, then corresponding distribution of the velocities $\vec{u}_*(\vec{u})$ of reflected from the surface gas atoms must be the same. In this case the function $\vec{u}_*(\vec{u})$ transforms Maxwellian distribution into itself. More general restrictions to the function $\vec{u}_*(\vec{u})$ can be represented as the principle of detailed balance in gas-surface interactions [3]. However, it is known from the papers of Barantsev and Miroshin (who considered the ray reflection originally) that the class of such functions $\vec{u}_*(\vec{u})$ is wide enough [2]. In our calculations only the functions $\vec{u}_*(\vec{u})$ are applied satisfying these restrictions. In spite of this, various analytical expressions of

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momentum exchange coefficients (depending on the angles of the incidence and of the reflection) can be obtained in the context. Correspondingly many different shapes of limit gas atoms trajectories are the advantages of the ray model. The diffuse addition (multiplied by the coefficient σ, $0 \le \sigma \le 1$) to the ray model gives us the more general ray-diffuse scattering function depending on the velocities $\vec{u}$ of incident upon the channel wall and $\vec{u}'$ of reflected from the surface gas atoms:

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

The diffuse addition causes a randomization and changes fundamentally the limit behavior of the studied dynamic system [4], [5]. The ray model has better experimental confirmation (especially combined with diffuse scattering) in comparison with other surface interaction models widely applied in practical DSMC calculations, in particular with the specular-diffuse model [2]. The approximation of real gas-surface characteristics by the ray model is good enough for different physical conditions. Therefore we assume the ray model to be valid also in considered flows.
The main purpose of this paper is the new analytic and numerical investigation of the limit behavior of this nonlinear dynamic system. Strange attractor can be observed in rarefied gas flows as a cascade of bifurcations. In usual applications of the chaos theory the corresponding chaotic behavior is the case of most interest. However, in a rarefied gas flow, unlike usual applications, most interesting is not chaotic behavior, but the transition from regular to chaotic behavior. Such transition indicates in practice the values of the parameters where the solution changes substantially by a very small deviation of these parameters. To study it not only for different values of the parameters, but also for different analytical approximations of momentum exchange coefficients is our main problem. From the point of view of nonlinear dynamics it corresponds to different iterative equations describing the trajectory of a gas atom.
Basic assumption that the number of gas-surface collisions exceeds the number of mutual gas atoms interactions can be expressed as Kn > 1 (Knudsen number is high). To take into account that Knudsen number is finite the local interaction approximations are applied [2]. The local interaction theory, being exact for free-molecular flow, gives the approximations of momentum and energy exchange coefficients which are confirmed by experiment for transition regime between free-molecular and continuum flows. Meanwhile we detect the bifurcations, the attractors and corresponding physical values in the flows. However, the problem of the empirical confirmation of the obtained numerically effect is still difficult, because the defined regions of empirical parameters (corresponding to the scattering conditions) are narrow enough. Therefore these scattering conditions are 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.
The parameters of rarefied gas flow in a channel are entirely determined by the scattering function $V(\vec{u},\vec{u}')$ (if the geometric shape is known) in a near free-molecular flow (Kn→∞). There is no need to eliminate possible mutual collisions of gas atoms in transitional regime (Kn > 1), because these collisions are taken into account by applyed local approximations [2]. Hence, similar connection between the parameters of scattering function V and the parameters of a rarefied gas flow in a channel can be obtained in this case. However, the solution cannot be extended to the whole region of Kn, because the influence of mutual collisions of gas atoms must be small: only in this case most of the incident gas atoms come according to the locality hypothesis from channel walls [2].
The rarefied gas flow is detected becoming unstable in our previous analytical and numerical investigations [1], [4]–[6] in long enough channels or nozzles for some transition parameter values of scattering function V under some specified conditions. The basic restriction is that the model describing scattering function V is close to the ray reflection. Corresponding momentum exchange coefficients for the ray scattering function V are expressed by $p = 2\cos\theta(\cos\theta + u'\cos\theta')$, $\tau = 2\cos\theta(\sin\theta - u'\sin\theta')$, where u and u' are absolute values of the velocities $\vec{u}$ and $\vec{u}'$, and θ and θ' are corresponding angles for incident and reflected gas atoms [2].

2. Approximations of momentum exchange coefficients in iterative equation

Simulating successive gas atoms reflections from channel walls, we obtain the nonlinear dynamic system (Fig. 1). Denoting $x_m = \tan\theta_m$, $x_{m+1} = \tan\theta_{m+1}$, where the subscript m indicates the number of reflections (x_m and x_{m+1} are successive values defining the trajectory of a gas particle in the channel), and expressing θ' from presented formulae of momentum exchange coefficients p and τ, we obtain iterative equation:

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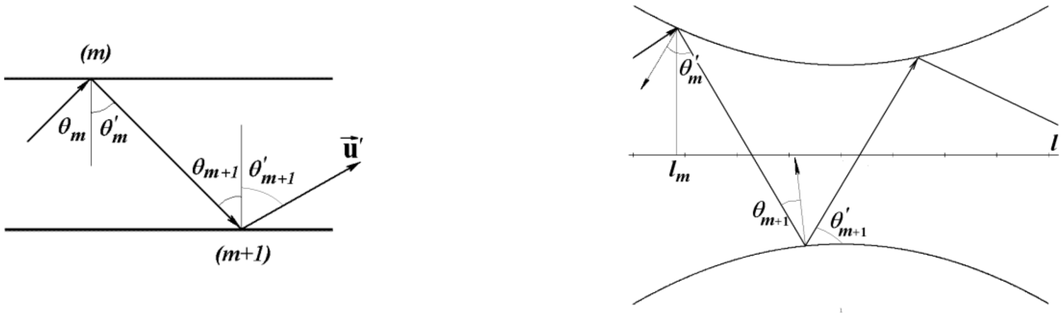
$$x_{m+1} = \tan\left[\psi\left(l_m, \arctan\frac{2x_m - \tau(1+x_m^2)}{p(1+x_m^2)-2}\right)\right] \tag{2}$$

Here the function ψ and the variable l_m are determined by the geometrical shape of the channel, and the momentum exchange coefficients p and τ are assigned by local approximations.



(a) (b)

Figure 1: The iterative scheme of successive reflections of a gas atom from the walls in a flat channel (a) or in a nozzle (b)

If the solutions of the equation (2) become unstable, then considered nonlinear dynamic system has many different limit solutions – attractors [1], [4]–[8]. Corresponding parameters of the scattering function V represent the values of singularity. In this case the problem is to find small regions of parameter values, where the Feigenbaum period-doubling cascade [7]–[8] can be observed. Numerical calculations of the trajectories of gas atoms in a channel demonstrate significant changes of the aerodynamic characteristics of the flow near the values of system parameters from the considered small regions. Iterative equation (2) describing the behavior of nonlinear dynamic system in these regions is more complicated than well-known equation for logistic map $x_{m+1} = rx_m(1-x_m)$. Therefore the investigation of its solutions becomes very difficult, and additional restrictions are taken into account.
First, we consider (following our previous papers [4]–[6]) two-dimensional flow, i. e. flat or cylindrical channel (Fig. 1). Then the function ψ in the equality (2) is identical, and the connection between the angles θ'_m and θ_{m+1} in successive m-th and $(m+1)$-th points of collisions of a gas atom with the surface becomes simple: $\theta'_m = \theta_{m+1}$.
Second, only three following most applied in practice local approximations are examined.

1. Depending on three parameters approximation based on the expansion of p and $\tau/\sin\theta$ in terms of the functions $\cos^n\theta$, n = 1, 2, … [4]–[6]. This model has been confirmed by experiment in many papers (cited in [2]) from St.-Petersburg State University and Central Aviation Institute (TSAGI, Moscow) and can be described by the equations $p = p_1\cos\theta + p_2\cos^2\theta$, $\tau = \tau_0\sin\theta\cos\theta$. Special cases of this approximation have been examined by Miroshin [8]: $p_2 = \tau_0$ ("model A") and $p_2 = 2$ ("model Z"). The coefficients p_1, p_2, τ_0 can be expressed in terms of aerodynamic values, such as Kn, Mach number, temperature factor etc. Substitution into iterative equation (2) reducing three coefficients p_1, p_2, τ_0 to two parameters a and b permits to transform it to:

$$x_{m+1} = \frac{x_m}{a(1+x_m^2)^{1/2} - b}, \text{ where } a = \frac{p_1}{2-\tau_0},\ b = \frac{2-p_2}{2-\tau_0}. \tag{3}$$

2. Another approximation suggested also by Miroshin [1] ("model B") reducing three coefficients p_2, p_4, τ_0 to two parameters a_1 and b_1 (p_2 and τ_0 remain the same, p_4 corresponds to higher power $\cos^4\theta$) transforms iterative equation (2) to:

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$$x_{m+1} = \frac{x_m\left[1-a_1+(1-b_1)x_m^2\right]}{a_1+b_1x_m^2}, \text{ where } a_1 = \frac{p_2+p_4-2}{p_2-\tau_0}, \ b_1 = \frac{p_2-2}{p_2-\tau_0} \quad \mathbf{(4)}$$

3. A more general approximation containing four coefficients p_1, p_2, τ_0, τ_1 and not yet been examined for nonlinear dynamic system parameters is corresponding to iterative equation with the same parameters *a* and *b* like in (3) and a new parameter *d*

$$x_{m+1} = \frac{x_m}{a\sqrt{1+x_m^2}-b}\left(1-\frac{d}{1+x_m^2}\right), \text{ where } d = \frac{\tau_1}{2-\tau_0} \quad \mathbf{(5)}$$

For $d = 0$ the equation (5) coincides with (3). Hence the first approximation (3) is particular case of the third (5). However, the second model (4) cannot be represented in the form (5), but the main properties are similar by corresponding values of the parameters. Fig. 2 illustrates the graphs of the functions (3)–(5) for the values of variables *a*, *b*, *c* and *d* (and corresponding momentum exchange coefficients) observed in real physical conditions of gas-surface interaction (and in the experiments). In particular, *a* = 2, *b* = 1.7 for the approximation (2) (dashed line), *a* = 0.2, *b* = 0.9 for (3) (dotted line), *a* = 2, *b* = 1.8, *d* = 0.3 for (4) (solid line).

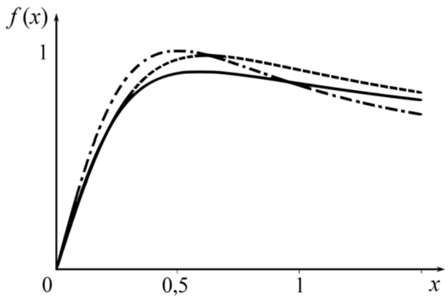

Figure 2: The functions in iterative equations (3)–(5) corresponding to successive reflections of a gas atom the walls in a channel

3. Attractors and Bifurcations in Rarefied Gas Flows

Studying the stability of rarefied gas flow in a channel we need to investigate the limit behavior of nonlinear dynamic system by $m \to \infty$ [4]–[8]. The necessary conditions for the existence of Feigenbaum cascade of bifurcations can be proven analytically for iterative equations (2)–(4). All three functions are unimodal for presented values of the parameters (as is shown on Fig. 2) – it follows from studying the sign of the first derivatives in a very large region of the variables *a*, *b* and *d*. Schwartz derivative is negative for all the functions $f(x_m)$ on the right side of iterative equations (3)–(5):

$$Sf(x) = \frac{f'''(x)}{f'(x)} - \frac{3}{2}\left(\frac{f''(x)}{f'(x)}\right) < 0 \quad \mathbf{(6)}$$

Miroshin has derived it analytically [8] for the equation (4), on the base of the representation of Schwartz derivative in the form:

$$Sf_2(x) = -6\,\frac{(b_1-a_1)\left(b_1(1-b_1)x^4-6a_1(1-b_1)x^2+a_1(1-a_1)\right)}{\left(b_1(1-b_1)x^4+(3a_1-2a_1b_1-b_1)x^2+a_1(1-a_1)\right)^2}, \text{ where } f_2(x) = x\,\frac{1-a_1+(1-b_1)x^2}{a_1+b_1x^2} \quad \mathbf{(7)}$$

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Similar representation and the proof of the inequality $Sf_1(x) < 0$ we have obtained for iterative equation (3), i.e. for $f_1(x) = x\left(a\left(1+x^2\right)^{1/2} - b\right)^{-1}$ [4]–[6], Schwartz derivative may be expressed as:

$$Sf_1(x) = -(3/2)\left(\left(a\left(1+x^2\right)^{1/2} - b\right)^2 + a^2 - b^2\right)\left(a - b\left(1+x^2\right)^{1/2}\right)^{-2}\left(1+x^2\right)^{-2} \quad \textbf{(8)}$$

The third model (5), i. e. $f_3(x) = x\left(a\left(1+x^2\right)^{1/2} - b\right)^{-1}\left(1 - d\left(1+x^2\right)^{-1}\right)$, does not allow simple formula for Schwartz derivative like (7) – it is much more complicated. However, the inequality $Sf_3(x) < 0$ can be proved analytically for $a > b$, $(d(3a-b)-a)(d-1) > 0$, and $x \in [0,\infty)$. For instance, the value for $x = 0$ is equal to $Sf_3(0) = -3\left(a/(a-b) + 2d/(d-1)\right)$.

Negative Schwartz derivative is necessary, but not sufficient for the initiation of Feigenbaum cascade of bifurcations – a numerical confirmation is needed. Our analytical and numerical investigation of limit solutions has shown that all the three iterative equations (3)–(5) can have attractors of different types depending on the parameters *a*, *b* and *d*. Limit cycles corresponding to the roots of the equation $f(x) = x$ and stationary point $x = 0$ (indicating direct flow along the axis of the channel) are obligatory. Iterative equations (3)–(4) can also have stationary points $x_1 = \left((b+1)^2/a^2 - 1\right)^{1/2}$, $x_2 = (2a-1)^{1/2}/(1-2b)^{1/2}$ and $x_0 = \infty$ respectively. The last value has a physical meaning of locking the channel, i.e. its conductivity reduces significantly near this point.

From numerical study of the third model (4) we can conclude that the attractors and bifurcations in this case are noticeably more various than for the first two models (2)–(3). In particular, up to three attractors exist corresponding to the roots of the equation $at^3 - (b+1)t^2 + d = 0$. The attractors of higher degree could be obtained from the equation $f \ldots f(x) = x$ (where $f(x)$ could be iterated many times) and the set of the solutions could be very rich for some values of *a*, *b* and *d*.

Thus, under certain conditions iterative equations (3)–(5) may have unstable solutions in some regions of the values of gas-surface interaction parameters *a*, *b* and *d*. In these regions (which can be found analytically in described way) comparative small modification of the parameters *a*, *b* and *d* causes significant difference between corresponding limit values $x_m = \tan\theta_m$. From aerodynamic point of view it has following interpretation: macroscopic parameters of the flow may fluctuate unsteady while the difference in microscopic values describing gas-surface interaction remains negligible. However, the flow becomes unstable only in very narrow regions, therefore it is difficult to find them numerically or experimentally. In the coordinate system (*a*, *b*) the regions of instability obtained analytically are concentrated near the line *a* = *b*.

Real physical setup of considered rarefied gas flows has not yet detailed experimental confirmation because of technical difficulties in performing such experiments. However, these analytical evaluations are confirmed by numerical calculations.

4. Numerical simulation

Monte Carlo simulation of the rarefied gas flow in the channel is applied to construct the bifurcation diagrams – it is the best way to study the limit behavior of unstable dynamic systems and their bifurcations.

The computation is similar to DSMC with the basic modification: the number of mutual gas atoms collision is assumed much less than the number of the gas atoms reflections from channel walls. In the mutual collisions the gas atoms have been considered as hard spheres, and in the gas-surface interactions (having the main effect to the solution) scattering function was supposed ray-diffuse.

In three bifurcation diagrams (Fig. 3) the appearing Feigenbaum period-doubling cascade is shown for three considered iterative equations: (3) (Fig. 3 (a)), (4) (Fig. 3 (b)), and (5) (Fig. 3 (c)). Fig. 3 (b) illustrates also Lyapunov exponent λ [2], [7]–[8] (parameter *r* is a combination of *a* and *b* in (3)), Fig. 3 (a) – a part of bifurcation diagram for $1.1 \le a \le 1.5$, and Fig. 3 (c) – a part of bifurcation diagram corresponding to $1.7 \le a \le 2.2$.

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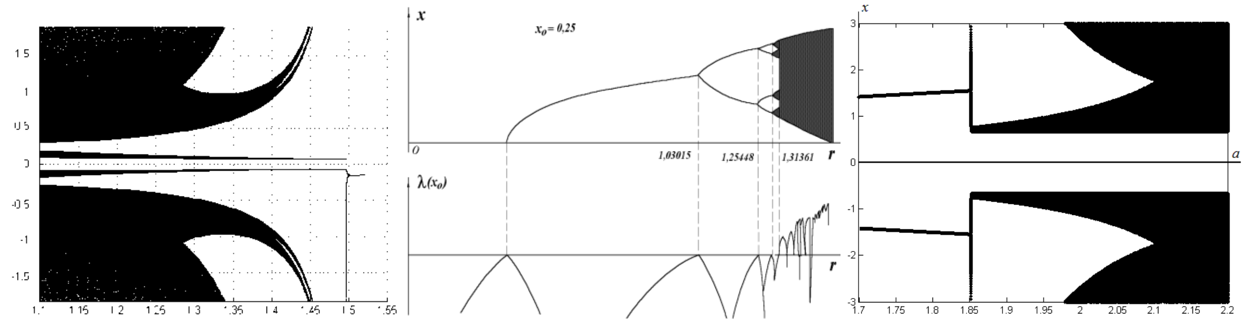

Figure 3: Bifurcation diagram for nonlinear dynamic system corresponding to rarefied gas flow in a channel and iterative equation (3) (a), (4) (b) and (5) (c)

The bifurcation diagrams shown in Fig.3 demonstrate the dependence of possible equilibrium (or long-term) values of a system on the bifurcation parameter *a*. Therefore nonrandom solutions are represented as lines (Figs. 3 (a) and 3 (b)) or as black regions.

To illustrate obtained results comparative graphs of the numerical density of gas atoms in some sections of a channel depending on the value *a* are presented (Fig. 4) for the first model (3).

The scattering function is assumed to be ray-diffuse with the identical value $\sigma = 0.1$. The parameters are changed gradually near the points of the instability to demonstrate the variation of the results. For instance, the variable *a* changes from 1.47 to 1.60 in four steps (Fig. 4). The largest difference between two graphs corresponding to nearest values *a* = 1.47 and *a* = 1.48 indicates the region of the instability in the segment $1.47 \le a \le 1.48$. Near the value *a* = 1.47 the conductivity of the channel reduces significantly – it has a physical meaning of locking the channel. Similar results have been obtained for other values of the parameters *a*, *b* and σ.

For increasing values of the coefficient σ, indicating the input of diffuse scattering into the function *V*, the bifurcation diagrams similar to presented in Fig.3 become dissolved like on Fig.5 because of the randomization. Random solutions can be observed on bifurcation diagram as distributed sets. At first sight the points on this diagram seem to be distributed randomly, but in fact a sharp structure is well seen in all diagrams of this type. The existence of this structure justifies our approach based on the nonlinear dynamics, and corresponding borders between the regions with different density of the points are the most interesting regions of the instability. The results of numerical calculations show that for relative small values of σ the effect of significant variation of flow parameters by a small modification of gas-surface interaction coefficients *a* and *b* remains qualitative the same as the effect for the ray scattering ($\sigma = 0$) and it can be observed by the same parameter values of *a* and *b*.

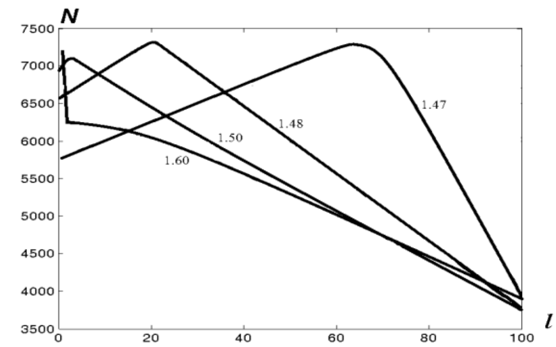

Figure 4: The change of the number N of gas atoms along the channel by the modification of the parameter a = 1.47, a = 1.48, a = 1.50, a = 1.60 by constant b = 1.7, $\sigma = 0.05$, iterative equation (3)

Near all the points of the bifurcation a negligible change of one of the parameters of the ray-diffuse model (less than 1%) causes also the substantial difference in gas flow in the channel (or in the nozzle).

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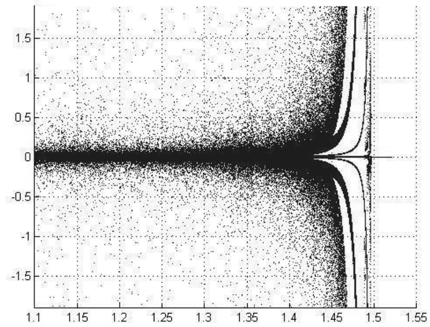

Figure 5: Bifurcation diagram for nonlinear dynamic system corresponding to rarefied gas flow in a channel and iterative equation (5) for a = 1.1 – 1.55 and σ = 0.1.

5. Conclusion

Monte Carlo simulation of different nonlinear dynamic systems corresponding to rarefied gas flows in channels has indicated various development of unstable behavior including cascades of period-doubling bifurcations. Analysis and comparison of the results leads to the following main conclusion.

1. Substantial difference in the characteristics of gas flow in a channel by negligible change of the parameters of ray-diffuse model of gas atoms scattering from surface is confirmed analytically and numerically. Most significant in applications is the possibility to use relatively simple analytical evaluations with the parameters found numerically corresponding to unstable rarefied gas flows. Hence our present study is numerically useful.
2. Comparing three models of rarefied gas-surface local interaction, we conclude that adding the extra parameter d of scattering function $f_3(x)$ allows us extending the region where considered dynamic system (related to rarefied gas flow) is unstable in the parametric space. Simulated unstable states of the system are close to physical situations observed in practice.
3. Obtained connection between the parameters of nonlinear dynamic system (a, b and θ_0) and momentum exchange coefficients (or accommodation coefficients) permits to express analytically the combinations of the gas dynamics characteristics (including Knudsen and Mach numbers, temperature factor etc.) specifying the unstable flows.
4. To verify the bifurcations of simulated type experimentally all considered physical values in the flows are to be set exactly to the same values as detected in our calculations. Defined regions of empirical parameters are very small therefore it is difficult to find them without special search. However, simulated unstable states of the system are close to physical situations observed in experiments.

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