

Scattering of Rarefied Gas Atoms from Poly-Gaussian Rough Surface

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Abstract

The dependence of the macro-parameters of the flow on surface roughness of the walls and on geometrical shape of the surface is investigated asymptotically and numerically in a rarefied gas molecular flow at high Knudsen numbers. Surface roughness is simulated on micro-level by a wide class of Poly-Gaussian (with probability density as the mixture of Gaussian densities) or Gaussian random processes. The results of rarefied gas flow Monte-Carlo simulation for both models of roughness are compared. Substantial difference is detected, as well in asymptotical expressions [3], as in numerical results. However, the results are substantially different from the calculations using more simple models of surface roughness. The properties of Poly-Gaussian model are studied allowing a better coincidence of its statistical parameters with the parameters of real polished surfaces, or rough surfaces processed by extrusion, pressing and other technologies. The comparison between Poly-Gaussian and Gaussian models shows more significant effect of roughness in aerodynamic values for Poly-Gaussian model as well in asymptotic as in numerical calculations; therefore the influence of surface roughness on momentum and energy exchange coefficients increases noticeably for Poly-Gaussian model compared to Gaussian one.

1. Introduction

The main purpose of this paper is to investigate the aerodynamic shadowing effect of a rough surface interacting with a rarefied gas flow at high Knudsen numbers as well in DSMC calculation as in analytic and asymptotic approximations.

Poly-Gaussian model of the roughness is studied [1], which is statistically verified on the base of experimental data on different surfaces [2]. This model is the generalization of Gaussian homogeneous isotropic random field applied in St.-Petersburg State University to simulate surface roughness in rarefied gas [3]–[4]. Poly-Gaussian model has several advantages [5] in comparison with other different more simple models of surface roughness applied in practice, including polygonal-line roughness [6], fractal [4], [7], conical-hole based model of the roughness [8], and the surface constructed of flat elements [9]. In particular, these simple models have no possibility to take into account the micro-roughness (the roughness of small scale), more than outweighing the input of large scale roughness into momentum and energy exchange coefficients on the surface [5].

Gaussian and Poly-Gaussian models have essential basic advantages, including:

- Corresponding random fields are differentiable, so that the local normal exists everywhere on the surface under simple conditions [1];
- Simulating numerically different real surfaces processed in various ways is easy simply varying the parameters (scale coefficients, correlation function and weighted function);
- Analytic representation of the probability of the absence of the crossings of inclined trajectory of a gas atom by the random field and of its other stochastic characteristics simplifies numerical Monte Carlo calculation of gas-surface interaction.

Poly-Gaussian model of roughness should be preferred to Gaussian one because of the reason explained in [10] and verified in [2]: “Non-Gaussian statistics have rough surfaces of mixed structure, modelled as a result of several stages of processing (by pressing, extrusion, grinding, honing etc.) of wearing surfaces after being operated, maintained and so on. Other reason for non-Gaussian relief is the deterministic component, which is typical for the processing by whetting, milling, polishing etc.”

2. Modelling gas atoms scattering from rough surface

Analytical expansion of scattering function V on a rough surface is based on its representation in the form $V = \hat{S} V_0$ [11], where the roughness operator \hat{S} depends only on the geometrical shape of a roughness and on the trajectory of a reflected gas atom [11], [12]. The operator \hat{S} does not depend on physical and chemical parameters of the gas and of the surface, which influence only the local scattering function V_0 (scattering function on smooth surface without roughness). Gas particles are called atoms because the structure of the molecule is also accounted by the local scattering function V_0 , so it does not affect the roughness operator \hat{S} .

New approach developed in our previous papers allows solving numerically the problem of simulating the gas atoms scattering from a rough surface [1], [5]. The expansion of the roughness operator considered for Gaussian [3] or Poly-Gaussian [1], [5] random field builds the base of this approach, and this expansion has good agreement with the DSMC methods. We have used the approximations of momentum and energy exchange coefficients on the rough surface to solve the problem [1], [3]–[5].

The simulation of gas-surface interaction applying fractal and deterministic models of a roughness (especially constructed of flat elements [9] or sine waves) seem to be simpler [5], [12]. However, the simplicity of rough surface simulation does not affect the computation time appreciably and gives no advantages. Most difficult part of the calculation is not the simulation of roughness, but the computation of gas atom scattering from rough surface. Moreover, the computation time is even reduced in our method in comparison to the methods based on simple roughness models. In fact, the roughness operator \hat{S} contains the whole information about the roughness geometry. If we obtain the correct representation of \hat{S} and corresponding numerical algorithm, then there is no need to simulate the shape of the rough surface in the DSMC calculations.

The scattering function $V(\mathbf{v}, \mathbf{v}') = \hat{S}_1 V_0(\mathbf{v}, \mathbf{v}', \mathbf{n})$ on the rough surface (taking into account only the first reflection from the surface, if there are multiple collisions [4]) can be rewritten as:

$$V(\mathbf{v}, \mathbf{v}') = \frac{1}{M_1} \iint_{z_y < \cot \theta} dz_x dz_y V_0(\mathbf{v}, \mathbf{v}', \mathbf{n}) \frac{(\mathbf{n} \cdot \mathbf{v}')}{(\mathbf{n} \cdot \mathbf{N})(\mathbf{N} \cdot \mathbf{v}')} \int_{-\infty}^{\infty} p(z, z_x, z_y) \Pi^{(1)}(\theta, \sigma_1, z, z_x, z_y) dz \quad (1)$$

Here \mathbf{v} and \mathbf{v}' are the velocities of incident and reflected gas atoms, $\mathbf{v} = (0, -\sin \theta, -\cos \theta)$, $V_0(\mathbf{v}, \mathbf{v}', \mathbf{n})$ is the local scattering function on a smooth area on the rough surface, M_1 is the normalizing factor [5], \mathbf{n} and \mathbf{N} are local and global normal unit vectors to the rough surface (\mathbf{n} – to the smaller area on a rough surface), \mathbf{N} and z -axis are directed perpendicular to the mean level of the roughness, and $(\mathbf{n} \cdot \mathbf{v}')$ designates a scalar product of the vectors \mathbf{n} and \mathbf{v}' .

The joined Poly-Gaussian probability density p of the field $z(x, y)$ and of its derivatives $z_x = \partial z / \partial x$ and $z_y = \partial z / \partial y$ in directions x and y is defined by the formula:

$$p(z, z_x, z_y) = \int_0^{\infty} g_{x_0, y_0}^{v^2 r} (z, z_x, z_y) dF(v) \quad (2)$$

Here $g_{x_0, y_0}^{v^2 r} (z, z_x, z_y)$ is the probability density of Gaussian process with correlation function $v^2 r(h)$ and its derivatives in the point (x_0, y_0) of a gas atom interaction with the surface, $F(v)$ is a non-decreasing on the interval $[0; \infty)$ weighted function, and the correlation function $r(h)$ must satisfy the restriction: its spectrum must contain continuous component [1].

The main difficulty in the calculation of scattering function (1) on rough surface and of aerodynamic macro-parameters of the flow is the computation of the conditional (assuming the values of z, z_x, z_y to be given) probability $\Pi^{(1)}$ of the absence of the level-crossings between the random field $z(x, y)$ and the trajectory of the gas atom [1], [3]–[5].

3. Aerodynamic shadowing effect and corresponding stochastic integrals

The conditional probability $\Pi^{(1)}$ is defined as :

$$\Pi^{(1)}(\theta_1, \sigma_1, z, z_x, z_y) = P\{z(0, y) \leq z + y \cdot \cot \theta \mid z(0, 0) = z, z_x = z'_x(0, 0), z_y = z'_y(0, 0)\} \quad (3)$$

This probability $\Pi^{(1)}$ allows us taking into account aerodynamic shadowing effect, which consists in the shadowing of a noticeable part of the area on a rough surface by the dimples of the relief for incident or reflected rarefied gas atoms, consequently, this area does not take part in the interaction of these gas atoms with the surface. The calculation of scattering function (1) becomes much more simple without the factor (3), because $\Pi^{(1)}$ depends on the values of a random field along the trajectory of a gas atom. So (3) is the integral in functional space (continuum integral), and it must be approximated by the integrals of high dimension (in practice, of dimension not less than 200 [4]):

$$\Pi^{(1)}(\theta_1, \sigma_1, z, z_x, z_y) = \lim_{h \rightarrow 0} \int_{-\infty}^{u_1} d\eta_1 \int_{-\infty}^{u_2} d\eta_2 \dots \int_{-\infty}^{u_n} p(0, h, 2h, \dots, nh, z, \eta_1, \eta_2, \dots, \eta_n, z_x, z_y) d\eta_n \quad (4)$$

The joined Poly-Gaussian probability density $p(0, h, 2h, \dots, nh, z, \eta_1, \eta_2, \dots, \eta_n, z_x, z_y)$ of the field $z(x, y)$ and its derivatives $\eta_1, \eta_2, \dots, \eta_n$ in n points u_1, \dots, u_n , has the arguments $0, h, 2h, \dots, nh$, where h is a pitch of movement along the y -axis in the computation, so that the values $0, h, 2h, \dots, nh$ correspond to the equation of the trajectory of a gas atom near the point $(0, 0, z)$ of the first collision with the surface.

The expression (4) requires too much computing time, and becomes useless for DSMC procedure. The difficulty of taking into account aerodynamic shadowing effect applying continuum integral computation is the reason why this approach is developed only in St.-Petersburg and is ignored in most calculations of rarefied gas flow interacting with rough surface. For example, the calculations of scattering functions based on the other models of random roughness in [6], [8], [9] (not Gaussian or Poly-Gaussian) are simpler only because applied models do not take into account aerodynamic shadowing effect. The same same computational problem remains if we consider aerodynamic shadowing effect. Even rough surface constructed of flat elements, if they are distributed randomly, requires calculating of continuum integrals (4) to take into account aerodynamic shadowing effect of the roughness (p becomes joined probability density of the field $z(x, y)$ with corresponding distribution).

Only most simple deterministic models of the roughness like sine waves or other regular periodic functions permit computing of rarefied gas-surface interaction without calculating continuum integrals. But deterministic models do not take into account the micro-roughness, therefore this approach reduces substantially the influence of the roughness on scattering function (about 2–3 times in practical calculations).

The conditional probability $\Pi^{(1)}$ of absence of its level-crossings with the trajectory of a gas atom (3) (or (4)) depends only on the values of the random field under the trajectory of a gas atom, so we can consider only the profile of the surface in the plane of two vectors: of the local normal \mathbf{n} and of the velocity \mathbf{v} (or \mathbf{v}') of gas particle. Thus the probability $\Pi^{(1)}$ for a random process can be studied instead of more complicated probability $\Pi^{(1)}$ for a random field. Therefore we consider the properties of Poly-Gaussian random processes.

4. Analytic and asymptotic properties of Poly-Gaussian random processes

The probability density of Poly-Gaussian random process in n points having the coordinates x_1, \dots, x_n , corresponding to time arguments t_1, \dots, t_n , is the mixture of Gaussian densities defined by the formula:

$$p_{t_1, \dots, t_n}(x_1, \dots, x_n) = \frac{1}{(2\pi)^{n/2}} \int_0^\infty \frac{1}{\sqrt{|R_n(v)|}} \exp\left\{-\frac{1}{2}(\mathbf{x} - \sigma(v))R_n^{-1}(v)(\mathbf{x} - \sigma(v))^T\right\} dF(v) \quad (5)$$

Here \mathbf{x} is the vector $\mathbf{x} = (x_1, \dots, x_n)$, the distribution parameters $\sigma(v)$ and $R_n(v)$ are the vector of a mean value and the correlation matrix of the values of random process in n points, $|R_n(v)|$ and $R_n^{-1}(v)$ are the determinant and the inverse of the correlation matrix, the upper index T denotes transposition. The non-decreasing weighted function $F(v)$ defined by (2) can be as continuous, as well discrete (stepped). The only restriction is the convergence of the integral (5) (or (2)).

Known advantage of Poly-Gaussian random process is that it can approximate an arbitrary random process with any desired accuracy [13]. Additional advantage – the sample relief of Poly-Gaussian random process can be simulated numerically by the simple algorithm based on the transformation of Gaussian distributions [2]. This algorithm is developed for many applications like light scattering on rough surface, growing of thin films for the micro-electronics, surface diagnostics by electronic spectroscopy, a friction in machinery etc. [2]. The possibility of precise approximation of real micro-reliefs is verified also in different technology processes. In particular, rough surfaces are simulated which have been modeled as well by ionic bombardment of the steel using nitrogen ions, as by chemical etching of the steel by alcohol solution of nitric acid. In both cases very good agreement with experimental measurements is confirmed.

The techniques of similar type are applied to model the surfaces of flying vehicles moving in rarefied gas. Taking it into account, we pay attention to the properties of Poly-Gaussian processes concerning the simulation of the roughness in rarefied gas-surface interaction. Most interesting are so-called spherically-invariant (or spherically symmetric) processes, representing the important particular case of Poly-Gaussian processes [14]. These processes are building a sufficiently wide class to approximate real rough profiles on the one hand, and they have the parameters similar to the parameters of well known Gaussian processes on the other. Spherically-invariant processes are determined by their characteristic functions $\varphi(\xi_1, \dots, \xi_n) = \mathbf{E} \exp(\boldsymbol{\xi} \cdot \mathbf{x})$ of the order n (\mathbf{E} denotes mathematical expectation). Characteristic function depend only on the norm of the vector argument $\boldsymbol{\xi} = (\xi_1, \dots, \xi_n)$:

$\varphi(\xi_1, \dots, \xi_n) = \varphi_1(\boldsymbol{\xi} R_n \boldsymbol{\xi}^T)$. The correlation matrix R_n is positive definite, therefore the quadratic form $\boldsymbol{\xi} R_n \boldsymbol{\xi}^T$ can be represented as the squared norm of the vector $\boldsymbol{\xi}$. The scalar function $\varphi_1(r)$ is determining the distribution and can be expressed in terms of the Poly-Gaussian distribution (1):

$$\varphi_1(r) = \Gamma\left(\frac{n}{2}\right) \int_0^\infty \left(\frac{2}{rv}\right)^{(n/2)-1} J_{(n/2)-1}(rv) dF(v) \quad (6)$$

Here $J_k(rv)$ is Bessel function of the first kind, $F(v)$ is an arbitrary non-decreasing function. So spherically-invariant processes build a wide enough class of Poly-Gaussian random processes to simulate real rough profiles. Some properties of spherically-invariant processes are similar to the properties of Gaussian processes. For example, spherically-invariant processes have linear regression; if a spherically-invariant process is ergodic, then it has Gaussian distribution, i. e. the weighted function $F(v)$ is the unit step; if a spherically-invariant process is Markov, then it is Gaussian process. The last proposition is not obvious and was first proved in our papers [1].

To calculate the conditional probability $\Pi^{(1)}$ we apply suggested by Miroschin [10] Rice expansion in terms of the factorial moments N_m of m -th order of the number of the intersections of the random field with the trajectories of gas atoms:

$$\Pi^{(1)} = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!} N_m \quad (7)$$

The values N_m can be expressed as the $2m$ -fold integrals of the joint probability density of $z(x,y)$ and its derivatives η_i ($i=1,2,\dots,m$). From the generalized expression (2) of the probability density of Poly-Gaussian random field and of its derivatives we have derived the representation of the factorial moments N_m of m -th order of the number $A_u[0; T]$ of the excursions of the random field above the level u of a trajectory of a gas atom:

$$N_m(u) = \int_0^{\infty} N_m^G(u/v) dF(v) \quad (8)$$

Here N_m^G are the factorial moments of m -th order of the number of the excursions of corresponding Gaussian random field above the level u/v on the same interval $[0; T]$.

Asymptotic evaluation of the factorial moments $N_m(u)$ for high level u is well-known for Gaussian processes [11], and for Poly-Gaussian processes it takes the form:

$$\lim_{u \rightarrow \infty} N_k(T, u) = \lambda_2^k / c_1^{k-1}, \quad k = 1, 2, \dots, \quad (9)$$

Here the constant value λ_2 is defined by the asymptotic expansion of correlation function:

$$r(h) = 1 - \lambda_2 h^2 / 2 + O(|h|^{2+a}), \quad h \rightarrow 0, \quad (10)$$

The weighted function $F(v)$ in (8) must have a step on the right side of the interval, i.e. there exist v_0 such that the function $F(v) = 1$ for all $v > v_0$, and the left-sided limit at this point v_0 is less than 1: $\lim_{v \rightarrow v_0 - 0} F(v) < 1$. The meaning of

the last inequality is that the probability mixture determining Poly-Gaussian field has a Gaussian component with the maximal value of the mixing variable v . So the asymptotic evaluation of the number of the excursions of Poly-Gaussian process above the high level is similar to corresponding Gaussian asymptotic evaluation only if the weighed function $F(v)$ defines Gaussian component with the maximal value $v = v_0$ of the mixing variable. In all other cases asymptotically all the moments are substantially different.

Thus, all aerodynamic characteristics of the surface simulated by Poly-Gaussian random field can be noticeably different from the characteristics of the surface simulated by Gaussian random field. Typical Poly-Gaussian profiles and probability densities are clearly different from Gaussian profiles and probability densities [1].

The factorial moments $N_m(u)$ can be computed numerically applying the expression of Gaussian random process as an integral of a Wiener process [1].

5. DSMC computation of rarefied gas flow near rough surface

Obtained results can be applied to the problem of studying the influence of surface roughness on aerodynamic characteristics in rarefied gas flow in two ways.

1. It is possible to derive asymptotic evaluations describing studied influence on smooth surface. However, in this case we need to take into account that similar evaluations in Gaussian case are very complicated and they are containing integrals in a functional space – continuum integrals. The computation of these integrals requires their approximation by the integrals of higher dimensions (4). Besides, real surfaces always contain micro-roughness (even by the best processing), which could not be considered as smooth surface. Therefore asymptotic evaluations on smooth surface are not widely applied in practice. The main practical conclusion that could be made from asymptotic investigations (8)–(10) is that the influence of surface roughness for Poly-Gaussian model of roughness may be more noticeable, than for Gaussian model. It follows from the statement: each next factorial moment N_{m+1} turns to infinity sooner, than each previous one.
2. Poly-Gaussian model could be applied in numerical calculations, first of all in DSMC. In this case appropriate random field could be selected on preliminary stage of the computation applying obtained results to guarantee that selected random field satisfies two basic conditions. First, the roughness profiles of real surfaces applied in practice must be approximated well by the random field. Second, numerical procedures are to be optimized depending on physical and chemical characteristics of the gas and of the surface. Hence, the model of the roughness must have necessary properties for the best simulating rarefied gas atoms scattering from the surface.

Expanding the local scattering function $V_0(\mathbf{v}, \mathbf{v}', \mathbf{n})$ in a series in terms of the orthogonal functions $\zeta_k(\mathbf{n})$:

$$V_0(\mathbf{v}, \mathbf{v}', \mathbf{n}) = \sum_{k=0}^{\infty} b_k(\mathbf{v}, \mathbf{v}') \zeta_k(\mathbf{n}), \quad (11)$$

we obtain the most general expansion of the scattering function V on a rough surface:

$$V(\mathbf{v}, \mathbf{v}') = \sum_{k=0}^{\infty} b_k(\mathbf{v}, \mathbf{v}') K_k(\mathbf{v}, \mathbf{v}') \quad (12)$$

Here $b_k(\mathbf{v}, \mathbf{v}')$ are the coefficients in the original expansion (11), and the roughness integral operator \hat{S}_1 is defined by (1). Continuum integrals $K_k(\mathbf{v}, \mathbf{v}') = \hat{S}_1 \zeta_k(\mathbf{n})$ depend only on the parameters of the random field simulating the rough surface:

$$K_k(\mathbf{v}, \mathbf{v}') = \frac{1}{M_1} \iint_{z_y < \cot \theta} dz_x dz_y \zeta_k(\mathbf{n}) \frac{(\mathbf{n} \cdot \mathbf{v}')}{(\mathbf{n} \cdot \mathbf{N})(\mathbf{N} \cdot \mathbf{v}')} \int_{-\infty}^{\infty} g(z, z_x, z_y) \Pi^{(1)}(\theta_1, \sigma_1, z, z_x, z_y) dz \quad (13)$$

The values $K_k(\mathbf{v}, \mathbf{v}')$ are completely defined by gas atom trajectory and by roughness parameters: mean-square tangent σ_1 of the local normal vector \mathbf{n} and normalized correlation function $\rho(r)$. Hence, it is possible to compute these integrals preliminary, before the main DSMC computation of a rarefied gas flow. This proposition is valid for an arbitrary local scattering function $V_0(\mathbf{v}, \mathbf{v}', \mathbf{n})$ satisfying only one condition.

The scattering function $V_0(\mathbf{v}, \mathbf{v}', \mathbf{n})$ in our approach must have an approximation in the form (11) with only a few parameters to describe the physical and the chemical features of the gas and of the surface. Applied in practice scattering functions (including diffuse, specular, Nochilla, Cercignani–Lampis and others) satisfy this condition.

After the coefficients of the expansion (12) are computed, the distribution of the scattered from rough surface gas atoms can be calculated. Knowing the analytical scattering model for the smooth surface without a roughness, the estimated parameters can be transformed according to the integrals $K_k(\mathbf{v}, \mathbf{v}')$, computed at preliminary step. From the equations (11)–(13), it follows that the parameters for the rough surface are linear combinations of the parameters on the smooth surface; and the coefficients of the linear expansion depend on $K_k(\mathbf{v}, \mathbf{v}')$. Simulating the calculated distribution, we obtain the velocities \mathbf{v}' of the gas atoms that are scattered by the rough surface. In terms of the computational speed, our algorithm has an advantage over the methods that use simple geometrical models to simulate the shape of the rough surface [6], [8], [9]. This advantage is achieved by eliminating the need for the geometrical-shape simulation in DSMC; all the shape information is accounted for at the preliminary steps.

5. Comparison with experiment

Computational results are compared for two different models of a surface roughness with experimental data obtained in TSAGI [9]. The result is presented for argon atoms scattering from Kapton surface for incidence angle $\theta = 60^\circ$ (Fig.1).

The scattering function (indicatrix) on smooth surface without roughness is shown by dotted line; it is closer to diffuse scattering, than to specular or ray reflection, and coincides well with Nochilla and Cercignani–Lampis models.

Numerical results obtained by Erofeev, Friedlander et.al. [8] are presented by dash-dotted line.

The results on Poly-Gaussian surface with the same roughness parameters applying our algorithm are shown by solid lines.

Experimental results [8] for smooth (white, 1) and rough (black, 2) Kapton surface are presented using different signs.

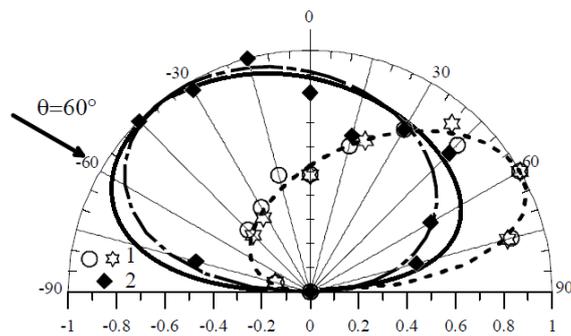


Figure 1: The argon scattering indicatrix on smooth and rough Kapton surfaces for incidence angle $\theta = 60^\circ$

Analyzing the graphs we can conclude that aerodynamic shadowing effect either has not been taken into account in [9], or considered partially: aerodynamic shadowing effect gives a wider indicatrix graph as well onwards, as in backwards direction. However, it is difficult to compare numerical results with the experiment because of large deviation in the scattering function experimental values in different directions. Both models demonstrate the effect of back scattering on a rough surface confirmed by the experiment.

Obtained by DSMC method results for momentum and energy exchange coefficients in this case are much closer to experimental results for both models and the difference between the results is not visible. But for some local scattering functions numerical DSMC computations show that the influence of surface roughness on momentum and energy exchange coefficients increases noticeably for poly-Gaussian model compared to Gaussian or to simple deterministic models.

5. Conclusion

Analytical and numerical investigation of the interaction of rarefied gas flows with a surface applying Gaussian, Poly-Gaussian and spherically-invariant models of surface roughness has discovered important advantages. Obtained results lead us to following conclusion.

1. Poly-Gaussian model of roughness allows to take into account aerodynamic shadowing effect on rough surface calculating the probability of absence of level-crossings and related functional integrals in scattering function. Suggested model is a generalization of Gaussian random field which is verified experimentally. Its statistical parameters have better coincidence with the parameters of real surfaces applied in practice. Basic statistical properties of the model are studied.
2. The results of direct simulation of rarefied gas flow with rough surface is carried out by Monte Carlo method for different models of roughness (including more simple models) are compared. The effect of aerodynamic shadowing effect on rough surface is studied for real surfaces and gases (for example Kapton surface and argon).
3. To reduce computing time in calculations the simulation of geometrical shape of the roughness must be taken into account preliminary in distribution coefficients before the main computation.
4. Applied statistical approach based on the Poly-Gaussian model is especially effective if surface roughness has noticeable influence on the macro-parameters of rarefied gas flows. The dependence of aerodynamics on surface roughness is more significant than for the Gaussian model.
5. The computational error increases with the main roughness parameter σ_1 – the mean-square tangent of the inclination angle.

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