DOI: 10.13009/EUCASS2022-4897
9TH EUROPEAN CONFERENCE FOR AERONAUTICS AND SPACE SCIENCES (EUCASS)

Aerodynamic Calculation of Rough Surface in Rarefied Gas Flow Applying the Solution of Inverse Problem

Olga A. Aksenova and Iskander A. Khalidov***
** St.-Petersburg Naval Polytechnic University, Department of Mathematics,*
17/1 Ushakovskaya Quai, 197045, St.-Petersburg, Russia; olga.a.aksenova@gmail.com
*** Peter the Great St.-Petersburg Polytechnic University, Department of Mathematics and Mechanics,*
195251, Polytechnicheskaya ul., 29, St.-Petersburg, Russia; iskander.khalidov@gmail.com

Abstract
The most effective method to determine the parameters of surface roughness in rarefied gas flow is the solution of the inverse problem, because applied in practical calculations profile diagrams show only the roughness of the largest scale. However, the main input into the influence of surface roughness on aerodynamic values takes the roughness of smaller scale [1]–[3], usually negligible on the profile diagram. Thus, the best way to find the roughness parameters is to calculate them from aerodynamic measurements, solving the inverse problem. Based on this solution algorithm allows us applying the results of our previous investigations concerning the problem of accounting surface roughness in aerodynamic calculation [1]–[3].

1. Introduction

Many aerodynamic experiments and calculations underestimate surface roughness. The influence of surface roughness on aerodynamic macroscopic parameters of rarefied gas flows is especially important because of two reasons. First, the velocities and other properties of gas molecules in rarefied gas flow without a boundary layer depend on the scattering kernel on the surface. Second, profile diagram measurement applied usually to obtain the parameters of surface roughness seems to be most simple and precise method to find the characteristics of the roughness. However, exact values of roughness parameters in rarefied gas could not be determined this way, because profile diagrams show only the roughness of the largest scale. Thus, the effect of surface roughness produced by the roughness of smaller scale remains unnoticed.

The main purpose of the present paper is to develop the algorithm of numerical calculation of rarefied gas flow near rough surface based on known solution of the inverse problem of determining the main surface roughness parameter from aerodynamic experimental data.

The main parameter characterizing surface roughness in basic technical applications is root-mean-square deviation of a rough surface $\sigma = (Mz^2)^{1/2}$. Here $z(x,y)$ is a deviation of random field simulating rough surface from its average level. Similar parameters of surface roughness are the average distance R_z between the highest peak and the lowest valley, and peak-to-peak distance. All these parameters are quite effective in different technical applications – like determining surface friction or destruction, and the interaction of rough surface with continuum flow. Nevertheless more relevant to the rarefied gas dynamics is the parameter $\sigma = \left(Mz_x^2\right)^{1/2} = \left(Mz_y^2\right)^{1/2}$ determined not by the height z, but by its partial derivatives $z_x = \partial z/\partial x$ and $z_x = \partial z/\partial y$ in directions x and y of a random field [1]–[6].

The parameter σ_1 describes root-mean-square values of the tangent of the angle θ_n between the local $\mathbf{n}$ and the global $\mathbf{N}$ normal vectors on rough surface. Hence, it is independent of the absolute values of the roughness amplitude. Usually the parameter σ_1 is obtained from statistical processing of profile diagram measurements, because it seems to be most exact method to find σ_1. However, the precision of determining the parameter σ_1 from experimental profile diagram measurements could be unsatisfactory, because profile diagrams show only the roughness of the largest scale. And the main input into the influence of surface roughness on aerodynamic values in rarefied gas is provided by the roughness of smaller scale, usually negligible on the profile diagram [1]–[4]. Moreover, the parameter σ_1 is not included in technical standard of surface quality. Hence, it is difficult to find the values of σ_1 in the literature. Therefore the only precise algorithm to determine the real values of the roughness parameter σ_1 is extracting it from aerodynamic measurements solving the inverse problem. The solution of this problem is based on analytical and numerical

DOI: 10.13009/EUCASS2022-4897

evaluation of the influence of surface roughness on scattering function and on momentum and energy exchange coefficients in rarefied gas flow.

2. Poly-Gaussian model of rough surface in rarefied gas flow

Analytical representation of scattering function V on a rough surface in the form $V = \hat{S} V_0$ allows deriving its expansion according to the number of gas atom collisions with the surface [5], [6]. Here the roughness operator $\hat{S}$ does not depend on physical and chemical parameters of the gas and of the surface. Consequently, it depends only on the geometrical shape of a roughness and on the trajectory of a reflected gas atom. Physical and chemical parameters influence only the local scattering function V_0 (scattering function on smooth surface without roughness). Gas particles are called atoms in considered problem, because the structure of the molecule is also accounted by the local scattering function V_0, and it does not affect the roughness operator $\hat{S}$.

The statement of the problem is based on the assumption that the number of rough irregularities in a small surface area dS is large, so that the scale of these irregularities is smaller than the aerodynamic scale of the flow [6]. Therefore, the characteristic scale of the roughness is smaller than the characteristic scale of the flow. Only this assumption permits to separate roughness operator $\hat{S}$ and local scattering function V_0.

The approach for solving the problem of simulating the gas atoms scattering from a rough surface numerically has been developed in our previous papers [1]–[4]. This approach is based on the expansion of the roughness operator considered for Gaussian [5] or poly-Gaussian random field. We have used the approximations of momentum and energy exchange coefficients on the rough surface to solve the problem [1]–[5]. DSMC method, applied together with discussed expansion, becomes especially effective.

It seems to be simpler to apply fractal and deterministic models of a roughness (especially constructed of flat elements [7] or sine waves) simulating gas-surface interaction [8]–[10]. However, most difficult part of the calculation is not the simulation of roughness, but the computation of gas atom scattering from rough surface. Thus, the simplicity of rough surface simulation does not affect the computation time appreciably [3] and gives no advantages. Moreover, our method reduces the computation time in comparison to the methods based on simple roughness models, because the whole information about the roughness geometry contains the roughness operator $\hat{S}$. 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.

Poly-Gaussian model of the roughness is more general, than Gaussian homogeneous isotropic random fields studied in St.-Petersburg State University [5], [6]. Both models have several advantages in comparison with other different more simple models of surface roughness applied in practice, including polygonal-line roughness [7], fractal [5], [11], conical-hole based model of the roughness [8], and the surface constructed of flat elements [9]–[10]. In particular, these simple models take into account only the input of large-scale roughness into momentum and energy exchange coefficients on the surface [5]. So simple models have no possibility to take into account the micro-roughness (the roughness of small scale) – it is the advantage of poly-Gaussian model. Moreover, this model is confirmed on the base of experimental data [12].

Gaussian and poly-Gaussian models have following additional basic advantages. First, Poly-Gaussian and Gaussian random fields are differentiable (unlike the surface constructed of flat elements), so that the local normal exists everywhere on the surface under simple conditions [4], [5]. Second, the simulation of different real surfaces processed in various ways is easy by simple variation of the parameters (scale coefficients, correlation function and weighted function). And, third, analytic representation of stochastic characteristics of the number of the crossings of inclined trajectory of a gas atom by the random field (such as the probability of the absence of the crossings) simplifies numerical Monte Carlo calculation of gas-surface interaction.

The reason to prefer poly-Gaussian model of roughness (to Gaussian one) is explained in [12] and in [4]: “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.”

Approximation of real micro-reliefs confirms the precision of poly-Gaussian model in different technology processes. In particular, the model has been applied to simulate rough surfaces produced as by ionic bombardment of the steel using nitrogen ions, as well as by chemical etching of the steel by alcohol solution of nitric acid. In both cases, a very good coincidence has been verified. If we compare with the profiles of real surfaces applied for space vehicles (for instance, metallic or synthetic), then we conclude that poly-Gaussian models are closer to reality.

DOI: 10.13009/EUCASS2022-4897

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 [5]) can be rewritten as

$$V(\mathbf{v},\mathbf{v}') = \frac{1}{M_1} \iint\limits_{z_y<\cot\theta} dz_x\, dz_y\; V_0(\mathbf{v},\mathbf{v}',\mathbf{n})\, \frac{(\mathbf{n}\cdot\mathbf{v}')}{(\mathbf{n}\cdot\mathbf{N})(\mathbf{N}\cdot\mathbf{v}')} \int\limits_{-\infty}^{\infty} p(z,z_x,z_y)\,\Pi^{(1)}(\theta,\sigma_1,z,z_x,z_y)\,dz. \qquad \textbf{(1)}$$

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, M_1 is the normalizing factor [3]. Scalar product of the vectors $\mathbf{n}$ and $\mathbf{v}'$ is denoted by $(\mathbf{n}\cdot\mathbf{v}')$, $\mathbf{n}$ 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 (Fig.1).

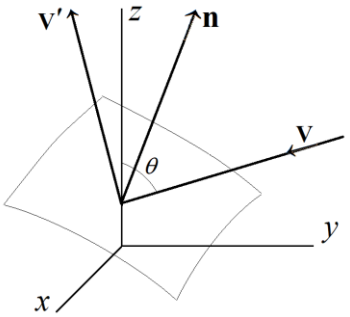

Figure 1: First reflection of a gas atom from smaller area on a rough surface

The expression (1) of scattering function contains two roughness parameters:

- the square mean derivative σ_1;
- functional roughness parameter: the normalized correlation function ρ of the random field $z(x,y)$.

The values σ_1 and ρ are most important for gas interaction, because all the other statistical parameters of the roughness (σ, R_z, skewness coefficient etc.) can be expressed in terms of main rough surface parameters σ_1 and ρ.
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

$$p(z,z_x,z_y) = \int\limits_0^{\infty} g^{v^2 r}_{x_0,y_0}(z,z_x,z_y)\,dF(v), \qquad \textbf{(2)}$$

where $g^{v^2 r}_{x_0,y_0}(z,z_x,z_y)$ is probability density of Gaussian process with correlation function $v^2 r(h)$ and its derivatives in the point t_0 of a gas atom interaction with the surface. Here $F(v)$ 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 [3].

3. Aerodynamic shadowing effect in rarefied gas on rough surface

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 probability $\Pi^{(1)}$ of the absence of the level-crossings between the random field $z(x,y)$ and the trajectory of the gas atom (assuming the values of z, z_x, z_y to be given) [1], [5], [6]

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

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

DOI: 10.13009/EUCASS2022-4897

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 [5])

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

Here (0, 0, z) is the point of the first collision of a gas atom with the surface, and p is joined poly-Gaussian probability density of the field $z(x,y)$ and its derivatives $\eta_1, \eta_2, \dots, \eta_n$ in n points u_1, ..., u_n, placed along the trajectory of the atom. Considered points are distributed uniformly along the x–axis ($x = 0, h, 2h, \dots, nh$), and h is a pitch of movement along the y–axis in the computation.

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, in [7], [8], [9]).

However, the same problem remains if other random models of the roughness are applied (not Gaussian or poly-Gaussian). 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. However, 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. Hence, only the profile of the surface can be considered in the plane of two vectors: of the local normal **n** and of the velocity **v** (or $\mathbf{v}'$) of gas particle. Thus, it is necessary to study only the probability $\Pi^{(1)}$ for a random process instead of more complicated probability $\Pi^{(1)}$ for a random field. Therefore, we consider the properties of poly-Gaussian random processes.

The probability density of poly-Gaussian random process in n points x_1, ..., x_n, corresponding to the arguments t_1, ..., t_n, is the mixture of Gaussian densities defined by the formula

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

where $\mathbf{x} = (x_1, \dots, x_n)$. Here $\sigma(v)$ and $R_n(v)$ are the vector of a mean value and the correlation matrix of the values of random process in n points, $|R_n(v)|$ is the determinant of the correlation matrix, $R_n^{-1}(v)$ – its inverse, the upper index T denotes transposition, $F(v)$ is a non-decreasing on the interval [0;∞) weighted function. The function $F(v)$ can be as continuous, as well discrete (stepped) – only the convergence of the integral is necessary.

In addition to discussed above merits of considered random fields, Poly-Gaussian random process has two more known advantages:

– it can approximate an arbitrary random process with any desired accuracy [13].

– the sample relief of poly-Gaussian random process can be simulated numerically by the simple algorithm based on the transformation of Gaussian distributions [12].

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. [12]. The possibility of precise approximation of real micro-reliefs is confirmed also in different technology processes. In particular, rough surfaces are simulated which have been modelled 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, experimental measurements confirmed numerical results with high precision. The techniques of similar type are applied to model the surfaces of flying vehicles moving in rarefied gas.

DOI: 10.13009/EUCASS2022-4897

4. Applying Rice expansion in numerical calculations of rarefied gas atoms scattering from rough surface

Suggested by Miroshin [6] Rice expansion we apply to calculate the conditional probability $\Pi^{(1)}$ in (1)–(4). This 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 has the form

$$\Pi^{(1)} = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!} N_m . \qquad \textbf{(6)}$$

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,…m). 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 has been derived in [14] from the generalized expression (2) of poly-Gaussian probability density of random field and of its derivatives

$$N_m(u) = \int_0^{\infty} N_m^G\left(\frac{u}{v}\right) dF(v) . \qquad \textbf{(7)}$$

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 $\frac{u}{v}$ 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 [6], and for poly-Gaussian (spherically-invariant [15]) processes it takes the form

$$\lim_{u\to\infty} N_k(T,u) = \frac{\lambda_2^k}{c_1^{k-1}}, \quad k = 1, 2, \ldots , \qquad \textbf{(8)}$$

where the constant value λ_2 is defined by the asymptotic expansion $r(h) = 1 - \frac{1}{2}\lambda_2 h^2 + O\left(|h|^{2+a}\right)$ of correlation function for $h \to 0$, and the weighted function $F(v)$ has a step on the right side of the interval, i. e. for some v_0 the function $F(v) = 1$ for all $v > v_0$, and the left-sided limit at this point v_0 is less than 1: $\lim_{v\to v_0-0} F(v) < 1$. This inequality means that the probability mixture determining poly-Gaussian field has Gaussian component with the maximal value of the variable v. Thus, 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 of the variable v_0. In all other cases asymptotically all the moments (8) are substantially different, i. e. 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 (5) are clearly different from Gaussian profiles and probability densities as presented in [12].

Numerically the factorial moments $N_m(u)$ (7) can be computed applying the expression of Gaussian random process as an integral of a Wiener process [5], [16].

There are two possibilities to apply obtained results to the problem of studying the influence of surface roughness on aerodynamic characteristics in rarefied gas flow.

On one hand, 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 high 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 is that the influence of surface roughness for poly-Gaussian model of roughness may be more noticeable, than for Gaussian model (because each next factorial moment N_{m+1} turns to infinity sooner, than each previous one).

DOI: 10.13009/EUCASS2022-4897

On the other hand, it is possible to apply poly-Gaussian model in numerical DSMC calculations. Obtained results allow us selecting appropriate random field on preliminary stage of the computation so that it could satisfy two conditions.
1. The random field must approximate well the roughness profiles of real surfaces applied in practice.
2. It must have necessary properties for optimizing numerical procedures (depending on physical and chemical characteristics of the gas and of the surface) for the best simulating rarefied gas atoms scattering from the surface.
The most general expansion of the scattering function V on a rough surface

$$V(\mathbf{v},\mathbf{v}') = \sum_{k=0}^{\infty} b_k(\mathbf{v},\mathbf{v}') K_k(\mathbf{v},\mathbf{v}'), \tag{9}$$

could be obtained from the expansion of the local scattering function $V_0(\mathbf{v},\mathbf{v}',\mathbf{n})$ in a series in terms of the orthogonal functions $\varsigma_k(\mathbf{n})$

$$V_0(\mathbf{v},\mathbf{v}',\mathbf{n}) = \sum_{k=0}^{\infty} b_k(\mathbf{v},\mathbf{v}') \varsigma_k(\mathbf{n}), \tag{10}$$

where $b_k(\mathbf{v},\mathbf{v}')$ are the coefficients in the expansion (9) or (10), and $K_k(\mathbf{v},\mathbf{v}') = \hat{S}_1 \varsigma_k(\mathbf{n})$ are continuum integrals depending only on the parameters of the random field simulating the rough surface

$$K_k(\mathbf{v},\mathbf{v}') = \frac{1}{M_1} \iint\limits_{z_y < \cot\theta} dz_x\, dz_y\; \varsigma_k(\mathbf{n}) \frac{(\mathbf{n}\cdot\mathbf{v}')}{(\mathbf{n}\cdot\mathbf{N})(\mathbf{N}\cdot\mathbf{v}')} \int_{-\infty}^{\infty} g(z,z_x,z_y)\,\Pi^{(1)}(\theta_1,\sigma_1,z,z_x,z_y)\,dz\,. \tag{11}$$

The values $K_k(\mathbf{v},\mathbf{v}')$ are completely defined by gas atom trajectory and by roughness parameters: σ_1 and $\rho(r)$. Thus, it is possible to compute these integrals preliminary, before the main DSMC computation of a rarefied gas flow. This proposition is valid in our approach for an arbitrary local scattering function $V_0(\mathbf{v},\mathbf{v}',\mathbf{n})$ with only one restriction. The scattering function $V_0(\mathbf{v},\mathbf{v}',\mathbf{n})$ must have an approximation in the form (10) 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. Fig.2 shows an example of computed integral (11) depending on roughness parameter σ_1. The decreasing of the accuracy for σ_1>1/3 and θ>70° could be explained by insufficient number of the realizations of random field in computation.

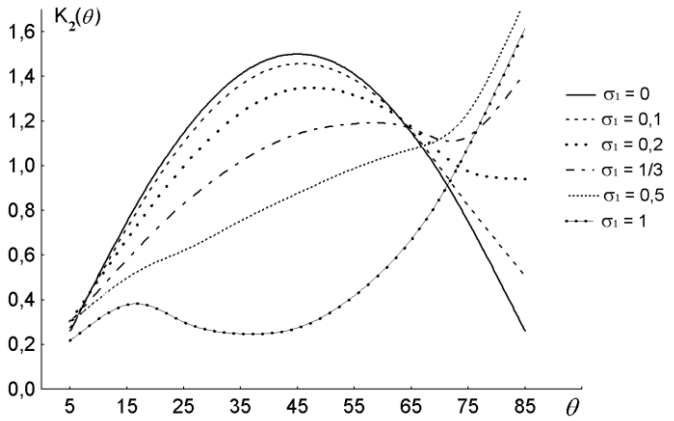

Figure 2: Continuum integral (11) depending on σ_1 and on the incidence angle θ (in deg.)

Knowing the analytical scattering model for the smooth surface without a roughness, the estimated parameters $b_k(\mathbf{v},\mathbf{v}')$ in (9) can be transformed according to the roughness operator in (11). The integrals (11) we must compute at preliminary step. From the equations (9)–(11), it follows that the parameters for the rough surface are linear combinations of the parameters on the smooth surface; the coefficients of the linear expansion depend on the values $K_k(\mathbf{v},\mathbf{v}')$. 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

DOI: 10.13009/EUCASS2022-4897

geometrical models to simulate the shape of the rough surface [7], [8], [9]. Eliminating the need for the geometrical-shape simulation in DSMC, and taking into account all the shape information at the preliminary steps allows us to achieve this advantage.

Applying all considered methods of the calculation of surface roughness effect in rarefied gas, we propose following solution algorithm for aerodynamic calculation of rarefied gas flow on the base of the solution of inverse problem.

1. Determining the set of the orthogonal functions $\varsigma_k(\mathbf{n})$ (we have applied trigonometric approximations used in the local interaction theory).
2. Expanding the local scattering function $V_0(\mathbf{v},\mathbf{v}',\mathbf{n})$ in a series in terms of the system $\varsigma_k(\mathbf{n})$; hence the coefficients $b_k(\mathbf{v},\mathbf{v}')$ are calculated.
3. Computing the integrals $K_k(\mathbf{v},\mathbf{v}')$ (11) in function space of the realizations of random field. The values (11) must be calculated for different number *k*, incidence angles, reflection angles and for different values of roughness parameter σ_1. Then it is necessary to expand obtained integrals $K_k(\mathbf{v},\mathbf{v}')$ in function space in a series in terms of the system $\varsigma_k(\mathbf{N})$ for different values of σ_1 and k (where **N** is the normal vector to the average level of rough surface).
4. Expanding the scattering function $V(\mathbf{v},\mathbf{v}')$ on rough surface (or the momentum and energy exchange coefficients obtained from the experimental data) in a series in terms of the system $\varsigma_k(\mathbf{N})$.
5. Calculating the values of $K_k(\mathbf{v},\mathbf{v}')$ from two expansions of $V(\mathbf{v},\mathbf{v}')$ in a series in terms of orthogonal functions $\varsigma_k(\mathbf{N})$ with the coefficients $b_k(\mathbf{v},\mathbf{v}')$. If the known experimental values of $V(\mathbf{v},\mathbf{v}')$ are here applied, then the solution of the inverse problem is obtained, finding as the roughness parameter σ_1, as well the correlation function from calculated $K_k(\mathbf{v},\mathbf{v}')$.
6. Computing the scattering function *V* on a rough surface by (9)–(11) gives finally the dependence of $V(\mathbf{v},\mathbf{v}')$ on surface roughness.
7. Substituting the expansion (9) into the integrals representing momentum *p*, τ and energy *q* exchange coefficients, we obtain the dependence of *p*, τ and energy *q* on surface roughness.

5. Rarefied gas atoms scattering from rough surface: DSMC computation

According to the proposed algorithm, it is necessary to solve the inverse problem on its first stage. Therefore, we need original experimental measurements of aerodynamic values (scattering function, momentum or energy exchange coefficients) on the same surface with different roughness parameters. Unfortunately, only few known experiments in rarefied gas satisfy these conditions. Testing our algorithm for the solution of the inverse problem, we have applied experimental data from [9] and [10].

The comparison of computational results for two different models of a surface roughness with experimental data obtained in TSAGI [9]–[10] is presented for argon atoms scattering from Kapton surface for incidence angles $\theta = 60°$ and $\theta = 60°$ (Fig.3).

Dotted line presents the scattering function (indicatrix) on smooth surface without roughness; it is closer to diffuse scattering, than to specular or ray reflection, and coincides well with Nochilla and Cercignani–Lampis models. Dash-dotted line shows the numerical results obtained by Erofeev, Friedlander et.al. [9]. Solid lines demonstrate our results on poly-Gaussian surface with the same roughness parameters. Different signs present experimental results [9] for smooth (white, 1) and rough (black, 2) Kapton surface.

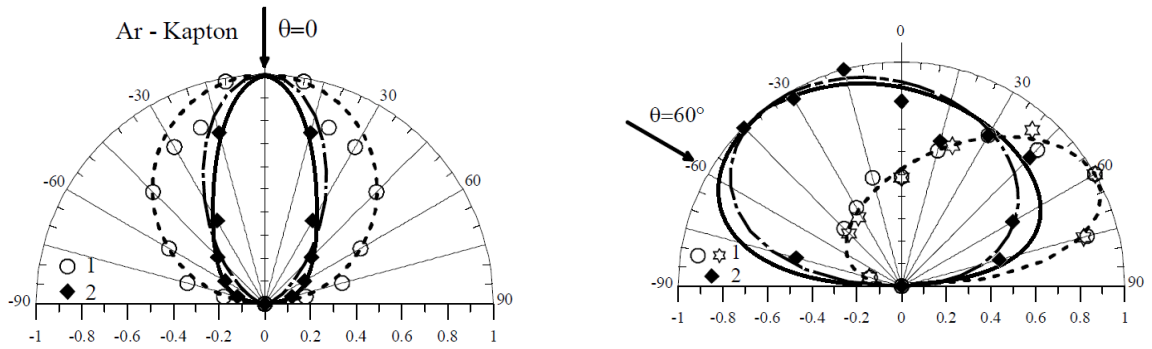

Figure 3: The argon scattering indicatrix on smooth and rough Kapton surfaces for incidence angles θ=0°; θ=60°.

DOI: 10.13009/EUCASS2022-4897

Comparing numerical results of direct simulation with the experiment and analysing the graphs we can conclude that either aerodynamic shadowing effect failed to take into account in [9], or considered partially: aerodynamic shadowing effect gives a wider indicatrix graph as well onwards, as in backwards direction.
The results depend on the local scattering kernel, and the solution of inverse problem shows that the value of σ_1 obtained by proposed algorithm from experimental data is 10%–30% higher than the value of σ_1 from the profile diagram measurements (or from direct measurements of geometrical parameters of artificial roughness). The difference is the input of the roughness of smaller scale not visible on profile diagrams.
Similar results are obtained from another experimental measurements in [9] and [10], for example from the normal momentum exchange coefficients of reflected gas flow (Ar and He) for different molecular energy E of incident molecular beam and different (Kapton or aluminium) surface roughness. The calculated value of σ_1 is 5%–35% higher in all computations than in profile diagram measurements.
Numerical DSMC computations for some local scattering functions have demonstrated, 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 one.

6. Conclusion

Considered Gaussian and poly-Gaussian models of surface roughness allow us precise accounting surface roughness in rarefied gas flow near rough surface. Necessary stage of the algorithm is analytical and numerical solution of the inverse problem of determining surface roughness parameter σ_1 in the interaction with rarefied gas flow. Obtained results lead us to following conclusion.

1. The solution of inverse problem is the best way to determine surface roughness parameters, because the roughness parameter σ_1 is not measured in the experiments: it is not included in technical standard of surface quality. Moreover, profile diagrams show only the roughness of the largest scale, hence the precision of measuring σ_1 from the profile diagram could be low. The computational error of proposed algorithm increases with σ_1.
2. Poly-Gaussian model of roughness, applied to take into account aerodynamic shadowing effect on rough surface, permits constructing the most effective solution of inverse problem. Taking into account aerodynamic shadowing effect on rough surface (which is usually underestimated), we need to calculate the probability of absence of level-crossings and related function space integrals in scattering function. Statistical parameters of this model (verified by experiment) have better coincidence with the parameters of real surfaces applied in practice. For instance, Poly-Gaussian model has been applied to simulate rough surfaces produced in different technology processes.
3. Solving both direct and inverse problems of surface roughness, the best way to reduce computing time is simulating the random field (modeling rough surface) preliminary, before the main DSMC computation of rarefied gas flow. This structure of computational algorithm allows obtaining time economy for the same precision even in comparison with more simple models of roughness.
4. Proposed algorithm is verified for different models of roughness, and the effect of aerodynamic shadowing on rough surface is studied for real surfaces (like Kapton and Al) and gases (like Ar and He).
5. The value of σ_1 obtained from the solution of inverse problem is substantially higher (up to 30–35%) than the value of σ_1 from the profile diagram measurements. Thus, this example confirms the advantage of our method of accounting surface roughness on the base of preliminary determining roughness parameter σ_1 from the solution of inverse problem.

References

[1] O. A. Aksenova, and I. A. Khalidov, 2019. Inverse Problem of Finding Surface Roughness Parameters in Rarefied Gas Flow. In: *Rarefied Gas Dynamics*, AIP Conference Proceedings 2132: 1700051–1700058.
[2] O. A. Aksenova, and I. A. Khalidov, 2016. Analytic Model of the Effect of Poly-Gaussian Roughness on Rarefied Gas Flow near the Surface. In: *Rarefied Gas Dynamics*, AIP Conference Proceedings 1786:1000071–1000078.
[3] I. A. Khalidov, 2014. Application of Poly-Gaussian Random Processes for the Simulation of Rough Surface in Rarefied Gas Flow. *St.Petersburg University Vestnik*. Ser.1, **59**, No.3: 428–436 (in Russian).
[4] I. A. Khalidov, 2014. Study of rarefied gas flow interaction with rough surface on the base of poly-Gaussian mathematical model. *St.Petersburg State Polytechnic University Journal*. No.4: 129–138 (in Russian).

DOI: 10.13009/EUCASS2022-4897

[5] O. A. Aksenova, and I. A. Khalidov, 2004. Comparison of Fractal and Statistical Models of Surface Roughness in the Problem of Rarefied Gas Atoms Scattering. *St.Petersburg University Vestnik*. Ser.1, No.1: 61–66 (in Russian).
[6] R. N. Miroshin, 1981. Intersections of Curves with Gaussian Processes. St.-Petersburg University Publishers, 1–280 (in Russian).
[7] A. Ukhov, B. Porodnov, and S. Borisov, 2009. Numerical Simulation of Gas Dynamics Conductivity of Micro Channels with Consideration of Surface Structure. In: *Rarefied Gas Dynamics*, AIP Conference Proceedings 1084, edited by Takashi Abe. 712–717.
[8] N. E. Gimelshein, T. C. Lilly, S. F. Gimelshein, A. D. Ketsdever, and I. J. Wysong, 2007. Surface Roughness Effects in Low Reynolds Number Nozzle Flows. In: *Rarefied Gas Dynamics*, edited by M. S. Ivanov and A. K. Rebrov (Novosibirsk: Siberian Branch of RAS): 695–702.
[9] A. I. Erofeev, O. G. Friedlander, et al., 2012. The Influence of Roughness of the Surface on the Interchange of Momentum between Gas Flow and Solid Surface. In: *Rarefied Gas Dynamics*, AIP Conference Proceedings 1501, edited by M. Mareschal. 1168–1174.
[10] A. I. Erofeev, A. P. Nikiforov, *et al.*, 2016. The Influence of the Roughness of the Surface on Scattering of Free-Molecular Gas Flow from Solid Bodies. TSAGI Journal, **47**, 4, pp. 12–27 (in Russian).
[11] O. A. Aksenova, 2001. *Mathematical Modeling* **13**, No.7, pp. 99–103 (in Russian).
[12] M. Litvak, and V. Malyugin, 2012. Poly-Gaussian Models of a non-Gaussian Randomly Rough Surface. *J. Technical Phys*. **57**, No.4:524–533.
[13] Sh. M. Chabdarov, and A. T. Trofimov, 1975. Poly-Gaussian Representations of Interferences and Descrete Signals Reception. *Radio Engineering and Electronics*, 20, No.4: 734–745 (in Russian).
[14] O. A. Aksenova, and I. A. Khalidov, 2004. Surface Roughness in Rarefied Gas Aerodynamics: Statistical and Fractal Models. St.Petersburg, St.Petersburg University Publishers:1–120 (in Russian).
[15] Kung Yao, 1973. IEEE Transactions on Information Theory, **19**, No.5., pp. 600–608.
[16] *Rough Surfaces*, 1982. Edited by N. R. Thomas, Longman Groups, London. 1–261.