Determination of roughness parameters of the surface interacting with rarefied gas flow

I A Khalidov
Peter the Great St. Petersburg Polytechnic University, 29 Polytechnicheskaya, St. Petersburg, 195251, Russia
E-mail: iskander.khalidov@gmail.com

Abstract. Numerical algorithm is proposed to determine the real values of surface roughness parameter \( \sigma_1 \) from aerodynamic measurements in rarefied gas flow. This algorithm is based on the solution of the inverse problem because the main input into the influence of surface roughness on aerodynamic values is contributed by the roughness of smaller scale. This roughness is usually negligible on the profile diagram, even if the roughness parameter \( \sigma_1 \) is measured in the experiment from the profile diagram. Moreover, the parameter \( \sigma_1 \) is not included in technical standard of surface quality: the main parameter defining surface roughness according to usual standard procedures is not \( \sigma_1 \), but the square mean deviation \( \sigma \) of the height of the surface. To solve the inverse problem we apply the simulation of surface roughness on micro-level by Gaussian or poly-Gaussian random field and the expansion of the scattering function on rough surface which has been applied earlier to solve the direct problem of studying the effect of surface roughness in rarefied gas flow. The value of roughness parameter \( \sigma_1 \) obtained from the solution of inverse problem is substantially higher than the value of \( \sigma_1 \) from the profile diagram measurements.

1. Introduction
Most of aerodynamic experiments in rarefied gas are performed without measuring surface roughness parameters. Therefore it is difficult to apply the results of our previous investigations concerning the problem of accounting surface roughness in aerodynamic calculation [1]–[3]. Rough surface is simulated here by random field, and \( z(x,y) \) is its deviation from its average level. The parameters of surface roughness are obtained usually from profile diagram measurements: it seems to be most simple and precise method to find the characteristics of the roughness. This approach is most effective in different technical applications including the interaction of rough surface with continuum flow, where surface roughness is characterized either by the main parameter – root-mean-square deviation of a rough surface \( \sigma = \sqrt{M_{z^2}} \) or by the average distance \( R_z \) between the highest peak and the lowest valley (or similar peak-to-peak distance).

In rarefied gas dynamics main roughness parameter \( \sigma_1 \) is independent of the absolute values of the roughness amplitude and describes root-mean-square values of the tangent of the angle \( \theta_n \) between the local \( \mathbf{n} \) and the global \( \mathbf{N} \) normal vectors on rough surface. This parameter \( \sigma_1 = \sqrt{M_{z_x^2}} = \sqrt{M_{z_y^2}} \) is determined by partial derivatives \( z_x = \frac{\partial z}{\partial x} \) and \( z_y = \frac{\partial z}{\partial y} \) in directions \( x \) and \( y \) of a random field [1]–[6]. Even if the roughness parameters are measured (like special aerodynamic experiments [4]–[5]), the
precision of measuring the roughness parameter $\sigma_1$ in the experiment could be unsatisfactory, because $\sigma_1$ is evaluated from the profile diagram. However, profile diagrams show only the roughness of the largest scale, and 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.

Therefore the only precise algorithm to determine the real values of the roughness parameter $\sigma_1$ is extracting it from aerodynamic measurements solving the inverse problem. The solution of this problem is based on analytical and numerical evaluation of the influence of surface roughness on scattering function and on momentum and energy exchange coefficients in rarefied gas flow.

2. Simulation of rough surface by Gaussian or Poly-Gaussian random field.

The algorithm of numerical simulation of gas atoms scattering from a rough surface has been developed in our previous papers [1]–[3]. This approach is based on the expansion of the roughness operator considered for Gaussian [6] or poly-Gaussian random field [1]–[3], [8]. 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], [6].

Gaussian model of rough surface has two main advantages.

- The parameters of the model have simple analytical expressions in terms of the basic statistical parameters of random field – for instance, in terms of its first and second moments (average value and variance). It allows us adjusting numerically the parameters of the model to approximate exactly the roughness parameters obtained from experimental profile measurements to compare numerical results with experimental data.

- The simple and effective numerical algorithm of random field simulation could be used to compute the mean values of the functionals (or of the operators) by averaging over the set of simulated surface realizations.

However, Gaussian model is insufficient for the approximation of all real surfaces used in practice. More universal approach based on Gaussian probability density mixtures leads us to more general poly-Gaussian model allowing approximation of an arbitrary random process with any desired accuracy [7].

The numerical algorithm for the approximation of poly-Gaussian random processes based on the transformation of Gaussian distributions is described in [8]. This algorithm is developed for applications like light scattering on rough surface, growing of thin films for the micro-electronics, surface diagnostics by electronic spectroscopy, friction and wear in machinery etc. The possibility of precise approximation of real micro-reliefs is confirmed in different technology processes. In particular, rough surfaces are simulated which have been produced 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 a very good coincidence is confirmed. Taking into account that the techniques of similar type are applied to produce the surfaces of flying vehicles moving in rarefied gas, we have confirmed numerically that poly-Gaussian random fields can be applied successfully to simulate the roughness in rarefied gas-surface interaction [1]–[2].

3. Application of poly-Gaussian model to the calculation of integrals in function space

The velocity distribution of gas atoms (or molecules) reflected from rough surface is described by the scattering function $V$. The expansion of scattering function $V$ on a rough surface is derived from its analytical representation in the form $V = \hat{S} V_0$, where the roughness operator $\hat{S}$ depends only on the geometrical shape of a roughness and on the trajectory of a reflected gas atom [6]. 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). Investigating the roughness operator $\hat{S}$ we can describe all gas particles as 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 $\hat{S}$. According to the random field theory the operator $\hat{S}$ can be expanded in a
series within the statistical model of the roughness [6]: $S = \sum_{m=1}^{\infty} S_m$. Taking into account the shading of the dimples of the relief makes the calculation of the integrals in roughness operator $\hat{S}$ very complicated. The main difficulty 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]–[3], [6]

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

Here $\theta_i$ is the incident angle of gas atoms, and roughness operator $\hat{S}$ contains this probability $\Pi^{(1)}$ even if we consider only the contribution $\hat{S}_i$ of the first collisions to the surface scattering function [6]. Originally the conditional probability $\Pi^{(1)}$ represents an integral in a function space of the samples of a random field, or so-called continuum integral. To compute the continuum probabilities of this type they have to be approximated by the integrals of high dimensions

$$\Pi^{(1)}(\theta, \sigma_1, z, z_x, z_y) = \lim_{n \to \infty} \prod_{i=1}^{n} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} p(0, h, 2h, \ldots, nh, z, \eta_1, \eta_2, \ldots, \eta_n, z_x, z_y) \, d\eta_n. \quad (2)$$

The computation of these multiple integrals of increasing dimensions is the most difficult part of the problem. The function $p(0, h, 2h, \ldots, nh, z, \eta_1, \eta_2, \ldots, \eta_n, z_x, z_y)$ in (2) is the joined probability density of the random field $z(x,y)$ and its derivatives $\eta_1, \eta_2, \ldots, \eta_n$ in the points $(0, h, 2h, \ldots, nh)$ placed uniformly under the trajectory of a gas particle (assuming the values of $z, z_x, z_y$ to be given).

If we apply the poly-Gaussian model of random field, this density is determined as a mixture of Gaussian probability densities [8], so we can derive 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 particle

$$N_m(u) = \int_0^u N_m^G \left( \frac{u}{v} \right) \, dF(v), \quad (3)$$

where $N_m^G$ are the factorial moments of $m$-th order of the number of the excursions of corresponding Gaussian random field above the level $u$ on the same interval $[0; T]$. From the eq. (3) similar representation of the conditional probability (1) can be obtained using Rice series [6].

4. **Numerical solution of inverse problem of determining the parameters of surface roughness**

More detailed representation of scattering function $V$ on a rough surface can be written in a form

$$V(v, v') = \sum_{k=0}^{\infty} b_k(v, v') K_k(v, v'), \quad (4)$$

if the local scattering function $V_0(v, v', n)$ is expanded in a series in terms of the orthogonal functions $\zeta_k(n)$

$$V_0(v, v', n) = \sum_{k=0}^{\infty} b_k(v, v') \zeta_k(n), \quad (5)$$
where \( \mathbf{v} \) and \( \mathbf{v}' \) are the velocities of incident and reflected gas atoms, \( b_k(\mathbf{v}, \mathbf{v}') \) are the coefficients in the expansions (4) and (5), and \( K_k(\mathbf{v}, \mathbf{v}') \) are continuum integrals depending only on the parameters of the random field simulating the rough surface

\[
K_k(\mathbf{v}, \mathbf{v}') = \frac{1}{M_1} \int_{z_i < \cot \theta} dz_i \int_{z_f} dz_f \frac{(n \cdot \mathbf{v}')}{(n \cdot \mathbf{N})(\mathbf{N} \cdot \mathbf{v}')} \int_{-\infty}^{\infty} g(z_i, z_i', z_f') \Pi^{(1)}(\theta, \sigma_1, z_i, z_f', z_f') dz_f'.
\]  

Here \( M_1 \) is the normalizing factor [6], \( (n \cdot \mathbf{v}') \) designates a scalar product of the local normal vector \( \mathbf{n} \) and the velocity \( \mathbf{v}' \) (scalar products \( (\mathbf{N} \cdot \mathbf{v}') \) are \( (\mathbf{n} \cdot \mathbf{N}) \) defined similar), \( g(z_i, z_i', z_f') \) is the joined probability density of \( z_i, z_i', z_f' \), and the conditional probability \( \Pi^{(1)} \) is defined by (1)–(2).

The function space integrals (6) are completely defined by gas atom trajectory and by roughness parameters: \( \sigma_1 \) and \( \rho(r) \), hence it is possible to compute these integrals preliminary, before the main DSMC computation of a rarefied gas flow. Moreover, it is valid for an arbitrary local scattering function \( V_0(\mathbf{v}, \mathbf{v}', \mathbf{n}) \). The only restriction to the scattering function \( V_0(\mathbf{v}, \mathbf{v}', \mathbf{n}) \) in our approach is the approximation (5) with only a few parameters describing 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 calculation of function space integrals (6), we can compute the coefficients of the expansion (4) of the distribution of the scattered from rough surface gas atoms. Knowing the analytical scattering model for the smooth surface without a roughness, we can transform the estimated parameters according to the integrals \( K_k(\mathbf{v}, \mathbf{v}') \), computed at preliminary step. From the equations (4)–(6), 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 [4], [5], [9], [10]. This advantage is achieved because the shape information is accounted for at the preliminary steps, so that the need for the geometrical-shape simulation in DSMC is eliminated.

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

- Determining the set of the orthogonal functions \( \zeta_k(\mathbf{n}) \) (in our calculations trigonometric approximations used in the local interaction theory are applied).
- Expanding the local scattering function \( V_0(\mathbf{v}, \mathbf{v}', \mathbf{n}) \) in a series in terms of the system \( \zeta_k(\mathbf{n}) \); hence the coefficients \( b_k(\mathbf{v}, \mathbf{v}') \) are calculated.
- Computing the integrals \( K_k(\mathbf{v}, \mathbf{v}') \) in function space for different angles of incidence and reflection and for different values of roughness parameter \( \sigma_1 \) and the number \( k \); obtained integrals \( K_k(\mathbf{v}, \mathbf{v}') \) in function space could be expanded in a series in terms of the system \( \zeta_k(\mathbf{n}) \) for different values of \( \sigma_1 \) and \( k \).
- 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 \( \zeta_k(\mathbf{n}) \).
- 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 \( \zeta_k(\mathbf{n}) \) with the coefficients \( b_k(\mathbf{v}, \mathbf{v}') \).
– Interpolating the array of calculated integrals $K_k(v, v')$ for different values of $\sigma_1$ and other roughness parameters, and finding the roughness parameter $\sigma_1$ and the correlation function.

According to the proposed algorithm, to solve the inverse problem 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 experiments in rarefied gas are known satisfying these conditions. We have applied experimental data from [4] and [5] to test the algorithm for the inverse problem. Experimental data are obtained in TSAGI for argon atoms scattering from Kapton surface.

5. Conclusion
Comparing numerical results of direct simulation with the experiment we can conclude that aerodynamic shadowing effect either has not been taken into account in [4]–[5], 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 numerical DSMC computations for some local scattering functions 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.

The results of the solution of inverse problem have shown that the value of $\sigma_1$ obtained by proposed algorithm from experimental data is 10%–30% higher than the value of $\sigma_1$ 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 [4]–[5], for example from the normal momentum exchange coefficients of reflected gas flow (He and Ar) for different molecular energy $E$ of incident molecular beam and different (Kapton or aluminium) surface roughness. In all computations the calculated value of $\sigma_1$ is 5%–35% higher than in profile diagram measurements.

Thus, the solution of inverse problem is the best way to determine surface roughness parameters, because profile diagrams show only the roughness of the largest scale, and the precision of measuring $\sigma_1$ from the profile diagram could be low. The most effective solution of inverse problem is based on poly-Gaussian model of roughness applied to calculate the probability of absence of level-crossings and related function space integrals in scattering function allowing taking into account aerodynamic shadowing effect on rough surface. This model is verified by experiment and its statistical parameters have better coincidence with the parameters of real surfaces applied in practice.

References
[1] Aksenova O A and Khalidov I A 2016 Analytic Model of the Effect of Poly-Gaussian Roughness on Rarefied Gas Flow near the Surface Rarefied Gas Dynamics AIP Conf. Proc. 1786 1000071–8
[2] Aksenova O A and Khalidov I A 2014 Poly-Gaussian Model of Randomly Rough Surface in Rarefied Gas Flow Rarefied Gas Dynamics AIP Conf. Proc. 1628 388–98
[3] Khalidov I A 2014 St. Petersburg Polytechnic University Journal 4 129–38 (in Russian)
[4] Erofeev A I, Friedlander O G, Nikiforov A P, Nesterov S B and Nezhmetdinova R A 2012 The Influence of Roughness of the Surface on the Interchange of Momentum between Gas Flow and Solid Surface Rarefied Gas Dynamics AIP Conf. Proc. 1501 1168–74
[5] Erofeev A I, Friedlander O G, Nikiforov A P, Nesterov S B and Nezhmetdinova R A 2016 TSAGI Journal 47 4 12–27
[6] Aksenova O A and Khalidov I A 2004 Surface Roughness in Rarefied Gas Aerodynamics: Statisical and Fractal Models (St.-Petersburg: St.-Petersburg University Publishers) (in Russian)
[7] Chabdarov Sh M and Trofimov A T 1975 Poly-Gaussian representation of arbitrary noises and the input of discrete signals Radio Engineering and Electronics 20 4 734–45 (in Russian)
[8] Litvak M and Malyugin V 2012 *Journal of Technical Physics* **82** 4 99–107 (in Russian)
[9] Ukhov A, Porodnov B and Borisov S 2009 Numerical Simulation of Gas Dynamics Conductivity of Micro Channels with Consideration of Surface Structure *Rarefied Gas Dynamics* *AIP Conf. Proc.* **1084** 712–7
[10] Gimelshein N E, Lilly T C, Gimelshein S F, Ketsdever A D and Wysong I J 2007 Surface Roughness Effects in Low Reynolds Number Nozzle Flows *Rarefied Gas Dynamics* (Novosibirsk: Siberian Branch of RAS) 695–702