Scattering of Rarefied Gas Atoms from Rough Surface Simulated with Fractals

Olga A. Aksenova

St.-Petersburg State University, St.-Petersburg, Russia

Abstract. The fractal approach to the model of surface roughness in the problem of gas-surface interaction is developed on the base of the generalization of two-dimensional model of roughness proposed by Blackmore and Zhou. The relation between the parameters of the model and the values influencing the aerodynamic coefficients is investigated. Computed results are compared with the values obtained using statistical model of roughness - the isotropic Gaussian random field.

ACCOUNT OF SURFACE ROUGHNESS IN RAREFIED GAS FLOW

The surface roughness is one of the most essential factors, which have to be taken into consideration in various problems of rarefied gas dynamics. These problems are the aerodynamic computation of bodies moving in a rarefied gas, the investigation of flows in channels and vessels and the interaction of gas jets with surfaces. A technique of the account of a statistical roughness in aerodynamic calculation of low-density flows is developed in Leningrad — St.-Petersburg University in papers of R.G. Barantsev, R. N. Miroshin and I.A. Khalidov since the sixtieth years. This technique is explained in the monographs [1], [2]. The results in statistical simulation and asymptotic research of a roughness are accumulated lately. These investigations permitted to find the dependence of aerodynamic values on basic parameters of a roughness [3], [4]. However statistical approach has a number of disadvantages. The most principal of them is the complexity of calculations because of the necessity of computation of so-called continuum integrals, which must be approximated by integrals of high dimension (up to 200). Another disadvantage is the difficulty of the account of a small-scale roughness. Nevertheless a small-scale roughness can make a considerable contribution to factors describing the influence of a roughness on gas-surface interaction.

In recent years in connection with the development of DSMC methods more often the determined (nonrandom) models of a roughness are used when simulating the interaction of gas with a rough surface. These models are constructed either of various systems of flat units, or of fingers, steps or sine waves. The determined models have advantage over statistical ones (in particular, over Gaussian [1] and diffusive [2]). The advantage consists in a simplicity of surface modeling at a Monte Carlo computation and in a possibility of analytical definition of a cross point of a trajectory of gas atom with a surface. Most convenient in rarefied aerodynamics appear fractal model (with the property of self-similarity). They allow to take into account the important contribution of a microroughness (irregularities of a smaller scale watched experimentally [4]). The determining role is played by the inclination of a rough surface to its average level [3].

The fractals were applied before to simulate a roughness in the applications only in a plane case (for example [5]), as the three-dimensional models are extremely complex [6]. The spatial case considered in the present paper is a nontrivial problem.

As well as in case of statistical model ([1], [2]) an area \( dS \) on a surface is considered so small in regard to characteristic aerodynamic scale, that its curvature can be neglected. It means that it is possible to consider an average level of a roughness on \( dS \) approximately as plane. At the same time in bounds of \( dS \) the large enough number of irregularities of a roughness should place. Then the scattering function \( V(v_1, v) \) of gas atoms dropping with speed \( v_1 \) on the area \( dS \) must be presented as an effect of the roughness operator \( \hat{S} \) on a local scattering function \( V_0(v_1, v, n) \):

\[
V(v_1, v) = \hat{S} V_0(v_1, v, n),
\]
where \( \mathbf{v} \) is the speed of outgoing atoms of gas, \( \mathbf{n} \) is an external normal to \( dS \) and \( V_0 (\mathbf{v}_1, \mathbf{v}, \mathbf{n}) \) is equal to the scattering function on smooth surface [2].

**GENERAL FRACTAL FUNCTIONAL MODEL**

The functional model for the rough surface profile is

\[
z(r, \varphi) = \alpha r^{-1} \sum_{n=1}^{\infty} \beta_n^{(s-2)n} \psi(\beta_n r + \gamma_n(\varphi))
\]  

(2)

The expression (2) at fixed value of a polar angle \( \varphi \) is equal to the two-dimensional profile model [5]. Here, as well as in [5], \( \alpha \) and \( \beta \) are constant parameters, \( \psi \) is a continuous \( 2\pi \)-periodic function, \( z \) is an altitude of a surface in regard to average level of an area \( dS \). Unlike offered in [5] model, the cylindrical coordinate system \((r, \varphi, z)\) is introduced with an axis \( z \) directed along a normal \( \mathbf{n} \), and a dependent on a polar angle \( \varphi \) shift \( \gamma_n(\varphi) \) of argument of function \( \psi \) is carried out.

Function \( z(r, \varphi) \) has, as well as the model from paper [5], following fractal property (self-affinity):

\[
z(\beta r, \varphi) = \beta^{2-s} z(r, \varphi)
\]  

(3)

where \( s \) is fractal dimension of the graph of the function (2) [5]. The self-affinity (3) of the graph (2) means that the roughness of a smaller scale is similar to the large-scale roughness if the horizontal size unit is multiplied with \( \beta \), and the vertical size unit — with \( \beta^{2-s} \).

In applications the constructed spatial fractal model of a rough surface must be reduced to a form which is most simply realizable in numerical aerodynamic calculations. Hence we have to take the function \( \psi \) so that the cross points of a trajectory of atom of gas with a surface could be easily defined analytically. Therefore we suggest selecting this function as a quadratic spline

\[
\psi(u) = \begin{cases} 
    a^2u^2 - b^2, & 0 < |u| < \frac{\pi}{2}, \\
    b^2 - a^2(\pi-|u|)^2, & \frac{\pi}{2} < |u| < \pi,
\end{cases}
\]  

(4)

and further continued periodic with period \( 2\pi \). By virtue of continuity here is \( a^2 \pi^2 = 4b^2 \).

The model (2), generally speaking, is determined, that means it does not contain stochastic elements. However a point of impact of a gas atom with the surface is arbitrary. So it is possible to discuss statistical characteristics of the model, which are received by averaging over the area \( dS \).

Let's find a relation between the parameters of model and the main characteristics of a roughness. The density function looks like [5]

\[
f(z) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(z-\mu)^2}{2\sigma^2}} \sum_{n=0}^{\infty} \omega_n \left( \frac{z - \mu}{\sqrt{2\sigma}} \right)^n.
\]  

(5)

Average value of the surface height \( z \) is \( \mu = 0 \) appropriate to selection of coordinate system, and the parameters of density \( \sigma \) and \( \omega_n \) vary depending on parameters of model \( \alpha, s \) and \( \beta \).
The main parameters of a roughness in aerodynamics, as is known [2], are $\sigma_1$ and $R(r)$. $\sigma_1$ is the mean quadratic deviation of a derivative $z'(r)$ and $R(r)$ is normalized correlation function. The computed values $\sigma_1$ are shown in fig. 1 and 2 at different values $s$ and $\beta$. The function $R(r)$ can be found as a sum of a Fourier series. Its typical graph taking into account first 10 terms of a series is shown in fig. 3.

Fig. 4 illustrates a typical view of a rough surface on an area $dS$ (appropriate to the introduced in a fig. 3 function $R(r)$) in Cartesian coordinate system $(x, y)$, corresponding to a polar system $(r, \varphi)$.
THE PROBABILITY OF FREE MOTION OF GAS ATOMS WITHOUT CROSSINGS OF THE TRAJECTORY WITH ROUGH SURFACE

The aerodynamic values contain the probability of the absence of the crossings of gas atoms trajectory with random function (2) modeling the rough surface. This probability can be written in the form of an integral

$$P_1(\theta, z_0, z_x, z_y) = \lim_{n \to \infty, h \to 0} \int_{-\infty}^{u_1} \int_{-\infty}^{u_2} p(r_0, r_0 + h i_1, r_0 + 2h i_1, \ldots, r_0 + h i_1, z_0, v_1, V_2, \ldots, V_n, z_x, z_y) \, dv_n,$$

where $r_1=(x_1, y_1), r_2=(x_2, y_2)$ are the coordinate vectors of two points in the plane $(x,y)$, $v = Z(x_1, y_1)$ and $w = Z(x_2, y_2)$ are the vertical coordinates of the surface at this points, $p(r_1, r_2, v, w)$ is the probability distribution of the model $Z(x,y)$ of rough surface, $i_1$ is unit vector of $x$-axis, over which lays the line $u_l(x) = z_0 + k (x - x_0) \tan \theta$ crossing the surface at the point $(x_0, y_0, z_0)$, and the function $p(r_0, r_0 + h i_1, r_0 + 2h i_1, \ldots, r_0 + h i_1, z_0, v_1, V_2, \ldots, V_n, z_x, z_y)$ is the joined probability distribution of surface heights $z_0, v_1, V_2, \ldots, V_n$ at the points over $x$-axis having the coordinates $x_0, x_0 + nh$ and the derivatives $z_x = \partial Z / \partial x$, $z_y = \partial Z / \partial y$ at the point $(x_0, y_0)$.

The probability $P_1(\theta, z_0, z_x, z_y)$ calculated by a Monte Carlo method is shown on fig. 5—6 for different values of roughness parameter $\sigma_1$ and of incident angle $\theta$.

![Figure 5](https://example.com/fig5.png)  ![Figure 6](https://example.com/fig6.png)

FIGURE 5. Probability $P_1(\theta, z_0, z_x, z_y)$ for $\sigma_1 = 0.1$

FIGURE 6. Probability $P_1(\theta, z_0, z_x, z_y)$ for $\sigma_1 = 0.5$

MOMENTUM EXCHANGE COEFFICIENTS ON A ROUGH SURFACE

The results of calculation of normal $p$ and tangent $\tau$ momentum exchange coefficients on a rough surface for elementary free-molecular gas flows using the fractal model are shown in fig. 5 — 8 at some values of parameters of model. The calculation is made by a Monte Carlo method. The single and twofold collisions of atoms of gas with a surface are accounted.
The scattering function $V_0(v_1, v, n)$ on a smooth surface is supposed specular (charts 7 and 9) or diffuse (figures 8 and 10).

The incident flow is assumed consisting of atoms of gas with identical velocity vectors $v_1$ so that $\theta_1$ is the angle between the vectors $v_1$ and $n$ ($n$ is a normal to an area $dS$ on a surface). The dashed lines show the results of calculations using statistical model of a roughness (the isotropic Gaussian random field [3]), and the dash-dotted lines — the values on a smooth surface.

REFERENCES