# Rarefied Gas Atoms Reflection on Rough Surfaces

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**Abstract.** The method for computation of aerodynamical characteristics for any convex axisymmetrical rough bodies in rarefied gas flows is proposed.

**Keywords:** Rarefied gas – rough surface interaction, normalization of scattering function.
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## Introduction

Surface roughness is one of essential factors, which influence on aerodynamical characteristics of bodies in rarefied gas flow. The statement of the problem of rarefied gas atoms reflection from a rough surface was made by R.G. Barantsev in [1]. There the problem was reduced to evaluation of some continual integrals. Numerical method for computation of these continual integrals was proposed in [2-3]. In case of a single reflection, calculations were carried out for the specular and the diffuse scattering function in a small area. The exchange coefficients and the aerodynamical resistance coefficients for the rough bodies of the simplest shape (sphere, cylinder, cone) were found in a free molecular flow. A contribution of the twofold reflections to aerodynamical characteristics was investigated in [4]. In the present paper aerodynamical characteristics for single and for both single and twofold reflections from a rough surface are compared. The contribution of the multiple reflections is taken into account by appropriate normalization of scattering function on a rough surface [5-6].

The rough surface is simulated by the homogeneous isotropic differentiable Gaussian random field with zero average and with given covariance function $\mathrm{B(x, y)} = \mathrm{B(r)} = \sigma^2 \rho(r)$, where $r^2 = x^2 + y^2$. The main roughness parameter $\sigma_1 = \sqrt{-B''(0)}$ is the inclination fluctuation of the rough surface. We consider the correlation functions $\rho_a(r) = \exp(-r^2/2)$ and $\rho_m(r) = (1+r)\exp(-r)$, describing extreme statistic models of differentiable rough surface: the former defines an analytic random field and the latter defines a field possessing only first order derivatives.

## Scattering Function and Exchange Coefficients on Smooth and Rough Surfaces

In the present paper we preserve the notation and terminology of [1-6]. We remind that *z*-axis is the external normal $\vec{N}$ to the mean level of the rough surface. Let an atom impinge upon a surface with the velocity

$$\vec{u}_1 = \{0, -u_1 \sin\theta_1, -u_1 \cos\theta_1\}, \qquad \theta_1 \in [0, \pi/2), \tag{1}$$

and emerge with the velocity

$$\vec{u} = \{u \sin\theta \cos\Phi, u \sin\theta \sin\Phi, u \cos\theta\}, \qquad \theta \in [0, \pi/2). \tag{2}$$

The probability of event Eq.2 under condition Eq.1 is denoted by $V(\vec{u} \mid \vec{u}_1)d\vec{u}$ where $V(\vec{u} \mid \vec{u}_1)$ is the scattering function on a rough surface. We represent $V$ by the series

$$V = \sum_{m=1}^{\infty} V_m, \qquad N_m = \iiint\limits_{u_z>0} V_m(\vec{u} \mid \vec{u}_1)d\vec{u}, \qquad \iiint\limits_{u_z>0} V(\vec{u} \mid \vec{u}_1)d\vec{u} = \sum_{m=1}^{\infty} N_m = 1, \tag{3}$$

where $V_m$ is the scattering function of the *m*-fold reflection, and $N_m$ is the *m*-fold reflection probability. The scattering functions $V_m$ are represented in the form of complicated multiple integrals involving the scattering function "in small" $V_0(\vec{u} \mid \vec{u}_1, \vec{n})$ - the scattering function on a smooth (non rough) surface, i.e. the scattering function from a small smooth area *ds* with random normal $\vec{n}$ [1-6]. We confine ourselves to single and twofold reflections in view of great computational difficulties for multiple reflections.

In case of a simple gas without trapping, sputtering and emission the momentum $p$, $\tau$ and the energy $q$ exchange coefficients on the rough surface are determined in terms of the scattering function $V(\vec{u}\,|\,\vec{u}_1)$ by

$$\vec{p}(\vec{u}_1) = \frac{2}{u_1}\cos\theta_1(\vec{u}_1 - \iiint_{u_z>0} V(\vec{u}\,|\,\vec{u}_1)\vec{u}d\vec{u}), \qquad q(\vec{u}_1) = \cos\theta_1(1 - \frac{2}{u_1^2}\iiint_{u_z>0} V(\vec{u}\,|\,\vec{u}_1)u^2 d\vec{u}). \tag{4}$$

The aerodynamical resistance coefficients $c_x$ are expressed in terms of $p$, $\tau$ by the formulae:

$$c_x = 2\int_0^{\pi/2}(p\cos\theta_1 + \tau\sin\theta_1)\sin\theta_1 d\theta_1, \tag{5}$$

for sphere;

$$c_x = 2\int_0^{\pi/2}(p\cos\theta_1 + \tau\sin\theta_1)d\theta_1, \tag{6}$$

for cylinder in cross flow.

Similarly, exchange coefficients $p_0, \tau_0, q_0$ on the smooth surface are defined by the scattering function in the small area $V_0(\vec{u}\,|\,\vec{u}_1, \vec{N})$

$$\vec{p}_0(\vec{u}_1) = \frac{2}{u_1}\cos\theta_1(\vec{u}_1 - \iiint_{u_z>0} V_0(\vec{u}\,|\,\vec{u}_1, \vec{N})\vec{u}d\vec{u}), \quad q_0(\vec{u}_1) = \cos\theta_1(1 - \frac{2}{u_1^2}\iiint_{u_z>0} V_0(\vec{u}\,|\,\vec{u}_1, \vec{N})u^2 d\vec{u}). \tag{7}$$

The aerodynamical resistance coefficients $c_{x0}$ on the smooth surface are obtained from Eq.5 and 6 by substituting $p_0, \tau_0$ instead of $p, \tau$. So, we have for the diffuse reflection from a smooth surface

$$V_{0d}(\vec{u}\,|\,\vec{u}_1, \vec{N}) = \tfrac{2h^2}{\pi} u\cos\theta\exp(-hu^2),$$

$$p_0 = \tfrac{\sqrt{\pi}}{\lambda}\cos\theta_1 + 2\cos^2\theta_1, \qquad \tau_0 = 2\sin\theta_1\cos\theta_1, \qquad q_0 = \cos\theta_1(1 - \tfrac{2}{\lambda^2}), \tag{8}$$

$c_{x0} = 2(\sqrt{\pi}/3\lambda + 1)$ for sphere, $c_{x0} = 2 + \pi\sqrt{\pi}/4\lambda$ for cylinder in cross flow, where $h=m/2kT$, $m$ is the atom mass, $k$ is the Boltzmann's constant, $T$ is the surface temperature, $\lambda = u_1/\sqrt{h}$. Analogously, we have for the specular reflection from a smooth surface

$$V_{0s}(\vec{u}\,|\,\vec{u}_1, \vec{N}) = \delta(\vec{u} - \vec{u}_1 + 2\vec{u}_{1N}), \qquad p_0 = 4\cos^2\theta_1, \quad \tau_0 = 0, \quad q_0 = 0, \tag{9}$$

$c_{x0} = 2$ for sphere, $c_{x0} = 8/3$ for cylinder in cross flow.

## Normalization of Scattering Function on a Rough Surface

In [2, 4] we have calculated aerodynamical characteristics in the following four approximations for $V$

$$V_c^{(1)} = V_1, \quad V_c^{(1,2)} = V_1 + V_2, \quad V_n^{(1)} = \tfrac{V_1}{N_1}, \quad V_n^{(1,2)} = \tfrac{V_1 + V_2}{N_1 + N_2}. \tag{10}$$

By using $V_c^{(1)}$ or $V_c^{(1,2)}$ we take only first or both first and second terms in the series Eq.3, i.e. we take into account only the contributions of single or both single and twofold reflections into aerodynamical characteristics. The inadequacy of this natural approach is that normalizing condition Eq.3 is not true for it. We note that for approximations $V_n^{(1)}$ or $V_n^{(1,2)}$ normalizing condition Eq.3 are valid. Using of $V_n^{(1)}$ (proposed in early work [1]) is equivalent to the hypothesis that multiply reflected atoms are distributed in the same way as single reflected ones. This assumption is not physically justified and, apparently, gives overstated values of $c_x$. To eliminate these defects, we propose the following new approximations for $V$

$$V_a^{(1)} = V_1 + (1 - N_1)V_0, \qquad V_a^{(1,2)} = V_1 + V_2 + (1 - N_1 - N_2)V_0, \tag{11}$$

where $V_0 = V_0(\vec{u}\,|\,\vec{u}_1, \vec{N})$ is the scattering function on smooth surface with normal $\vec{N}$, coinciding with normal to the mean level of the rough surface. Normalizing condition Eq.3 for $V_a^{(1)}$ and $V_a^{(1,2)}$ is obviously valid. Using $V_a^{(1)}$ or $V_a^{(1,2)}$, we assume that multiply reflected atoms scatter as in case of smooth surface, coinciding with mean level of rough surface. In other words, for multiply reflected atoms we neglect surface roughness. This assumption is also physically unjustified, but in contrast to approximations $V_c^{(1)}$ and $V_c^{(1,2)}$ it enables us to take into account multiple reflections at least in the first approximation.

Below we derive formulae for exchange coefficients under approximation $V_a^{(1)}$. Inserting in Eq.4 $V_a^{(1)}$ from Eq.11 instead of $V(\vec{u}\mid\vec{u}_1)$ we obtain

$$\vec{p}_a^{(1)} = \vec{p}_c^{(1)} - \frac{2}{u_1}\cos\theta_1(1-N_1)\iiint\limits_{u_z>0} V_0(\vec{u}\mid\vec{u}_1,\vec{N})\vec{u}d\vec{u}. \qquad (12)$$

According to Eq.7, we have

$$\frac{2}{u_1}\cos\theta_1\iiint\limits_{u_z>0} V_0(\vec{u}\mid\vec{u}_1,\vec{N})\vec{u}d\vec{u} = \frac{2}{u_1}\cos\theta_1\vec{u}_1 - \vec{p}_0. \qquad (13)$$

Substituting Eq.13 into Eq.12, we arrive at

$$\vec{p}_a^{(1)} = \vec{p}_c^{(1)} + (1-N_1)(\vec{p}_0 - \frac{2}{u_1}\cos\theta_1\vec{u}_1). \qquad (14)$$

Similarly, we obtain from Eq.4, 7 and 11

$$\vec{p}_a^{(1,2)} = \vec{p}_c^{(1),2} + (1-N_1-N_2)(\vec{p}_0 - \frac{2}{u_1}\cos\theta_1\vec{u}_1),$$

$$q_a^{(1)} = q_c^{(1)} + (1-N_1)(q_0 - \cos\theta_1), \quad q_a^{(1,2)} = q_c^{(1,2)} + (1-N_1-N_2)(q_0 - \cos\theta_1). \qquad (15)$$

Projecting $\vec{p}$ in Eq.14 and 15 on *z*-axis and plane *(x, y)*, we finally obtain

$$p_a^{(1)} = p_c^{(1)} + (1-N_1)(p_0 - 2\cos^2\theta_1), \quad \tau_a^{(1)} = \tau_c^{(1)} + (1-N_1)(\tau_0 - 2\sin\theta_1\cos\theta_1),$$

$$p_a^{(1,2)} = p_c^{(1,2)} + (1-N_1-N_2)(p_0 - 2\cos^2\theta_1), \quad \tau_a^{(1,2)} = \tau_c^{(1,2)} + (1-N_1-N_2)(\tau_0 - 2\sin\theta_1\cos\theta_1). \quad (16)$$

## Results and Discussion

For the diffuse reflection "in small" from Eq.8, 15 and 16 we obtain

$$p_a^{(1)} = p_c^{(1)} + (1-N_1)\sqrt{\pi}/\lambda\cos\theta_1, \qquad \tau_a^{(1)} = \tau_{c,}^{(1)}$$
$$q_a^{(1)} = q_c^{(1)} - 2/\lambda^2(1-N_1)\cos\theta_1,$$
$$p_a^{(1,2)} = p_c^{(1,2)} + (1-N_1-N_2)\sqrt{\pi}/\lambda\cos\theta_1, \qquad \tau_a^{(1,2)} = \tau_c^{(1,2)}, \qquad (17)$$
$$q_a^{(1,2)} = q_c^{(1,2)} - 2/\lambda^2(1-N_1-N_2)\cos\theta_1.$$

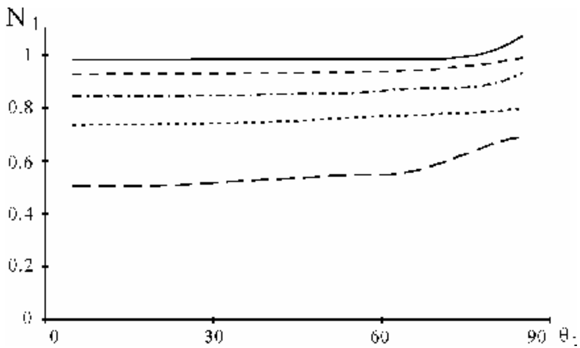


**FIGURE 1.** $N_1(\theta_1)$ (diffuse).

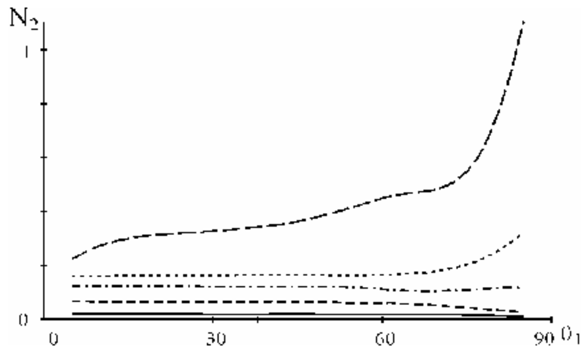


**FIGURE 2.** $N_2(\theta_1)$ (diffuse).

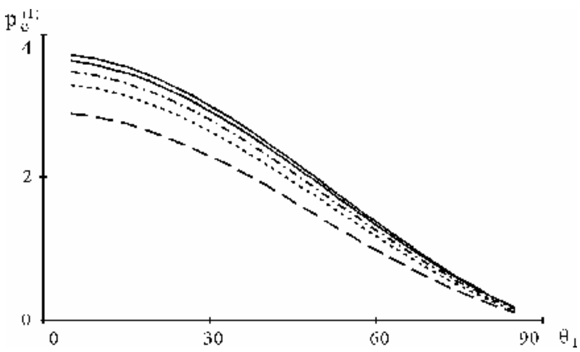


**FIGURE 3.** $p_c^{(1)}(\theta_1)$ at $\lambda = 1$.

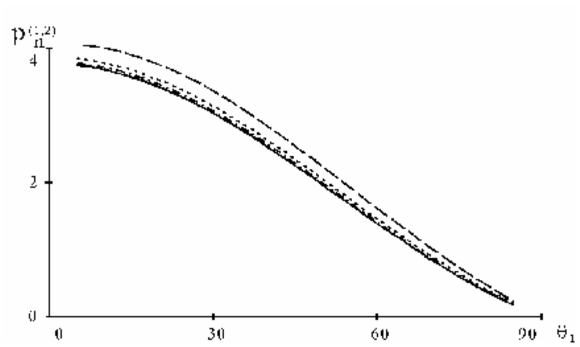


**FIGURE 4.** $p_n^{(1,2)}(\theta_1)$ at $\lambda = 1$.

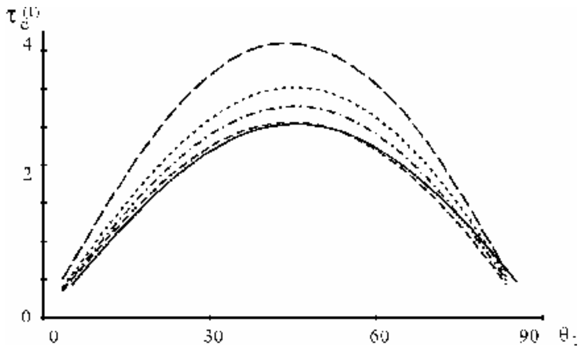


**FIGURE 5.** $\tau_c^{(1)}(\theta_1)$ at $\lambda = 1$.

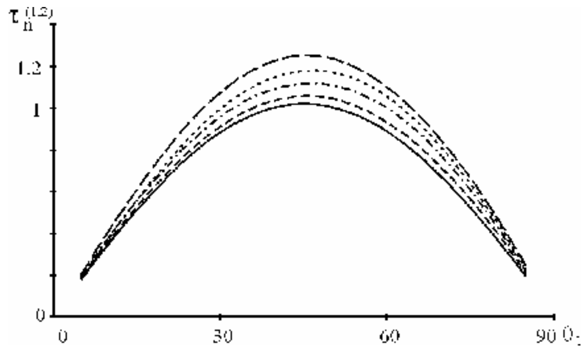


**FIGURE 6.** $\tau_n^{(1,2)}(\theta_1)$ at $\lambda = 1$.

The dependence of $N_1$, $N_2$, $p_c^{(1)}$, $p_n^{(1,2)}$, $\tau_c^{(1)}$, $\tau_n^{(1,2)}$ on the incidence angle $\theta_1$ and on the roughness parameter $\sigma_1$ at $\lambda = 1$ is shown in Figs 1-6. Values of these functions are plotted by solid lines at $\sigma_1 = 0.1$, by dashed ones at $\sigma_1 = 0.2$, by dash dotted ones at $\sigma_1 = 1/3$, by dotted ones at $\sigma_1 = 0.5$ and by long dashed ones at $\sigma_1 = 1$. One can see that $N_1 + N_2 > 1$ at large values of $\sigma_1$ and $\theta_1$. The failure of normalizing condition Eq.3 is explained by the error of our method of computation: it is too large at large values of $\theta_1$ and $\sigma_1$ (cf. [2, 4]). The dependence of the aerodynamical resistance coefficient $c_x$ on $\sigma_1$ at $\lambda = 1$ and $\lambda = 5$ is shown in Figs 7,9 for sphere and in Figs 8,10 for cylinder in cross flow for all six approximations given in Eq.10 and 11. Values of $c_{xc}$ are plotted by dashed lines, of $c_{xn}$ by solid ones and of $c_{xa}$ by dotted ones, $\sigma_1$ is graduated at the logarithmic scale. For slight roughness (i.e. small $\sigma_1$) the results obtained for all six approximations are well agreed, but for large $\sigma_1$ the results are in striking disagreement: values of $c_{xc}$ are strongly understated; values of $c_{xn}$ are somewhat overstated; intermediate values of $c_{xa}$ are most reliable.

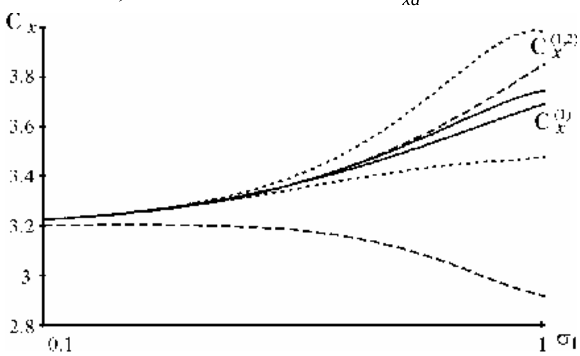


**FIGURE 7.** $C_x(\sigma_1)$ at $\lambda = 1$.

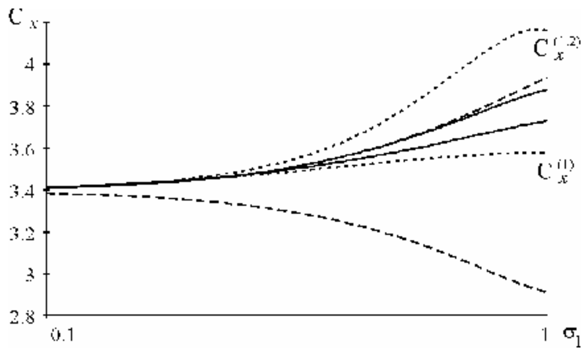


**FIGURE 8.** $C_x(\sigma_1)$ at $\lambda = 1$.

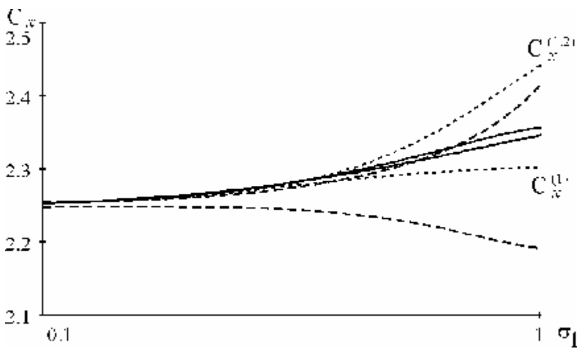


**FIGURE 9.** $C_x(\sigma_1)$ at $\lambda = 5$

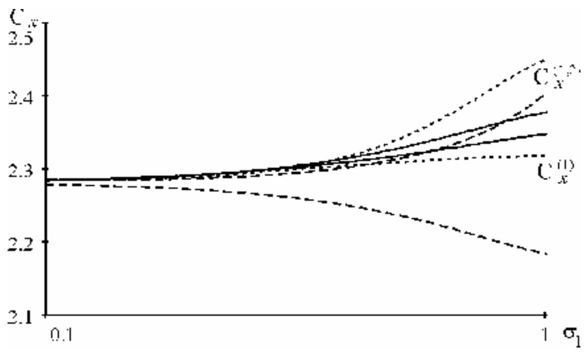


**FIGURE 10.** $C_x(\sigma_1)$ at $\lambda = 5$

For the specular reflection "in small", substituting $V_{0s}$ from Eq.9 in Eq.11 in place of $V_0$ we get following two approximations

$$V_s^{(1)} = V_1 + (1 - N_1)V_{0s}, \quad V_s^{(1,2)} = V_2 + V_1 + (1 - N_1 - N_2)V_{0s}. \qquad (18)$$

From Eq.9 and 16, we obtain exchange coefficients in these approximations

$$p_s^{(1)} = p_c^{(1)} + 2(1-N_1)\cos^2\theta_1, \quad \tau_s^{(1)} = \tau_c^{(1)} - (1-N_1)\sin 2\theta_1,$$

$$p_s^{(1,2)} = p_c^{(1,2)} + 2(1-N_1-N_2)\cos^2\theta_1, \quad \tau_s^{(1,2)} = \tau_c^{(1,2)} - (1-N_1-N_2)\sin 2\theta_1. \quad (19)$$

Here we assume that for multiple collisions the reflection from corresponding smooth surface is also specular one. However, admissible alternative is that for multiple collisions reflection from corresponding smooth surface is diffuse one. In this case we must choose parameter $\lambda$ to satisfy the condition that energy $q_0$ exchange coefficient equals zero, i.e. $\lambda = \sqrt{2}$ (cf. Eq.9). It corresponds to the assumption that after first or after both first and second collisions from a rough surface atom "forgets" his velocity $\vec{u}_1$ and takes velocity $\vec{u}$, magnitude of which corresponds to zero energy exchange with surface ($q_0 = 0$ for specular reflection) and its direction corresponds to "cosine law"(cf. Eq.8). In this case substituting $V_{0d}$ from Eq.8 into Eq.11 instead of $V_0$ gives two additional approximations

$$V_d^{(1)} = V_1 + (1-N_1)V_{0d}, \qquad V_d^{(1,2)} = V_1 + V_2 + (1-N_1-N_2)V_{0d}. \quad (20)$$

From Eq.8, 16 and 20 at $\lambda = \sqrt{2}$, we find

$$p_d^{(1)} = p_c^{(1)} + \sqrt{\pi/2}(1-N_1)\cos\theta_1, \quad \tau_d^{(1)} = \tau_{c,}^{(1)}$$

$$p_d^{(1,2)} = p_c^{(1,2)} + \sqrt{\pi/2}(1-N_1-N_2)\cos\theta_1, \quad \tau_d^{(1,2)} = \tau_c^{(1,2)}. \quad (21)$$

Figs 11-16 show the dependence of $N_1$, $N_2$, $p_c^{(1)}$, $p_n^{(1,2)}$, $\tau_c^{(1)}$, $\tau_n^{(1,2)}$ on $\sigma_1$ and $\theta_1$. The dependence of aerodynamical resistance coefficient $c_x$ on $\sigma_1$ in a free molecular flow is shown in Figs 17, 19 for sphere and in Figs 18, 20 for cylinder in cross flow for all eight approximations given in Eq.10, 18 and 20. Values of $c_{xs}$ are plotted by long dashed lines and of $c_{xd}$ by dashdotted ones [5, 6]. From the above results one can estimate the contribution of the twofold reflections to aerodynamical characteristics. One can also see the limits of applicability of mentioned approximations at various values of roughness parameter $\sigma_1$. Using the local interaction theory [7] allows us to determine the aerodynamical characteristics for any convex axisymmetrical rough bodies in the transitional flow regime [8].

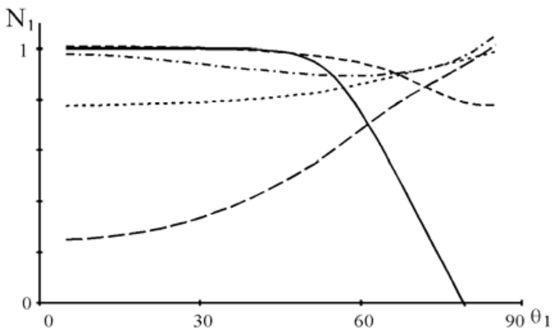


**FIGURE 11.** $N_1(\theta_1)$ (specular).

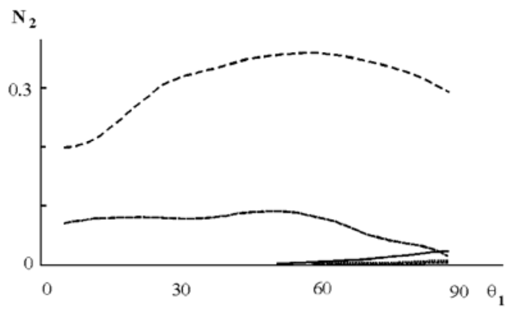


**FIGURE 12.** $N_2(\theta_1)$ (specular).

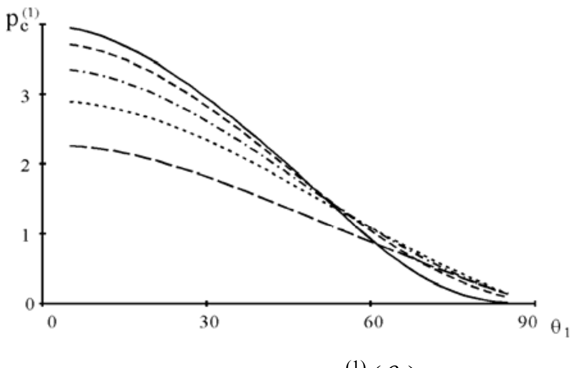


**FIGURE 13.** $p_c^{(1)}(\theta_1)$.

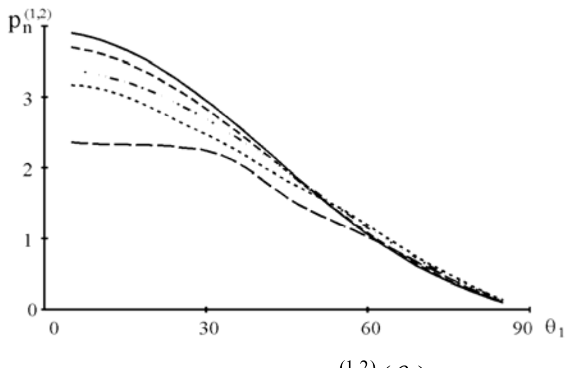


**FIGURE 14.** $p_n^{(1,2)}(\theta_1)$.

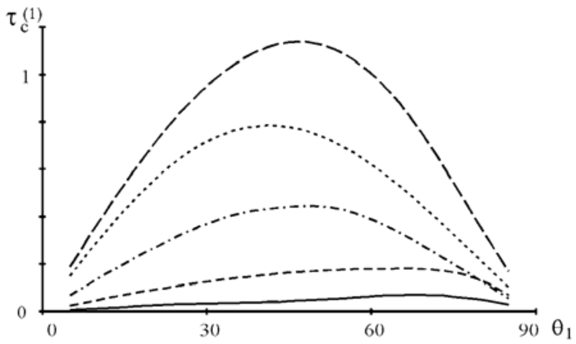


**FIGURE 15.** $\tau_c^{(1)}(\theta_1)$.

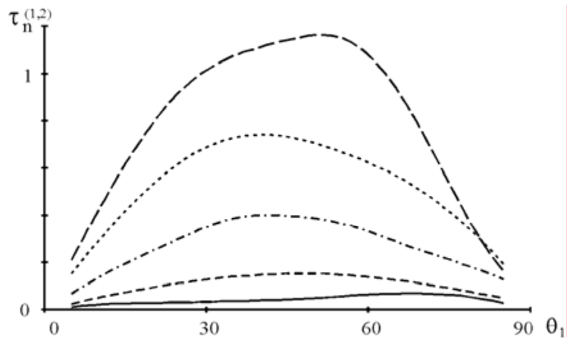


**FIGURE 16.** $\tau_n^{(1,2)}(\theta_1)$.

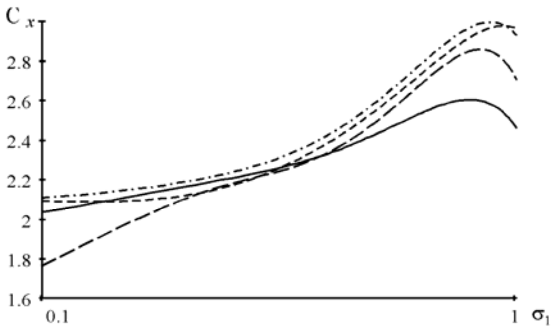


**FIGURE 17.** $C_x^{(1)}(\sigma_1)$ (sphere).

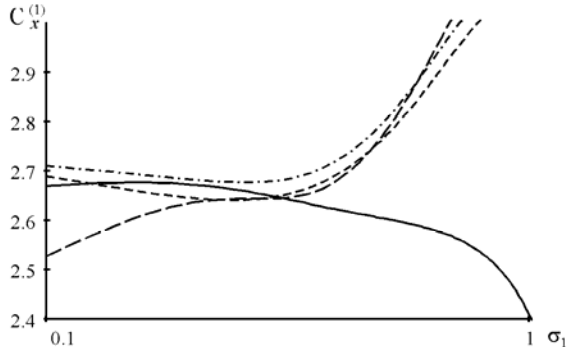


**FIGURE 18.** $C_x^{(1)}(\sigma_1)$ (cylinder).

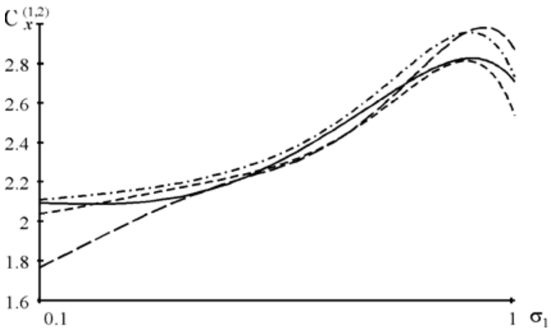


**FIGURE 19.** $C_x^{(1,2)}(\sigma_1)$ (sphere).

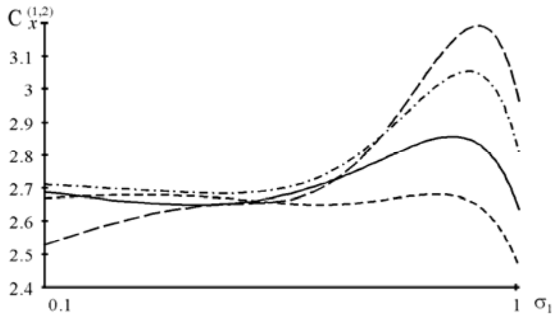


**FIGURE 20.** $C_x^{(1,2)}(\sigma_1)$ (cylinder).

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