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Regarding a Benchmark Problem: Rarefied Gas Flow Through a Rough-Surfaced Channel[1]

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Abstract—Rarefied gas flow through a modeled rough-surfaced channel is presented as a benchmark problem in rarefied gas dynamics. To meet the benchmark problem requirements, a short set of problem-solving parameters were employed, in particular, a fairly simple model of surface roughness and a free molecular regime of gas flow. A test particle Monte Carlo method was applied for a high-accuracy computation of the gaseous transmission probability through a modeled rough-surfaced channel. For the gas-surface scattering law, the diffuse as well as Maxwell and Cercignani–Lampis models have been used. A comparison was carried out between our results and theoretical and numerical data available in the open literature.

Keywords: benchmark problem, rough-surfaced channel, gaseous transmission probability, test particle Monte Carlo method.

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Benchmark problems in rarefied gas dynamics were presented by Felix Sharipov during the 64th IUVSTA Workshop on Practical Applications and Methods of Gas Dynamics for Vacuum Science and Technology [1, 2]. The attendees were invited to solve fairly simple tasks on rarefied gas dynamics, using the same short set of problem-solving parameters. Then, having compared the experimental and computation results obtained by different methods, it is possible to identify the most effective and reliable computation methods for solving more complex problems regarding rarefied gas dynamics. Furthermore, a benchmark problem may be applied for testing new program codes and software.

One of the workshop highlights was a benchmark problem of rarefied gas flow through a channel of finite length [2, 3]. The following set of problem-solving parameters was proposed: rarefaction parameter, reduced length (length to channel height or radius ratio) and pressure ratio (output pressure to input pressure of the channel).

However, the workshop did not pay much attention to such an important factor as surface roughness. Indeed, quite a lot of numerical studies have been devoted to the influence of the surface roughness on the rarefied gas flow in channels, in particular [4–14]. Typically, these works use a different problem-solving set of parameters, more specifically, different models of roughness. This fact makes the comparison of the computation results much more difficult. Therefore, a benchmark problem is required for testing program codes and verifying computation results.

For a benchmark problem of rarefied gas flow through a rough-surfaced channel, a simple and intuitive roughness model should be used with a short set of defining parameters, such as a saw-shaped model of roughness. While reducing the set of problem-solving parameters, it is expedient to perform the computation in an easily computable free molecular flow regime in which the rarefaction parameter becomes zero [15]. Indeed, this flow regime does not require taking into account the gas molecule-molecule interaction, which greatly facilitates the computation. In a free molecular regime, the gas flow through the channel is typically characterized as transmission probability W. Its physical meaning lies in the following: after entering the channel input connecting two large containers, the molecule with probability W will pass through the channel from one container to another.

The aim of this paper is to define the gaseous transmission probability through the modeled rough-surfaced channel as a solution to the benchmark problem in rarefied gas dynamics.

[1] The article is published in the original.

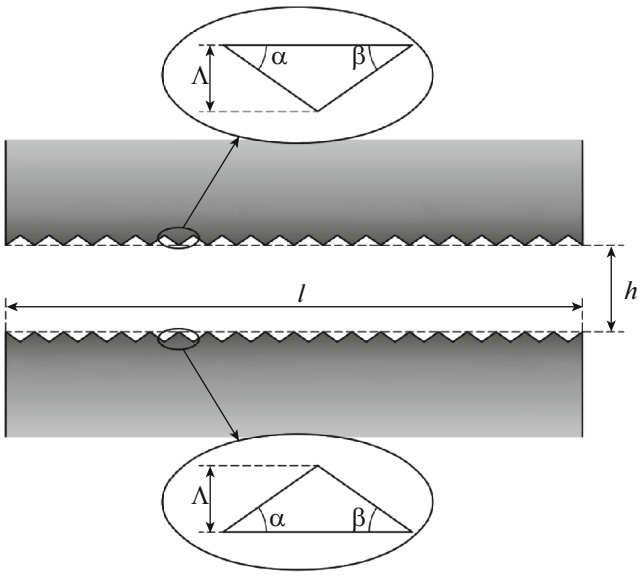

Fig. 1. Geometry of the modeled rough-surfaced channel: l—channel length, h—channel height, Λ—roughness height, α and β—inclination angles.

Let us consider two containers containing the equilibrium gas and connected by a rough-surfaced channel. We chose the rectangular shape of the channel and limited ourselves to the two-dimensional statement of the problem. The geometry of the modeled channel is shown in Fig. 1. As can be seen from the figure, the channel of length l and height h has a surface roughness in the form of a "saw" with identical teeth; Λ is the saw tooth height, α and β are the angles of inclination. To perform computation, it is advisable to use the test particle Monte Carlo method (TPMC) [16].

Let us recall that the TPMC method is based on modelling the movement of a large number of particles. Since under free-molecular regime molecules do not interact with one another, it is possible to model the movement of each particle separately.

Comprehensive study of gas flows in channel-connected containers generally presents a fairly significant challenge requiring high computational resources. In the free molecular regime, however, it would be sufficient to only consider gas flow inside the channel. The presence of the containers in this case may be included through boundary conditions at the channel ends. The following assumption should be made in this case: the containers are infinitely large, and the gas flow inside them is viscous. In this case, one can confidently assume that the gas molecules entering the channel from the container through the end have a distribution function of molecules crossing a certain plane in an equilibrium gas. This fact excludes the containers from the geometry under consideration. We emphasize that this is all valid only for the free molecular flow regime in the channel; as in the case with the transition regime, the simulation of the corresponding problem requires inclusion of a certain pre-channel region into the geometry under consideration [17, 18]. Thus, it is necessary to generate a particle on the entrance cross section of a channel, then calculate the particle's trajectory and locate the point of the particle's contact with the channel wall.

There is the possibility of the particle passing through the channel without any contact with the wall, in which case a new particle on the channel's entrance cross section is generated. If the particle does contact with the wall, its reflection is simulated according to the gas-surface scattering model – in particular the particle's post-contact velocity is computed. Then a new point of the particle's contact with the wall is found. The sequence is repeated until the particle exits the channel. After that, a new particle on the entrance cross section is generated.

A particle may exit the channel either via the entrance cross section (in which case it has not passed through) or via the opposite cross section (the particle has passed through). When the behaviour of a sufficiently high number of particles is modelled, the probability of a molecule passing through the channel from the entrance cross section to the exit cross section (transmission possibility) is calculated as $W = N_p/N$, where N_p is the number of particles that have passed through the channel and N is the total number of generated particles.

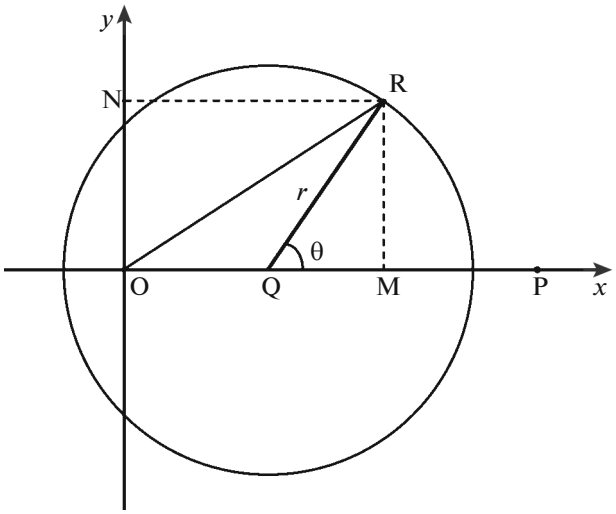

Fig. 2. Geometry of the Cercignani–Lampis model according to [22].

In this paper, with the total number of generated particles $N = 10^9$, N_p was no less than 10^8, which guarantees a computation error of no more than 0.1% [16]. Indeed, we evaluated our results by running at least 10 modelling tests of the particle movement in the channel for each individual case. In each case, the scatter of the results was insignificant, and value of $(W_{\max} - W_{\min})/\bar{W}$ did not exceed 0.001.

For the gas-surface scattering law, the diffuse as well as Maxwell [19] and Cercignani–Lampis [20] models have been used. The Maxwell model is the most frequently used model for practical calculations and scattering kernel reads as

$$R_M(\mathbf{v}' \to \mathbf{v};\varepsilon) = (1-\varepsilon)\cdot\delta(\mathbf{v} - (\mathbf{v}' - 2v_n'\mathbf{n})) + \varepsilon\frac{m^2 v_n}{2\pi(kT_s)^2}\exp\left(-\frac{mv^2}{2kT_s}\right),$$

where $\mathbf{v}'$ and $\mathbf{v}$ are velocities of the incident and reflected molecule, respectively; v_n is a normal component velocity; m is molecule mass; T_s is surface temperature; $\mathbf{n}$ is the unit vector normal to the surface; k is Boltzmann constant, and $\delta(x)$ is the delta function.

The Cercignani–Lampis (CL) model is more physically sound. In particular, we showed that, unlike the Maxwell model, the application of the Cercignani–Lampis model allows an accurate description of the gas-surface scattering process under a non-isothermal rarefied gas flow [21]. In the case of isotropic gas-surface scattering in the plane tangential to the surface, the mathematical form of the Cercignani–Lampis scattering kernel is written as

$$R_{CL}(\mathbf{v}' \to \mathbf{v};\alpha_n;\alpha_\tau) = \frac{m^2 v_n}{2\pi\alpha_n\alpha_\tau(2-\alpha_\tau)(kT_s)^2}\exp\left\{-\frac{m(v_n^2 + (1-\alpha_n)v_n'^2)}{2\alpha_n kT_s} - \frac{m(\mathbf{v}_\tau - (1-\alpha_\tau)\mathbf{v}_\tau')^2}{2\alpha_\tau(2-\alpha_\tau)kT_s}\right\}$$
$$\times I_0\left(\frac{\sqrt{1-\alpha_n}}{\alpha_n}\frac{mv_n v_n'}{kT_s}\right) \quad (0 \le \alpha_n \le 1;\ 0 \le \alpha_\tau \le 2),$$

where $I_0(x) = (2\pi)^{-1}\int_0^{2\pi}\exp(x\cos\varphi)d\varphi$, $\mathbf{v}_\tau$ is the two-dimensional vector of the tangential velocity, α_n is the accommodation coefficient of the kinetic energy corresponding to the normal molecular velocity, and α_τ is the accommodation coefficient of the tangential momentum.

In order to simulate the gas-surface scattering according to the Maxwell model, the superposition method was used: fraction ε of the incident molecules comes to equilibrium with the surface and reflects off that surface diffusely, while the remainder $(1-\varepsilon)$ is reflected specularly. The gas-surface scattering simulation on the Cercignani–Lampis model was performed based on the approach suggested by Lord [22], who offered an ingenious geometrical representation of this model (Fig. 2). The figure may represent the magnitudes of both the normal and tangential velocity components of incident $\mathbf{v}'$ and reflected $\mathbf{v}$ molecules.

Table 1. Transmission probability W through a modeled rough-surfaced channel vs the relative roughness height Λ/h and the gas-surface scattering law in the case of the length to height ratio $l/h = 10$ and inclination angle $\alpha = \beta = 45°$

Gas-surface scattering	W				
	$\Lambda/h = 1 \times 10^{-1}$	1×10^{-2}	1×10^{-3}	1×10^{-4}	1×10^{-5}
Diffuse	0.19056	0.18483	0.18427	0.18420	0.18421
Maxwell ($\varepsilon = 0.8$)	0.19158	0.18553	0.18495	0.18489	0.18489
CL ($\alpha_n = \alpha_\tau = 0.8$)	0.19177	0.18573	0.18515	0.18509	0.18506

The point P represents the state of an incident molecule. According to Lord, without loss of generality the representation must be transformed from the original coordinate system to the system within which the velocity components of an incident molecule $\mathbf{v}'$ look like $(v_n'; \sqrt{v_{\tau 1}'^2 + v_{\tau 2}'^2}; 0)$, where v_n' is the normal velocity component, whereas $v_{\tau 1}'$ and $v_{\tau 2}'$ are tangential velocity components within the original coordinate system. In this case, the distance OP represents the magnitude of v_n' or $\sqrt{v_{\tau 1}'^2 + v_{\tau 2}'^2}$.

The point Q represents the average state of reflected molecules and is located on the OP segment in such a way that the ratio OQ/OP equals either $(1 - \alpha_n)^{1/2}$ or $(1 - \alpha_\tau(2 - \alpha_\tau))^{1/2}$. The point R represents the actual state of a reflected molecule. The probability of this state lying within element $rdr d\theta$ at point $(r; \theta)$ is either $(r/\pi\alpha_n)\exp(-r^2/\alpha_n)drd\theta$ or $(r/\pi\alpha_\tau(2 - \alpha_\tau))\exp(-r^2/\alpha_\tau(2 - \alpha_\tau))drd\theta$, where r is the distance QR and θ is the angle PQR. The distance OR represents the magnitude of the normal component v_n or $\sqrt{v_{\tau 1}^2 + v_{\tau 2}^2}$, where $v_{\tau 1}$ and $v_{\tau 2}$ are the tangential components represented by projections onto the axes OM and ON, respectively.

Thus, solving the geometrical problem, one can model the velocity components $\mathbf{v}$ of a reflected molecule as follows: the normal component $v_n = (r^2 + (1 - \alpha_n)v_n'^2 + 2r(1 - \alpha_n)^{1/2}v_n' \cos\theta)^{1/2}$, where $r = (-\alpha_n \ln(1 - R_1))^{1/2}$ and $\theta = 2\pi R_2$; the tangential components $v_{\tau 1} = (1 - \alpha_\tau(2 - \alpha_\tau))^{1/2}\sqrt{v_{\tau 1}'^2 + v_{\tau 2}'^2} + r\cos\theta$ and $v_{\tau 2} = r\sin\theta$, where $r = (-\alpha_\tau(2 - \alpha_\tau)\ln(1 - R_3))^{1/2}$ and $\theta = 2\pi R_4$. Here, R_i are random numbers uniformly distributed between 0 and 1; all velocity components of both the incident and the reflected molecule are normalized to the most probable velocity at the surface temperature. For the next stage of computation, the velocity components of the reflected molecule must be then transformed back into the original coordinate system.

In our computations, the value of the diffuse fraction $\varepsilon = 0.8$ in the Maxwell model as well as the parameters of the Cercignani–Lampis model $\alpha_n = \alpha_\tau = 0.8$ are equivalent to the values commonly encountered in reality [23].

Prior to our computations, we conducted a peculiar verification of our program code. An isolated system was used consisting of two identical containers connected by a thin channel with a substantially unsymmetrical model of surface roughness (asymmetric "saw"), in particular with $\alpha = 90°$ and $\beta = 10°$ (Fig. 1). Since the system is isolated, the number of molecules in the first and second containers should be the same, according to the second law of thermodynamics. As a consequence, transmission probabilities from the first container to the second and backwards must be equal.

We computed the following parameters: transmission probability, mean path in the channel and time of traveling through the channel for the particles that passed through the entire channel and made at least one contact with the wall; also, the mean quantity of particle's collisions with the rough surface during contact. The test was carried out specifically so that some particles started from one inlet section of the channel (Case 1), whereas others started from the opposite one (Case 2).

We conducted a sufficient number of tests, specifying different channel sizes and parameters of an asymmetric "saw", and demonstrated that the calculated parameters with accuracy to computation error are the same in both simulation cases even if the height of the "saw" is the same as that of the channel [24]. This fact, hopefully, speaks of correctness of our further computations.

Table 1 presents transmission probability W through a modeled rough-surfaced channel versus relative roughness height Λ/h and the gas-surface scattering law in case of the length to height ratio $l/h = 10$ and inclination angle $\alpha = \beta = 45°$. As the table suggests, once roughness height Λ becomes negligibly small

Table 2. Transmission probability W through a modeled rough-surfaced channel vs inclination angle $\alpha = \beta$, gas-surface scattering law and length to height ratio l/h in case of relative height of roughness $\Lambda/h = 1 \times 10^{-4}$

l/h	Gas-surface scattering	W				
		$\alpha = \beta = 0°$	15°	30°	45°	60°
1	Diffuse	0.68438	0.66454	0.63146	0.60996	0.60567
	Maxwell ($\varepsilon = 0.8$)	0.72462	0.70101	0.62983	0.58704	0.60455
	CL ($\alpha_n = \alpha_\tau = 0.8$)	0.72801	0.69668	0.63763	0.60392	0.60633
10	Diffuse	0.24056	0.21615	0.19388	0.18420	0.18228
	Maxwell ($\varepsilon = 0.8$)	0.32351	0.24474	0.20228	0.18489	0.17886
	CL ($\alpha_n = \alpha_\tau = 0.8$)	0.28068	0.24206	0.20244	0.18509	0.18105

compared to channel height h, gaseous transmission probability W becomes independent of value Λ. The same behavior of W was observed in the Monte Carlo calculation of a free molecular gas flow in a rough-surfaced tube [25]. This fact agrees with the classical theoretical work [26], which determines gas scattering on a rough surface with certain limitations using just one parameter – inclination of microareas which make up the rough surface. Value $\Lambda/h = 1 \times 10^{-4}$ was used for further computations.

Table 2 shows computed transmission probability W versus inclination angle $\alpha = \beta$, the gas-surface scattering law and length to height ratio l/h. It is to be recalled that in the case of a smooth channel surface ($\alpha = \beta = 0°$) and the diffuse scattering law, transmission probability W can be calculated, using the reliable Berman's formula [27]

$$W = \frac{1}{2}[1 + (1 + L^2)^{1/2} - L] - \frac{\frac{3}{2}[L - \ln(L + (1 + L^2)^{1/2})]^2}{L^3 + 3L^2 + 4 - (L^2 + 4)(1 + L^2)^{1/2}},$$

where L is the reduced length ($L = l/h$). According to this formula, W is 0.68438 and 0.24080 for $l/h = 1$ and 10, respectively. As can be seen from the table, our results agree perfectly well with this formula. It also follows from the table that minimum transmission probability W is observed at inclination angle $\alpha = \beta = 45°$. This minimum was first recorded in [28] during Monte Carlo calculations of the transmission probability through a rough-surfaced tube.

In the case of diffuse scattering, our data agree with reliable results [29]. Unfortunately, they are presented only in the form of figures, which is why we can only acknowledge the qualitative agreement. In Fig. 3, we graphically combined figures from [29] in the case of $l/h = 10$ with the corresponding figure, reflecting the Table 2 data.

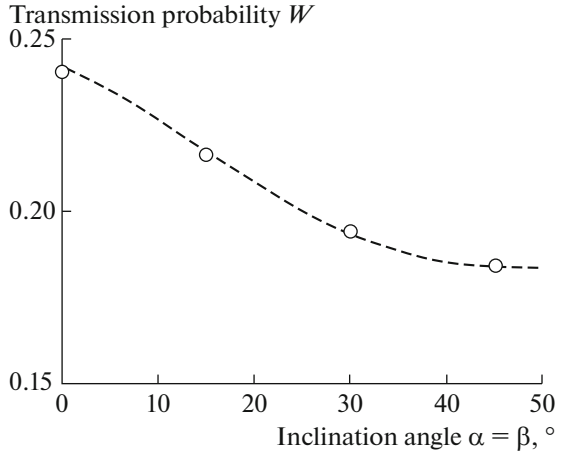

Fig. 3. Transmission probability W through a modeled rough-surfaced channel vs inclination angle $\alpha = \beta$ in the case of the diffuse scattering and the length to height ratio $l/h = 10$ (dash line—[29], circles—Table 2).

In conclusion, using the test particle Monte Carlo method, gaseous transmission probability W through a modeled rough-surfaced channel was determined with computation error less than 0.1%. The results obtained are in excellent agreement with the theoretical and numerical data available in the open literature. We hope that our results can be used as benchmark data for testing new models, methods and software in rarefied gas dynamics. Our next step is to develop a program code for modeling gas flow through a rough-surfaced channel, not only for the free molecular, but also for the transition and almost continuum flow regimes. In this case, it is necessary to model not only gas-surface scattering, but also gas molecule-molecule interaction.

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