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Short communication

Influence of gas–surface interaction on gaseous transmission probability through conical and spherical ducts

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ABSTRACT

Gas flows through ducts are used in the metrology of vacuum in order to develop a continuous flow standard. Usually, the diffuse scattering is assumed for those particles which undergo collisions with the duct surface. However, many experiments pointed out a significant deviation from the diffuse scattering especially for light gases like helium. As a consequence, the conductance calculated on the basis of the diffuse scattering can be different from the real one leading to an additional uncertainty which is usually neglected. In the present work, the conductance of conical and spherical ducts applying the Cercignani–Lampis model of the gas–surface interaction is calculated. It is shown that in contrast to previous works, the energy accommodation can significantly affect isothermal gas flows. Moreover, a decrease of the accommodation coefficients not always leads to an increase of the transmission probability, but in some situations a smaller energy accommodation coefficient corresponds to a smaller conductance.

When a rarefied gas is modeled, the diffuse gas–surface interaction, i.e. complete accommodation, is usually assumed. However, many experimental works, see e.g. Refs. [1–8], pointed out a significant deviation from the diffuse scattering especially for light gases like helium and neon. The diffuse-specular scattering is the easiest way to take into account a non-complete accommodation. As was pointed out in Refs. [9], the diffuse-specular model of the gas–surface interaction having just one adjustable parameter contradicts to experimental data on the so-called thermomolecular pressure difference [1–3]. At the same time, the Cercignani–Lampis (CL) model [10] describes more physically the gas–surface interaction due to the fact that it contains two adjustable parameters, viz., accommodation coefficients (AC) of tangential momentum α_t and that of kinetic energy of molecular motion normal to a surface α_n. Nowadays, the CL model of the gas–surface interaction is also widely used, see e.g. the papers [7–9,11–17]. The ACs α_t and α_n can be extracted by comparing theoretical results and experimental data as was done in Refs. [12–14]. According to these comparisons, the ACs are very sensitive to many factors especially to mechanical and chemical properties of a surface so that only general tendency for these coefficients can be pointed out. First, the lighter gases, like helium and neon, have smaller ACs. The momentum AC varies in the range from 0.8 to 1 and the energy AC can vary in a larger range, namely, from 0.1 to 1. Since, the value of AC for a specific surface is hardly known, it is important to estimate its influence on gas flows. According to the papers [12–14], an isothermal gas flow is determined basically by momentum AC and a heat transfer through a gas depends on both momentum and energy ACs.

The vacuum metrology is based on numerical or analytical solutions of some problems on gas flows. For instance, a continuous flow standard is based on gas flows through conical and spherical ducts shapes [18,19]. In the free-molecular regime, the flow rate through an aperture is expressed in terms of the transmission probability (TP) [20]. Its values for many kinds of aperture shape for the diffuse gas–surface interaction are given in the book by Saksaganskii [21]. Since the ducts are usually very short, the most part of gaseous molecules passes through the duct without a collision with its surface so that the fraction of particles undergoing collisions with the surface is small. Usually, it is assumed the diffuse scattering for this part of particles, but this assumption is not always fulfilled. The conductance calculated on its basis can be different from the real one that leads to an additional uncertainty which is not included in the total uncertainty calculated in Ref. [19].

The aim of the present work is to calculate the conductance through conical and spherical ducts based on the CL model using the ACs extracted from experimental data. A comparison of these

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data with those obtained for the diffuse scattering will give us the uncertainty related to the gas–surface interaction.

Consider a partition of thickness L separating two vacuum chambers. A gas flows from the left chamber to the right one through a duct of radius R on the left side of the partition. It is assumed that the pressure in the left chamber is so small that the regime of flow is free-molecular. The pressure in the right chamber is negligibly small when compared with that in the left one. Since the flow is free-molecular, the distribution function of particles entering into the duct through its left side corresponds to an equilibrium state at a temperature T_0.

The calculation will be carried out in term of the dimensionless molecular velocity defined as $\mathbf{c} = (m/2k_B T_0)^{1/2}\mathbf{v}$, where m is the molecular mass of gas, k_B is the Boltzmann constant, and $\mathbf{v}$ is the dimensional molecular velocity. Two shapes of the axisymmetrical duct shown in Fig. 1 will be considered here, viz., conical and spherical ducts. Besides the aspect ratio L/R, the conical duct is characterized by the angle β between its axis and lateral surface. The spherical duct is characterized by the sphere radius R_S.

The gas–surface interaction law can be written in a general form via a scattering kernel $R(\mathbf{c}',\mathbf{c})$ as [20,22,23] $c_n f(\mathbf{c}) = -\int_{c'_n<0} c'_n f(\mathbf{c}')R(\mathbf{c}',\mathbf{c})\mathrm{d}\mathbf{c}'$, where $f(\mathbf{c})$ is the velocity distribution function, $\mathbf{c}'$ and $\mathbf{c}$ are the molecular velocity of incident and reflected particles, respectively. According to the definition of the scattering kernel $R(\mathbf{c}',\mathbf{c})$, it represents the distribution of velocity $\mathbf{c}$ of scattered particles having its incident velocity equal to $\mathbf{c}'$. It can be decomposed on the kernels for each velocity component $R(\mathbf{c}',\mathbf{c}) = R_n(c'_n,c_n)R_t(c'_{t1},c_{t1})R_t(c'_{t2},c_{t2})$, where c_n is the component normal to the surface, while c_{t1} and c_{t2} are two tangential components.

When the surface temperature is equal to T_0, the CL kernel [10] is represented by the following components

$$R_n(c'_n,c_n) = \frac{c_n}{\pi\alpha_n}\int_0^{2\pi}\exp\Big[-\Big(c_n^2+(1-\alpha_n)c_n'^2 + 2\sqrt{1-\alpha_n}\,c_n c'_n\cos\theta\Big)\Big/\alpha_n\Big]d\theta, \qquad (1)$$

$$R_t(c'_t,c_t) = \frac{1}{\sqrt{\pi\alpha_t(2-\alpha_t)}}\exp\left[-\frac{\left(c_t-(1-\alpha_t)c'_t\right)^2}{\alpha_t(2-\alpha_t)}\right], \qquad (2)$$

where α_t is the tangential momentum AC and α_n is the AC of the kinetic energy related to the normal component of molecular velocity c_n.

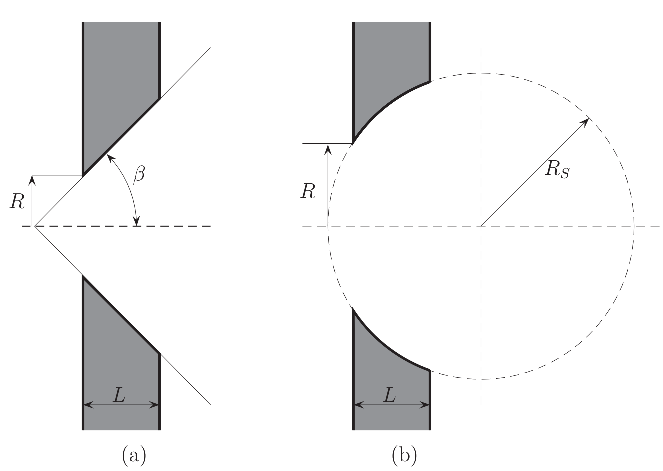

Fig. 1. Shapes and sizes of ducts: a) conical; b) spherical.

We are going to calculate the TP denoted as W through the conical and spherical ducts as function of the ACs α_t and α_n for various values of the aspect ratio L/R, angle β and radii ratio R_S/R.

The TP is calculated by the test particle Monte Carlo method which consists of a generation of model particles at the duct entrance uniformly distributed over its cross section and with the velocities obeying the Maxwellian distribution function. Then, the trajectory of each particle is simulated. When a particle hits the duct wall, its scattering is simulated according to the assumed gas–surface interaction law. As a results, some particles leave the duct through its inlet and other via its outlet. The TP is calculated as the ratio $W = N_{out}/N_{tot}$, where N_{out} is the number of particles leaving the duct through its outlet, and N_{tot} is the total number of model particles generated at the duct inlet. The method is well described in the book by Bird [24] for the diffuse-specular gas–surface interaction. Here, only the procedure to model the gas–surface interaction according to the CL law (1) and (2) will be given.

To generate the tangential components c_{t1} and c_{t2}, two variables c_* and θ are generated as

$$c_* = \sqrt{-\ln R_f}, \quad \theta = 2\pi R'_f, \qquad (3)$$

where R_f and R'_f are two different random fractions varying from 0 to 1. Then the tangential velocity components c_{t1} and c_{t2} after the collision with the wall are calculated via the corresponding components c'_{t1} and c'_{t2} before the collision as

$$c_{t1} = \sqrt{\alpha_t(2-\alpha_t)}c_*\cos\theta + (1-\alpha_t)c'_{t1}, \qquad (4)$$

$$c_{t2} = \sqrt{\alpha_t(2-\alpha_t)}c_*\sin\theta + (1-\alpha_t)c'_{t2}. \qquad (5)$$

It is checked that at $\alpha_t = 0$ the tangential velocity remains the same after the scattering, while it corresponds to the diffuse scattering at $\alpha_t = 1$.

The normal velocity component c_n is calculated independently of the tangential one following the procedure proposed by Lord [25]. First, the variables c_* and θ are generated according to (3) using random fractions R_f and R'_f generated anew. Then, the normal component of reflected particle is related to the variables c_*, θ and the normal velocity of incident particle c'_n as

$$c_n = \left[\alpha_n c_*^2 + (1-\alpha_n)c_n'^2 + 2\sqrt{\alpha_n(1-\alpha_n)}c_* c'_n\cos\theta\right]^{1/2}. \qquad (6)$$

Again, if $\alpha_n = 0$ then the normal component does not change its value, i.e. $c_n = |c'_n|$, that happens at the specular reflection. When $\alpha_n = 1$, the distribution of c_n corresponds to the diffuse scattering law, i.e. $c_n = c_*$.

Note, the TP of particles from the right chamber to the left one denoted as $W_{\leftarrow}$ is related to that calculated here as $A_{out}W_{\leftarrow} = A_{in}W$, where A_{in} and A_{out} are the areas of the inlet and outlet cross sections, respectively. It is valid for any ACs values under the assumption of the present work, i.e. the temperatures of the duct and gas are the same. Otherwise, a pumping effect would arise without any effort. Thus, the quantity $W_{\leftarrow}$ will have the same dependence on the ACs as that calculated here.

The numerical calculation were carried out for four values of the angle, viz., $\beta = 0$, 15°, 30° and 45°. The first value represents an ordinary cylinder. Eight values of the aspect ratio L/R varying between 0.1 and 20 were considered. Three values of each AC were assumed, i.e. $\alpha_t = 0.8, 0.9, 1$ and $\alpha_n = 0.1, 0.5, 1$. The smallest values