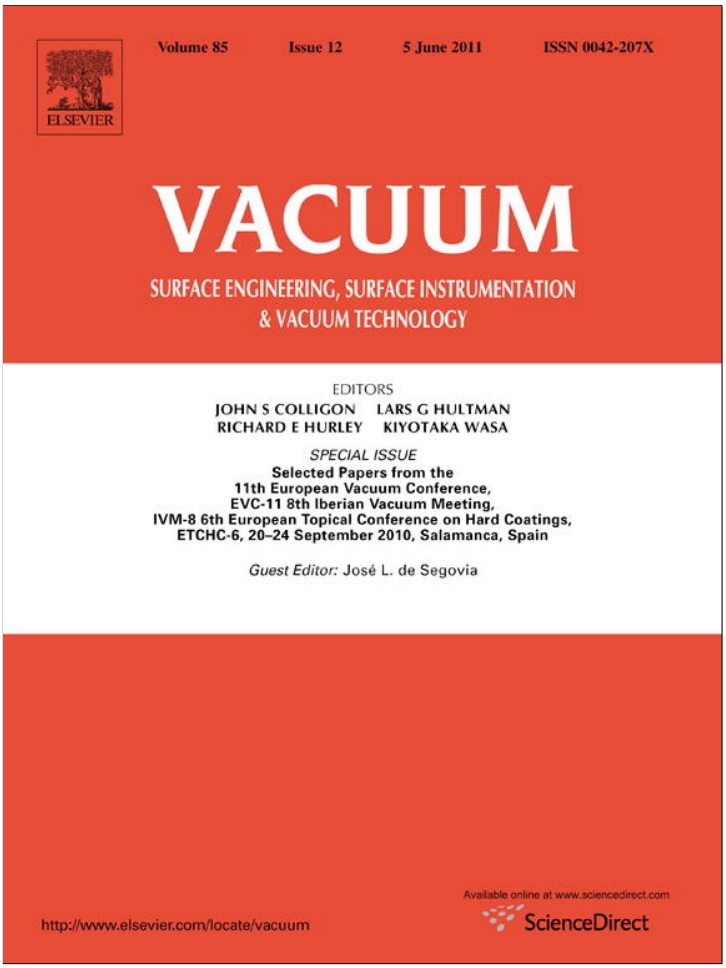

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Gas-surface scattering effect on vacuum gas flows through rectangular channels

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ABSTRACT

Flow of a rarefied gas through a channel of rectangular cross section is investigated numerically and experimentally. Emphasis is given on the study of the molecular scattering law influence at the wall boundary surfaces. The Cercignani-Lampis boundary conditions are considered in detail for the current problem, along with the linearized BGK kinetic model and the discrete velocity method. Numerical conductance values are tabulated for certain aspect ratios and accommodation coefficients in the whole range of the Knudsen number and compared with corresponding experimental results for certain gas-surface combinations. Compared to the classical Maxwell diffuse boundary conditions, the Cercignani-Lampis gas-surface interaction allows a better agreement with the measurements.

1. Introduction

It is known that the design and optimization of a gas vacuum system is a task of high complexity. This is partly due to the lack of experimental and numerical data in the literature regarding the flow behavior of gases under the pumping stage rarefied conditions. The Knudsen number in the pumping system may vary in the whole range of rarefaction, thus requiring a unified methodology for the flow simulation. Because of the low values of the pressure, the Navier-Stokes-Fourier formulation is not valid, while the free-molecular (collisionless) description of the gas fails to provide realistic results for an important range of pressure, defining the so-called transition regime. Therefore, modeling approaches based on kinetic theory should be employed due to their ability to capture the correct behavior of the gas in the whole range of the Knudsen number and for a wide variety of practical situations in vacuum systems, including pumping systems in DT fusion reactors. The vacuum network can then be studied in a tractable and efficient manner by considering each component, mostly channels of various lengths and cross-sections, separately and by constructing the numerical solution through a combination of these piping elements.

An important part of this physical description, often overlooked or oversimplified, are the boundary conditions. The commonly used Maxwell diffuse-specular kernel [1] is based on the hypothesis that a part of the molecules arriving at a wall surface depart from it having a Maxwellian distribution according to the wall temperature, while the rest of them are reflected specularly. This gas-surface interaction model is simple, easily understood at both microscopic and macroscopic level, while the associated numerical effort for its implementation is minimal. Furthermore, in a variety of physical systems, it provides reliable results in very good agreement with corresponding experimental findings [2,3].

However, it has been found that in several occasions this type of scattering law is not physically realistic. As stated in [4,5], discrepancies are found between numerical and experimental data [6]. In particular, the mass flow rate is in reality lower than it was expected by numerical calculations and the required value of the so-called tangential momentum accommodation coefficient $0 < \alpha \leq 1$ would be outside of its physical range. Also it has been reported that the value of α may depend on the rarefaction degree [6,7]. Therefore, an attempt to examine a variety of gases and surfaces and store the corresponding values of α in tables would not be effective. It seems that trying to integrate all types of interaction mechanisms in only one free parameter is not correct and cannot be physically justified.

Another gas-surface scattering kernel has been proposed in [8] and applied in several problems in the literature [9–11]. There are several advantages of this approach: Two parameters are involved, namely α_t and α_n, to quantify the accommodation of tangential momentum and the kinetic energy of the normal velocity component, respectively. The diffuse and specular scattering kernels are easily retrieved by setting the two coefficients equal to unity or zero respectively. Furthermore, the case of

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Table 1
Reduced flow rate G for some indicative cases.

δ	α_t	H/W = 1			H/W = 0.5			H/W = 0.1		
		α_n = 0.50	0.75	1.00	0.50	0.75	1.00	0.50	0.75	1.00
0.00	0.50	1.738	1.721	1.708	2.363	2.335	2.316	2.983	2.936	2.905
	1.00	0.839	0.839	0.839	1.152	1.152	1.152	1.500	1.500	1.500
	1.50	0.497	0.508	0.517	0.693	0.710	0.725	0.940	0.968	0.991
0.10	0.50	1.686	1.672	1.662	2.271	2.251	2.236	2.817	2.781	2.757
	1.00	0.793	0.793	0.793	1.073	1.073	1.073	1.354	1.354	1.354
	1.50	0.456	0.464	0.473	0.622	0.636	0.648	0.809	0.832	0.851
0.50	0.50	1.640	1.634	1.629	2.206	2.197	2.190	2.696	2.681	2.669
	1.00	0.762	0.762	0.762	1.028	1.028	1.028	1.261	1.261	1.261
	1.50	0.434	0.438	0.442	0.592	0.599	0.605	0.740	0.752	0.763
1.00	0.50	1.639	1.637	1.635	2.215	2.212	2.209	2.695	2.689	2.683
	1.00	0.768	0.768	0.768	1.043	1.043	1.043	1.265	1.265	1.265
	1.50	0.445	0.447	0.449	0.615	0.618	0.621	0.755	0.761	0.766
5.00	0.50	1.870	1.869	1.868	2.624	2.622	2.620	3.171	3.169	3.167
	1.00	0.987	0.987	0.987	1.416	1.416	1.416	1.698	1.698	1.698
	1.50	0.668	0.669	0.669	0.987	0.988	0.989	1.189	1.191	1.192
10.00	0.50	2.221	2.219	2.216	3.202	3.197	3.193	3.863	3.857	3.852
	1.00	1.317	1.317	1.317	1.959	1.959	1.959	2.360	2.360	2.360
	1.50	0.993	0.996	0.998	1.520	1.524	1.528	1.841	1.846	1.851

backscattering, i.e. the reversal of the velocity vector after a collision with a wall, is simulated using $\alpha_t = 2$, $\alpha_n = 0$. These boundary conditions also allow values of the TPD exponent in better agreement with experiments.

In this work the flow of a gas through a duct of rectangular cross section is solved subject to CL boundary conditions in the whole range of the Knudsen number. Detailed results of the conductance are tabulated in terms of the channel aspect ratio and certain values of the CL accommodation coefficients. Furthermore, a comparison with experimental results is provided to demonstrate the applicability of the CL boundary conditions. The TRANSFLOW vacuum facility, which has provided reliable experimental results in previous works [2], has been used for this purpose.

2. Kinetic formulation

2.1. Governing equations

The flow of a rarefied gas through a long rectangular duct of height H and width W has been formulated in previous works [12,13], based on kinetic model equations. The flow is driven by a pressure gradient in the longitudinal direction z, while the rectangular cross section lies on the x-y plane. Isothermal wall conditions at reference temperature T_0 are assumed.

The problem can be described in the whole range of the Knudsen number by the Boltzmann equation, where the collision term is substituted by the BGK model. After a well-known mathematical procedure [12,14] we get the governing equation

$$c_x\frac{\partial\phi}{\partial x}+c_y\frac{\partial\phi}{\partial y}+\delta\phi = \delta u_z-\frac{1}{2} \tag{1}$$

where ϕ is a reduced distribution function, c_i, $i = x,y$ are the components of the molecular velocity and u_z is the macroscopic velocity along the duct. All quantities in (1) are in dimensionless form. The rarefaction parameter δ is defined as

$$\delta = \frac{PH}{\mu v_0} \tag{2}$$

with $P = P(z)$ being the pressure along the channel, μ the dynamic viscosity at reference temperature T_0 and $v_0 = \sqrt{2RT_0}$ the most probable molecular velocity, where R is the gas constant. It is noted that the rarefaction parameter is inversely proportional to the Knudsen number. The macroscopic velocity is calculated through

$$u(x,y) = \frac{1}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\phi\exp\Big(-c_x^2-c_y^2\Big)dc_xdc_y, \tag{3}$$

while the reduced flow rate is estimated by

$$G(\delta) = 2\frac{H}{W}\int_{-W/(2H)}^{W/(2H)}\int_{-1/2}^{1/2}u(x,y)dydx \tag{4}$$

Once the kinetic problem is solved, following a standard procedure based on mass conservation along the channel the dimensionless kinetic quantities are converted to dimensionalized bulk quantities of practical interest [1]. In particular, the conductance of the flow is obtained according to [2]

$$C = \frac{4(H\times W)^2}{2(H+W)v_0m}\frac{RT_0}{L}G^*, \tag{5}$$

where

Table 2
Conductance C [l/sec] dependence on the accommodation coefficients for N_2 flow through a duct (H=W=16 mm, L=1277 mm) into vacuum at 296 K.

δ	α_t	α_n = 0.50	0.75	1.00
0.00	0.50	1.065	1.055	1.047
	1.00	0.514	0.514	0.514
	1.50	0.305	0.311	0.317
0.10	0.50	1.033	1.025	1.019
	1.00	0.486	0.486	0.486
	1.50	0.279	0.285	0.290
0.50	0.50	1.005	1.002	0.998
	1.00	0.467	0.467	0.467
	1.50	0.266	0.269	0.271
1.00	0.50	1.005	1.003	1.002
	1.00	0.471	0.471	0.471
	1.50	0.273	0.274	0.275
5.00	0.50	1.146	1.146	1.145
	1.00	0.605	0.605	0.605
	1.50	0.409	0.410	0.410
10.00	0.50	1.362	1.360	1.358
	1.00	0.808	0.808	0.808
	1.50	0.609	0.610	0.612

$$G^* = \frac{1}{\delta_1 - \delta_2} \int_{\delta_2}^{\delta_1} G(\delta) d\delta. \quad (6)$$

Here δ_1 and δ_2 correspond to the inlet and outlet conditions, while m denotes the molecular mass. The integrodifferential system of (1) and (3) may be solved provided that boundary conditions along the perimeter of the rectangular cross section are properly imposed.

2.2. Boundary conditions

In the case of linearized kinetic equations, boundary conditions are modeled by [5]

$$\phi^+ = A\phi^- + \phi_0 - A\phi_0 \quad (7)$$

with the subscript 0 denoting the reduced Maxwellian distribution at the surface conditions and the superscripts +, − denoting the distributions of molecules departing from and impinging on the wall. The operator A is defined as

$$A\phi(\mathbf{c}) = \int_{c_n'<0} R\left(-\mathbf{c} \rightarrow -\mathbf{c}'\right)\phi\left(\mathbf{c}'\right) d\mathbf{c}' \quad (8)$$

and the scattering kernel $R(\mathbf{c}' \rightarrow \mathbf{c})$ represents the probability density function that a molecule approaching a wall with velocity $\mathbf{c}'$ will be reflected with $\mathbf{c}$.

Here, we focus on the Cercignani-Lampis scattering kernel

$$R\left(\mathbf{c}' \rightarrow \mathbf{c}\right) = \frac{2c_n}{\pi\alpha_n\alpha_t(2-\alpha_t)} \exp\left\{-\frac{c_n^2 + (1-\alpha_n)c_n'^2}{\alpha_n}\right\} \times \exp\left\{-\frac{[\mathbf{c}_t - (1-\alpha_t)\mathbf{c}_t']^2}{\alpha_t(2-\alpha_t)}\right\} I_0\left(\frac{2\sqrt{1-\alpha_n}c_n c_n'}{\alpha_n}\right) \quad (9)$$

where $I_0(x) = (1/2\pi)\int_0^{2\pi} exp(x\cos\psi)d\psi$ is the modified Bessel function of the first kind and zeroth order. It can be seen that by setting in (9) $\alpha_n = \alpha_t = 1$ or $\alpha_n = \alpha_t = 0$, the diffuse and specular scattering kernels are reduced, respectively.

The governing Equations (1) and (3), subject to CL boundary conditions (9), are solved numerically using a central difference scheme in the physical space and the discrete velocity algorithm in the molecular velocity space. The resulting discretized equations are solved in an iterative manner. This typical computational scheme has been repeatedly used in the past with great success and is described in detail in previous works (e.g. [14].).

3. Experimental setup

It would be useful to compare the current numerical simulations with relevant experimental data in order to obtain the accommodation coefficients, thereby characterizing the specific gas-surface combinations. For this purpose, the TRANSFLOW (Transitional Flow Range Experiments) test facility, set up by the KIT research team, has been employed. The basic principle of the TRANSFLOW test rig is the measurement of the conductance of different channels in the transitional and near transitional flow regime at isothermal conditions, based on the direct dynamic approach: a constant flow is adjusted and the pressure difference is measured. The constant flow into the test rig is provided by a dosing unit. The temperature and pressure of the injected gas can be measured in the dosing dome, which is directly connected to the dosing unit. The test channel follows the dosing dome in the flow direction. At the downstream end it is connected with the pump dome. The pump dome serves to measure temperatures and pressures at the outlet side of the test channel. It is also equipped with turbomolecular pumps, which are further connected to the forepumps, to maintain the vacuum conditions inside the system. A complete description can be found in [2]. In this work, a long duct with length L = 1277 mm and H = W = 16 mm has been used. The inner surface of the channel was of standard clean technical quality without special treatment. Gas nitrogen (N_2) was used in average temperature $T_0 = 296$ K.

4. Results

The numerical results have been obtained using a uniform grid of 200 intervals in both x and y directions, 20 magnitudes, distributed in $[0, c_{max}]$ according to the Legendre polynomial roots, and 120 polar angles, uniformly distributed in $[0, 2\pi]$. The validity of the code has been benchmarked for $\alpha_t = \alpha_n = 1$ by comparing with corresponding results in the literature [12] obtained using Maxwell diffuse boundary conditions and good agreement has been found. Also, the qualitative behavior of the CL results is similar to the one observed in other geometrical configurations, such as flow through a cylindrical tube [5].

In Table 1 the reduced flow rate G is shown for three aspect ratios H/W in the whole range of the rarefaction parameter δ. It is seen that it highly depends on the value of the tangential momentum accommodation coefficient. Lower values of conductance are observed for higher α_t, occurring due to a higher probability of bouncing-back molecular behavior. Furthermore, the variation of α_n does not play a significant role. In more detail, the influence of α_n on G depends on the degree of tangential accommodation: for $\alpha_t < 1$ an increase in α_n causes a decrease in the flow rate, while for $\alpha_t > 1$ the opposite tendency is demonstrated. The flow rate is also highly dependent on the aspect ratio of the orthogonal cross section and increases as the ratio decreases. Finally, it is noted that in every case, the Knudsen minimum occurs for values of δ around unity.

Based on the dimensionless results, in Table 2, the conductance is provided for nitrogen flow through a square duct used in the experimental part of this work. It is seen that the dependency of the conductance on the CL accommodation coefficients is similar to the one observed for the reduced flow rate.

In Fig. 1, the computational results based on the CL and Maxwell diffuse boundary conditions have been compared with corresponding experimental data from previous work [2]. In order to

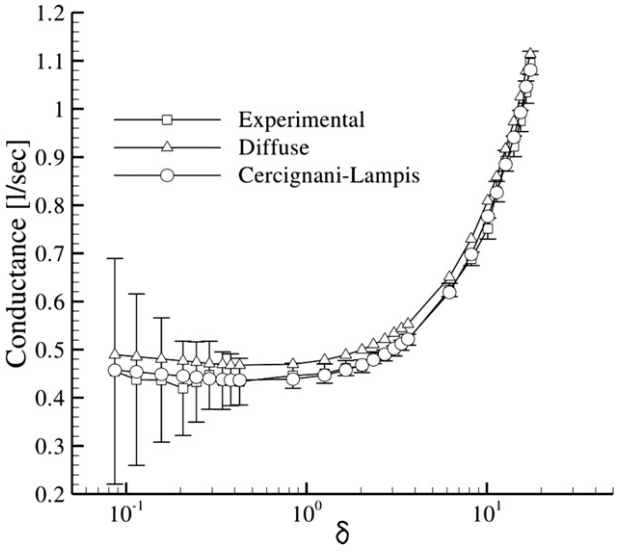

Fig. 1. Comparison between experimental and numerical results (nitrogen, 296 K).

obtain the values of the CL accommodation coefficients, it is observed that in the Tables 1 and 2 the dependence of the flow rates on α_n, for this pressure driven flow, is negligible. Therefore, it is safely assumed that $\alpha_n = 1$, while the value of α_t is varied until a very good agreement with the experimental results is obtained. It is found that by setting $\alpha_t = 1.06$ an excellent agreement is obtained with the corresponding experimental results in the whole range of δ. It is also seen that the previously implemented Maxwell diffuse boundary conditions slightly overestimate the experimental results [2]. It can be thus stated that for the specific combination of nitrogen and technically clean steel surface the backscattering phenomenon may occur, producing flow rates slightly lower than the ones predicted using the Maxwell diffuse kernel.

5. Concluding remarks

Pumping of a gas through a rectangular channel component has been considered numerically and experimentally. The Cercignani-Lampis scattering kernel has been applied and the accommodation coefficients have been extracted for specific combinations of gas and surface. Results in terms of conductance have also been tabulated for the current configuration and a wide range of rarefaction levels. It has been found that, compared to the classical Maxwell diffuse-specular boundary conditions, the implementation of the CL boundary conditions allows a better agreement with the experimental results.

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