

# **THE CERCIGNANI-LAMPIS BOUNDARY CONDITIONS IN RECTANGULAR MICRO-CHANNEL FLOWS**

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## **Abstract**

The Cercignani-Lampis boundary conditions are considered in detail for the problem of rarefied gas flow through a channel of rectangular cross-section. The linear BGK kinetic model and the discrete velocity method are employed for this study. The results are in good qualitative agreement with similar configurations for other cross-sections in the literature. The flow rate is tabulated for various values of the side ratio, the accommodation coefficients and the rarefaction parameter. The required computational effort is compared to a similar case using the Maxwell diffuse-specular kernel.

## **1 Introduction**

Kinetic calculations employing Maxwell diffuse boundary conditions are often used for practical applications, including gas flows in microchannels. The Maxwell model (Ferziger & Kaper, 1974) is based on the hypothesis that all molecules arriving at a wall surface depart from it having a Maxwellian distribution according to the wall temperature. 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 (Varoutis et al., 2009; Pitakarnnop et al., 2009). However, in several occasions it has been observed that the Maxwell scattering law is not adequate.

As stated in (Sharipov, 2002; 2003), discrepancies between numerical and experimental data are found in flows through rectangular ducts and tubes. Reliable numerical data on the rarefied gas flow through a cylindrical capillary (Cercignani & Sernagiotto, 1966; Aoki, 1989; Sharipov, 1996; Siewert, 2000), assuming diffuse reflection, are available in the literature. An extensive list of works on these types of the flows is found in the review paper by (Sharipov & Seleznev, 1998). In some cases they are in disagreement with experimental data (Porodnov et al., 1974). In particular, the mass flow rate is in reality larger than it was expected by numerical calculations. As an alternative approach, the diffuse-specular boundary conditions have been introduced. It is assumed that a percentage of molecules equal to  $\alpha \in [0,1]$  is reflected diffusely, while, the remaining percentage equal to  $(1-\alpha)$  is reflected specularly. This kernel has been used in many works (e.g., Sharipov, 1996; Porodnov et al., 1978; Breyiannis et al., 2008) and, in some cases (Porodnov et al., 1974; 1978; Borisov et al., 1999), the so-called tangential momentum accommodation coefficient, taking values between zero and unity, has been chosen so that the numerical and experimental data would fit well. In other cases however, the diffuse-specular scattering model cannot describe properly the gas-surface interaction. As it is noted in (Sharipov, 2002; 2003), performing various types of experimental measurements of i) the Poiseuille flow rate ii) the thermal creep flow rate and iii) the viscous slip coefficient, but always with the same gas and surface yields different values of  $\alpha$ . It seems that trying to integrate in only one free parameter all types of interaction mechanisms is not correct and cannot be physically justified.

Also, the implementation of the diffuse-specular model does not provide good estimates of the thermomolecular pressure difference (TPD) exponent  $\omega$ . The TPD physical system is the one where the temperature driven flow is counterbalanced by the pressure driven flow deducing a zero net flow rate (Ritos, 2009). In the free molecular limit, the kinetic solution with diffuse-specular boundary conditions yields  $\omega=1/2$  independent of  $\alpha$ , while it has been shown based on experimental work that values of  $\omega < 1/2$  may be observed (Edmonds & Hobson, 1965). It may also be worth mentioning that the value of  $\alpha$  may differ for the free-molecular and hydrodynamic regimes. For example, the interaction between helium and glass has been examined in (Porodnov et al. 1974; 1978) and three different values of  $\alpha$  have been used to fit the experimental data in the whole range of rarefaction. Therefore, an attempt to examine a variety of gases and surfaces and store the corresponding values of  $\alpha$  in tables for practical purposes would not be effective.

Another scattering kernel has been proposed in (Cercignani & Lampis, 1971). There are several advantages of their approach: Two parameters are involved, namely  $\alpha_t \in [0, 2]$  and  $\alpha_n \in [0, 1]$ , 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 backscattering, i.e. the reversal of the velocity vector after a collision with a wall, is simulated using  $\alpha_t = 2$ ,  $\alpha_n = 0$ . It is clearly seen that the lobular distributions produced by the Cercignani-Lampis (CL) model, shown in Figure 1 of (Santos, 2007), are more physically realistic in comparison to the corresponding distributions of the diffuse-specular model. These boundary conditions also allow values of the TPD exponent lower than  $1/2$ . A rigorous verification of this kernel should include a set of experiments investigating different transport phenomena for the same gas-surface combination.

An adequate number of works employing the CL kernel in a variety of problems now exists in the literature (Frezzotti, 1989; Sharipov & Bertoldo, 2006; Santos, 2007). Lord also extended the CL model (Lord, 1991; Lord, 1995), including polyatomic gas flows and the case of diffuse scattering with incomplete energy accommodation. He has also applied it in the widely used Direct Simulation Monte Carlo (DSMC) method. However, implementation of the CL boundary conditions to gas flows through microchannels is limited so far in cylindrical tubes only.

In this paper, the application of the CL kernel in gas flow through a channel of rectangular cross-section is discussed. This may be useful to the microfluidics community since microflows through rectangular channels have been extensively studied and in some cases discrepancies between computational and experimental results have been observed.

## 2 Scattering kernels

In general, the boundary conditions are imposed using the expression

$$|\xi_n| f(\underline{\xi}) = \int_{\xi'_n < 0} |\xi'_n| R(\underline{\xi}' \rightarrow \underline{\xi}) f(\underline{\xi}') d\underline{\xi}', \quad (1)$$

with  $\underline{\xi}$  and  $\underline{\xi}'$  being the velocity vectors of the departing and impinging molecules, respectively, and  $f(\underline{\xi}) \equiv f(\hat{\underline{r}}_B, \underline{\xi})$  is the molecular distribution function, where  $\hat{\underline{r}}_B$  is the position vector of the boundary point being considered. The scattering kernel  $R(\underline{\xi}' \rightarrow \underline{\xi})$  represents the probability that a molecule approaching a wall with velocity  $\underline{\xi}'$  will be reflected with  $\underline{\xi}$ . Also, the  $n$  subscript denotes the normal component of the corresponding velocity. The meaning of expression (1) is that

if we sum the molecules moving to the wall with any possible  $\underline{\xi}'$  and scatter to  $\underline{\xi}$  with probability  $R(\underline{\xi}' \rightarrow \underline{\xi})$ , we obtain the flow of particles leaving with  $\underline{\xi}_n$ , displayed in the left hand side of (1).

All scattering kernels must obey certain general rules. Since  $R$  denotes a probability it should be positive, i.e.,

$$R(\underline{\xi}' \rightarrow \underline{\xi}) \geq 0. \quad (2)$$

Also, assuming that the wall is not porous or absorbing, all molecules are scattered to some velocity after they collide with the wall and therefore the normalization property

$$\int_{\xi_n > 0} R(\underline{\xi}' \rightarrow \underline{\xi}) d\underline{\xi} = 1 \quad (3)$$

applies. Finally, the reciprocity condition

$$|\xi_n'| \exp\left(-\frac{m\xi'^2}{2k_B T_w}\right) R(\underline{\xi}' \rightarrow \underline{\xi}) = |\xi_n| \exp\left(-\frac{m\xi^2}{2k_B T_w}\right) R(-\underline{\xi} \rightarrow -\underline{\xi}') \quad (4)$$

holds, with  $m$  being the molecular mass,  $k_B$  the Boltzmann constant and  $T_w$  the wall temperature. Equation (4) expresses a “detailed balance” and is clarified in (Cercignani & Lampis, 1971; Cercignani, 1975).

The commonly used Maxwell diffuse-specular kernel is

$$R(\underline{\xi}' \rightarrow \underline{\xi}) = \alpha \frac{m^2 \xi_n}{2\pi (k_B T_w)^2} \exp\left(-\frac{m\xi'^2}{2k_B T_w}\right) + (1-\alpha) \delta[\underline{\xi}' - \underline{\xi} + 2\underline{n}(\underline{n} \cdot \underline{\xi}')] \quad (5)$$

where  $\delta$  is the Dirac delta function and  $\underline{n}$  is the outward normal vector on the wall surface. Here, we focus on the Cercignani-Lampis scattering kernel

$$R(\underline{\xi}' \rightarrow \underline{\xi}) = \frac{m^2 \xi_n}{2\pi \alpha_n \alpha_t (2-\alpha_t) (k_B T_w)^2} \exp\left(-\frac{m[\xi_n^2 + (1-\alpha_n)\xi_n'^2]}{2k_B T_w \alpha_n} - \frac{m[\xi_t^2 - (1-\alpha_t)\xi_t'^2]}{2k_B T_w \alpha_t (2-\alpha_t)}\right) I_0\left(\frac{\sqrt{1-\alpha_n} m \xi_n \xi_n'}{\alpha_n k_B T_w}\right) \quad (6)$$

where  $I_0(x) = \frac{1}{2\pi} \int_0^{2\pi} \exp(x \cos \phi) d\phi$  is the modified Bessel function of the first kind and zeroth order. It can be seen that by setting in (6)  $\alpha_t = \alpha_n = 1$  or  $\alpha_t = \alpha_n = 0$ , the diffuse and specular scattering kernels are reduced, respectively.

### 3 Problem formulation with the CL boundary conditions

Here, the flow of a rarefied gas through a long duct of rectangular microchannel of height  $H$  and width  $W$  is formulated, based on a kinetic model equation associated with the Cercignani-Lampis boundary conditions. The flow is isothermal at reference temperature  $T_w$ , it is due to a pressure gradient along the longitudinal  $z$  direction, while the rectangular cross section lies in the  $(x, y)$  plane, with  $-W/(2H) \leq x \leq W/(2H)$  and  $-1/2 \leq y \leq 1/2$ .

#### 3.1 Kinetic equations

It has been shown that the fully developed flow through channels of rectangular cross section can be accurately simulated by the linearized BGK equation, written as (Sharipov, 1999)

$$c_x \frac{\partial h}{\partial x} + c_y \frac{\partial h}{\partial y} = \delta [2c_z u - h] - c_z, \quad (7)$$

where  $h \equiv h(x, y, \underline{c})$  is the unknown linearized distribution function,  $\underline{c} = (c_x, c_y, c_z)$  is the molecular and  $u \equiv u_z(x, y)$  is the macroscopic velocity along the duct. All quantities in (7) are in dimensionless form. The rarefaction parameter  $\delta$  is defined as

$$\delta = \frac{PH}{\mu v_0}, \quad (8)$$

with  $P = P(z)$  being the pressure along the channel,  $\mu$  the dynamic viscosity at reference temperature  $T_0$  and  $v_0 = \sqrt{2(k_B/m)T_0}$  the most probable molecular velocity. It is noted that the rarefaction parameter is inversely proportional to the Knudsen number.

Furthermore, to reduce the computational effort, the projected distribution function

$$\phi(x, y, c_x, c_y) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} h(x, y, c_x, c_y, c_z) \exp(-c_z^2) c_z dc_z \quad (9)$$

is introduced. By acting properly on equation (7) we obtain the final expression

$$c_x \frac{\partial \phi}{\partial x} + c_y \frac{\partial \phi}{\partial y} + \delta \phi = \delta u - \frac{1}{2} \quad (10)$$

and the macroscopic velocity is calculated through

$$u(x, y) = \frac{1}{\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi \exp(-c_x^2 - c_z^2) dc_x dc_z. \quad (11)$$

Once the kinetic problem, described by (10) and (11) and the appropriate boundary conditions, is solved, the dimensionless flow rate is estimated as

$$G = 2 \frac{H}{W} \int_{-W/(2H)-1/2}^{W/(2H)-1/2} \int u(x, y) dy dz. \quad (12)$$

The formulation of the problem is completed and the integrodifferential system (10) and (11) may be solved provided that boundary conditions along the perimeter of the rectangular cross section are properly imposed. This issue is discussed in the next subsection.

### 3.2 Boundary conditions

In the case of linear kinetic models, the starting point for boundary conditions is (Cercignani, 1975)

$$h^+ = Ah^- + h_0 - Ah_0, \quad (13)$$

with the superscripts  $+, -$  denoting the distribution of particles leaving and approaching the boundary surface, respectively. The operator  $A$  is defined by (Cercignani et al., 2004)

$$[Ah](c_n, c_{t1}, c_{t2}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_0^{\infty} R(-\underline{c} \rightarrow -\underline{c}') h(c'_n, c'_{t1}, c'_{t2}) dc'_n dc'_{t1} dc'_{t2}. \quad (14)$$

The velocity component vertical to the wall is  $c_n$ , while the two tangential components parallel to the wall are  $c_{t1}$  and  $c_{t2}$ .

For the present flow configuration the Maxwellian perturbation term  $h_0$  vanishes because the walls are isothermal and their temperature is equal to the reference value. To simplify, for clarity purposes, the mathematical manipulation of the CL boundary conditions, the methodology will be presented for one of the four boundaries of the problem, namely the lower one, i.e. for  $y = -1/2$ . Also, at the lower boundary  $c_n \equiv c_y$ ,  $c_{t1} \equiv c_x$  and  $c_{t2} \equiv c_z$ . Applying the projection procedure as it is defined by (9) into (13) it is reduced that

$$\phi\left(x, -\frac{1}{2}, c_x, c_y\right) = A\phi\left(x, -\frac{1}{2}, c_x, -c_y\right), \quad c_y > 0 \quad (15)$$

Using Equation (9), the above expression can be rewritten as

$$\phi\left(x, -\frac{1}{2}, c_x, c_y\right) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} Ah\left(x, -\frac{1}{2}, c_x, -c_y, c_z\right) c_z \exp(-c_z^2) dc_z, \quad c_y > 0. \quad (16)$$

In the case of diffuse-specular boundary conditions, substituting kernel (5) into (16) yields

$$\phi\left(x, -\frac{1}{2}, c_x, c_y\right) = (1-\alpha)\phi\left(x, -\frac{1}{2}, c_x, -c_y\right), \quad c_y > 0 \quad (17)$$

where  $\alpha \in [0,1]$  is the so-called accommodation coefficient. The two limiting values  $\alpha = 0$  and  $\alpha = 1$  correspond to purely diffuse or specular scattering respectively.

In the case of the Cercignani-Lampis boundary conditions substituting (14) into (16) yields

$$\phi\left(x, -\frac{1}{2}, c_x, c_y\right) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^0 \left[ \int_{-\infty}^{\infty} R(-c \rightarrow -c') c_z e^{-c_z^2} dc_z \right] h\left(x, -\frac{1}{2}, c'_y, c'_x, c'_z\right) dc'_y dc'_x dc'_z, \quad (18)$$

for  $c_y > 0$ . Equation (18) will be simplified by estimating the integral

$$E(\underline{c}' \rightarrow \underline{c}) = \int_{-\infty}^{\infty} R(-\underline{c} \rightarrow -\underline{c}') c_z \exp(-c_z^2) dc_z. \quad (19)$$

The CL kernel, given by (6), can be decomposed as  $R = R_{t1} \times R_{t2} \times R_n$ , where the two tangential parts are

$$R_t(c'_t \rightarrow c_t) = \frac{1}{\sqrt{\pi(1-\gamma^2)}} \exp\left[-\frac{(c_t - \gamma c'_t)^2}{(1-\gamma^2)}\right] \quad (20)$$

and the normal part is

$$R_n(c'_n \rightarrow c_n) = \frac{2c_n}{\alpha_n} \exp\left[-\frac{c_n^2 + (1-\alpha_n)c_n'^2}{\alpha_n}\right] I_0\left[\frac{2\sqrt{1-\alpha_n}c_n c'_n}{\alpha_n}\right]. \quad (21)$$

Following (Cercignani et al., 2004), we have substituted  $\gamma = 1 - \alpha_t$  and  $1 - \gamma^2 = \alpha_t(2 - \alpha_t)$  in order to reduce the size of the tangential components. Therefore, the integral

$$J = \frac{E(\underline{c}' \rightarrow \underline{c})}{R_t(-c_x \rightarrow -c'_x) R_n(-c_y \rightarrow -c'_y)} = \int R_t(-c_z \rightarrow -c'_z) c_z \exp(-c_z^2) dc_z \quad (22)$$

must be estimated. Substituting (20) into (22) for  $c'_t = -c_z$  and  $c_t = -c'_z$  it is found that

$$J = \alpha c'_z \exp(-c_z'^2) \quad (23)$$

Using this result, equation (18) is rewritten in the more compact form

$$\phi^+\left(x, -\frac{1}{2}, c_x, c_y\right) = \frac{\gamma}{\sqrt{\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^0 R_n(-c_y \rightarrow -c'_y) R_t(-c_x \rightarrow -c'_x) c'_z \exp(-c_z'^2) h\left(x, -\frac{1}{2}, c'_y, c'_x, c'_z\right) dc'_y dc'_x dc'_z \quad (24)$$

Finally, substituting the scattering kernel components (20) and (21) into (24) and changing back from  $\gamma$  to  $\alpha_t$  results to the final expression for the projected distribution function at  $y = -1/2$ :

$$\begin{aligned} \phi\left(x, -\frac{1}{2}, c_x, c_y\right) = & -\frac{2(1-\alpha_t)}{\alpha_n \sqrt{\pi \alpha_t (2-\alpha_t)}} \int_{-\infty}^{\infty} \int_{-\infty}^0 \phi^-\left(x, -\frac{1}{2}, c'_x, c'_y\right) c'_y \\ & \times \exp\left\{-\frac{c_y'^2 + (1-\alpha_n)c_y'^2}{\alpha_n} - \frac{[(1-\alpha_t)c_x - c'_x]^2}{\alpha_t(2-\alpha_t)}\right\} I_0\left(\frac{2\sqrt{1-\alpha_n}c_y c'_y}{\alpha_n}\right) dc'_y dc'_x, \quad c_y > 0 \end{aligned} \quad (25)$$

It is noted that since the normal component of the impinging velocity takes only negative values at the specific boundary we have used in the manipulation  $c'_n = c_y$ .

The procedure for the other three boundaries is similar. At the upper boundary, i.e.,  $y=1/2$  the impinging particles are moving in the positive direction and this has an effect on the sign of the corresponding equation. The boundary condition at  $y=1/2$  is:

$$\phi^+\left(x, \frac{1}{2}, c_x, c_y\right) = \frac{2(1-\alpha_t)}{\alpha_n \sqrt{\pi\alpha_t(2-\alpha_t)}} \int_{-\infty}^{\infty} \int_0^{\infty} \phi^-\left(x, \frac{1}{2}, c'_x, c'_y\right) c'_y \times \exp\left\{-\frac{c_y^2 + (1-\alpha_n)c_x^2}{\alpha_n} - \frac{[(1-\alpha_t)c_x - c'_x]^2}{\alpha_t(2-\alpha_t)}\right\} I_0\left(\frac{2\sqrt{1-\alpha_n}c_y c'_y}{\alpha_n}\right) dc'_y dc'_x, \quad c_y < 0 \quad (26)$$

The corresponding boundary conditions for the left and right wall are obtained by (25) and (26), respectively, by exchanging  $c_x, c'_x$  with  $c_y, c'_y$  on the right hand side.

The governing equations (10) and (11), subject to diffuse-specular or CL boundary conditions, 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 it is described in detail in several previous works (e.g. Naris & Valougeorgis, 2005).

## 4 Results

The presented results are obtained using  $I=J=100$  nodes in the  $x$  and  $y$  directions and  $M \times N = 32 \times 100$  molecular velocities with  $M$  denoting and  $N$  the polar angles. The dimensionless flow rates, shown in Table 1, are calculated for three rectangular cross sections in the whole range of the rarefaction parameter.

In the case of complete accommodation, that is  $\alpha_t = 1$  and  $\alpha_n = 1$ , the results have been compared with the corresponding ones in the literature (Sharipov, 1999) obtained with Maxwell diffuse boundary conditions and good agreement has been found. In fact, these particular results are obtained for any value of  $\alpha_n$ , since the boundary conditions (25) and (26) for the distribution function are independent of this parameter for  $\alpha_t = 1$ .

Table 1: Dimensionless flow rates  $G$

$\delta$	$\alpha_t$	H/W = 1			H/W = 0.5			H/W = 0.25		
		$\alpha_n = 0.5$	0.75	1	0.5	0.75	1	0.5	0.75	1
0	0.5	1.7381	1.7205	1.7078	2.3628	2.3350	2.3158	2.9825	2.9355	2.9051
	1	0.8387	0.8387	0.8387	1.1523	1.1523	1.1523	1.5003	1.5003	1.5003
	1.5	0.4969	0.5076	0.5174	0.6934	0.7104	0.7253	0.9403	0.9681	0.9914
0.1	0.5	1.6856	1.6718	1.6616	2.2714	2.2506	2.2356	2.8165	2.7812	2.7573
	1	0.7934	0.7934	0.7934	1.0734	1.0734	1.0734	1.3544	1.3544	1.3544
	1.5	0.4558	0.4644	0.4725	0.6224	0.6359	0.6480	0.8092	0.8317	0.8513
0.5	0.5	1.6400	1.6339	1.6288	2.2056	2.1970	2.1902	2.6963	2.6810	2.6692
	1	0.7621	0.7621	0.7621	1.0277	1.0277	1.0277	1.2609	1.2609	1.2609
	1.5	0.4338	0.4381	0.4424	0.5920	0.5987	0.6051	0.7403	0.7522	0.7633
1	0.5	1.6392	1.6368	1.6346	2.2153	2.2119	2.2090	2.6954	2.6889	2.6834
	1	0.7677	0.7677	0.7677	1.0426	1.0426	1.0426	1.2645	1.2645	1.2645
	1.5	0.4449	0.4469	0.4489	0.6145	0.6176	0.6207	0.7550	0.7606	0.7662
5	0.5	1.8700	1.8690	1.8684	2.6235	2.6217	2.6203	3.1707	3.1688	3.1673
	1	0.9871	0.9871	0.9871	1.4156	1.4156	1.4156	1.6983	1.6983	1.6983
	1.5	0.6680	0.6688	0.6694	0.9865	0.9879	0.9891	1.1894	1.1911	1.1923
10	0.5	2.2214	2.2185	2.2160	3.2015	3.1968	3.1926	3.8630	3.8572	3.8521
	1	1.3174	1.3174	1.3174	1.9587	1.9587	1.9587	2.3601	2.3601	2.3601
	1.5	0.9930	0.9957	0.9981	1.5199	1.5243	1.5283	1.8406	1.8461	1.8511

It can be seen that the flow rate highly depends on the value of the tangential momentum accommodation coefficient. In particular, as  $\alpha_t$  increases, the flow rate is reduced. Three values of this coefficient have been studied and one of them is higher than unity, indicating a partial bouncing-back behaviour which results in reduced flow rates. Also, it is observed that  $\alpha_n$  does not cause large variations in the flow rate. The influence of  $\alpha_n$  on  $G$  is related to the values of  $\alpha_t$ : for  $\alpha_t < 1$  an increase in  $\alpha_n$  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  $\delta$  around unity.

A comparison of the required CPU time has been performed between the diffuse-specular and the CL boundary conditions. In the first case the accommodation coefficient is  $a = 0.5$ , while in the latter the CL coefficients are  $\alpha_t = 0.5$ ,  $\alpha_n = 1$ . Since both types of boundary conditions are used to fit numerical with experimental data, it is interesting to have an estimation of the total time required for each model. The CPU time (in hours) needed to solve the flow of a rarefied gas through a square channel with Maxwell and CL BCs is shown in Table 2. It is seen that the computational cost of the CL kernel is about one order of magnitude larger than the one required by the diffuse-specular kernel. This is mainly due to the additional computational effort needed in every iteration, in order to estimate the complicated integrals at the right hand side of the boundary conditions.

Table 2: CPU time (in hours) for  $H/W=1$  with i) Diffuse-specular BCs ( $a = 0.5$ ) and ii) Cercignani-Lampis BCs ( $\alpha_t = 0.5$ ,  $\alpha_n = 1$ ).

$\delta$	0	0.05	0.1	0.2	0.5	1	2	5	10	20
Maxwell	0.0461	0.0472	0.0506	0.0556	0.0686	0.0914	0.1347	0.2881	0.6253	1.6050
CL	0.7006	0.7258	0.7778	0.8553	1.0628	1.4253	2.1506	4.5853	9.8939	25.3817

Closing this work, it is noted that the CL scattering kernel has been successfully applied to solve the rarefied gas flow through a channel of rectangular cross-section. The results corresponding to Maxwell diffuse boundary conditions are in good agreement with previous work (Pitakarnnop et al., 2009; Sharipov, 1999), despite the relatively sparse numerical grid. Also, the qualitative behaviour of the CL results is similar to the one observed in other geometrical configurations such as flow through a cylindrical tube. The present work will be used to estimate the TPD exponent in rectangular channels and specify the CL coefficients for certain gas-surface interaction by comparison with experimental work.

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## References

- Aoki, K., 1989, Numerical analysis of rarefied gas flows by finite-difference method, In Rarefied Gas Dynamics, edited by E. P. Muntz, D. P. Weaver and D. H. Campbell, AIAA, Washington, DC, Volume 118
- Breyiannis, G., Varoutis, S. and Valougeorgis, D., 2008, Rarefied gas flow in concentric annular tube: Estimation of the Poiseuille number and the exact hydraulic diameter, Eur. J. Mech. B/Fluids, 27, 609-622
- Borisov, S.F., Sazhin, O.V., Sharipov, F. and Grachyov, I.A., 1999, Tangential momentum accommodation on atomic clean and contaminated surface, Rarefied Gas Dynamics 1, edited by R. Brun, R. Campargue, R. Gatignol, J.C. Lengrand, CEPAD, Toulouse, 333-339

- Cercignani, C. and Sernagiotto, F., 1966, Cylindrical Poiseuille flow of a rarefied gas, *Phys. Fluids*, 9, 40–44
- Cercignani, C. and Lampis, M. 1971, Kinetic models for gas-surface interactions, *Transport theory and statistical physics*, 1(2), 101–114
- Cercignani, C., 1975, *Theory and application of the Boltzmann equation*, Elsevier, New York
- Cercignani, C., Lampis, M. and Lorenzani, S., 2004, Plane Poiseuille Flow with Symmetric and Nonsymmetric Gas-Wall Interactions, *Transport Theory and Statistical Physics*, 33, 545–561
- Edmonds, T. and Hobson, G.P., 1965, A study of thermal transpiration using ultrahigh-vacuum techniques, *J. Vac. Sci. Technol.*, 2, 182–197
- Ferziger, J.H. and Kaper, H.G., 1972, *Mathematical Theory of Transport Processes in Gases*, North-Holland Publishing Company, Amsterdam
- Frezzotti, A., 1989, Numerical simulation of supersonic rarefied gas flow past a flat plate: effects of the gas-surface interaction model on the flow field, *Rarefied Gas Dynamics: Theoretical and computational techniques*, edited by E. P. Muntz, D. P. Weaver and D. H. Campbell, AIAA, Washington, DC, Volume 118
- Lord, R.G., 1991, Some extensions to the Cercignani-Lampis gas-surface scattering kernel, *Phys. Fluids A* 3 (4), 706–710
- Lord, R.G., 1995, Some further extensions to the Cercignani-Lampis gas-surface scattering kernel, *Phys. Fluids A* 7 (5), 1159–1161
- Naris, S. and Valougeorgis, D., 2005, The driven cavity flow over the whole range of the Knudsen number, *Phys. Fluids*, 17, 097106
- Pitakarnnop, J., Varoutis, S., Valougeorgis, D., Geoffroy, S., Baldas, L. and Colin, S., 2009, A novel experimental setup for gas microflows, *Microfluid Nanofluid*, 10.1007/s10404-009-0447-0
- Porodnov, B.T., Suetin, P.E., Borisov, S.F. and Akinshin, V.D., 1974, Experimental investigation of rarefied gas flow in different channels, *J. Fluid Mech.* 64, 417–437
- Porodnov, B.T., Kulev, A.N. and Tukhvetov, F.T., 1978, Thermal transpiration in a circular capillary with a small temperature difference, *J. Fluid Mech.*, 88, 609–622
- Ritos, K., Lihnaropoulos, J., Naris, S. and Valougeorgis, D., 2009, Study of the thermomolecular pressure difference phenomenon in thermal creep flows through microchannels of triangular and trapezoidal cross sections, 2<sup>nd</sup> Micro and Nano Conference, West London, UK
- Santos, W.F.N., 2007, Gas-Surface Interaction Effect on Round Leading Edge Aerothermodynamics, *Brazilian Journal of Physics*, 37, 2A, 337–348
- Sharipov, F., 1996, Rarefied gas flow through a long tube at any temperature difference, *J. Vac. Sci. Technol.*, A 14, 2627–2635
- Sharipov, F. and Seleznov, V., 1998, Data on internal rarefied gas flows, *J. Phys. Chem. Ref. Data*, 27, 657–706
- Sharipov, F., 1999, Rarefied gas flow through a long rectangular channel, *J. Vac. Sci. Technol. A* 17 (5), 3062–3066
- Sharipov, F., 2002, Application of the Cercignani–Lampis scattering kernel to calculations of rarefied gas flows. I. Plane flow between two parallel plates, *Eur. J. Mech. B/Fluids* 21, 113–123
- Sharipov, F., 2003, Application of the Cercignani–Lampis scattering kernel to calculations of rarefied gas flows. III. Poiseuille flow and thermal creep through a long tube, *Eur. J. Mech. B/Fluids* 22, 145–154
- Sharipov, F. and Bertoldo, G., 2006, Heat transfer through a rarefied gas confined between two coaxial cylinders with high radius ratio, *J. Vac. Sci. Technol. A*, 24, 6, 2087–2093
- Siewert, C.E., 2000, Poiseuille and thermal-creep flow in cylindrical tube, *J. Comp. Phys.*, 160, 470–480
- Varoutis, S., Naris, S., Hauer, V., Day, C. and Valougeorgis, D., 2009, Computational and experimental study of gas flows through long channels of various cross sections in the whole range of the Knudsen number, *J. Vac. Sci. Technol. A* 27 (1), 89–100