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The Boltzmann Equation: Mathematics and Applications

CARLO CERCIGNANI (*)

Sunto. – Il lavoro è suddiviso in due parti. La prima presenta un risultato recente dell'autore riguardante l'esistenza della soluzione dell'equazione di Boltzmann per molecole maxwelliane, senza alcun taglio nel nucleo del termine d'urto, quando la soluzione dipende da una sola variabile spaziale. A differenza del ben noto teorema di Di Perna-Lions, si dimostra che vale anche la conservazione dell'energia. La seconda parte presenta problemi di dinamica dei gas rarefatti, retti dall'equazione di Boltzmann riguardanti la teoria delle micromaxxhine (MEMS) e nanomacchine (MEMS).

Summary. – The paper is subdivided into two parts. The first presents a recent result by the author concerning the existence of the solution of the Boltzmann equation for Maxwell molecules, without any cutoff in the collision kernel, when the solution depends on just one variable. At variance with the well-known theorem of DiPerna-Lions, conservation of energy is also shown to hold. The second part will concern rarefied gas dynamics problems, governed by the Boltzmann equation and concerning the theory of micromachines (MEMS) and nanomachines (NENS).

1. - Introduction

The present paper is subdivided into two parts. The first presents a recent result by the author concerning the existence of the solution of the Boltzmann equation for Maxwell molecules, without any cutoff in the collision kernel, when the solution depends on just one variable. At variance with the well-known theorem of DiPerna-Lions, conservation of energy is also shown to hold. The second part will concern rarefied gas dynamics problems, governed by the Boltzmann equation and concerning the theory of micromachines (MEMS) and nanomachines (NENS). These devices are increasingly applied to a great variety of industrial and medical problems. In these problems, given the small dimensions of the devices, it is necessary to use the kinetic theory, instead of the usual fluid dynamics, based on the Navier - Stokes equations, to describe the motion of

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air in the gaps of the devices. Some variational and simple numerical solutions will be discussed and compared with costly Monte Carlo simulations in the second part of the paper. In the rest of this introduction we shall introduce the problem discussed in the first part.

In 1989, DiPerna and Lions [8] used various previous results and remarks, together with their new concept of renormalized solution to prove the first general global existence theorem for the Boltzmann equation in the non-homogeneous case. It was soon clear [2] that solutions depending on just one space variables are special in the sense that one may hope to obtain existence in a more traditional sense; the final step was recently performed by the author [4], who eliminated a truncation for small relative speeds in the collision term.

Here we are concerned with the initial value problem for the nonlinear Boltzmann equation for Maxwell molecules without cutoff, when the solution depends on just one space coordinate which might range from $-\infty$ to $+\infty$ or from 0 to 1 (with periodicity boundary conditions); for definiteness we stick to the latter case. Easy modifications, in the vein of Ref. [6], are necessary to deal with the case of different boundary conditions. The x-, y- and z- component of the velocity $v \in \mathbb{R}^3$ will be denoted by ξ , η and ζ respectively, and the equation reads

(1.1)
$$\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial x} = Q(f, f)$$

with

$$(1.2) Q(f,f)(x,v,t) = \int \int B(\boldsymbol{n} \cdot (\boldsymbol{v} - \boldsymbol{v}_*), |\boldsymbol{v} - \boldsymbol{v}_*|) (f'f'_* - ff_*) \sin\theta \, d\theta d\phi \, d\boldsymbol{v}_*.$$

$$v' = \boldsymbol{v} - \boldsymbol{n}[\boldsymbol{n} \cdot (\boldsymbol{v} - \boldsymbol{v}_*)]$$

$$v'_* = \boldsymbol{v}_* + \boldsymbol{n}[\boldsymbol{n} \cdot (\boldsymbol{v} - \boldsymbol{v}_*)]$$

For a detailed explanation of the structure of the collision term, see [3], [7], or [8]. The angles θ and ϕ are the polar and azimuthal angles of the collision parameter $n \in S^2$ relative to a polar axis in direction $V = v - v_*$.

We introduce as in [4] the weak form of the collision term, Q(f,f). We shall henceforth use the latter notation for the operator defined by:

$$(1.3) \int_{[0,T]\times[0,1]\times\mathbb{R}^3} Q(f,f)(x,\boldsymbol{v},t)\,\varphi(x,\boldsymbol{v},t)\,d\boldsymbol{v}\,dx\,dt$$

$$= \frac{1}{2} \int_{[0,T]\times[0,1]\times\mathbb{R}^3\times\mathbb{R}^3\times S^2} B(\boldsymbol{n}\cdot(\boldsymbol{v}-\boldsymbol{v}_*),|\boldsymbol{v}-\boldsymbol{v}_*|)\,(\varphi'+\varphi'_*-\varphi-\varphi_*)ff_*d\mu dt\,.$$

for any test function $\varphi(x, \boldsymbol{v}, t)$ which is twice differentiable as a function of \boldsymbol{v} with second derivatives uniformly bounded with respect to x and t. In Eq. (1.4) we

have used the notation

$$(1.4) d\mu = \sin\theta \, d\theta d\phi \, d\mathbf{v}_* d\mathbf{v} dx$$

We remark that for classical solutions the above definition is known to be equivalent to that in (1.2). The main reason for introducing it is that it may produce weak solutions (as opposed to renormalized solutions in the sense of DiPerna and Lions [8]) even if the collision term is not necessarily in L^1 . This also avoids cutting off the small relative speeds, as done in [6].

For a function f to be a weak solution of the Boltzmann equation, it must satisfy Eq. (1.1), where the derivatives in the left hand side are distributional derivatives and the right hand side has been defined above.

We assign an initial value $f(x, \mathbf{v}, 0) = f_0(x, \mathbf{v})$, and we shall assume that $f_0 \in L^1_+([0, 1] \times \mathbb{R}^3)$ with the normalization

$$(1.5) \qquad \qquad \iint f_0 \, dx \, dv = 1.$$

The association of the solution with the weak formulation is standard. The objective of this paper is to show that the initial value problem for the Boltzmann equation without angular cutoff has a global weak solution in the sense defined above. The main step in proving this is a proof that collision term Q(f,f) is such that the expression in Eq. (1.3) is finite.

2. – The collision term for weak solutions in the case of noncutoff potentials

In this section we want to prove that the definition of Sect. 1 makes sense for inverse power potentials without introducing Grad's angular cutoff, as hinted at in the previous paper [4]. To this end we consider the following identity:

$$(2.1) \qquad \int_{0}^{1} ds \int_{0}^{1} dt \frac{\partial^{2}}{\partial s \partial t} \left[\varphi(\boldsymbol{v} + s(\boldsymbol{v}' - \boldsymbol{v}) + t(\boldsymbol{v}_{*} - \boldsymbol{v}')) \right]$$

$$= \int_{0}^{1} ds \left\{ \frac{\partial}{\partial s} \left[\varphi(\boldsymbol{v} + s(\boldsymbol{v}' - \boldsymbol{v}) + (\boldsymbol{v}_{*} - \boldsymbol{v}')) \right] - \frac{\partial}{\partial s} \left[\varphi(\boldsymbol{v} + s(\boldsymbol{v}' - \boldsymbol{v})) \right] \right\}$$

$$= \varphi(\boldsymbol{v}_{*}) - \varphi(\boldsymbol{v}') - \varphi(\boldsymbol{v}'_{*}) + \varphi(\boldsymbol{v})$$

Hence

$$(2.2) \qquad \varphi(\boldsymbol{v}) + \varphi(\boldsymbol{v}_*) - \varphi(\boldsymbol{v}') - \varphi(\boldsymbol{v}'_*) = \int_0^1 ds \int_0^1 dt \sum_{i,j=1}^3 \frac{\partial^2 \varphi}{\partial v_i \partial v_j} (v_i' - v_i) (v_j^* - v_j')$$

If K is an upper bound for the second derivatives, we obtain the following

estimate

$$(2.3) |\varphi(v) + \varphi(v_*) - \varphi(v') - \varphi(v'_*)| \le 9K|v' - v||v^* - v'| \le 9K|V||n \cdot V|$$

Hence if the kernel B diverges for $\theta = \pi/2$, but $B\cos\theta$ is integrable, then the integral with respect to θ does not diverge. We recall that, if the intermolecular force varies as the n-th inverse power of the distance, then

$$(2.4) B(\boldsymbol{n} \cdot (\boldsymbol{v} - \boldsymbol{v}_*), |\boldsymbol{v} - \boldsymbol{v}_*|) = B(\theta)|V|^{\frac{n-5}{n-1}}$$

where $B(\theta)$ is a non-elementary function of θ which for θ close to $\pi/2$ behaves as the power -(n+1)/(n-1) of $|\pi/2-\theta|$. In particular, for n=5 one has the Maxwell molecules, for which the dependence on V disappears.

We conclude that for power-law potentials, $B\cos\theta$ behaves as the power -2/(n-1) of $|\pi/2-\theta|$ and the definition of a weak solution given in Sect. 1 makes sense for n > 3.

Henceforth we shall consider just Maxwell molecules, for which we state the main result of this section as

Lemma 2.1. – The following estimate holds

$$(2.5) \qquad \left| \int\limits_{[0,T]\times[0,1]\times\mathbb{R}^3} Q(f,f)(x,\boldsymbol{v},t)\,\varphi(x,\boldsymbol{v},t)\,d\boldsymbol{v}\,dx\,dt \right| \\ \leq \beta_0 K \int\limits_{[0,T]\times[0,1]\times\mathbb{R}^3\times\mathbb{R}^3} |\boldsymbol{V}|^2 f f_* d\boldsymbol{v} d\boldsymbol{v}_* dx\,dt\,.$$

where K is un upper bound for the second derivatives of ϕ and β_0 a constant that only depends on molecular parameters.

3. - Basic estimates

We recall from a previous paper [4] that if we cutoff the values of θ close to $\pi/2$ then there is a weak solution in the sense defined in Sect. 1.

THEOREM 3.1. – Let $f_0 \in L^1(\mathbb{R} \times \mathbb{R}^3)$ be such that

(3.1)
$$\int f_0(\cdot)(1+|v|^2)dvdx < \infty; \qquad \int f_0|\ln f_0(.)|dvdx < \infty.$$

Also, assume that the collision kernel for Maxwell molecules B is cutoff for $|\theta - \pi/2| \le \varepsilon$ ($\varepsilon > 0$). Then there is a weak solution f(x, v, t) of the initial value problem (1.1), (1.4), such that $f \in C(\mathbb{R}_+, L^1(\mathbb{R} \times \mathbb{R}^3)), f(.,0) = f_0$. This solution conserves energy globally.

We now set out to prove the crucial estimates for the solution of the initial value problem and for the collision term. It is safe to assume that we deal with a sufficiently regular solution of the problem, because this can always be enforced by truncating the collision kernel and modifying the collision terms in the way described in earlier work, in particular in [8]. If we obtain strong enough bounds on the solutions of such truncated problems, we can then extract a subsequence converging to a renormalized solution in the sense of DiPerna and Lions; and the bounds which we do get actually guarantee that this solution is then a solution in the weak sense defined above.

Consider now the functional

(3.2)
$$I[f](t) = \int_{x < y} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} (\xi - \xi_*) f(x, \mathbf{v}, t) f(y, \mathbf{v}_*, t) d\mathbf{v}_* d\mathbf{v} dx dy$$

where the integral with respect to x and y is over the triangle $0 \le x < y \le 1$. This functional was in the one-dimensional discrete velocity context first introduced by Bony [1]. The use of this functional is the main reason why we have to restrict our work to one dimension; no functional with similar pleasant properties is known, at this time, in more than one dimension (for a discussion of this point see a recent paper of the author [5]). Notice that if we have bounds for the integral

with respect to x of $\rho = \int_{\mathbb{R}}^{3} f(x, \boldsymbol{v}, t) d\boldsymbol{v}$ and for

$$E(t) = \int_{0}^{1} \int |\boldsymbol{v}|^{2} f \ d\boldsymbol{v} dx,$$

then we have control over the functional I[f](t).

A short calculation with proper use of the collision invariants of the Boltzmann collision operator shows that

(3.3)
$$\frac{d}{dt}I[f] = -\int_{[0,1]} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} (\xi - \xi_*)^2 f(x, \boldsymbol{v}_*, t) f(x, \boldsymbol{v}, t) \, d\boldsymbol{v} d\boldsymbol{v}_* dx$$

Notice that the first term on the right, apart from the factor $(\xi - \xi_*)^2$, has structural similarity to the collision term of the Boltzmann equation, and the integrand is nonnegative. This is the reason why the functional I[f] is a powerful tool.

After integration from 0 to T > 0 and reorganizing,

(3.4)
$$\int_{0}^{T} \int_{[0,1]} \int_{r} \int_{r} (\xi - \xi_{*})^{2} f(x, \boldsymbol{v}_{*}, t) f(x, \boldsymbol{v}, t) d\boldsymbol{v} d\boldsymbol{v}_{*} dx dt = I[f](0) - I[f](T).$$

According to a previous remark, the right-hand side of (3.4) is bounded. Since the total energy is conserved, we have proved

LEMMA 3.2. – If f is a sufficiently smooth solution of the initial value problem given by (1.1) and (1.4) with initial value f_0 , then

$$\int_{0}^{t} \int_{0}^{1} \int_{r} \int_{r} (\xi - \xi_{*})^{2} f(x, \boldsymbol{v}_{*}, \tau) f(x, \boldsymbol{v}, \tau) d\boldsymbol{v} d\boldsymbol{v}_{*} dx d\tau$$

are bounded.

The idea of the basic estimates was given in Ref. [2]; we will repeat some details here to make this paper self-contained.

We have now the following

Lemma 3.3. – Under the above assumptions, we have, for the weak solutions of the Boltzmann equation for noncutoff Maxwell molecules:

(3.7)
$$\int_{\mathbb{R}^{3} \times \mathbb{R}^{3} \times [0,T] \times [0,1]} |\boldsymbol{v} - \boldsymbol{v}_{*}|^{2} f(\boldsymbol{x}, \boldsymbol{v}, t) f(\boldsymbol{x}, \boldsymbol{v}_{*}, t) dt d\mu < K_{0}$$

where K_0 is a constant, which only depends on the initial data (and molecular constants).

In fact, we can take $\varphi = \xi^2$ as a test function and remark that the contribution of the left hand side is bounded in terms of the initial data because $\xi^2 \leq |v|^2$. Hence the integral in the right hand side is also bounded. When computing this integral, we use as polar angles θ (the angle between \boldsymbol{n} and \boldsymbol{V}) and ϕ (a suitable angle in the plane orthogonal to \boldsymbol{V}) so that the components n_i (i=1,2,3) of \boldsymbol{n} are given by

$$\begin{split} n_1 &= \frac{V_1}{V}\cos\theta - \frac{V_0}{V}\sin\theta\cos\phi \\ n_2 &= \frac{V_2}{V}\cos\theta + \frac{V_1V_2}{VV_0}\sin\theta\cos\phi - \frac{V_3}{V}\sin\theta\sin\phi \\ n_3 &= \frac{V_3}{V}\cos\theta + \frac{V_1V_3}{VV_0}\sin\theta\cos\phi + \frac{V_2}{V}\sin\theta\sin\phi \end{split}$$

where V_i (i=1,2,3) are the components of \emph{V} and $V_0=\sqrt{V_2^2+V_3^2}$. Then we have

$$\xi' = \xi - V_1 \cos^2 \theta + \frac{1}{2} V_0 \sin 2\theta \cos \phi$$

$$\xi_*' = \xi_* + V_1 \cos^2 \theta - \frac{1}{2} V_0 \sin 2\theta \cos \phi$$

We have:

$$\begin{split} \varphi(\boldsymbol{v}) + \varphi(\boldsymbol{v}_*) - \varphi(\boldsymbol{v}') - \varphi(\boldsymbol{v}'_*) &= 2V_1^2\cos^2\theta \\ -V_1V_0\sin2\theta\cos\phi - 2V_1^2\cos^4\theta - \frac{1}{2}V_0^2\sin^22\theta\cos^2\phi + 2V_0V_1\cos^2\theta\sin2\theta\cos\phi \end{split}$$

Then after integrating with respect to ϕ :

$$(3.9) \int_{[0,T]\times[0,1]\times\mathbb{R}^3} Q(f,f)(x,v,t)\xi^2 dv dx dt$$

$$= \int_{[0,T]\times[0,1]\times\mathbb{R}^3\times\mathbb{R}^3\times S^2} B(\theta)\{\pi[-2V_1^2\cos^2\theta + 2V_1^2\cos^4\theta] + \frac{\pi}{4}V_0^2\sin^22\theta)ff_*d\mu dt$$

$$= \int_{[0,T]\times[0,1]\times\mathbb{R}^3\times\mathbb{R}^3\times S^2} B(\theta)\{\frac{\pi}{4}(V^2 - 3V_1^2\})\sin^22\theta ff_*d\mu dt.$$

We can separate the contributions from the two terms, since they separately converge and obtain

$$(3.10) \int_{[0,T]\times[0,1]\times\mathbb{R}^{3}} Q(f,f)(x,\boldsymbol{v},t)\xi^{2}d\boldsymbol{v} dx dt = -3B_{0} \int_{[0,T]\times[0,1]\times\mathbb{R}^{3}\times\mathbb{R}^{3}} (\xi-\xi_{*})^{2} f f_{*}d\boldsymbol{v} d\boldsymbol{v}_{*} dx dt + B_{0} \int_{[0,T]\times[0,1]\times\mathbb{R}^{3}\times\mathbb{R}^{3}} |\boldsymbol{V}|^{2} f f_{*}d\boldsymbol{v} d\boldsymbol{v}_{*} dx dt.$$

where if the force between two molecules at distance r is κr^{-5} , then

(3.11)
$$B_0 = a\sqrt{\frac{\kappa}{2m^3}} \quad (a = 1.3703...).$$

The constant a was first computed by Maxwell [10]; the value given here was computed by Ikenberry and Truesdell [9]. Since we know that the left hand side of Eq. (3.10) is bounded and the first term in the right hand side is bounded, it follows that the last term is also bounded by a constant depending on initial data (and molecular constants, such as m and κ).

4. - Existence of weak solutions for noncutoff potentials

In order to prove the existence of a weak solution, we shall assume that this has been proved for Maxwell molecules with an angular cutoff ([4]), as stated in Theorem 3.1; actually to make the paper self-contained and the proof more explicit, we shall assume that the proof is available when a cutoff for small relative speed is introduced. In this case, in fact the proof

immediately follows from the DiPerna-Lions existence theorem with the estimate of Lemma 3.4; it is enough to remark that a solution exists when we renormalize by division by $1 + \varepsilon f$ (f independent of $\varepsilon > 0$) and we case to the limit $\varepsilon \to 0$ thanks to (3.7), which, of course, holds in the cutoff case as well.

In the noncutoff case we approximate the solution by cutting off the angles close to $\pi/2$ and the small relative speeds. In this way we can obtain a sequence f_n formally approximating the solution f whose existence we want to prove.

LEMMA 4.1. – Let $\{f^n\}$ be a sequence of solutions to an approximating problem. There is a subsequence such that for each T > 0

i)
$$\int f^n \ dm{v} o \int f \ dm{v} \ a.e. \ and \ in \ L^1((0,T) imes \mathbb{R}^3),$$
 ii)
$$\int\limits_{\mathbb{R}^3} |V|^2 f_{n*} dm{v}_* o \int\limits_{\mathbb{R}^3} |V|^2 f_* dm{v}_*$$

in $L^1((0,T) \times \mathbb{R}^3 \times B_R)$ for all R > 0, and a.e., iii)

$$(4.1) g_n(x,t) = \frac{\int\limits_{\mathbb{R}^3 \times \mathbb{R}^3} |V|^2 f_n f_{n*} d\boldsymbol{v} d\boldsymbol{v}_*}{1 + \int f_n d\boldsymbol{v}} \to \frac{\int\limits_{\mathbb{R}^3 \times \mathbb{R}^3} |V|^2 f f_* d\boldsymbol{v} d\boldsymbol{v}_*}{1 + \int f d\boldsymbol{v}} = g(x,t)$$

weakly in $L^1((0,T)\times(0,1))$.

PROOF. – i) is immediate. ii) uses an argument well-known in DiPerna-Lions proof with the estimate $\sup_n \int f_n(1+|v|^2) dv < \infty$ to reduce the problem to bounded domains with respect to v_* .

For iii) we use i) and the fact that f_n converges weakly, but the factor multiplying it in the integral converges a.e. because of ii).

Now we remark that $g_n(x,t)$ converges weakly to g(x,t) and $\rho_n(x,t)$ converges a.e. to $\rho(x,t)$ and the integral $\int \rho_n g_n dx dt$ is uniformly bounded to conclude with the following Lemma:

Lemma 4.2. – Let $\{f_n\}$ be a sequence of solutions to an approximating problem. There is a subsequence such that for each T > 0

$$(4.2) \qquad \int\limits_{(0,T)\times(0,1)\times\mathbb{R}^3\times\mathbb{R}^3} |V|^2 f_n f_{n*} d\mu dt \to \int\limits_{(0,T)\times(0,1)\times\mathbb{R}^3\times\mathbb{R}^3} |V|^2 f f_* d\mu dt$$

We can now prove the following, basic result:

Lemma 4.3. – Let $\{f_n\}$ be a sequence of solutions to an approximating problem, weakly converging to f. There is a subsequence such that for each T > 0

$$(4.3) \qquad \int\limits_{(0,T)\times(0,1)\times\mathbb{R}^3} \phi Q_n(f_n,f_n)dtdxd\boldsymbol{v} \to \int\limits_{(0,T)\times(0,1)\times\mathbb{R}^3} \phi Q(f,f)dtdxd\boldsymbol{v}$$

where Q_n and Q are given by the weak form of the collision operator, as defined in Eq. (1.4).

PROOF. — In fact the integrand in the left hand side of Eq. (4.3) is dominated by the integrand of Eq. (4.2) which weakly converges and we can take the limit.

Thanks to this result, we can now pass to the limit in the approximating problem to obtain

THEOREM 4.4. – Let $f_0 \in L^1(\mathbb{R} \times \mathbb{R}^3)$ be such that

$$(4.4) \qquad \int f_0(\cdot)(1+|\boldsymbol{v}|^2)d\boldsymbol{v}dx < \infty; \qquad \int f_0|\ln f_0(.)|d\boldsymbol{v}dx < \infty.$$

Then there is a weak solution $f(x, \mathbf{v}, t)$ of the initial value problem (1.1), (1.4), such that $f \in C(\mathbb{R}_+, L^1(\mathbb{R} \times \mathbb{R}^3)), f(., 0) = f_0$.

An immediate consequence of Theorem 4.4 is

THEOREM 4.5. – The solution whose existence has been proved in the previous theorem conserves energy globally.

In fact we can take $\varphi = |v|^2$ as a test function and this immediately yields the result. The lack of this property is one of the drawbacks of the DiPerna-Lions renormalized solutions.

It is, of course, easy to prove that momentum is conserved globally. But we can prove more, i.e.

Theorem 4.6. – The solution whose existence has been proved above conserves momentum locally.

In fact we can take $\varphi = vg(x)$ as a test function, where g(x) is a smooth periodic function of the space coordinate: the result follows.

5. - Introduction to the second part

The presence of a fluid film is known to reduce the sliding friction between solid objects. Although one usually thinks of a liquid (typically, oil), the case of a gas lubricant (typically, air) is also very important in several applications. Sometimes, problems of gas lubrication are not so obvious, because air is so easily available that one tends to disregard its presence. As technology expands and the size of components becomes smaller and smaller, the role of rarefied gases as lubricants becomes increasingly important. A typical example is provided by modern computers: the read/write head must be as close as possible to a rotating disk, and the air in between has accordingly a thickness of the order of a mean free path.

In lubrication theory, the thickness of the gas layer is extremely small compared with its lateral dimensions. Properly handled, this observation can be used to eliminate from the equations the dependence upon one of the three space variables. This possibility was exploited since long time by the famous hydrodynamicist Osborne Reynolds [12] to integrate the mass balance equation across the layer and to use the linearized Navier—Stokes equation for momentum balance to evaluate the quantities appearing as integrands. Fortunately, Reynolds's argument can be extended to rarefied gases; the only difference is that the linearized Boltzmann equation must now be used to evaluate the averaged velocity components in the mass balance equation.

From a very superficial consideration of the matter one might expect that the main problem of lubrication theory is to predict the friction which results from a given configuration of solid objects. However, a little more reflection reveals that the real problem is quite different. Lubricating layers are usually found between two solid bodies which are acted upon by forces (such as gravity) tending to push them together. To carry this load, the gas layer must develop normal stresses, largely dominated by pressure. Thus the first task of lubrication theory is to predict the pressure distribution and from it the load-carrying capacity. Thus we must relate the velocity components to the pressure gradients and to the motion of the solid surfaces bounding the gas layer. Since the variations of thickness are very slow, this result is obtained by solving highly idealized problems between parallel plates, such as plane Couette and Poiseuille flows, which will be considered in Sect. 8. Thus these problems, far from being didactic exercises, play a very important role in applications of enormous practical importance.

6. - The Linearized Boltzmann Equation and the BGK model

The solutions describing equilibria of the Boltzmann equation are the socalled Maxwellians, *i.e.* distributions of the form

(6.1)
$$M = \rho_0 (2\pi R T_0)^{-3/2} \exp\left[-|\xi - v_0|^2/(2R T_0)\right]$$

where ρ_0 , v_0 , T_0 are parameters having the meaning of density, bulk velocity and temperature in an equilibrium state. The vector v_0 is usually taken to be zero.

We can look for solutions in the form

$$(6.2) f = M(1+h).$$

Then the Boltzmann equation takes on the form:

(6.3)
$$\frac{\partial h}{\partial t} + \xi \cdot \frac{\partial h}{\partial \mathbf{x}} = Lh + \Gamma(h, h)$$

where L is the linearized collision operator:

(6.4)
$$Lh = 2M^{-1}Q(Mh, M)$$

and $\Gamma(h,h)$ the nonlinear part (assumed to be small compared to the linear one):

(6.5)
$$\Gamma(h,h) = M^{-1}Q(Mh,Mh).$$

Here Q(f,g) is the bilinear symmetric operator uniquely associated with Q(f,f). The rigorous theory for solutions of the form (6.2) was given by S. Ukai (see Refs. [7] and [11] for more details).

In many applications, the collision term in the Boltzmann equation is replaced by the so-called BGK model (see Refs. [3] and [11] for more details):

(6.6)
$$J(f) = v[\Phi(\xi) - f(\xi)]$$

where the collision frequency v depends on the local density ρ and the local temperature T, whereas Φ is the local Maxwellian:

(6.7)
$$\Phi = \rho (2\pi RT)^{-3/2} \exp\left[-|\xi - v|^2/(2RT)\right]$$

having the same density, temperature and bulk velocity v. Notice that from the viewpoint of nonlinearity the BGK model is worse than the Boltzmann equation, but offer the advantage tat one can derive integral equations for ρ , v, T. The linearized form reads:

(6.8)
$$L_{BGK} = v_0 \left[\int \hat{M}(\xi_*) h(\xi_*) d\xi_* + \frac{\xi}{RT_0} \cdot \int \xi_* \hat{M}(\xi_*) h(\xi_*) d\xi_* + \left(\frac{|\xi|^2}{2RT_0} - \frac{3}{2} \right) \int \left(\frac{|\xi_*|^2}{2RT_0} - \frac{3}{2} \right) \hat{M}(\xi_*) h(\xi_*) d\xi_* - h \right]$$

and is extremely useful, as we shall see.

7. – The Modified Reynolds Equation

The starting point to obtain the rarefied version of the Reynolds equation for lubrication is the mass balance equation, a consequence of the Boltzmann equation. This equation is considerably simplified by the fact that the variations of density do not show up for slow motion in the steady case, which is the most important in applications and we shall consider henceforth. Thus

(7.1)
$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0,$$

where the three velocity components are denoted by u, v, w.

Let us consider a layer of gas between two walls located at z=0 and z=D(x,y); the lower wall moves in its own plane (see Fig. 1, where, for simplicity, the z-direction has been suppressed). If we integrate Eq. (7.1) across the layer, we obtain

(7.2)
$$\frac{\partial}{\partial x} \int_{0}^{D} u dz + \frac{\partial}{\partial y} \int_{0}^{D} v dz = 0.$$

Since the problem is linear and the pressure gradient is assumed to be constant across the layer, each component u, v is proportional to the sum of the velocities given by a Poiseuille flow with pressure gradient dp/dx, dp/dy respectively and a Couette flow with the lower wall moving with velocity components U and V. We refer to Fig. 1 where, for simplicity, the y-axis has been suppressed.

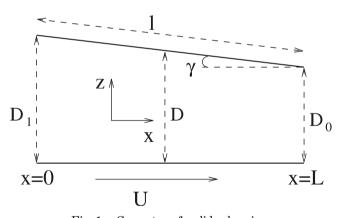


Fig. 1 – Geometry of a slider bearing.

In the case of Couette flow the evaluation of the integral: $F_C^{(1)} = \int\limits_0^D u_C dz$ is easy, if the walls are assumed to be identical. In fact, in this situation the profile is antisymmetric with respect to the midpoint and $F_C^{(1)} = \frac{UD}{2}$ Similarly $F_C^{(2)} = \int\limits_0^D v_C dz = \frac{VD}{2}$ The behavior of the flow rate for plane Poiseuille flow is

much more complicated and is given by

(7.3)
$$F_P^{(1)} = \int_0^D u_P dz = -\frac{1}{\rho_0 \sqrt{2RT_0}} \frac{\partial p}{\partial x} D^2 Q(\delta);$$

$$F_P^{(2)} = \int_0^D v_P dz = -\frac{1}{\rho_0 \sqrt{2RT_0}} \frac{\partial p}{\partial y} D^2 Q(\delta)$$

where δ is the ratio between the distance and the (unperturbed) mean free path.

$$\delta = \frac{pD}{\mu\sqrt{2RT}}$$

and $Q(\delta)$ is the nondimensional flow rate which can be obtained by solving the problem of plane Poiseuille flow. Thus the modified Reynolds equation reads as follows

(7.4)
$$\frac{\partial}{\partial x} \left[\frac{\partial p}{\partial x} D^2 Q(\delta) \right] + \frac{\partial}{\partial y} \left[\frac{\partial p}{\partial y} D^2 Q(\delta) \right] = \rho_0 \sqrt{2RT_0} \left[\frac{U}{2} \frac{\partial D}{\partial x} + \frac{V}{2} \frac{\partial D}{\partial y} \right].$$

Given D = D(x, y), this is an (elliptic) partial differential equation for p which must be solved for an assigned value of p (usually constant) at the boundary.

We have assumed so far that the linearization assumption holds everywhere. It may turn out, however, that the pressure undergoes a significant change. In this case, one can still utilize the linearized Boltzmann equation to compute the local flow rate, but one should use the local pressure p throughout, rather than the unperturbed pressure p_0 . The modified Reynolds equation then reads as follows

(7.5)
$$\frac{\partial}{\partial x} \left[\frac{D^2 Q(\delta)}{\sqrt{2RT}} \frac{\partial p}{\partial x} \right] + \frac{\partial}{\partial y} \left[\frac{D^2 Q(\delta)}{\sqrt{2RT}} \frac{\partial p}{\partial y} \right] = \frac{1}{2} \left[U \frac{\partial (\rho D)}{\partial x} + V \frac{\partial (\rho D)}{\partial y} \right].$$

In the continuum limit we have

$$Q(\delta) = \frac{1}{6} \, \frac{pD}{\mu \sqrt{2RT}}$$

and Eq. (7.5) becomes

(7.6)
$$\frac{\partial}{\partial x} \left[\frac{\rho D^3}{\mu} \frac{\partial p}{\partial x} \right] + \frac{\partial}{\partial y} \left[\frac{\rho D^3}{\mu} \frac{\partial p}{\partial y} \right] = 6 \left[U \frac{\partial (\rho D)}{\partial x} + V \frac{\partial (\rho D)}{\partial y} \right].$$

which is essentially the equation originally given by Reynolds [12].

8. - The Reynolds Equation and the Poiseuille-Couette Problem

The micromachinery fabrication techniques have become more and more mature in the last ten years. In particular, the micro-electro-mechanical systems (MEMS) developed rapidly and found many applications in microelectronics, medicine, biology, optics, aerospace and other high technology fields. Both experimental and computational efforts have been undertaken to understand the specific features of the microscale flows. A basic constituent of the MEMS devices is the microchannel, the region between two parallel plates that can reveal many specific features of the low speed internal flows in microdevices. Typically the first devices were integrated micro-channel/pressure sensor systems. The Knudsen number at the outlet of the channel at room conditions is 0.05 for nitrogen, and even higher for helium; hence the flow is surely beyond the slip flow regime. The pressure distribution along the channel and the flow rates across these channels are found to deviate from the linear distribution of the Poiseuille flow. Monte Carlo methods were used to simulate microchannel flows but they meet with the excessively high demands to the storage and computation time. The gradual regulation of the inlet and outlet boundary conditions of the channel seems to be tremendously difficult for DSMC in solving the long channel flows. In fact the typical DSMC simulation of the micro channel flow is limited to high speeds. Recently, the so called information preservation (IP) method was proposed [13, 14]; it uses a conservative scheme and a superrelaxation technique, with results in excellent agreement with experimental data.

However, the kinetic theory of MEMS does not require heavy computational tools. The generalized Reynolds equation can be used to calculate the gas film lubrication problem provided that the flow rate of Poiseuille flow is calculated from the linearized Boltzmann equation.

Following Ref. 15, let us consider again two plates separated by a distance D and a gas flowing parallel to them, in the x direction, due to a pressure gradient. The lower boundary (z=-D/2) moves to the right with velocity U, while the upper boundary (z=D/2) is fixed. Both boundaries are held at a constant temperature T_o . However, at variance with our previous discussions, we assume the gas-surface interaction to be different at the wall.

As usual, if the pressure gradient and the velocity U are taken to be small, it can be assumed that the Boltzmann equation can be linearized about a Maxwellian. If we assumes the linearized BGK model for the collision operator, the Boltzmann equation reads:

(8.1)
$$\frac{1}{2}k + \zeta \frac{\partial Z}{\partial z} = \frac{1}{\ell} \left[\pi^{-\frac{1}{2}} \int_{-\infty}^{+\infty} e^{-c_{z_1}^2} Z(z, c_{z_1}) dc_{z_1} - Z(z, \zeta) \right]$$

where by definition

$$egin{align} Z(z,\zeta) &= \pi^{-1} \int \limits_{-\infty}^{+\infty} \int \limits_{-\infty}^{+\infty} e^{-c_x^2 - c_y^2} c_x h(z,m{c}) \, dc_x \, dc_y \ &k = rac{1}{p} rac{\partial p}{\partial x} = rac{1}{
ho} rac{\partial
ho}{\partial x} \end{split}$$

with p and ρ being the gas pressure and density, respectively, and ℓ is the mean free path. Consequently, the bulk velocity of the gas is given by:

$$(8.2) \hspace{1cm} q(z) = \pi^{-\frac{1}{2}} \int\limits_{-\infty}^{+\infty} e^{-c_{z_{1}}^{2}} Z(z, c_{z_{1}}) \, dc_{z_{1}}$$

From Eq. (8.1) we obtain the integral equation:

(8.3)
$$Z(z,\zeta) = \exp\left(-\left(z + \frac{D}{2}\operatorname{sgn}\zeta\right)/(\zeta\ell)\right)Z\left(-\frac{D}{2}\operatorname{sgn}\zeta,\zeta\right) + \int_{-\frac{D}{2}\operatorname{sgn}\zeta}^{z} \exp\left(\frac{-|z-t|}{|\zeta|\ell}\right)[q(t) - k\ell/2]/(\zeta\ell) dt$$

with the values at the boundary, $Z\left(-\frac{D}{2}\operatorname{sgn}\zeta,\zeta\right)$, depending on the model of boundary condition chosen. In the following, we will consider the Maxwell boundary conditions and consider two walls having different physical properties, i.e. with two accommodation coefficients (a_1,a_2) . In this case, the boundary conditions can be written as:

$$Z^{+}(D/2,\zeta) = (1 - a_1)Z^{-}(D/2, -\zeta)$$

$$Z^{+}(-D/2,\zeta) = a_2U + (1 - a_2)Z^{-}(-D/2, -\zeta)$$

where U is expressed in units of $(2RT_o)^{1/2}$; $Z^-(-D/2,\zeta)$, $Z^-(D/2,\zeta)$ are the distribution functions of the molecules impinging upon the walls; similarly, $Z^+(-D/2,\zeta)$, $Z^+(D/2,\zeta)$ are the distribution functions of the molecules reemerging from the same walls.

Once the function at the boundary, $Z\left(-\frac{D}{2}\operatorname{sgn}\zeta,\zeta\right)$, has been evaluated following the analytical procedure reported in Refs. 7 and 5, the substitution of the integral formula (8.3) in the definition (8.2) of q(z) gives the following expression for the bulk velocity of the gas:

(8.4)
$$q(z) = \frac{1}{2}k\ell[1 - \psi_p(u)] + U\psi_c(u)$$

Eq. (8.4) shows that the gas velocity is induced by the superposition of two

distinct effects. The gas moves by an imposed pressure gradient (Poiseuille flow) and by the shear driven flow due to the motion of the bottom surface (Couette flow). The non-dimensional functions $\psi_p(u)$ and $\psi_c(u)$, giving the Poiseuille and Couette contributions, respectively, satisfy the following integral equations:

$$(8.5) \ \psi_p(u) = 1 + \frac{1}{\sqrt{\pi}} \int_{-\delta/2}^{\delta/2} dw \psi_p(w) \{ (1 - a_1) S_{-1}(\delta - u - w) + (1 - a_2) S_{-1}(\delta + u + w) + (1 - a_1) (1 - a_2) [S_{-1}(2\delta - u + w) + S_{-1}(2\delta + u - w)] + T_{-1}(|u - w|) \}$$

$$(8.6) \ \psi_c(u) = \frac{a_2}{\sqrt{\pi}} \left[T_o(\delta/2 + u) + (1 - a_1)S_o(3/2\delta - u) + (1 - a_1)(1 - a_2)S_o(5/2\delta + u) \right]$$

$$+ \frac{1}{\sqrt{\pi}} \int_{-\delta/2}^{\delta/2} dw \psi_c(w) \left\{ (1 - a_1)S_{-1}(\delta - u - w) + (1 - a_2)S_{-1}(\delta + u + w) + (1 - a_1)(1 - a_2)[S_{-1}(2\delta - u + w) + S_{-1}(2\delta + u - w)] + T_{-1}(|u - w|) \right\}$$

where $T_n(x)$ is the Abramowitz function defined by

$$T_n(x) = \int_0^{+\infty} t^n \exp(-t^2 - x/t) dt$$

 $S_n(x)$ is a generalized Abramowitz function defined by

$$S_n(x,\delta,a_1,a_2) = \int_0^{+\infty} \frac{t^n \exp(-t^2 - x/t)}{1 - (1 - a_1)(1 - a_2) \exp(-2\delta/t)} dt$$

and the following non-dimensional variables have been introduced:

$$\delta = D/\ell$$
, $w = t/\ell$, $u = z/\ell$.

Using Eq. (8.4), the flow rate (per unit time through unit thickness) defined by:

(8.7)
$$F = \rho \int_{-D/2}^{D/2} q(z) dz$$

can be expressed as the sum of the Poiseuille flow $({\cal F}_p)$ and the Couette flow $({\cal F}_c)$ as follows:

(8.8)
$$F = F_p + F_c = -\frac{\partial p}{\partial x} D^2 Q_p(\delta, a_1, a_2) + \frac{\rho UD}{2} Q_c(\delta, a_1, a_2)$$

where

$$Q_p(\delta,a_1,a_2) = -rac{1}{\delta} + rac{1}{\delta^2} \int\limits_{-\delta/2} \delta/2 \psi_p(u) du$$

$$Q_c(\delta, a_1, a_2) = rac{2}{\delta} \int\limits_{-\delta/2}^{\delta/2} \psi_c(u) du$$

are the non-dimensional volume flow rates.

9. - The Generalized Reynolds equation for Unequal Walls

One can easily extend the generalized Reynolds equation to the case of unequal walls:

(9.1)
$$\frac{d}{dx} \left(\frac{dp}{dx} D^2 Q_p(\delta, a_1, a_2) - \frac{\rho UD}{2} Q_c(\delta, a_1, a_2) \right) = 0$$

For the purpose of a direct comparison with the classical Reynolds equation (7.6), let us introduce the Poiseuille relative flow rate:

(9.2)
$$\tilde{Q}_p(\delta, a_1, a_2) = \frac{Q_p(\delta, a_1, a_2)}{Q_{con}}$$

where $Q_{con} = \delta/6$. Furthermore, the rarefaction parameter δ can be expressed as: $\delta = \delta_o PH$, where δ_o is the characteristic inverse Knudsen number defined by the minimum film thickness, D_o , and the ambient pressure p_o as:

$$\delta_o = \frac{p_o D_o}{\mu \sqrt{2RT_o}}$$

Finally, assuming that the heat generation in the gas is very small, so that an isothermal process can be considered, the non-dimensional generalized Reynolds equation reads:

$$(9.3) \qquad \frac{d}{dX} \left(\tilde{Q}_p(\delta_o PH, a_1, a_2) PH^3 \frac{dP}{dX} - Q_c(\delta_o PH, a_1, a_2) \Lambda PH \right) = 0.$$

Here the bearing number Λ is defined as

(9.4)
$$\Lambda = \frac{6\mu Ul}{p_o D_o^2}$$

where μ is the viscosity coefficient. If the two walls are identical ($a_1 = a_2 = a$), the Couette flow rate is independent of the Knudsen number regardless of the

value of the accommodation coefficient a and Eq. (9.3) reduces to the generalized Reynolds equation introduced by Fukui and Kaneko [16, 17].

Writing the non-dimensional film thickness H in terms of the longitudinal coordinate X,

$$(9.5) H = \frac{D_1}{D_0} - \frac{l}{L} \left(\frac{D_1}{D_0} - 1 \right) X$$

such that

$$\frac{dP}{dX} = -\frac{l}{L} \left(\frac{D_1}{D_0} - 1 \right) \frac{dP}{dH}$$

Eq. (9.3) can be immediately integrated to give:

$$(9.6) \qquad \frac{l}{L} \left(\frac{D_1}{D_o} - 1 \right) \tilde{Q}_p(\delta_o PH, a_1, a_2) PH^3 \frac{dP}{dH} + Q_c(\delta_o PH, a_1, a_2) \Lambda PH = K_1$$

where K_1 is a constant of integration. The substitution of

$$(9.7) PH = \zeta$$

in Eq. (9.6) gives:

(9.8)
$$\frac{d\zeta}{dH} = \frac{\zeta}{H} - \frac{[Q_c(\delta_o\zeta, a_1, a_2)A\zeta - K_1]}{l/L(D_1/D_o - 1)\tilde{Q}_p(\delta_o\zeta, a_1, a_2)H\zeta}$$

Eq. (9.8) can be solved numerically using relaxation methods. To apply this numerical scheme, the differential equations have to be replaced by finite-difference equations on a point mesh. The solution of the resulting set of equations is determined by starting with a guess and improving it iteratively using Newton's method. The Poiseuille flow rate coefficient $Q_p(\delta, a_1, a_2)$ has been evaluated by means of the numerical method described in Ref. 18 and the variational technique for the integrodifferential form of the Boltzmann equation

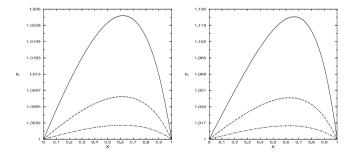


Fig. 2 – Pressure profile for $\delta_o = 0.5$. The line styles indicate a = 0.8 (solid), a = 0.3 (dashed), and a = 0.1 (dot dashed). The bearing number Λ is 10 (left) and 50 (right)

based on the BGK model. In order to compute the Couette flow rate $Q_c(\delta, a_1, a_2)$ one can solve numerically Eq. (8.6), extending a finite difference technique first introduced by Cercignani and Daneri [19].

Once $\zeta(H)$ has been numerically evaluated on a grid that spans the domain of interest, Eqs. (9.5) and (9.7) give the pressure field in the gas film as a function of X. Furthermore, a prediction of the vertical force acting on the upper surface of the slider bearing, crucial for practical design, may be obtained from the load carrying capacity W, defined as

$$(9.9) W = \frac{l}{L} \int_{0}^{\infty} L/l(P-1) dX$$

In order to investigate the effects of the rarefaction parameter δ_o and the bearing number Λ on the basic lubrication characteristics (pressure distribution and load carrying capacity), the parameters describing the gas film geometric configuration were fixed at the following values: $D_1/D_o=2$, $L/D_o=100$. Figure 2 shows the pressure field as a function of the longitudinal coordinate X at three different bearing numbers: $\Lambda=10$, 50, 200. To assess the influence of the boundary conditions, the profiles corresponding to different accommodation coefficients (for bounding walls supposed physically identical) are drawn in Figs. 2 and 3.

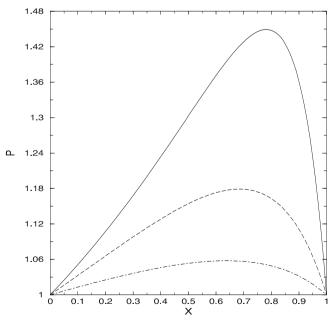


Fig. 3 – Pressure profile for $\delta_o=0.5$. The line styles indicate a=0.8 (solid), a=0.3 (dashed), and a=0.1 (dot dashed). The bearing number Λ is 200.

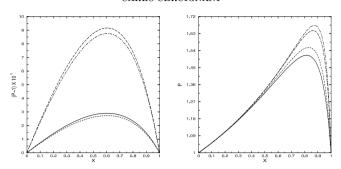


Fig. 4 – Pressure profile for $\delta_o=0.5$. The line styles indicate $a_1=0.5$ $a_2=0.8$ (solid), $a_1=0.5$ $a_2=0.3$ (dashed), and $a_1=0.5$ $a_2=0.1$ (dot dashed). The bearing number Λ is 10 (left) and 50 (right).

Looking at the pictures, one sees that the pressure distribution in the gas film increases with increasing Λ . Furthermore, at fixed bearing number, the pressure field reduces by increasing the fraction of gas molecules specularly reflected by the walls. Fig. 3 reports the pressure profiles for the same parameters as in Fig. 2, except that now the two bounding plates are allowed to re-emit the impinging gas molecules differently, so that two accommodation coefficients can be defined. We keep the accommodation coefficient of the upper wall (a_1) fixed and vary the other one (a_2) .

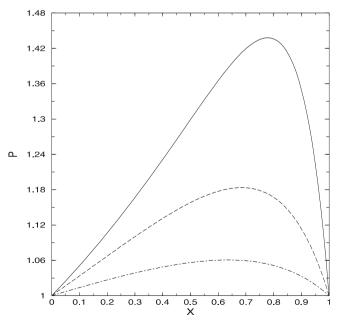


Fig. 5. – Pressure profile for $\delta_o=0.5$. The line styles indicate $a_1=0.5$ $a_2=0.8$ (solid), $a_1=0.5$ $a_2=0.3$ (dashed), and $a_1=0.5$ $a_2=0.1$ (dot dashed). The bearing number Λ is 200.

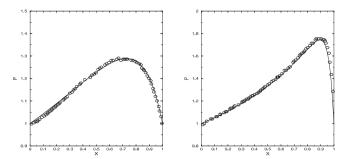


Fig. 6. – Pressure profile versus X. Comparison between the results obtained with the modified Reynolds equation (solid line) and DSMC data ¹ (open circles). The parameters are: $\delta_o = 0.7$, $\Lambda = 61.6$, $\alpha = 1$ (left); $\delta_o = 0.2$, $\Lambda = 1264$, $\alpha = 1$ (right).

A comparison with Fig. 2 shows that, for every Λ , the pressure distribution significantly depends on a_2 and only weakly on a_1 . This picture remains true at different Knudsen numbers progressing from free molecular, through transitional, to continuum regions (see Fig. 4).

It is worth noting that, when Λ increases, the Couette contribution to the lubrication flow rate becomes dominant compared with the Poiseuille flow. Therefore, if the two walls are identical, the influence of the Knudsen number on

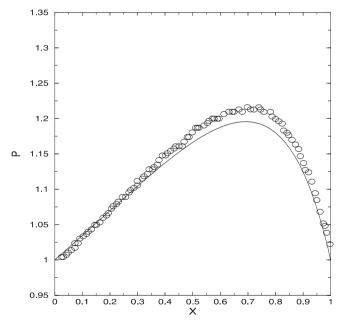


Fig. 7. – Pressure profile versus X. Comparison between the results obtained with the modified Reynolds equation (solid line)and DSMC data¹ (open circles). The parameters are: $\delta_o = 0.7$, $\Lambda = 61.6$, a = 0.7.

the load carrying capacity decreases as Λ increases, since Q_c is independent of δ and a. On the contrary, if the two walls have a different physical structure the load carrying capacity shows a dependence on both the Knudsen number and the accommodation coefficients a_1 , a_2 . For the validation of the code, the results obtained with the modified Reynolds equation have been compared with the results from DSMC (Direct Simulation Monte Carlo) simulations published by Alexander et al. [20] in the case of Maxwell's boundary conditions on two physically identical walls (see Fig. 5).

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