Komponente des amorphen Bi von der Fourier-Analyse nicht geliefert. So sind in aufgedampftem amorphem, glasigem und geschmolzenem Se auch Bereiche mit großer Ordnung und mit $2\,r_2 = 7{,}38\ \text{Å}$ als bevorzugtem Atomabstand vorhanden, sie streuen nach DEBYE[21]; ihr Anteil ist jedoch gering. Über diese Bereiche sagt die Fourier-Analyse der Intensitätskurve nichts aus. Um ein vollständiges Bild vom Aufbau nichtkristalliner Stoffe zu erhalten, hat man die Ergebnisse aus der Fourier-Analyse und aus der Diskussion der Intensitätskurve heranzuziehen.

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On Boundary Conditions Method in the Kinetic Theory of Gases

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It is shown that the work of Cercignani and Tironi on Maxwell's boundary conditions method can be improved in a simple and logical way. The technique for improvement is illustrated by a study of the linearized plane Couette flow problem and it is found that the proposed modification yields results that are identical with some highly accurate variational results.

I. Introduction

Theoretical interest in the kinetic theory of gases dates back to the classical work of MAXWELL[1], who, in his attempts to explain the experimental results of Kundt and Warburg and Reynolds, developed a simple and reasonably effective approach. In essence, Maxwell noticed the discontinuity of the distribution near the surface, made some simple and plausible approximations for the distribution incident on the surface, and then by using the momentum or heat transfer considerations he arrived at some fairly accurate results for the slip or the jump terms. These ideas of

Maxwell were further pursued by Von-Smoluchowski, Langmuir, Weber, Knudsen etc. and an interesting account of these approaches can be found in the books by KENNARD[2] and LOEB[3].

More recently, with the increased interest in the kinetic theory of rarefied gases, several exact solutions of the linearized model equations[4-8] and some very effective and highly accurate approximate solutions of the linearized Boltzmann equation (or the linearized Wang Chang Uhlenbeck equation for the polyatomic gases) with general forms of the boundary conditions have been given[9-15]. This latter work has indicated that for the

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Kramer's problem and the temperature jump problem, Maxwell's approach is quite satisfactory; however for the thermal creep[10] or the diffusion slip problems[11,16] Maxwell's approach can lead to results that are, in certain limits, not even qualitatively correct. This situation has led to a closer examination of Maxwell's arguments, and in a very recent paper[17] it has been shown that by a simple and very logical modification of Maxwell's ideas highly accurate results for all slip problems can be derived. In fact these results are identical to those obtained by the variational methods.

In two recent papers, CERCIGNANI and TIRONI[18,19] (CT) have shown how Maxwell's approach can be used to treat flow of arbitrary rarefaction with reasonable success using a technique they have termed the "Boundary Conditions Method" (BCM). Although not explicitly demonstrated in their work (due to several algebraic arrors), the method is quite satisfactory for the problems they treated. However, the boundary conditions method as presented by Cercignani and Tironi would suffer from the same defects as Maxwell's slip calculations when applied to such cross-effects as thermal transpiration or diffusion. Thus it seems natural to examine the feasibility of the modified approach at all rarefactions. Further, since CT indicate that the boundary conditions method could be useful in treating non-linear problems, a basic improvement in the development of the method should be of interest.

It is, therefore, the purpose of this paper to investigate the possibilities of modifications in the boundary conditions method. Specifically linearized Couette flow[9,20] problem is considered and it is shown that by a simple and logical modification of the work of Cercignani and Tironi highly accurate results are obtained. Once again, the expression obtained for the stress is identical to that derived using a variational method[9]. Since similar considerations apply to other widely studied problems (Poiseuille flow, thermal creep, etc.), and since detailed numerical results for these problems are already available, they will not be pursued in detail here.

II. Linearized Plane Couette Flow

This problem is among the most widely studied problems in the kinetic theory and it has, in a sense, been a test bed for the accuracy of various approximate methods[9,20]. One is interested here in the stress in a gas enclosed between two parallel plates located at $x = \mp d/2$ and moving with velocities $\mp u_0/2 \ll 1$ in the z-direction. If $\Phi(x, c)$ is a measure of the perturbation in the distribution function $f(x, c)$ from an absolute maxwellian f_0 (corresponding to the conditions at $x = 0$), then, for the diffuse reflection at the plates, it is easily shown that Φ is determined by the linearized Boltzmann equation

$$c_x \frac{\partial \Phi(x, c)}{\partial x} = L \Phi(x, c) \qquad (1)$$

and the boundary conditions

$$\Phi\left(\mp \frac{d}{2}, c\right) = \mp u_0 c_z, \qquad c_x \gtrless 0. \qquad (2)$$

Here $x = (x, y, z)$ is the position vector and $c = (c_x, c_y, c_z)$ is the velocity vector. Also, the non-dimensional and the actual (with tildes) quantities are related by

$$c = (m/2kT_0)^{1/2} \tilde{c}, \qquad u_0 = (m/2kT_0)^{1/2} \tilde{u}_0$$

and

$$x = \tilde{x}/l_p, \qquad d = \tilde{d}/l_p$$

where

$$l_p = \frac{2\mu}{\varrho} \left(\frac{m}{2kT_0}\right)^{1/2}$$

is a viscosity mean free path. Here μ is the viscosity of the gas and ϱ is the density. Note that in the linearized problem $(1)-(2)$ the non-homogeniety is only due to the u_0 term. Thus without loss of generality, we shall, for simplicity, set $u_0/2 = 1$. (It should be clear that this has nothing to do with the earlier statement $u_0/2 \ll 1$, which was used to arrive at the linear problem from the non-linear Boltzmann equation.)

For the BGK model (to which we shall confine our attention here) it is sufficient to consider the function

$$g(x, c_x) = \frac{1}{\pi} \int\!\!\int\limits_{-\infty}^{\infty} dc_y \, dc_z \exp(-c_y^2 - c_z^2) \, c_z \, \Phi(x, c)$$

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which, then, is determined by the equations

$$c_x \frac{\partial g(x, c_x)}{\partial x} = - g(x, c_x)$$

$$+ \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} dc_x' \exp(- c_x'^2) g(x, c_x') \quad (3)$$

$$g\left(\mp \frac{d}{2}, c_x\right) = \mp 1 \qquad c_x \gtrless 0. \quad (4)$$

For later use, it is convenient now to introduce the integral equation corresponding to the Eqs. (3) and (4). It is easily shown that

$$g(x, c_x) = U(q(x)) + UE(- \operatorname{sgn} c_x) \quad (5)$$

where the operators U and E are given by

$$U f(x, \boldsymbol{c}) = \frac{1}{c_x} \left[\eta(c_x) \int_{-d/2}^{x} dx' \exp\left\{ - \frac{x - x'}{c_x} \right\} f(x', \boldsymbol{c}) \right.$$

$$\left. - \eta(- c_x) \int_{x}^{d/2} dx' \exp\left\{ - \frac{x - x'}{c_x} \right\} f(x', \boldsymbol{c}) \right] \quad (6)$$

and

$$E = \delta\left(x + \frac{d}{2}\right) \eta(c_x) c_x - \delta\left(x - \frac{d}{2}\right) \eta(- c_x) c_x. \quad (7)$$

In this, $\eta(c_x) = 1, c_x > 0; \eta(c_x) = 0, c_x < 0$.

Also, $q(x)$, the mass velocity is defined by

$$q(x) = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} dc_x \exp(- c_x^2) g(x, c_x). \quad (8)$$

It is well known that the Eq. (3) possesses a particular solution (an additive constant is ruled out by virtue of the anti-symmetry in the problem.)

$$g(x, c_x) = \alpha(x - c_x). \quad (9)$$

Where α is an arbitrary constant. Expression (9) is, in fact, the Chapman-Enskog solution corresponding to the BGK model and is realized in the bulk of the gas where the effect of the kinetic layers is not large.

Now we note two constraints that must be satisfied by any solution of the problem (as we shall see in the sequel, these two constraints play the central role in the approximation method to be discussed here). Multiplying Eq. (3) by $\exp(- c_x^2)$ and integrating we find that

$$\frac{\partial}{\partial x} (c_x, g(x, c_x)) = 0$$

i.e.

$$(c_x, g(x, c_x)) = \text{constant} \quad (10)$$

where for the scalar product we have used the notation

$$(g_1(x, c_x), g_2(x, c_x)) \quad (11)$$

$$= \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} dc_x \exp(- c_x^2) g_1(x, c_x) g_2(x, c_x).$$

Next, taking scalar product (11) of Eq. (3) on c_x, we get

$$\frac{\partial}{\partial x} (c_x^2, g(x, c_x)) = - (c_x, g(x, c_x)) = \text{constant}$$

i.e.

$$(c_x^2, g(x, c_x)) \approx \text{linear in } x. \quad (12)$$

Relations (10) and (12) indicate that the two scalar products $(c_x, g(x, c_x))$ (which really corresponds to stress) and $(c_x^2, g(x, c_x))$ can be adequately described by the asymptotic solution (9). Thus we could write

$$(c_x, g(x, c_x)) \approx (c_x, g_{\text{asy}}(x, c_x)) = - \alpha/2, \quad (13)$$

$$(c_x^2, g(x, c_x)) \approx (c_x^2, g_{\text{asy}}(x, c_x)) = (\alpha/2) x. \quad (14)$$

Where α is, as yet, an unknown constant. From the above equations, it is quite clear that at $x = - d/2$ we should have,

$$(c_x, g(- d/2, c_x)) = - \alpha/2, \quad (15)$$

$$(c_x^2, g(- d/2, c_x)) = - (\alpha/4) d. \quad (16)$$

These two equations, in a way, constitute boundary conditions that should be satisfied by any solution of the problem. It is further noted that the ratio of stress p_{xz} to its value in the free molecular limit $(p_{xz, fm})$ is given by

$$\frac{p_{xz}}{p_{xz, fm}} = \frac{(c_x, g(x, c_x))}{(c_x, g_{fm}(x, c_x))} = \frac{\pi^{1/2}}{2} \alpha. \quad (17)$$

Thus it is sufficient to construct an approximate procedure for the evaluation of α. Maxwell's approach, as extended by Cercignani and Tironi, consists in using the boundary condition (15) alone for this purpose. Following Maxwell, CT reason that an approximation for $g(- d/2, c_x)$, $c_x < 0$ can be obtained by assuming that in the gas the hydrodynamic velocity profile $q(x) = \alpha x$ prevails. Thus CT write

$$q(x) = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} dc_x' \exp(- c_x'^2) \alpha(x - c_x') = \alpha x \quad (18)$$

and, thus, they assume

$$\eta(-c_x)\,g\left(-\frac{d}{2},c_x\right)$$
$$=\eta(-c_x)\,[U(\alpha x)+UE(-\operatorname{sgn}c_x)]_{x=-d/2} \quad (19)$$

i.e., at $x=-d/2$ the distribution is assigned the form

$$g\left(-\frac{d}{2},c_x\right)=\eta(-c_x)\left[\alpha\left\{\left(-\frac{d}{2}-c_x\right)-\left(\frac{d}{2}-c_x\right)\right.\right.$$
$$\left.\left.\cdot\,e^{d/c_x}\right\}+e^{d/c_x}\right]-\eta(c_x) \quad (20)$$

and, this is then used in the Eq. (15) to determine α. This procedure yields

$$\frac{p_{xz}}{p_{xz,fm}}=\pi^{1/2}\frac{[1+2\,T_1(d)]}{[\pi^{1/2}+d\,\{1-2\,T_1(d)\}+4\,\{T_2(d)+d\,T_1(d)\}]} \quad (21)$$

Where $T_\eta(x)$ are the well studied Abramowitz functions,

$$T_\eta(x)=\int_0^\infty dt\,t^\eta\,e^{-t^2-x/t}. \quad (22)$$

The result (21), however, is different from the one reported by CERCIGNANI and TIRONI[18]. It appears that Cercignani and Tironi committed an algebraic error in their Eq. (3.5), and that their corrected results should agree with the Eq. (21) given above. Numerical results corresponding to Eq. (21) are given in the Table 1 and indicate that while CT found a difference of up to 12% from the exact results (obtained via numerical methods or the variational methods), the corrected results in fact differ from the exact results by a maximum of 5%. In what follows, we show how even this difference can be removed by modifying the above approach in a simple and meaningful way.

Essentially, we wish to use the additional information that is provided by the Eq. (16). Clearly, this should allow the determination of a second adjustable constant. Since the kinetic layers contain deviations from the continuum profile, a better approximation for the incident distribution can be made by stipulating that, on the average, the velocity profile in the whole gas may be more reasonably described as $q(x)=\alpha' x \triangleq (\alpha+\beta)\,x$, where β is at present some other unknown constant. Thus we write,

$$g\left(-\frac{d}{2},c_x\right)=\eta(-c_x)\left[(\alpha+\beta)\left\{\left(-\frac{d}{2}-c_x\right)\right.\right.$$
$$\left.\left.-\left(\frac{d}{2}-c_x\right)e^{d/c_x}\right\}+e^{d/c_x}\right]-\eta(c_x) \quad (23)$$

and then use the Eqs. (15) and (16) to determine α and β. We immediately find

$$\left(\frac{d}{4}+\frac{\pi^{1/2}}{4}+\frac{d}{2}\,T_1(d)+T_2(d)\right)\alpha$$
$$+\left(\frac{d}{4}-\frac{\pi^{1/2}}{4}+\frac{d}{2}\,T_1(d)+T_2(d)\right)\beta=\tfrac{1}{2}+T_1(d), \quad (24)$$

$$\left(\frac{\pi^{1/2}}{8}\,d+\frac{1}{2}-\frac{d}{2}\,T_2(d)-T_3(d)\right)\alpha$$
$$+\left(-\frac{\pi^{1/2}}{8}\,d+\frac{1}{2}-\frac{d}{2}\,T_2(d)-T_3(d)\right)\beta \quad (25)$$
$$=\frac{\pi^{1/2}}{4}-T_2(d).$$

These two equations may be readily solved for α, and after some simple algebraic manipulations we can write the final result in the form

$$\frac{p_{xz}}{p_{xz,fm}}=\frac{1}{2}+T_1(d)-\frac{1}{4}$$
$$\cdot\frac{(d[1+2\,T_1(d)]+[4\,T_2(d)-\pi^{1/2}])^2}{d^2[\tfrac{1}{2}+T_1(d)]+4\,d\,T_2(d)+[4\,T_3(d)-2]}. \quad (26)$$

Table 1. Stress $p_{xz}/p_{xz,fm}$ in the plane Couette Flow.

Inverse Knudsden Number d	Lees and Liu Moment Method	Boundary Conditions Eq. (3.5) Ref. [18]	Method Eq. (21)	Numerical Eq. (26)	Method Willis[20]
.01	.9944	.9859	.9914	.9914	.9913
.1	.9466	.8836	.9261	.9261	.9258
1.0	.6393	.5298	.6129	.6008	.6008
1.25	.5864	.4922	.5652	.5512	.5517
1.50	.5416	.4622	.5248	.5097	.5099
1.75	.5032	.4370	.4850	.4743	.4745
2.0	.4698	.4151	.4598	.4438	.4440
2.5	.4149	.3780	.4085	.3935	.3938
3.0	.3714	.3468	.3675	.3537	.3539
5.0	.2617	.2566	.2611	.2524	.2526
7.0	.2020	.2009	.2019	.1964	.1964
10.0	.1506	.1504	.1505	.1474	.1474
20.0	.0814	.0814	.0814	.0805	.0807

Which, in fact, is precisely the variational result (derived with the help of linear trial functions) reported in Ref. [9]. This result is known to be remarkably accurate. Though numerical values corresponding to this expression have been given earlier, for the purpose of completeness, these results are again reported in the Table 1, where the moment method results of Lees and Liu and the accurate numerical results of WILLIS [20] are included. In fact, as noted by CERCIGNANI and PAGANI [9], the variational result [and hence the expression (28)] is more accurate than the results of Willis.

III. Discussions and Conclusions

We have shown that the boundary conditions method is capable of yielding remarkably accurate results. It is rather interesting to find that as for the slip problems, this approach leads to results that are identical with the variational results. This situation indicates that it should be possible to construct a simple physical interpretation of the variational approach. Also the boundary conditions method may be, perhaps, given a better mathematical foundation.

We may note that while in this paper we have confined our attention to the Couette flow problem, the problems of Poisseuille flow or the thermal creep flow can also be treated with equal ease. In fact in each case, it should be possible to obtain results that are identical to the variational results. Since the numerical results for these problems are already available, it seems advisable to not to pursue these questions in detail here. It should be noted, however, that for the Poiseuille flow problem CERCIGNANI and TIRONI [18] again seem to have committed algebraic errors. Thus, we believe that their Eq. (4.8) should be

$$Q(d) = \frac{2}{d} \frac{\frac{1}{2} - 2\,T_3(d) + T_1(d) - d\,T_2(d) + \frac{\pi^{1/2}}{4}\,d + \frac{1}{8}\,d^2 - \frac{1}{4}\,d^2\,T_1(d)}{1 - 2\,T_1(d)} - \frac{d}{12} \qquad (27)$$

and this corrected equation predicts a Poiseuille flow rate that is with in 5% of the variational results — as compared to 17% deviation obtained by Cercignani and Tironi.

It seems to us that it will be quite interesting to investigate the feasibility of the boundary conditions method for non-linear problems. Since this method is already superior to Lees and Liu moment method in the linear case, it would not be surprising if a similar situation occurs in the non-linear case. Investigations on the non-linear Couette flow [21, 22] problem have been initiated and if the technique proves efficient, these results would be given in a subsequent work.

No doubt, the method could also find some use in the study of gas-mixtures, polyatomic gases etc. Similar problems in neutron transport and radiative heat transfer should also be susceptible to the method.

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