

MONTE CARLO SOLUTIONS OF NONLINEAR BOLTZMANN EQUATION FOR PROBLEMS OF HEAT TRANSFER IN RAREFIED GASES

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NOMENCLATURE

a ,	gain term of the collision integral;
$(a - bf)$,	collision integral;
bf ,	loss term of the collision integral;
d ,	distance between the parallel plates;
f ,	molecular velocity distribution function;
k ,	Boltzmann constant;
Kn ,	Knudsen number, equation (1);
m ,	molecular mass;
M_T ,	gradient parameter, equation (2);
n ,	number density;
n_1 ,	twice the number density of the molecules reflected from the cold wall;
\bar{n} ,	dimensionless number density, $(n/n_1 - T_1/T_2)/(1 - T_1/T_2)$;
q ,	heat flux;
T ,	temperature;
x ,	x coordinate;
α ,	thermal accommodation coefficient = $(T_i - T_r)/(T_i - T_w)$;
τ ,	integration variable, equation (4).

Subscripts

1,	at cold plate;
2,	at hot plate;
i ,	incident molecules;
r ,	reflected molecules;
w ,	plate;
x ,	x -coordinate;
\perp ,	at right angle to x .

Superscripts

($\bar{\quad}$), ($\bar{\quad}$) average quantity.

Symbols set in bold type are vector quantities.

basic equation of kinetic theory. The major difficulty in solving the nonlinear Boltzmann equation is the intractable form of the collision integral in it. The collision integral represents the rate of change of velocity distribution due to intermolecular collisions. It is directly related to the local departure from thermal equilibrium, and its evaluation is essential in studying non-equilibrium phenomena in rarefied gases as well as in solving the nonlinear Boltzmann equation.

Nordsieck's Monte Carlo method of evaluating the Boltzmann collision integral [1] has been used to solve the non-linear Boltzmann equation for the heat transfer problem between two plates at different temperatures [2]. A small part of the results of the problems of heat transfer in rarefied gases was presented at the Sixth and Seventh International Symposiums on Rarefied Gas Dynamics [2, 3]. We shall describe in this paper the application of Nordsieck's method to these problems and some typical results.

Solutions have been obtained for these problems by solving the Krook equation [4], by solving the Boltzmann transport equations [5, 6], or by using the Monte Carlo simulation technique [5-7]. We have compared the Boltzmann solutions with two of these solutions that we reproduced and with an experiment [8].

We consider the problem of heat transfer between parallel plates having two different temperatures, T_1 and T_2 ($T_2 > T_1$), and at distance d apart. The physical system is characterized by two parameters: a length parameter Kn and a gradient parameter, M_T , related to the departure from thermal equilibrium:

$$Kn = \sqrt{[(2kT_1)/m] / \int_0^d \bar{b}_{eq} dx} \quad (1)$$

in which \bar{b}_{eq} = average local equilibrium collision frequency.

$$M_T = [2(T_2 - T_1)/(T_2 + T_1)] Kn. \quad (2)$$

The parameter Kn may be interpreted as the reciprocal of the number of mean free paths between the two plates and the parameter M_T as the gradient in each mean free path. In order to study the detailed non-equilibrium gas behavior

IN ANY flow region having large property gradients, the gas is far from thermal equilibrium. The gas in such a flow region can be described by the Boltzmann equation, the

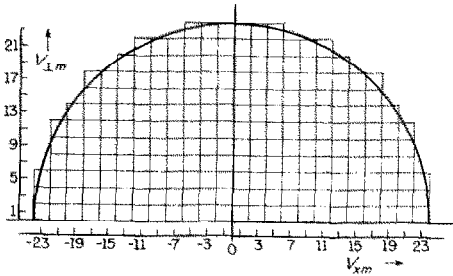


FIG. 1. Velocity space for axially symmetrical molecular flows. v_x = velocity in x -direction, v_1 = velocity at right angle to x . Subscript m denotes machine unit used in the computer program.

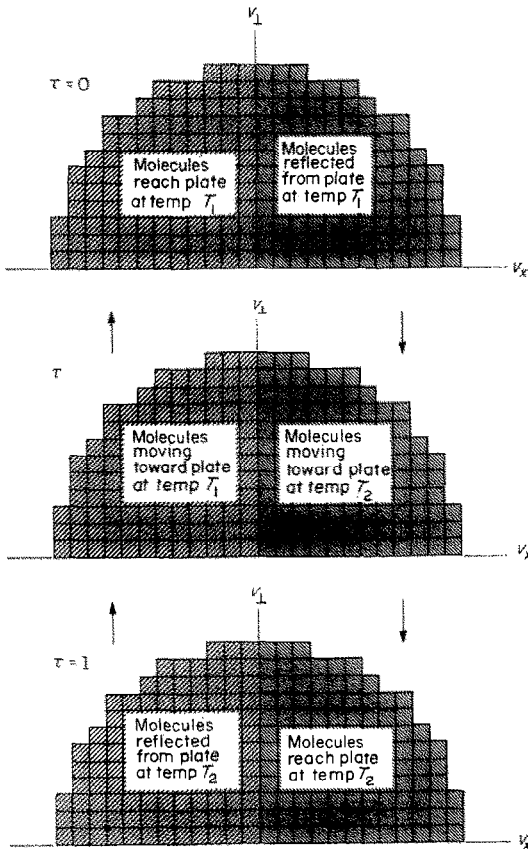


FIG. 2. Schematic representation, in velocity space, of two groups of molecules that move in opposite directions. Arrows represent the direction of motion and of integration.

of the heat transfer problem, solutions should be obtained for a large range of *both* parameters. Let us consider, for example, cases with the same M_T but different values of Kn , i.e. the temperature gradient per mean free path is the same but the number of mean free paths between the two plates differs. The behavior of the gas in a mean free path is expected to change with the Knudsen number and it is of interest to study the difference in this behavior for different values of Kn . Also, it is quite clear that the linearized solutions which have been obtained for small temperature differences yield results only for a narrow range of non-equilibrium conditions.

The Boltzmann equation for one-dimensional flows may be written as

$$v_x(df/dx) = (a - bf) \quad (3)$$

in which $f = f(v, x)$ = velocity distribution function and $(a - bf)$ = collision integral. $a(v, x)$, the gain term in the collision integral; is the rate of scattering of molecules in dv of velocity space. $b(v, x) f(v, x)$, the loss term, is the rate of scattering of molecules out of dv of velocity space.

The direct evaluation of the thousands of collision integrals needed, each one of which is a nonlinear, five-dimensional integral, would require months on the fastest present-day computer. Nordsieck [1] devised a statistical sampling technique closely resembling the real statistical collision phenomena in the gas. With his method, the computation time of the integrals is reduced to the order of an hour, with accuracy of the order of one per cent.

The molecular flow in the heat transfer problem is axially symmetrical, that is, the velocity distribution function $f = f(v_x, v_1)$. v_1 = velocity in the direction at right angle to x . The velocity space considered is therefore two-dimensional. As shown in Fig. 1, the velocity space in Nordsieck's method is quantized by covering the semi-circular region with 226 fixed cells. The Monte Carlo calculations produce 226 values of each of the functions "a" and bf for each iteration for a given set of $f(v_x, v_1)$.

In our iterative scheme for integrating the Boltzmann equation we replace the position variable x by τ with

$$(d\tau/dx) = Kn(\sqrt{2/\pi}) nT^{\frac{1}{2}} \quad (4)$$

in which n = local number density and T = local temperature.

The boundary condition used corresponds to isotropic emission with either complete or incomplete energy accommodation. The accommodation coefficient α is defined as follows.

$$\alpha = (T_i - T_r)/(T_i - T_w) \quad (5)$$

in which T_i and T_r are the temperatures of the incident and reflected molecules respectively and T_w = plate temperature.

In order to explain the numerical method, it is convenient to show schematically in Fig. 2 the velocity space at three

τ -positions. Each semi-circular region has two quadrants. The quadrant with $v_x > 0$ is for the molecules moving toward the hot plate and that with $v_x < 0$, for the molecules moving toward the cold plate. There are 113 velocity points in each quadrant. One Boltzmann equation is associated with each velocity point. The integration of 113 Boltzmann equations of the right-moving molecules is from $\tau = 0$ to $\tau = 1$, while, for the left-moving molecules, the integration of the 113 Boltzmann equations starts from $\tau = 1$. The form of the distribution function at each starting position is determined by the boundary conditions at each plate and is thus known; however, the density is unknown. The distribution function at the terminating position is also unknown. The integration scheme of the 226 Boltzmann equations is also divided into two parts for the two groups of molecules. The computation scheme was designed according to the following conditions peculiar to the heat transfer problem:

- (1) The boundary conditions at $\tau = 0$ and $\tau = 1$ are half-range Maxwellians with T_1 and T_2 equal to either the wall temperatures or a fraction of them (for $\alpha < 1$). The ratio n_2/n_1 is unknown. n_1 and n_2 are twice the number density of reflected molecules at the cold plate and the hot plate respectively.

- (2) There is no mass motion of the molecules.

The iterative procedure consists of the following steps:

- Step 1—Divide the variable τ into J intervals.
- Step 2—Assume initial distribution function $f = f^0(\mathbf{v}, \tau)$.
- Step 3—Evaluate the collision integral for this f at each τ .
- Step 4—Integrate the resulting differential equation for each of the 226 velocity bins to get $f^1(\mathbf{v}, \tau)$. The integration of the 113 Boltzmann equations in the right quadrant is from 0 to 1, and in the left quadrant, from 1 to 0.
- Step 5—The half range moments of $f^1(\mathbf{v}, 1)$ (i.e. at the hot plate) are computed and the values of $f^1(\mathbf{v}, 1)$ at the left quadrant (i.e. for $v_x < 0$) adjusted to insure zero mean flow of the gas.
- Step 6—Repeat steps (3), (4) and (5) to perform successive iterations.

We use the rms difference of successive iterates to measure the residual δf and to monitor the convergence of the iterative process.

As indicated above, our method of solving the Boltzmann equation consists of two parts: evaluating the collision integrals by a Monte Carlo method and integrating the Boltzmann equation. These two parts are carried out separately in two computer programs. We also have a subprogram for evaluating the Krook model of the collision integral and incorporated it in the program so that we may use it in place of the Monte Carlo program to solve the Krook equation. In essence, therefore, we tackle the Krook equation by using the same iterative scheme we designed for solving the Boltzmann equation. Since any systematic error due to integration for the solutions of the two equations is comparable, it would be more meaningful to make com-

parative studies. It should be pointed out here that it is difficult to make compatible comparison with other solutions obtained by other researchers who used different definitions of Kn .

We have used Lavin's scheme to obtain 4-moment solutions of the Boltzmann transport equations; however, his scheme had to be modified slightly due to the difference in the definition of Kn used.

Boltzmann solutions have been obtained for the case of complete energy accommodation ($\alpha = 1$) for the following ranges of parameters: (1) K_n : 0.1–100, (2) M_T : 0.03529–35.29, (3) T_1/T_2 : 0.1–0.9.

Nine stations dividing the variable τ were generally used; however, in order to get more detailed information in the

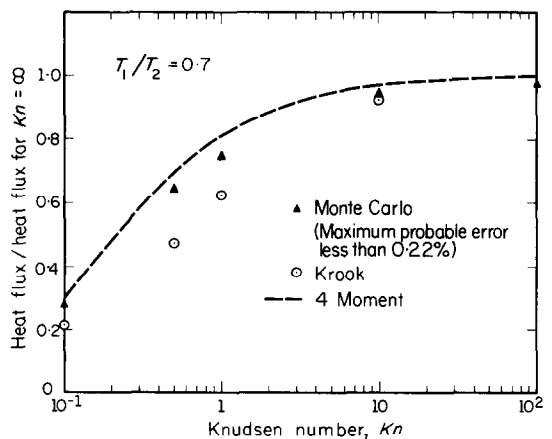


FIG. 3. Comparison of the results on heat flux.

Knudsen layer, fifteen stations were selected for solutions of less Kn . Monte Carlo samples of 2^{13} collisions were used. Four independent runs were made to obtain the statistical errors.

Figure 3 shows the heat flux as a function of Kn for $T_1/T_2 = 0.7$. In the transition regime, the Monte Carlo values are slightly smaller than the 4-moment values but appreciably larger than the Krook values. Similar differences were found for other values of T_1/T_2 and for the normal stress in x -direction.

The temperature and density profiles for two values of Kn (10 and 0.5) and $T_1/T_2 = 0.7$ are compared with the corresponding results of the Krook solution and the 4-moment solution. As shown in Figs. 4 and 5 there are appreciable differences between the Monte Carlo results and the other two calculations. The most significant difference is that, for the case of $Kn = 0.5$, both temperature

and density profiles obtained from the Monte Carlo solutions exhibit nonlinearities near each boundary (much more near the hot boundary) and thus show the presence of the Knudsen layer. The corresponding profiles obtained from the 4-moment and Krook solutions are practically linear.

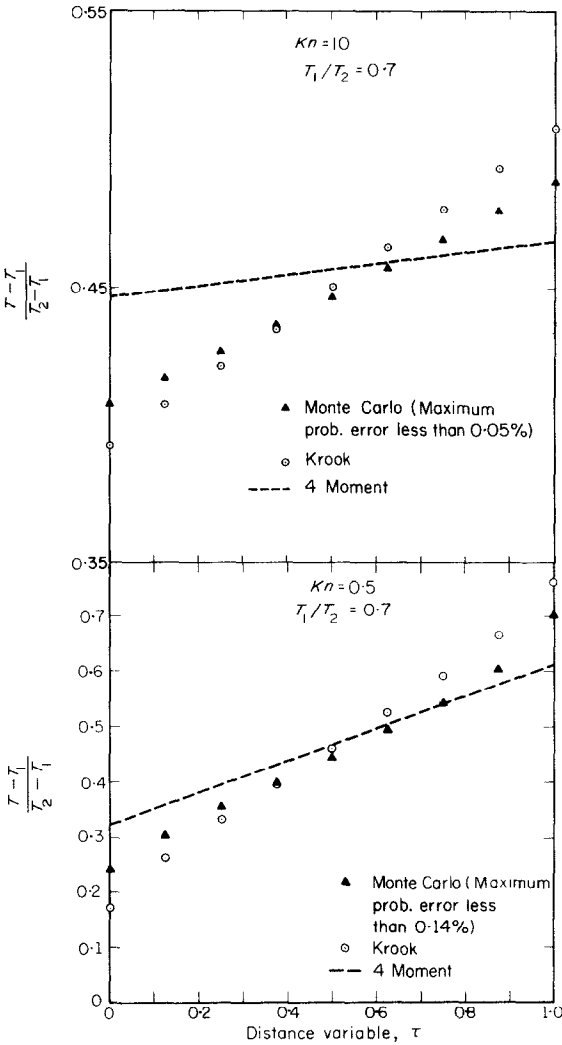


FIG. 4. The temperature as a function of distance variable τ . $Kn = 10$ and 0.5 . $T_1/T_2 = 0.7$.

Calculations of the functionals of the collision integral make it possible to study in detail the local departure from equilibrium. For example, we have found that several moments of the collision integral exhibit sharper forms of nonequilibrium behavior in the Knudsen layer than either the temperature or the density profile [2].

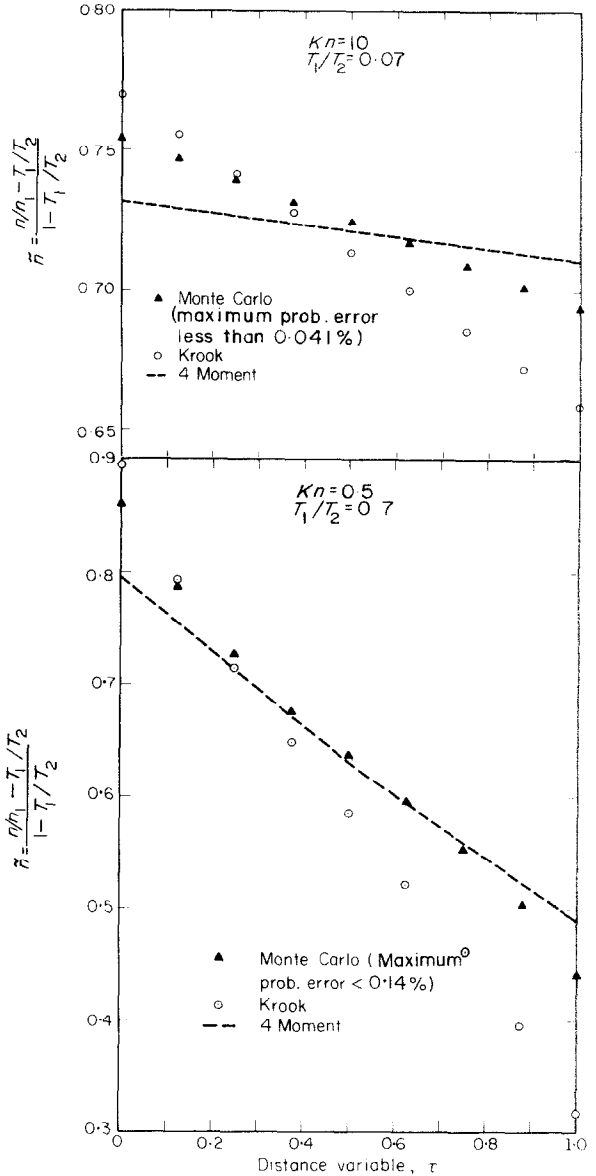


FIG. 5. The reduced density \tilde{n} as a function of distance variable τ . $Kn = 10$ and 0.5 . $T_1/T_2 = 0.7$.

We have compared the density profiles with those determined in an experiment [8] for the following cases: $Kn = 0.6313, 0.2493$ and 0.0548 ; $T_1/T_2 = 0.783$; $\alpha = 0.826$. Figure 6 illustrates the result for $Kn = 0.2493$. This agreement is an indication that we are able to make accurate calculations

under near-equilibrium as well as far-from-equilibrium conditions.

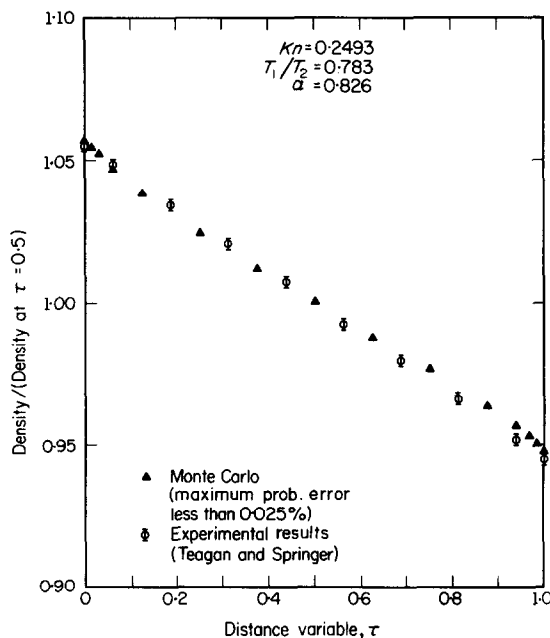


FIG. 6. Comparison of a density profile with that determined in an experiment.

ACKNOWLEDGEMENT

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REFERENCES

1. A. NORDSIEK and B. L. HICKS, Monte Carlo evaluation of the Boltzmann collision integrals, Proc. Fifth Intl. Symp on Rar. Gas Dyn., Vol. 1, pp. 695-710 (1967).
2. S. M. YEN and H. J. SCHMIDT, Monte Carlo solutions of the Boltzmann equation for heat transfer problems, Proc. Sixth Intl. Symp. on Rar. Gas Dyn., Vol. 1, pp. 205-213 (1969).
3. S. M. YEN, Solutions of the Boltzmann and Krook equations for heat transfer problems with Maxwell boundary conditions, Proc. Seventh Intl. Symp. on Rar. Gas Dyn. (to be published).
4. D. G. ANDERSON and H. K. MACOMBER, Numerical experiments in kinetic theory, Proc. Fourth Intl. Symp. on Rar. Gas Dyn., Vol. 1, pp. 96-111 (1965).
5. M. LAVIN, A Monte Carlo solution for heat transfer in rarefied gases, M.S. Thesis, MIT (1961).
6. J. K. HAVILAND, The solution of two molecular flow problems by the Monte Carlo method, *Meth. Comp. Phys.* 4, 109-209 (1965).
7. M. PERMUTTER, Analysis of Couette flow and heat transfer between two parallel plates enclosing rarefied gas by Monte Carlo, Proc. Fifth Symp. on Rar. Gas Dyn., Vol. 1, pp. 455-480 (1967).
8. W. P. TEAGEN and C. P. SPRINGER, Heat transfer and density distribution measurements between parallel plates in the transition regime, *Physics Fluids* 11, 497-506 (1968).

Int. J. Heat Mass Transfer. Vol. 14, pp. 1869-1873. Pergamon Press 1971. Printed in Great Britain

MASS TRANSFER DURING FILM BOILING ON VERTICAL FIBERS

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NOMENCLATURE

A ,	fiber cross-sectional area [cm ²];	D_w ,	diameter of the tungsten wire [cm];
A_s ,	final fiber cross-sectional area [cm ²];	f ,	a function defined by equation (10) [cm ⁻¹];
A_w ,	tungsten wire cross-sectional area [cm ²];	g ,	gravitational constant [cm min ⁻²];
D ,	mass diffusivity [cm ² min ⁻¹];	h ,	thickness of a fiber slice [cm];
D_{av} ,	average diameter of the deposit [cm];	k_z ,	rate constant [g moles cm ⁻² min ⁻¹ in. ^{0.246}];
D_s ,	diameter of the deposit [cm];	E ,	liquid evaporation rate [cm min ⁻¹];
		M_s ,	molecular weight of SiC;