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NUMERICAL STUDIES OF STRONG SHOCK WAVES PART VIII: PROPERTIES OF A SHOCK WAVE FOR A MACH NUMBER OF 2.5

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Numerical Studies of Strong Shock Waves

Part VIII: Properties of a Shock Wave for a Mach Number of 2.5

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ABSTRACT

This report describes a study of the structure of a shock wave in a gas of hard spheres for a Mach number $M_1 = 2.5$. The characteristics of the velocity distribution function f, of the collision integral, and of moments of these functions are discussed in detail for nine stations within the shock wave.

The structure was calculated by solving the (non-linear) Boltzmann difference equation by an iterative numerical method that includes Monte Carlo evaluation of the collision integral and a number of other new techniques. The 12th iterate is taken to be the solution of the difference equation. The average convergence error of this iterate is estimated to be not more than 0.5% of f.

It is found that although departures of the calculated solution from the Mott-Smith shock are generally small they are the smallest on the upstream side of the shock. The most important specific results are the following:

1. The largest deviation of the calculated velocity distribution functions from the Mott-Smith functions occurs near the hot side of the shock and near the "cold peak" in velocity space and amounts to 21% of f. The rms deviations at any given station in the shock are from four to ten times larger than the likely error at that station and eleven times larger than the estimated convergence error of the

iteration method. The deviations form regular patterns in velocity space at each station in the shock.

2. The collision integral (a-bf) calculated by the Monte Carlo method smooths rapidly during the first few iterations. The residual $[v_{xa}(df/dx)-a+bf]$ is two to five times smaller for the twelfth than for the first iterate. Earlier studies show that the random and systematic errors of the Monte Carlo evaluation of the collision integral lie in the range 1-3% for a Monte Carlo sample of the size used here.

3. The calculated reciprocal shock thickness is 0.301 ± 0.009, in units of the reciprocal upstream mean free path, a value not significantly different from the "u^2-moment" value obtained by Mott-Smith. The density gradient dn/dx, however, is an asymmetrical function of the reduced density $\hat{n} = (n-n_1)/(n_2-n_1)$ unlike the symmetrical function obtained by Mott-Smith. Thus the maximum of the gradient occurs at $\hat{n} = 0.41$ rather than 0.5; there is a significant difference between the upstream and downstream half-thicknesses of the shock; and the density gradient is a parabolic function of $\hat{n}$ only on the upstream side of the shock.

4. The calculated collision rate deviates significantly from the equilibrium value calculated from the local density and temperature in the shock, but never by more than 2.5%. Three moments of (a-bf) behave very much like dn/dx, as functions of n, which possibly suggests a source of difficulty in the six moment method of estimating shock structure.

5. Five moments of f including the Boltzmann flux, approach their equilibrium values on the hot side of the shock more rapidly than do the Mott-Smith values of the same moments. The maximum deviations between the calculated and Mott-Smith values of these moments are consistently six to nine times larger than the likely errors of the calculated moments. The moment $\mathcal{M}_9$, proportional to the lateral temperature $t_\perp$, shows the largest maximum deviation, namely 1.8% and is a quadratic function of $\hat{n}$ on the upstream side of the shock. The deviations of other moments are asymmetrical, the maximum deviations occurring near the hot side of the shock.

LIST OF SYMBOLS

1. Basic Set

Variables and Functions (Nordsieck units used throughout)

$a = a(\bar{v},n)$ $b = b(\bar{v},n)$	parts of the collision integral, (a-bf)
$f = f(\bar{v},n)$	velocity distribution function
f',F,F'	$f(\bar{v}',n), f(\bar{V},n), f(\bar{V}',n)$
I	number of iterations
J	number of stations in the shock wave
j	ordinal number of stations in the shock wave — $j=0,1,\ldots(J-1)$
$K_1 = v_m/v$	scaling parameter
M_1	upstream Mach number
N_7	2^{N_7} = number of collisions in the Monte Carlo sample
n	particle density
$\hat{n}$	reduced particle density, $(n-1)/(n_2-1)$
$\delta\underline{n}$	$(n_2-1)/(J-1)$
n'	dn/dx
$\underline{n}'$	Monte Carlo value of n'
r	ordinal number of the collision sample
s	ordinal number of velocity bin — $s=0,1,\ldots,226$
v_x	component of $\bar{v}$ perpendicular to the shock wave
v_{xa}	value of v_x measured relative to the shock wave

$v_\perp$	component of $\bar{v}$ parallel to the shock wave
$\bar{v}$	molecular velocity
$\bar{v}, \bar{v}'$	velocities of molecules entering a collision
$\bar{V}, \bar{V}'$	velocities of molecules leaving a collision
x	position coordinate measured perpendicular to the shock wave

Subscripts, etc.

c or 1	indicates "cold" or upstream side of shock wave
h or 2	indicates "hot" or downstream side of shock wave
m	refers to "machine" units of velocity, $v_m = K_1 v$
MC	Monte Carlo
M-S	Mott-Smith
$\rightarrow(\leftarrow)$	indicates $v_{xa} > (<) 0$
j	station j
s	velocity bin s
I	number of iterations

2. Special Symbols Used in This Report

G(n)	Boltzmann flux
H(n)	Boltzmann function
$\mathcal{M}_k(n)$, $\mathcal{M}'_k(n)$	k-th moments of f and of df/dx
$t_\perp$	"lateral" temperature
$\delta f = \delta f_{js}$	$[AV_{js}\, f_{I=12} - f_{I=0}]_{MC}$

f_{js}	value of f for the j-th station and s-th velocity bin
$AV_{js}f$	mean value of f_{js} for a set of four Monte Carlo runs
$\epsilon_{js}f$	"likely" error of $AV_{js}f$
$\epsilon_{j}f$	rms value, taken w.r.t. s, of $\epsilon_{js}f$
ν_a	twice the collision frequency
$\rho_j(\delta f)$, $\rho_j f$	rms values, taken w.r.t. s, of δf_{js} and of f_{js}
$\sigma_{js}f$	sample standard deviation of f_{js}
$\sigma_j f$	rms value, taken w.r.t. s, of $\sigma_{js}f$
max (v_{xm}), θ_I, θ_{II}	parameters describing the distribution of f_{js} in velocity space

The operators AV, σ, and ϵ refer to the mean, sample standard deviation and "likely" error computed from a set of four, statistically independent values of an operand.

INTRODUCTION

In this report we shall describe in detail the solution of the Boltzmann differential equation for a strong shock wave ($M_1 = 2.5$). The method of solution was first described in a paper[1] for the Oxford Symposium and illustrated there by brief discussions of a strong shock wave and of a pseudo-shock. The accuracy of the method of solution for a strong shock wave is discussed in a recent CSL report.[2]

Our solution of the Boltzmann equation involves the following major steps:

1) Replace the Boltzmann differential equation by a set of 226 difference equations, one for each velocity bin $\bar{v} = (v_x, v_\perp)$. The difference equations are derived by using a Monte Carlo evaluation of the collision integral (a-bf) and a stable numerical integration with respect to the variable n, the particle density, as an independent variable.

2) Solve this set of difference equations for 226(J - 2) values of the velocity distribution function $f(\bar{v},n)$ and also of $a(\bar{v},n)$ and of $[b(\bar{v},n)f(\bar{v},n)]$, where J is the number of stations in the shock. The solution is obtained by an iterative method which permits close control of the errors.[2]

3) Calculate physically interesting moments of the velocity distribution function f and of the collision integral

(a-bf). Numerical integration methods are used that are more accurate than the individual values of the integrand.

The results discussed in this report were obtained at the twelfth iteration, I = 12, for $M_1 = 2.5$ using fixed sets of Monte Carlo samples,[2] each sample containing 2^{N_7} collisions. Most of the results refer to $N_7 = 15$ and to J = 9 stations in the shock. The starting values (zero-th iterate) were Mott-Smith velocity distribution functions. Four independent runs were made corresponding to four independent sets of collision samples. The results output during each computer run include the following numbers, in Nordsieck units,[1] for each of nine stations in the shock and for any specified iteration: 226 values of f, a, and bf; 11 moments of f; 9 moments of a; and 9 moments of (a-bf). The moments mentioned include the Boltzmann function H, the Boltzmann flux G, and their derivatives. We note that all of these quantities are known at the two boundaries before we solve the Boltzmann equation for the shock wave.

We shall use Nordsieck units throughout the report unless otherwise stated. In these units the maximum value of the velocity distribution function and the values of density and temperature are equal to one at the upstream boundary of the shock wave. The unit of length is $2^{-\frac{1}{2}}\chi$ (upstream mean free path). The unit of velocity is $(\pi/2)\chi$ (upstream mean molecular speed).

We shall describe only what appears to be the most interesting of the characteristics of this large set of results for $M_1 = 2.5$. In

particular, we shall discuss the mean value and "likely" error[3] of each of the physically interesting quantities. These means and errors are derived from the four independent runs. This description of the shock wave for $M_1 = 2.5$ may then serve as a model for similar analyses at other Mach numbers.

OUTLINE OF TECHNIQUES USED IN SOLVING THE BOLTZMANN EQUATION

Our method of solving the Boltzmann equation for a shock wave is successful because it combines a number of new techniques that overcome earlier difficulties. These techniques may be summarized as follows.

1) Derivation of the difference equations

1.1) Use of an efficient Monte Carlo method (1962)[4] of evaluating the collision integral in the Boltzmann equation.[1,5] Although the Monte Carlo method has so far only been applied for elastic sphere molecules, this restriction is not necessary to the success of the method. Its accuracy has been carefully studied in two CSL reports.[2,6] The method has been successfully applied to several problems.[7,8]

1.2) Least squares adjustment of the collision integral (1964). This adjustment forces the conservation equations to be satisfied, prevents positive values of the gradient dG/dx of the Boltzmann flux, and prevents drift owing to unavoidable bias in our quadrature method used to evaluate the collision integral. (No quadrature method is free from bias.)

These two steps of the derivation define, for a "fixed" set of collision samples defined earlier,[2] an algorithm for calculating the collision integral at each station and velocity bin.

1.3) Use of n as an independent variable in place of x (1963). The variable n is generated during the solution of the Boltzmann difference equations and is used as the independent variable. This choice of the independent variable makes possible an appropriate variation of the interval Δx through the shock wave for any Mach number; stabilizes the shock by eliminating the artificial origin on the x axis; separates the problem of determining those functions like f and its moments that vary slowly with n and show small Monte Carlo fluctuations, from the problem of determining those functions such as (a-bf) and dn/dx that show more rapid variation with n and larger fluctuations. The function $dn/dx = n'(n)$ is obtained directly by integration of the collision integral (a-bf) so that its "likely" error can be calculated more easily than if this derivative were obtained by differentiation of n(x). The function n'(n) contains all the physically interesting information about the density profile. In particular, its maximum value is inversely proportional to the (density) shock thickness.

The first three steps of the derivation replace, for a given number of stations J and a fixed set of collision samples, the Boltzmann differential equation by the Boltzmann difference equations.

2. Solution of the difference equations. A rapidly converging, iterative method of solution of the Boltzmann difference

equations is obtained through the use of a stable numerical integration with respect to n which "homes" on the boundary values (1958, Nordsieck), and by completing separate iterative sequences for each of four fixed sets of independent, random collisions (1966). Averaging the solutions for these four sets of collisions gives the final, mean values of f and estimates of the statistical errors.

If, for given J, sample set, and starting values, the rms difference between the iterates for iterations (I-1) and I is less than say 2×10^{-4} we call the I-th iterate a solution, $f_A(\bar{v},n)$, of class A of the Boltzmann difference equations. If, for given J, both the estimated rms convergence error[2] and the rms variation of $f_A(\bar{v},n)$ with starting values are less than the rms variation of $f_A(\bar{v},n)$ across the four runs, then we call the mean of $f_A(\bar{v},n)$ across the four runs a solution of class B. It is solutions of class B of the difference equations that we shall discuss in this report.

REQUIREMENTS TO BE SATISFIED BY SOLUTIONS OF THE BOLTZMANN EQUATION FOR A SHOCK WAVE

There is at present no theory of the convergence of the solutions of our Boltzmann difference equations to solutions of the Boltzmann differential equation, as the sample size 2^{N_7}, number of iterations I, number of velocity bins S, and number of stations J are increased. In the absence of such theory we can at least require that the solutions of the difference equations satisfy a number of requirements that the solutions of the differential equations would themselves

satisfy. Some of these requirements[9] are listed below, and the solutions we discuss in this report satisfy all of them within the limitations of accuracy imposed by finite values of N_7, I and S.

1. Monotonic decrease of the Boltzmann flux G.
2. Constant values in the shock of the three conserved moments of f.
3. Non-positive values of dG/dx.
4. Zero values of the x derivatives of the three conserved moments.
5. Agreement with values of three moments of (a-bf) calculated analytically.[10]
6. Agreement with known boundary values of f, a, bf and their moments.
7. (a-bf) = 0 on $v_{xa} = 0$, that is, for molecules whose x component of velocity is zero relative to the shock.
8. Iterative solution independent of starting values (that is, of the zero-th iterate).

BEHAVIOR OF THE VELOCITY DISTRIBUTION FUNCTION

The unknown function in the Boltzmann difference equations is the velocity distribution function $f(\bar{v}_s, n_j) = f_{js}$ $(j=1,2\cdots(J-2);$ $s=0,1,2\cdots225)$. Once this function is known we can calculate the two parts of the collision integral a, bf by the Monte Carlo method and any moments of f, a or bf. We shall therefore first discuss the behavior of f_{js} before turning to the other functions.

For purposes of orientation it is useful to have before us the rms values of f at the j-th station,[2] that is, $\rho_j f$, $\overrightarrow{\rho_j f}$, $\overleftarrow{\rho_j f}$. The quantity $\rho_j f$ is the rms value of f_{js} at the j-th station. The notations $\rightarrow$ and $\leftarrow$ refer, respectively, to molecules moving forward or backward with respect to the shock, that is, to $v_{xa} > 0$ or $v_{xa} < 0$. The rms values are given in Table 1.

Table 1

Rms Values of f - (J = 9)

j	$\rho_j f$	$\overrightarrow{\rho_j f}$	$\overleftarrow{\rho_j f}$
0	0.1396	0.1793	0.00026
1	0.1286	0.1650	0.0109
2	0.1206	0.1540	0.0206
3	0.1157	0.1464	0.0312
4	0.1135	0.1420	0.0413
5	0.1143	0.1408	0.0514
6	0.1178	0.1429	0.0614
7	0.1240	0.1484	0.0718
8	0.1349	0.1593	0.0843

In our discussion of f_{js} it is convenient, for several reasons, to use the Mott-Smith velocity distribution functions[11] as reference functions: for $M_1 = 2.5$ they are good approximations to the solution of the Boltzmann equation; they are simple (linear)

functions of the independent variable n; and they are the zero-th approximations used in our iterative, numerical solutions of the Boltzmann difference equations. We therefore shall use the difference function

$$\delta f = \delta f_{js} = [AV_{js} f\big|_{I=12} - f_{js}\big|_{I=0}] \qquad (1)$$

in our discussion.

In accordance with the conventions in Report IX the first term on the right-hand side of this equation is the mean value of f_{js}, for each bin s and station j, taken over the four independent collision samples for the twelfth iteration. The second term on the right-hand side is the Mott-Smith or starting value of the velocity distribution function for the same bin and station. We shall use δf as an abbreviation for δf_{js}.

We find that we can define the most important characteristics of the variation of δf in velocity space by describing, in each of <u>four</u> regions in velocity space and for each j (or station), the bins for which $|\delta f| > 10\, \epsilon_{js} f$, that is, the bins for which $|\delta f|$ is statistically very significant. The "likely error"[3] $\epsilon_{js} f$ is that corresponding to the Monte Carlo fluctuations[2] and is equal to $0.442\sigma_{js} f$ where $\sigma_{js} f$ is the sample standard deviation of f_{js} across the four independent runs.

The four regions, numbered I – IV, are shown schematically in Figs. 1 a, b and can be used to describe the behavior of the differences δf at any station by appropriate parameterization, as shown in Table 2. In many individual bins outside these four regions the

differences are also significantly different from zero, though by less than $10\epsilon_{js}f$. Since they are highly correlated with respect to j and s, the differences in these regions outside I – IV are also quite significant in the aggregate, but we shall not discuss them further here.

In discussing Table 2 we note first that the departures of the characteristics of the shock from Mott-Smith behavior are nearly the same for j = 1, 2 (and sometimes 3), a result also found in the behavior of some of the moments to be discussed later. Also, the total number of significant bins, that is those bins in which $|\delta f| \geq 10\epsilon_{js}f$, increases from 29% for j = 1 and 2 to 38% for j = 3 - 7.

The total number of significant bins in regions I and II is almost constant as j changes, but the numbers of bins in each of these two regions changes drastically with j. Regions III and IV contain most of the large values of f (i.e. most of the molecules) so that the characteristics of these two regions should strongly affect the moments and also the rms value of δf, that is, $\rho_j \delta f$. In most of the bins in Regions III and IV, for j = 7, the values of f are nearer to the equilibrium values on the hot side of the shock ($n = n_2$) than are the Mott-Smith values. In Region IV the largest value of δf occurs near $v_{xm} = 11$ and $v_{\perp_m} = 9$ at j = 4 and amounts to +14% of f. In Region III the largest $|\delta f|$ occurs near the cold peak ($v_{xm} \sim 10$ and $v_{\perp_m} = 1$) at j = 7 and amounts to 21% of f. The subscript m refers here to "machine" units of velocity in which $(v_{xm}/v_x) = (v_{\perp_m}/v_\perp) = 8.40$ for $M_1 = 2.5$.

We note certain further correlations indicated by our calculations: the number of significant bins in Region III at the j-th

Table 2

Difference δf between Monte Carlo Solution and Mott-Smith Functions

	j = 1	2	3	4	5	6	7
Region I: $\delta f > 0$							
no. of bins	9	12	10	14	25	36	56
$\sim \theta_I$	140	135	125	125	105	85	60
max δf	2.5×10^{-4}	2.8×10^{-4}	1.5×10^{-4}	2.5×10^{-4}	3.9×10^{-4}	2.8×10^{-4}	7.4×10^{-4}
Region II: $\delta f < 0$							
no. of bins	42	43	49	46	37	18	3
$\sim \theta_{II}$	120	115	105	110	85	75	25
max $\lvert\delta f\rvert$	1.0×10^{-3}	4.5×10^{-4}	7.4×10^{-4}	3.5×10^{-4}	2.7×10^{-4}	5.4×10^{-4}	3.1×10^{-5}
Region III: $\delta f < 0$							
no. of bins	6	6	9	10	11	14	14
$\sim$ max v_{xm}^*	9	11	9	11	13	13	13
max $\lvert\delta f\rvert$	2.6×10^{-2}	4.3×10^{-2}	5.5×10^{-2}	6.2×10^{-2}	6.2×10^{-2}	5.6×10^{-2}	9.3×10^{-2} a)
Region IV: $\delta f > 0$							
no. of bins	9	6	13	14	17	15	12
max δf	5.8×10^{-3}	6.0×10^{-3}	7.3×10^{-3}	1.2×10^{-2}	1.2×10^{-2}	7.5×10^{-3}	5.3×10^{-3}

*The subscript m refers to machine units[1] in which $v_{xm}/v_x = 8.40$.

a) An anomalous velocity bin.

Table 2 (continued)

	j						
no. of significant bins*	1	2	3	4	5	6	7
in I & II	51	55	59	60	62	54	59
in III & IV	15	12	22	24	28	29	26
for $v_{xa} < 0$	13	16	12	17	26	34	33
for $v_{xa} > 0$	53	51	69	68	65	52	55
total (all v_{xa})	66	67	81	85	91	86	88

*Significant bins are those for which $|\delta f| \geq 4.6\sigma_{js}f$, a difference of "two letters" or more between corresponding velocity bins in the isoline plots of $\delta f(j,s)$ and of $\sigma_{js}f$.

station correlates well with the quantity $\overrightarrow{\sigma_j f}/\overrightarrow{\rho_j \delta f}$, and the total number of significant bins for which $v_{xa} < 0$ at the j-th station correlates well with the quantity $\overleftarrow{\sigma_j f}/\overleftarrow{\rho_j \delta f}$, results that are not unexpected, in view of our definition of "significant bins."

In the calculation of (a-bf) in both Regions I and II for an equilibrium gas, there is known to be a small positive bias[6] produced by discarding the "unsuccessful collisions." There is also presumably some (unknown) bias in calculating (a-bf) in Regions I and II for the non-equilibrium gas in the shock wave and a corresponding bias in the values of f obtained by the iteration process. In these regions there is, however, no similarity between the bias pattern of (a-bf) for the equilibrium gas and the patterns of δf for the seven stations in the shock wave.

A quantitative summary of the values of δf that are significantly different from zero can be made by comparing $\rho_j \delta f$ (the rms value of δf at the j-th station) with $\epsilon_j f$ (the rms likely error at the j-th station). The comparison is given in Table 3. The bottom row of numbers in Table 3 measures the fractional uncertainty in $\rho_j \delta f$. The numbers indicate that the "likely" error in f is small, compared to $\rho_j \delta f$, at each station. Further calculation shows that the rms "likely" error for all bins and stations is only 15% of $\rho \delta f$, the rms δf for all bins and stations.[12] Note that $\epsilon_j f$ is almost constant across the shock but that $\rho_j \delta f$ increases substantially from the cold to the hot side of the shock. The fractional uncertainty in $\rho_j \delta f$ therefore decreases from the cold to the hot side of the shock.

Table 3

Properties of f and δf for each station

j	1	2	3	4	5	6	7
$10^3 \times \epsilon_j f$	0.98	1.22	1.33	1.21	1.04	0.98	0.94
$10^3 \times \rho_j \delta f$	3.73	6.09	7.40	8.20	8.50	8.32	9.11
$\epsilon_j f / \rho_j \delta f$	0.26	0.20	0.18	0.15	0.12	0.12	0.10

We have observed a small anomaly in the iterative solutions of the Boltzmann difference equations. As I increases from 1 to 12 the values of f and of (a-bf) in certain ("maverick") velocity bins seem to slowly diverge. (This behavior does not prevent finding solutions of class B, as defined earlier.) The anomaly occurs for several sample sets for J = 9 but only near the hot side of the shock and for two or three bins at most. A phenomena possibly related to that of the maverick bins is the lack of convergence, within $I \leq 12$, of the iterative sequence for $N_7 = 11$. Both phenomena appear to be characteristic of the Monte Carlo sampling and will be investigated further.

BEHAVIOR OF THE COLLISION INTEGRAL

During the first few iterations the isolines of the collision integral (a-bf) become much smoother than they are for I = 0, but this increase of smoothness is less for J = 9 than for J = 3. Similarly, the variation of dn/dx with n is smoother for I = 12 than for I = 0. (In the last section of the paper we shall make a distinction between dn/dx and $d\underline{n}/dx = \int (a\text{-}bf)_{MC}\, d\bar{v}/v_{xa}$. This distinction is not needed here.) Several pieces of evidence thus indicate that the early iterations serve to adjust, in a subtle way, the values of f at each station to the collision samples, both at that station and at neighboring stations.

The smallness of $\delta_I f$, the change in f from iteration (I - 1) to iteration I, was used in Report IX as <u>one</u> measure of the degree of convergence of the iterations. This measure corresponds to the "second

test"[8] of a proposed solution of the Boltzmann equation for a shock wave. In the "first test," given in the same reference, the ratio of the two terms in the Boltzmann equation is used instead as a measure of accuracy of the proposed solution. We can use a second measure of convergence here that is similar to the "first test." In this second measure of convergence we use the difference of the two terms in the Boltzmann equation; namely, $[v_{xa}(df/dx)-a+bf]$, where v_{xa} is the x component of molecular velocity measured relative to the shock. We find that the values of this difference are two to five times smaller for I = 12 than for I = 0. Note that the iteration method that produces $f_{js}/_{I=12}$ works to reduce δf progressively and does not necessarily reduce as rapidly the rms value of $[v_{xa}(df/dx)-a+bf]$ (or its finite difference equivalent).

The errors in the Monte Carlo calculation of the two parts, a and bf, of the collision integral have been discussed in some detail[6] for gases in equilibrium. For purposes of orientation we quote several of these errors here. The mean systematic error in determining (a-bf), near equilibrium, is 1.2% of a or of bf, for a well-filled velocity space. The standard deviation of the systematic error of (a-bf) is 1.8% of a or of bf. For $N_7 = 15$ (the value used in the calculations described here) the standard deviation of the random error of (a-bf) is 2.6% of a or of bf.

We can compare $(a\text{-}bf)_{MC}$, the Monte Carlo value of (a-bf) for the shock wave with $(v_{xa}\ df/dx)_{M\text{-}S}$, the Mott-Smith[11] value of $(v_{xa}\ df/dx)$. (The subscript a in v_{xa} indicates a velocity component

measured relative to the shock.) For this purpose we use the Monte Carlo value of (a-bf) for the twelfth iteration of one of the four runs for J = 9, N_7 = 15. We calculate $(v_{xa}\ df/dx)_{M-S}$ from the equation

$$(df/dx)_{M-S} = B(n-1)(n_2-n)\cdot(f_2-f_1)/(n_2-1) \qquad (2)$$

where B = 0.5049 (corresponding to Mott-Smith's use of the "u^2" moment), n and n_2 have the values calculated in our Monte Carlo Boltzmann program, and all quantities are in Nordsieck units.

The two functions, as we would expect from the comparison of Monte Carlo and Mott-Smith values of f earlier in the report, are quite similar. Indeed, the sign of the difference $[(a-bf)_{MC} - (v_{xa}\ df/dx)_{M-S}]$ can be predicted, for the regions III and IV of Figs. 1a, b, from the values of δf. Near the hot side of the shock, at j = 7, the difference is positive for every bin for which $v_{xa} > 0$, and the isoline pattern of the difference resembles that of $(-v_{xa}\ df/dx)_{M-S}$ throughout the velocity space. This behavior of the difference for j = 7 is caused by the fact that $(a-bf)_{MC}$ is roughly proportional to $(v_{xa}\ df/dx)_{M-S}$ there but is much smaller in absolute value. Various moments of $(a-bf)_{MC}$ and of $(v_{xa}\ df/dx)_{M-S}$ behave in similar fashion.

THE DENSITY PROFILE

For several years we have found it desirable to use n, the particle density, as the independent variable in place of x. We use a related variable $\hat{n} = j(J-1)^{-1}$ here and plot $dn/dx = \int (a-bf)\ d\bar{v}/v_{xa}$

against $\hat{n}$ as in Fig. 2. The mean values and 50% confidence limits (corresponding to the "likely errors") for dn/dx are shown for each value of $\hat{n}$.

The maximum value of dn/dx in Nordsieck units is 0.362 ± 0.011,[13] and it occurs at $\hat{n} = 0.41$. The reciprocal shock thickness $(dn/(n_2-1)dx)$ is then 0.301 ± 0.009,[13] in units of (upstream mean free path)$^{-1}$, and the thickness is 3.32 ± 0.10[13] in units of the upstream mean free path. The Mott-Smith value[11] of the reciprocal shock thickness, derived from his "u^2" moment method and in units of (upstream mean free path)$^{-1}$, is 0.303, not significantly different from the Monte Carlo value.

The dn/dx *vs* $\hat{n}$ profile in Fig. 2 is decidedly asymmetrical, unlike the Mott-Smith profile. Thus, for example, $(dn/dx)_{M-S}$ is 50% larger than $(dn/dx)_{MC}$, for $j = 7$. This asymmetry corresponds to a less obvious asymmetry of the $\hat{n}$ *vs* x profile (Fig. 3) calculated by numerical integration. We can describe the asymmetry of this density profile as follows. Consider the three points, 1, 2, 3 on the density profile defined by three values of $\hat{n}$, namely, $\hat{n} = 0.0625$, 0.500 and 0.9375. The "upstream half-thickness" of the shock is measured by $(x_2-x_1) = 2.18 \pm 0.03$[13] in units of the upstream mean free path. The "downstream half-thickness" of the shock is measured by $(x_3-x_2) = 2.83 \pm 0.05$,[13] in the same units. The difference between these half-thicknesses is 0.64 ± 0.006[13] which is 19% of the shock thickness.

On the left side of the density gradient curve ($j = 1,2,3,4$) we find that $(dn/dx)/[\hat{n}(1-\hat{n})]$ is not significantly different from the

constant value 1.445 ± 0.047.[13] For j = 5, 6, 7 the departures from this value are significant and are consistently negative. We note that Mott-Smith's velocity distribution functions imply that the quadratic dependence of dn/dx upon $\hat{n}$ should hold for the entire shock. His value of the proportionality constant (in Nordsieck units, calculated from the "u^2" moment equations) is 1.461. We can compare these values with two others. The values of the proportionality constant calculated for J = 3, N_7 = 17 and I = 0 and 12 are 1.4712 ± 0.029[13] and 1.4792 ± 0.046.[13] The first of these values is calculated from Mott-Smith velocity distribution functions using the moment $dn/dx = \int(a-bf)d\bar{v}/v_{xa}$. The second value is calculated from Monte Carlo velocity distribution functions at I = 12, i.e., after solution of the Boltzmann difference equation has been obtained, and uses the same formula for calculating dn/dx.

The similarity of the four values of the ratio $(dn/dx)/[\hat{n}(1-\hat{n})]$ is remarkable. We may conclude, as we did after examination of $\delta f(j,s)$, that the Mott-Smith values of f and the values of a-bf derived from them, correspond more closely to the solution of the Boltzmann equation on the upstream than on the downstream side of the shock.

VARIOUS OTHER MOMENTS OF a AND OF (a-bf). (J=9, N_7=15, I=12)

In Fig. 4 the mean values and 50% confidence limits of the Boltzmann flux $G(\hat{n}) = \int v_{xa} f \log f \, d\bar{v}$ are plotted <u>vs</u> $\hat{n}$ for I = 12. For comparison, the values of $G(\hat{n})$ are also shown for I = 0 (Mott-Smith).

The difference between the two curves is much larger than the likely error. Note that the curve for I = 12, corresponding to solution of the Boltzmann equation, approaches the hot side of the shock ($\hat{n} = 1$) with a much more nearly horizontal slope than does the Mott-Smith curve. The deviations between Monte Carlo and Mott-Smith values again are in the direction of more rapid approach to equilibrium values on the hot side. Each curve decreases monotonically and therefore, because dn/dx is positive within the shock wave, each corresponding function satisfies the Boltzmann Theorem.

The quantity $\nu_a = \int a \, d\bar{v}$ is twice the collision frequency and, for an equilibrium gas, equals $\sqrt{2} n^2 T^{1/2}/\pi$. We find that the Monte Carlo values of ν_a differ at most by 2.5% from the values calculated from this equilibrium formula using the local values of density and temperature. The likely error in ν_a is less than 1.1% at each station in the shock.

The derivatives

$$\eta_2' = \nu_{a,b} = \int (a-bf) d\bar{v} \tag{3}$$

$$\eta_3' = \int v_{xa} (a-bf) d\bar{v} \tag{4}$$

$$\eta_4' = \int v_a^2 (a-bf) d\bar{v} \tag{5}$$

of the three conserved fluxes are identically zero because of the (a-bf) correction used in our calculations. (Note that $v_a^2 = v_{xa}^2 + v_\perp^2$.)

Three other moments of (a-bf) used in Yen's description of shock structure[14] derived by the six-moment method are

$$\mathcal{M}_6' = \int v_{xa}^2 (a\text{-}bf)\, d\bar{v} \tag{6}$$

$$\mathcal{M}_{11}' = \int v_{xa}^3 (a\text{-}bf)\, d\bar{v} \tag{7}$$

$$\mathcal{M}_{711}' = \mathcal{M}_7' - \mathcal{M}_{11}' = \int v_{xa}\, v_\perp^2 (a\text{-}bf)\, d\bar{v} \,. \tag{8}$$

We calculated the values of these moments from the (a-bf) tables obtained in our Monte Carlo solutions of the Boltzmann equation. The three moments exhibit a striking similarity to the moment $dn/dx = \int (a\text{-}bf)\, d\bar{v}/v_{xa}$. In

Table 4

Behavior of Three Moments of a-bf

	j = 1	2	3	4	5	6	7
$\mathcal{M}_6'/(dn/dx)$	-0.463	-0.442	-0.432	-0.452	-0.445	-0.433	-0.341
	$\pm$0.019[13]	0.010	0.015	0.009	0.014	0.016	0.030
$\mathcal{M}_{11}'/(dn/dx)$	-0.649	-0.625	-0.616	-0.635	-0.620	-0.591	-0.419
	$\pm$0.029	0.015	0.020	0.017	0.022	0.027	0.050
$\mathcal{M}_{711}'/(dn/dx)$	0.670	0.618	0.601	0.646	0.636	0.613	0.426
	0.024	0.011	0.022	0.012	0.019	0.021	0.047

fact each ratio, $\mathcal{M}_k/(dn/dx)$, (k = 6,11,711) does not vary significantly as j varies from 1 to 6, as seen in Table 4. Also, $\mathcal{M}_7' = \int v_{xa} v_a^2 (a\text{-}bf)\, d\bar{v} = \mathcal{M}_{711}' + \mathcal{M}_{11}'$ is not significantly different from zero. These several results may clarify numerical problems that are inherent in the six-moment method of estimating shock structure.

VARIOUS MOMENTS OF f

The independent variable $\underline{n}$ actually used in our numerical integration of the Boltzmann equation is slightly different from the particle density n. The variable $\underline{n}$ is defined implicitly by giving its derivative $d\underline{n}/dx$ as a function of $\underline{n}$. The derivative is calculated by a numerical quadrature

$$d\underline{n}/dx = \int [(a-bf)_{MC}/v_{xa}]d\bar{v} \tag{9}$$

where the collision integral $(a-bf)_{MC}$ is calculated by the Monte Carlo sampling. The variable n is defined by a second numerical quadrature

$$n(\underline{n}) = \int f(\bar{v},\underline{n})d\bar{v} \tag{10}$$

over the velocity distribution function $f(\bar{v},\underline{n})$ calculated by our Monte Carlo solution of the Boltzmann equation. We find that the deviation of n from $\underline{n}$ may be neglected except at j = 7 where it amounts to -0.42%. Corresponding corrections of other computed moments of f, at j = 7, were made so that they may truly be considered to be functions of n rather than of $\underline{n}$.

The three conserved moments of the Monte Carlo f's (fluxes of mass, momentum and energy) are constant within 0.38, 0.31 and 0.46%, respectively. Errors of the numerical integrations in velocity space are, for these same moments, at most 0.11, 0.19 and 0.26%. The near constancy of these moments is enforced by our (a-bf) correction method. If these three moments were exactly conserved, the values of each of the other moments might be changed by a fraction of a percent from the values obtained in our calculations.

Five non-constant moments of f are:

$$\mathcal{M}_5 = \int f \log f \, d\bar{v} \qquad \text{the Boltzmann function} \qquad (11)$$

$$\mathcal{M}_6 = \int v_{xa}{}^3 f \, d\bar{v} \qquad (12)$$

$$\mathcal{M}_9 = \int v_\perp{}^2 f \, d\bar{v} = nt_\perp/\pi \qquad (13)$$

$$\mathcal{M}_{10} = \int v_{xa} f \log f \, d\bar{v} \qquad \text{the Boltzmann flux} \qquad (14)$$

$$\mathcal{M}_{11} = \int v_{xa}{}^4 f \, d\bar{v} \qquad \text{a moment used in the six-moment method .} \qquad (15)$$

We shall be interested primarily in the deviations of the Monte Carlo values of these moments from the Mott-Smith values. Note that, as usual, we are considering f and each moment to be a function of n, the particle density. The Mott-Smith f and the non-logarithmic moments of the Mott-Smith f are linear functions of n that depend only upon the boundary conditions and not upon knowledge of Mott-Smith's parameter B. Note also that in calculation of these deviations the numerical quadrature error (in forming the moments) cancels out to a large extent because both Monte Carlo and Mott-Smith moments were calculated by the same quadrature process, and the integrands are very similar. For $\mathcal{M}_5$, $\mathcal{M}_6$, $\mathcal{M}_9$ and $\mathcal{M}_{11}$ the correction, at j = 7, of $\underline{n} \rightarrow n$ (see Subsect. 1) makes each of these Monte Carlo moments closer, by a small but significant amount, to its equilibrium value at the hot side of the shock, and, as in the case of the f's, the Monte Carlo values were already closer (or as close) to the equilibrium values than were the Mott-Smith ones. The correction of $\underline{n} \rightarrow n$ produces no significant change in the value of $\mathcal{M}_{10}$ because the $\mathcal{M}_{10}$ vs n curve is nearly horizontal at j = 7.

The deviations from Mott-Smith values are summarized in Table 5. The maximum deviations are consistently six or seven times larger than the likely errors of the Monte Carlo moments. Although no deviation is larger than 1.8%, each of the maximum deviations is statistically significant.

Table 5

Deviations of Monte Carlo Moments from Mott-Smith Moments

Moment	$\mathcal{M}_5$	$\mathcal{M}_6$	$\mathcal{M}_9$	$\mathcal{M}_{10}$*	$\mathcal{M}_{11}$
Largest % Deviation	-0.93	-0.59	+1.8	-1.6	-0.45
% Likely Error	0.14	0.10	0.2	0.2	0.06

*Plotted in Fig. 4.

The deviations between Monte Carlo and Mott-Smith moments show interesting properties as functions of $\hat{n}$ or j. The deviations are significant, for all $\hat{n} > \frac{1}{2}$ for all of the five moments, and are significant, for $n < \frac{1}{2}$ for all of the five moments except $\mathcal{M}_9$. This one Monte Carlo moment, which is proportional to $t_\perp$, therefore behaves like dn/dx and the other moments of (a-bf) in being similar to Mott-Smith moments only on the upstream side of the shock. The deviations of $\mathcal{M}_{11}$ are approximately parabolic in $\hat{n}$. The deviations of the other moments are asymmetrical, with the maximums located near the hot side of the shock wave.

FOOTNOTES AND REFERENCES

1. Monte Carlo Evaluation of the Boltzmann Collision Integral. Arnold Nordsieck and Bruce L. Hicks. CSL Report R-307, July, 1966. Also to be published in the Proceedings of the Fifth International Symposium on Rarefied Gas Dynamics.

2. Numerical Studies of Strong Shock Waves. Part IX: Error Analysis for a Mach Number of 2.5. B. L. Hicks and M. A. Smith. CSL Report R-348, April 1967.

3. The "likely" error is one-half of the difference between the 50% confidence limits for a small sample, in our case a sample of four.

4. Our first use of each technique is indicated by the year in parentheses.

5. Nordsieck developed the principal part of this Monte Carlo method before 1959.

6. Numerical Studies of Strong Shock Waves. Part VII: Study of Monte Carlo Errors in the Evaluation of the Collision Integral. M. A. Smith and B. L. Hicks. CSL Report I-131, November, 1965.

7. The Pseudo-Shock: A Non-Linear Problem of Translational Relaxation. B. L. Hicks. CSL Report R-236, June 1965.

8. On the Accuracy of Approximate Solutions of the Boltzmann Equation. S. M. Yen and Bruce L. Hicks. CSL Report R-308, July 1966. Also to be published in the Proceedings of the Fifth International Symposium on Rarefied Gas Dynamics.

9. These requirements are independent when they are applied to solutions of the difference equations. Similar requirements were satisfied by our solution of the pseudo-shock problem.(7)

10. This requirement was developed by Dr. S. M. Yen.

11. The Solution of the Boltzmann Equation for a Shock Wave. H. M. Mott-Smith, Phys. Rev. 82, 885 (1951).

12. The convergence error, defined in Report IX, is only, on the average, 9% of the rms value of δf.

13. "Likely" error.

14. Approximate Solution of the Boltzmann Equation for a Shock Wave. S. M. Yen. AVCO RAD-TM-66-9, March 17, 1966.

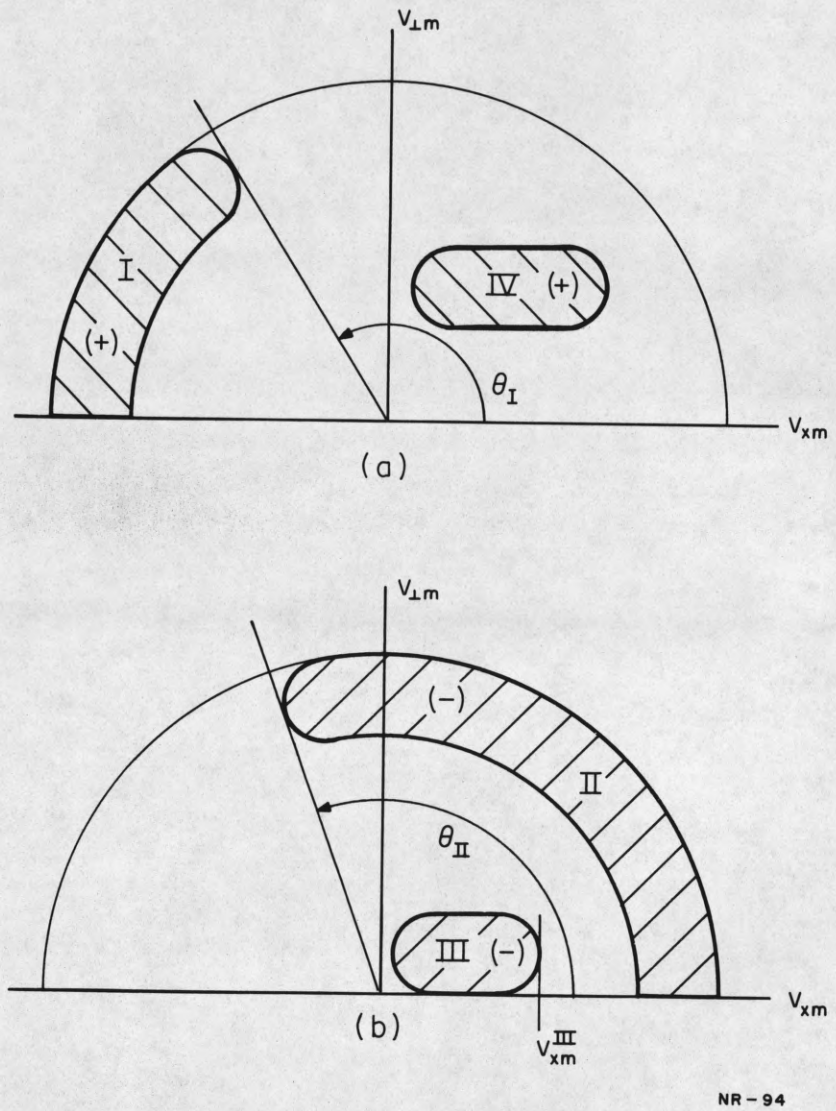

Fig. 1. Deviations between Monte Carlo and Mott-Smith Values of the Velocity Distribution Function $f(v_x,v_\perp)$ for a Strong Shock Wave. The Monte Carlo Calculations were made for a gas of elastic spheres for a Mach number $M_1 = 2.5$. These deviations $\delta f = f_{MC}(v_x,v_\perp) - f_{M\text{-}S}(v_x,v_\perp)$ are represented qualitatively by indicating the regions I and IV, in Fig. 1a, in which $\delta f > 0$ and the regions II and III, in Fig. 1b, in which $\delta f < 0$. The values of the parameters θ_I, θ_{II}, v_{xm}^{III} and other characteristics of these regions are summarized in Table 2 for each station in the shock wave.

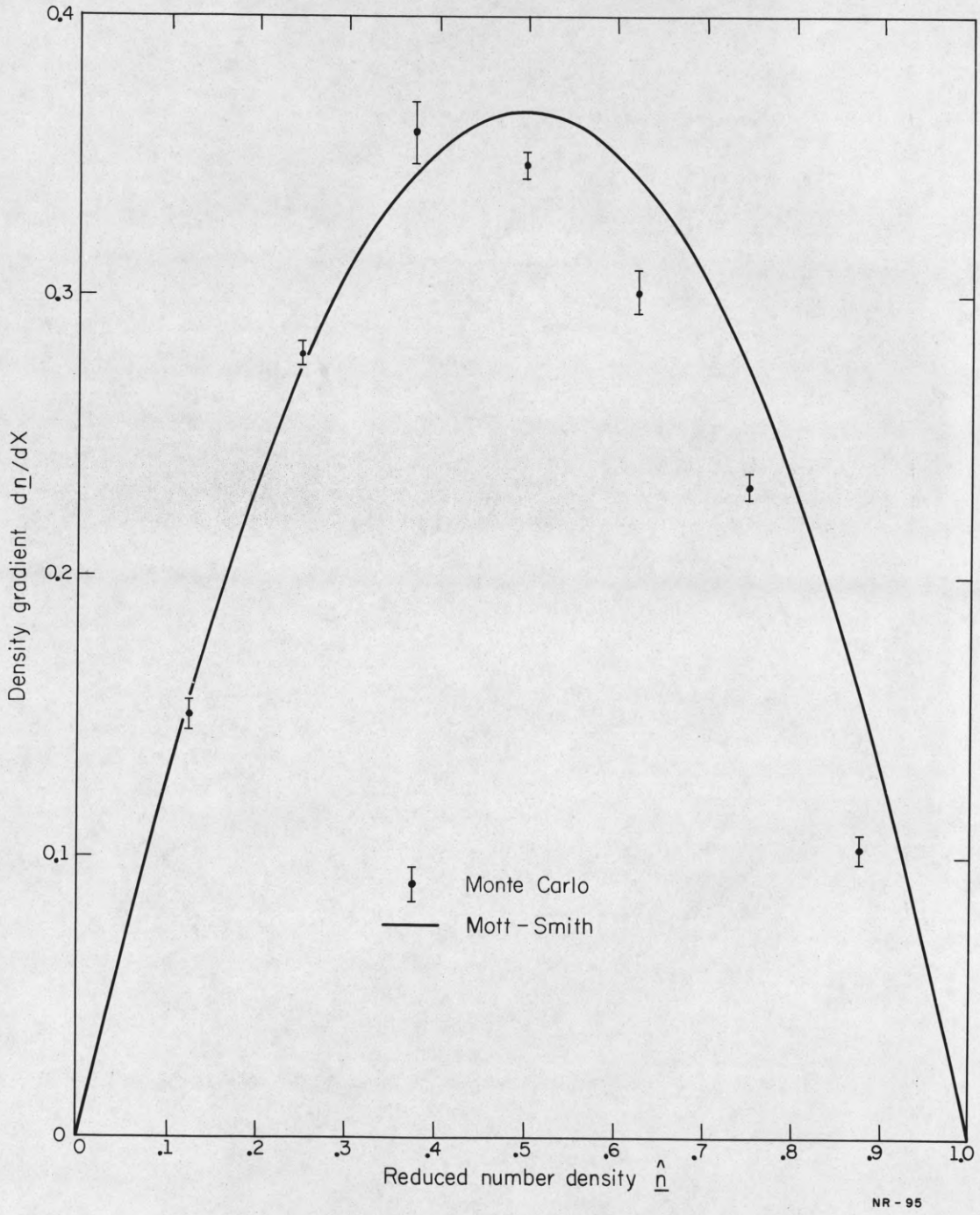

Fig. 2. The density gradient dn/dx as a function of reduced number density $\hat{n}$ in a shock wave (Mach number $M_1 = 2.5$). The units are Nordsieck units.[1] The symbols Φ indicate the 50% confidence limits.

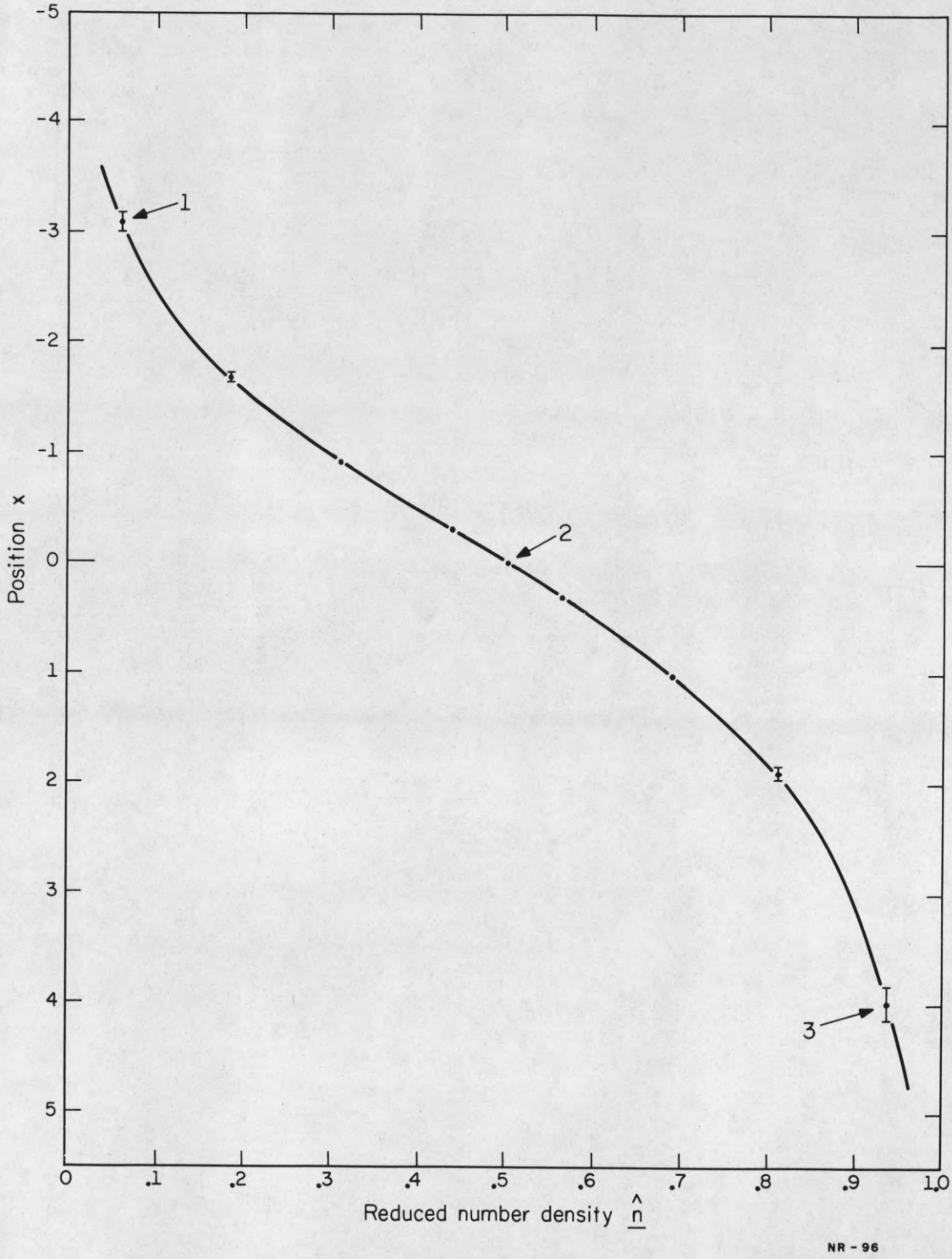

Fig. 3. The density profile: x coordinate in the shock as function of reduced density $\hat{n}$. The units are Nordsieck units.[1] The Mach number $M_1 = 2.5$. The symbols Φ indicate the 50% confidence limits.

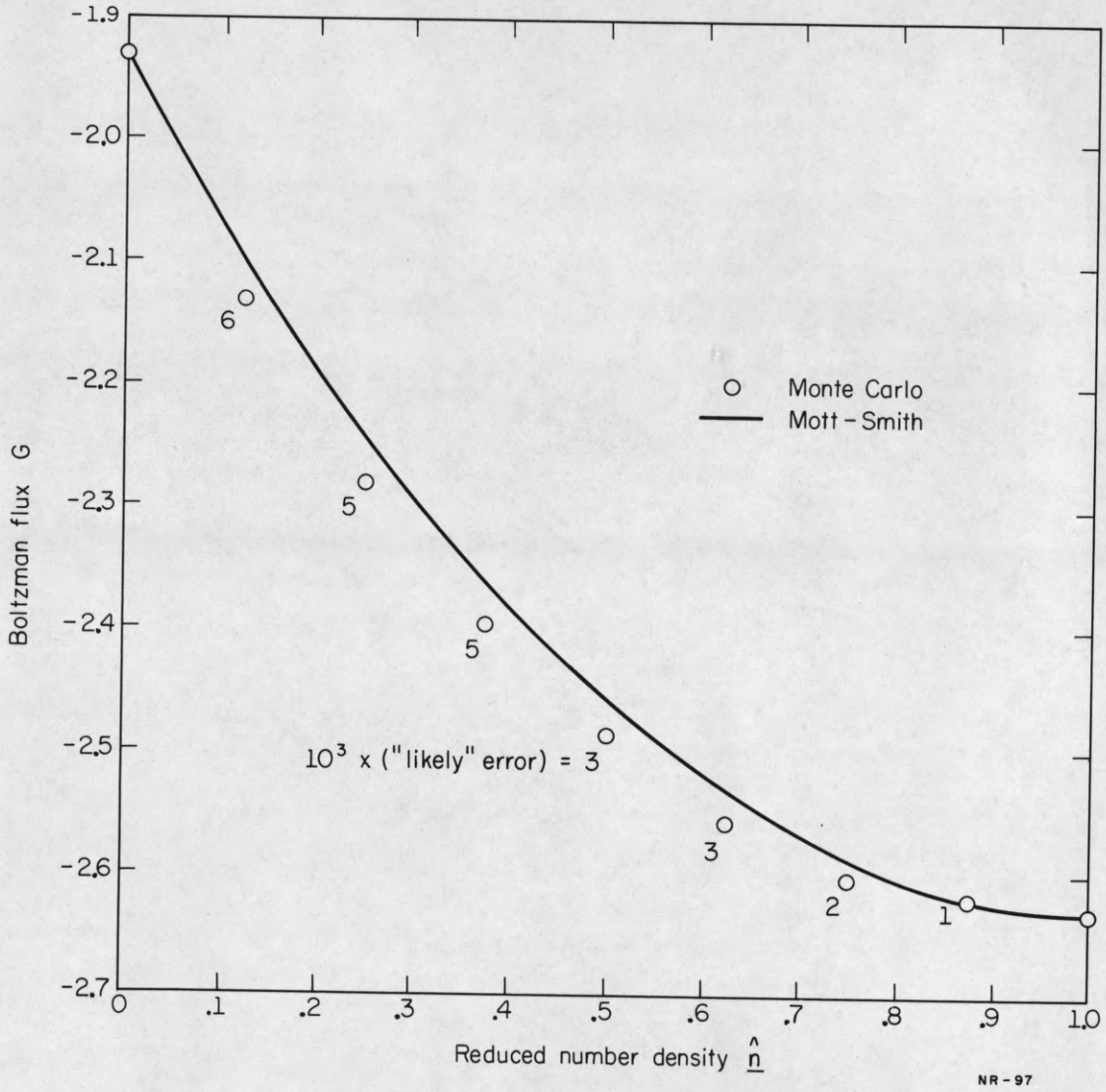

Fig. 4. The Boltzmann flux G as a function of reduced number density $\hat{n}$ in a shock wave (Mach number $M_1 = 2.5$). The units are Nordsieck units.[1] The "likely error" is one-half the difference between the 50% confidence limits.

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13. ABSTRACT

This report describes a study of the structure of a shock wave in a gas of hard spheres for a Mach number $M_1 = 2.5$ The characteristics of the velocity distribution function f, of the collision integral, and of moments of these functions are discussed in detail for nine stations within the shock wave.

The structure was calculated by solving the (non-linear) Boltzmann difference equation by an iterative numerical method that includes Monte Carlo evaluation of the collision integral and a number of other new techniques . The 12th iterate is taken to be the solution of the difference equation. The average convergence error of this iterate is estimated to be not more than 0.5% of f.

It is found that although departures of the calculated solution from the Mott-Smith shock are generally small they are generally small they are the smallest on the upstream side of the shock. The most important specific results are the following:

1. The largest deviation of the calculated velocity distribution functions from the Mott-Smith functions occurs near the hot side of the shock and near the "cold peak" in velocity space and amounts to 21% of f. The rms deviations at any given station in the shock are from four to ten times larger than the likely error at that station and eleven times larger than the estimated convergence error of the iteration method. The deviations for regular patterns

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ABSTRACT (continued)

in velocity space at each station in the shock.

2. The collision integral (a-bf) calsulated by the Monte Carlo method smooths rapidly during the first few iterations. The residual $[v_{xa}(df/dx)-a+bf]$ is two to five times smaller for twelfth than for the first iterate. Earlier studies show that the random and systematic errors of the Monte Carlo evaluation of the collision integral lie in the range 1-3% for a Monte Carlo sample of the size used here.

3. The calculated reciprocal shock thickness is 0.301 ± 0.009, in units of the reciprocal upstream mean free path, a value not signigicantly different from the "u^2-moment" value obtained by Mott-Smith. The density gradient dn/dx, however, is an asymmetrical function of the reduced density $\hat{n} = (n-n_1)/(n_2-n_1)$ unlike the symmetrical function obtained by Mott-Smith. Thus the maximum of the gradient occurs at $\hat{n} = 0.41$ rather than 0.5; there is a significant difference between the upstream and downstream half-thickness of the shock; and the density gradient is a parabolic function of $\hat{n}$ only on the upstream side of the shock.

4. The calculated collision rate deviates significantly from the equilibrium value calculated from the local density and temperature in the shock, but never by more that 2.5%. Three moments of (a-bf) behave very much like dn/dx, as functions of n, which possibly suggests a source of difficulty in the six moment method of estimating shock structure.

5. Five moments of f including the Boltzmann flux, approach their equilibrium values on the hot side of the shock more rapidly than do the Mott-Smith values of the same moments. The maximum deviations between the calculated and Mott-Smith values of these moments are consistently six to nine times larger than the likely errors of the calculated moments. The moment m_9 proportional to the lateral temperature $t_\perp$, shows the largest maximum deviation, namely 1.8% and is a quadratic function of n on the upstream side of the shock. The deviations of other moments are asymmetrical, the maximum deviations occurring near the hot side of the shock.