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NUMERICAL STUDIES OF THE NON-LINEAR BOLTZMANN EQUATION

PART I: SUMMARY OF PROGRAMS AND THEORY USED IN MONTE CARLO SOLUTIONS OF THE BOLTZMANN EQUATION

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I. DESCRIPTION OF THE PRINCIPAL COMPUTER PROGRAMS

1. The Boltzmann Program (in CODAP, Assembly Language)

1.1 The Monte Carlo Program

Uses tables of f (and of local equilibrium f when using M-B corrections: Sect II 8) for J stations (J = 1 to 17) to calculate and store values of a_d and $(bf)_d$ in separate tables. In calculations before 1967 a new sample of 2^{N_7} collisions was used for each station. Since then the same sample has been used for each station. The program also calculates moments of a and bf for use in least squares corrections.

1.2 The Moment Program

Uses tables of f, a_d, and a_d-$(bf)_d$ for calculation by numerical integration of 11 moments of each of these functions for each of J stations; prints or punches these moments and also $\sigma_j \delta a$, $\delta \nu_a \mid_j$, $\rho_j \delta_I f$, $\rho_j \delta_I \vec{f}$, $\rho_j \delta_I \overleftarrow{f}$ for each station; prints and punches the average of these last three quantities over all interior stations, namely, $\rho \delta_I f$, $\rho \delta_I \vec{f}$, $\rho \delta_I \overleftarrow{f}$.

1.3 The Integration Program

Uses tables of f, a_d, $(bf)_d$ for one iteration (for the shock and heat transfer problems) or for one time (for relaxation problems) to calculate by numerical integration with respect to n, x, τ (as time variable for pseudoshock) or τ (as space variable for heat transfer problems), the values of f for the next iterate or time.

1.4 Control Programs

Physical Problems. Each of these control programs provide, in a manner specified by parameter tape and by jump switches, for the execution of a series of calculations for a given physical problem. Control programs exist for the following problems:

1. Shock waves (Boltzmann)
2. Shock waves (Krook)
3. Pseudo-shock (Boltzmann)
4. Relaxation (Boltzmann)
5. Heat Transfer (Boltzmann)
6. Heat Transfer (Krook)

As an illustrative example we list the successive steps in the control program for the Boltzmann shock wave:

(1) Input of parameters from paper tape.

(2) Calculation of constants that depend on Mach number and the output of some of these.

(3) Calculation of the initial velocity distribution function f (usually Mott-Smith).

(4) Output of moments of the initial f.

(5) Calculation of a and bf by the Monte Carlo program.

(6) Least squares correction of a and bf and calculation of moments of the corrected a and bf.

(7) Calculation of a new f by the integration program.

(8) Calculation and output of moments of the new f, and output of moments of a and a-bf.

(9) Output of f numbers, f, a, a-bf and $\psi(a/bf)$ isoletters.

(10) Output of tables for each station of the mean, rms and sigma $[\psi(a/bf)]$.

(11) Return to (5) for next iteration.

Note: The amount of output can be regulated by jump switches, and there is a choice of output medium.

Data Analysis. The principal programs in this category are:

a. FAV: Calculates the likely error, mean value and their ratio for each velocity bin of the value of f or of a-bf for four Monte Carlo runs for each station. Also outputs the rms values of these tables for each station.

b. FCOMPAR: Outputs in numerical and isoline form for each velocity bin at each station the difference between and ratio of values of f calculated by two different procedures or from two different theories. Also outputs the mean, rms and standard deviation of the difference between the two f tables for each station.

c. BJ (f test): Compares the values of an initial f with the values of f after one iteration.

d. DFDXCONT: Compares $(df/dx)v_{xa}$ and (a-bf), both calculated from the input f numbers.

e. ABCONØ: Compares a and bf calculated by the Monte Carlo program with analytical a and bf on the cold and hot sides of the shock wave.

1.5 Input-Output

Parameters. Each set of parameters defines a calculation completely, when used with a given control program. Though the list varies somewhat from one problem to another, the important parameters are:

M_1 Mach number

J number of stations in the shock wave

$\delta\tau$ reduced time interval

N_7 2^{N_7} is the number of collisions in a Monte Carlo sample

u_{2m} downstream velocity in the shock wave in "machine units" ($u_{2m} = K_1 u_2$)

r_o initial random number

K_n Knudsen number

T_1/T_2 temperature ratio of two plates in heat transfer problem

The parameters are input initially on a parameter tape and are printed at intervals during output to identify the different parts of a series of calculations.

Tables. There are many fixed, auxiliary tables in the Monte Carlo and moment programs to make possible fast and accurate calculations. In the Monte Carlo program, for example, the principal tables are a) values of $\sin\varphi$ and $\cos\varphi$ defining cells in velocity space; b) values of α, β, γ corresponding to cells in the space of the line of centers vector $\bar{k}$; and c) an auxiliary table which makes possible fast and accurate calculations of $(A^2+B^2)^{\frac{1}{2}}$.

In the moment program there are several tables of weight functions used to make possible accurate numerical integrations over velocity space for both singular and non-singular integrands.

ISOLET. This program prints a character, corresponding to the value of a function, for each of 226 bins in velocity space. Each character represents a range of values of the function. From the printed characters it is easy to sketch isolines of the function. The present program uses separate tables to give ISOLET characters for f; for a or a-bf; and for $\psi(X_1/X_2)$, used to get isolines of the ratio of two functions. (See Table 1 and Table 2.)

PROGSAVE. This program saves everything in the core memory so that it is easy to interrupt and later to continue a Monte Carlo run.

2. FORTRAN Programs

AVERR

Provides a mean value and likely error of each of the 40 quantities in the moment output for each station and also of about 60 quantities derived from the moment output for each of four Monte Carlo runs (See III 1,2).

AVERR2

Calculates additional quantities as well as those in AVERR for heat transfer problem (see III 3).

AVERR3

Calculates all the functions for the heat transfer problem for imperfect accommodation, with equivalent temperature ratio as input parameter (see II 10,11; III 4).

MOMNTFN

Calculates, from the Mach number and the mean value and likely error of six moments, the values and maximum errors of 13 derived quantities.

MOMENTS

Calculates moments for the equilibrium gases at the cold and hot sides of the shock wave.

NSBOLTZ

Calculates Chapman-Enskog distribution functions [$f_{C.E.} = f_o(1+\phi)$] corresponding to the Navier-Stokes description of the shock wave for input into the Boltzmann program.

NSBOLTZO

Calculates $f_o\phi$ of the Chapman-Enskog distribution function for input into the Boltzmann program.

NSBOLTZF

Calculates f_o of the Chapman-Enskog distribution function for input into the Boltzmann program.

KROOK1

Calculates the distribution function and its moments for the Krook equation for a parallel-plates heat transfer problem. One application is the calculation of the Krook distribution function for input into the Boltzmann heat transfer program.

FT4MOM

Calculates the 4-moment distribution function for input into the Boltzmann heat transfer program.

II. THEORY AND EQUATIONS - Boltzmann Program

1. Units

The unit of x is $\lambda/\sqrt{2}$, the unit of velocity v is $\pi c/2$ and the unit of f is f_m where λ, c and f_m are, respectively, the values of the mean free path, the mean molecular speed and the maximum value of f in an appropriate reference gas. The units of all other quantities can be expressed in terms of the units of x, v and f.

2. Symbol List

$\mathcal{A}, \mathcal{A}'$	constants in MC program
$a = a(\bar{v},n)$ $b = b(\bar{v},n)$	parts of the collision integral, (a-bf)
$a_d, a'; b_d, b'$	scaled values of a and b
$B(w)$	$b(\bar{v})$ for the cold, equilibrium gas
c_1	velocity unit
c_s	velocity of sound
$f = f(\bar{v},n)$	velocity distribution function
f', F, F'	$f(\bar{v}',n), f(\bar{V},n), f(\bar{V}',n)$
$\mathcal{F}_h$	fraction of molecules ignored (on hot side of shock)
g	weight factor for $\bar{v}$ quadrature
$-\mathcal{M}_{10}$	flux of "entropy"
$H = \mathcal{M}_5$	Boltzmann function per unit volume ("negative entropy")
I	ordinal number of iteration
j	ordinal number of stations in the shock wave - $j = 0,1,\ldots(J-1)$
J	number of stations
k	ordinal number of moment
$\bar{k}$	unit vector along line of centers
$K_1 = v_m/v$	velocity scaling parameter
K_n	Knudsen number
M	Mach number
$\mathcal{M}_k(x)$	moments of the velocity distribution function

$\mathcal{M}'_{ka}, \mathcal{M}'_{k}$	moments of a/v_{xa} and $(a-bf)/v_{xa}$.
$n(x)$	number density
n'	dn/dx
$\underline{n}'$	Monte Carlo value of n'
N_7	2^{N_7} is the number of collisions in Monte Carlo sample
s	ordinal number of velocity bin - $s = 0,1,...225$
t	reduced temperature
T_1/T_2	temperature ratio of two plates in heat transfer problem
u	mass velocity (relative to shock)
u_{2m}	$K_1 u_2$
$\bar{v}$	molecular velocity relative to center of mass of gas on hot side
$\bar{v}, \bar{v}'$	velocities of molecules entering a collision
$\bar{V}, \bar{V}'$	velocities of molecules leaving a collision
$\bar{v}_r$	$\bar{v} - \bar{v}' = -\bar{V} + \bar{V}'$
$\bar{w}$	peculiar velocity relative to center of mass of gas at one station
x	Cartesian coordinate in direction of flow (from cold plate to hot plate for the heat transfer problem)
y, z	Cartesian coordinates perpendicular to x.
ν_a	twice the collision rate (for unit volume)
$\Psi(X_1/X_2)$	$(X_1 - X_2) / (X_1 + X_2)$

Subscripts

a	(on a velocity symbol) - measured with respect to the shock ("absolute" velocity)
m	refers to "machine" units of velocity; thus v_m (in machine units) = $K_1 v$
x, y, z	associated with the Cartesian components of velocity
$\perp$	associated with the velocity components perpendicular to x axis
c, h or 1, 2	cold and hot side of shock (equilibrium conditions) or cold and hot plates in heat transfer problems

Superscripts

$\longrightarrow$ ($\longleftarrow$)	indicates $v_{xa} > (<) \; 0$

3. Description of Gas in Equilibrium

a. Velocity Variables

$$\bar{w} = \bar{v}_a - \bar{i}_x u = \bar{i}_x [v_{xa} - u] + \bar{i}_\perp v_\perp \qquad \text{(any station)}$$

$$\bar{v} = \bar{v}_a - \bar{i}_x u_2$$

$$\bar{w}_1 = \bar{v}_a - \bar{i}_x u_1 = \bar{i}_x (v_{xa} - u_1) + \bar{i}_\perp v_\perp = \bar{v} + \bar{i}_x (u_2 - u_1) \qquad \text{(cold side)}$$

$$\bar{v} = \bar{w}_2 = \bar{v}_a - \bar{i}_x u_2 = \bar{i}_x (v_{xa} - u_2) + \bar{i}_\perp v_\perp = \bar{i}_x v_x + \bar{i}_\perp v_\perp \qquad \text{(hot side)}$$

$$v^2 = v_x^2 + v_\perp^2 \quad ; \quad v_a^2 = v_{xa}^2 + v_\perp^2$$

b. Velocity Distribution Functions

$$f_c = f_c(w_1) = e^{-\pi w_1^2}$$

$$f_h = f_h(w_2) = n_2 t_2^{-3/2} e^{-\pi w_2^2/t_2}$$

c. Functions Related to a and bf

$$B(w) = \left(\frac{w}{2} + \frac{1}{4\pi w}\right)\mathrm{erf}(\sqrt{\pi} w) + \frac{1}{2\pi} e^{-\pi w^2}$$

$$b_{cn}(\bar{v}) = B(w_1)$$

$$b_{hn}(\bar{v}) = (n_2/n_1) t^{1/2} B(w_2 t^{-1/2})$$

4. Functions of Upstream Mach Number M_1

(monatomic gas)

$$u_1 = M_1(5/6\pi)^{1/2} \qquad n_1 = 1$$

$$n_2 = 4M_1^2/(3 + M_1^2) \qquad u_2 = u_1/n_2 = u_1(3+M_1^2)/4M_1^2$$

$$p_2/p_1 = 1 + 5(M_1^2-1)/4$$

$$t_2 = 1+(M_1^2-1)(3+5M_1^2)/16M_1^2 = \frac{(5M_1^2-1)(M_1^2+3)}{16M_1^2}$$

$$K_1 = u_{2m}/u_2$$

$$M_2^2 = (3+M_1^2)/(5M_1^2-1)$$

$$\frac{c_1}{c_s} = \sqrt{6\pi/5}$$

$$\left.\begin{aligned} u_1 &= n_2 u_2 \\ u_1^2 + \frac{1}{2\pi} &= n_2\left(u_2^2 + \frac{1}{2\pi}\, t_2\right) \\ u_1^2 + \frac{5}{2\pi} &= u_2^2 + \frac{5}{2\pi}\, t_2 \end{aligned}\right\} \quad \text{Rankine - Hugoniot}$$

5. Moments of f, a and a-bf.

$$v_{xa}\, df/dx = a - bf$$

Moments of f

$$\left.\begin{aligned} \mathcal{M}_k &= \int f \Phi_k(\bar{v})\, d\bar{v} \\ \mathcal{M}'_{ka} &= \int a \Phi_k(\bar{v})\, d\bar{v}/v_{xa} \end{aligned}\right\} \quad k = 1, \ldots 11$$

Moments of (df/dx)

$$\mathcal{M}'_k = \int (a-bf)\Phi_k(\bar{v})\, d\bar{v}/v_{xa}$$

where

$$\Phi_1(\bar{v}) = 1$$

$$\Phi_2(\bar{v}) = v_{xa}$$

$$\Phi_3(\bar{v}) = v_{xa}^2$$

$$\Phi_4(\bar{v}) = v_{xa} v^2$$

$$\Phi_5(\bar{v}) = \ln f$$

$$\Phi_6(\bar{v}) = v_{xa}^3$$

$$\Phi_7(\bar{v}) = v_{xa}^2 v^2$$

$$\Phi_8(\bar{v}) = v_{xa} v^4$$

$$\Phi_9(\bar{v}) = v_\perp^2$$

$$\Phi_{10}(\bar{v}) = v_{xa} \ln f$$

$$\Phi_{11}(\bar{v}) = v_{xa}^4$$

The program calculates these moments using the quadrature formulae in Sect. II 7.

6. "Cut-Off" Errors and Choice of Values of K_1.

In the Boltzmann Program many of the parameters are derived from M_1 and from $u_{2m} = K_1 u_2$, where u_{2m} must be an even integer in order to permit an optimum method of numerical integration for those integrals containing v_{xa}^{-1} in the integrand. The parameter K_1 is calculated for each M_1 after choosing for u_{2m} an integer value that is small enough to give an acceptable "cut-off" error. This error is measured by $\mathcal{F}_h$, the fraction of the molecules on the hot side of the shock that have large speeds and are ignored in the numerical integration. Figure 1 can be used to choose an appropriate value of u_{2m} for each M_1. For heat transfer problems, K_1 is calculated for each value of T_1/T_2. (u_{2m} is not a parameter.)

7. Quadrature in the v_x-$v_\perp$ Plane.

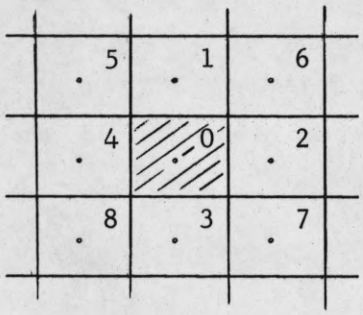
Integration in velocity space is needed to evaluate each of the 11 moments of f, and a and of a-bf. The quadrature formula is

$$\int_{\substack{\text{all}\\ \text{velocity}\\ \text{space}}} z\,d\bar{v} \;\tilde{=}\; 8\pi K_1^{-3} \sum_{s=0}^{225} (g z v_{\perp m})_s$$

The integrand z is assumed to vanish outside a semi-circular region in velocity space and to be proportional to $v_\perp$ as $v_\perp \to 0$.

The values of the weight function g are calculated by superposing local quadrature formulae for individual velocity cells. The local quadrature formulae must be derived for several different cases.

(a) Non-singular Integrands: Two local quadrature formulae are needed here. Consider first a cell whose center (point 0) is $(v_x^o, v_\perp^o)$ where $v_\perp^o > 1$. The neighboring centers 1,2...8 are numbered as shown in the figure:



The coordinates of point 5, for example, are $(v_x^o-2,\ v_\perp^o+2)$. We use five values of the integrand, namely, z_0, z_1, z_2, z_3, z_4 to calculate the integral over the cell containing point 0.

If we represent z by a polynomial of the second degree in v_x and $v_\perp$, then we find that

$$I = \int_{\substack{\text{cell}\\0}} z d\bar{v} = 4z_0 + \frac{1}{6}(z_1+z_2+z_3+z_4-4z_0)$$

where z_i is evaluated at the center of each cell.

Now consider a cell whose center (point 0) lies at $v_\perp = 1$. We use four values of the integrand, namely, z_0, z_1, z_2, z_4 to calculate the

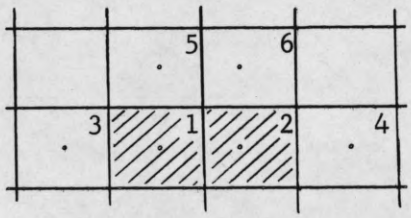
integral over the cell containing the point 0, and choose a polynomial of the second degree that goes to zero for $v_\perp = 0$.

We now find that

$$I = \int_{\substack{\text{cell}\\0}} z d\bar{v} = 3z_0 + \frac{1}{6}(z_0+z_1+z_2+z_4).$$

With a local quadrature formula thus defined for each cell, we obtain by addition the values of the weight function $g(v_x, v_\perp)$ for each of the 226 cells.

(b) Singular Integrands: Two more local quadrature formulae are necessary for integration past the pole at $v_x = -u_{2m}$ in six of the integrals over a and over a-bf. The method of derivation is similar to that of the other formulae except that the integral is calculated over two bins rather than one.



For the case when $v_\perp \neq 1$ we find that

$$I = \int z d\bar{v} = \frac{1}{6}(23z_1+23z_2+z_3+z_4)$$

over the two cells in x, y space containing points 1 and 2, and when

$v_\perp = 1$ we find that

$$I = \int z d\bar{v} = \frac{19}{6}(z_1+z_2)+\frac{1}{6}(z_3+z_4)+\frac{2}{9}(z_5+z_6) \ .$$

By addition we find the weight factors for integration of the singular integrands for $u_{2m} = 2$, 4, and 6, the three values of interest for our Boltzmann calculations.

8. Monte Carlo Calculation of the Collision Integral.

$$\partial f/\partial\tau + v_x \partial f/\partial x = a-bf = \int (FF'-ff')|\bar{k}\cdot\bar{v}_r| d\bar{v}'(d\bar{k}/4\pi) \quad (a)$$

$$v_\perp m a = \alpha\Sigma\varkappa_1 FF' \quad (b)$$

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[a] Monte Carlo Evaluation of the Boltzmann Collision Integral. Arnold Nordsieck and Bruce L. Hicks, Proceedings of the Fifth International Symposium on Rarefied Gas Dynamics, p. 695, Pergamon Press (1967).

[b] Maxwell-Boltzmann (MB) correction has been used since early 1968. These equations are changed to

$$v_\perp m a = \alpha\Sigma\varkappa_1 (FF'-1/2(F_{eq}F_{eq}'-f_{eq}f_{eq}'))$$

$$v_\perp m bf = \alpha\Sigma\varkappa_1 (ff'+1/2(F_{eq}F_{eq}'-f_{eq}f_{eq}'))$$

where n, u and t for the local equilibrium f, f_{eq}, are calculated from $\mathcal{M}_k$, the moments of f.
In effect, we subtract from the collision integral of f the collision integral of the corresponding Maxwell-Boltzmann f (approximately zero).

$$v_{\perp m}bf = \mathcal{A}\Sigma\varkappa_1 ff'$$

where

$$\varkappa_1 = |\bar{k}\cdot\bar{v}_r| v_{\perp m} v'_{\perp m}$$

$$\mathcal{A} = 226^2\pi 2^{-N_7} K_1^{-4}$$

and the summation is over all "hits" for a given velocity bin.

Scale $\mathcal{A}$ by the equation

$$K_1\mathcal{A} = \mathcal{A}'2^{N_8-N_7}$$

where N_8 is the smallest integer such that $\mathcal{A}' < 1$. Then

$$\mathcal{A}'2^{N_8} = 226^2\cdot\pi\cdot K_1^{-3} = 160{,}459.9864K_1^{-3}$$

Scale $\Sigma\varkappa_1 FF'$ by the equation[c]

$$\begin{aligned} a_d &= 2^{N_5-N_3-N_7}\Sigma\varkappa_1 FF' \\ &= 2^{N_5-N_3-N_7} v_{\perp m} a 2^{N_7-N_8} K_1/\mathcal{A}' \\ &= 2^{N_5-N_3-N_8} v_{\perp m} a K_1/\mathcal{A}' = K_2 a \end{aligned}$$

where N_3 scales $\varkappa_1$ by

$$2^{-N_3-N_7}\varkappa_1 < 1 \qquad \text{(satisfied by } N_3+N_7 \geq 15\text{)}$$

Usually $N_3 = 8$ and $N_5 = 5$.

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[c] Similarly for $\Sigma\varkappa_1 ff'$ and bf.

9. Integration of the Boltzmann Equation.

The equation for forward integration is

$$f_{j+1} = [f_j(\eta_{j+\frac{1}{2}}-b'_j)+a'_j+a'_{j+1}]/(\eta_{j+\frac{1}{2}}+b'_{j+1})$$

with a similar equation for backward integration. It is understood that f_{j+1}, f_j in this equation correspond to iteration (I+1) whereas a'_j, a'_{j+1}, b'_j, b'_{j+1} are calculated from values of f_j, f_{j+1} for iteration I. In the above difference equation

$$\eta_{j+\frac{1}{2}} = \tfrac{1}{2}(\underline{n}'_j+\underline{n}'_{j+1})$$

$$\underline{n}'_j = \int (a-bf)_j v_{xa}^{-1} d\bar{v} \qquad \text{(iteration I)}$$

Also

$$a'_j/a_j = b'_j/b_j = \delta\underline{n}/2 \mid v_{xa} \mid ,$$

$$\delta\underline{n} = (n_h-n_c)/(J-1)$$

The Boltzmann equation in terms of $\underline{n}$ as independent variable now reads

$$v_{xa}\underline{n}'\frac{df}{d\underline{n}} = a-bf.$$

For heat transfer problems τ is used as the independent variable,

and the Boltzmann equation reads

$$v_{xa} \frac{df}{d\tau} \cdot \frac{d\tau}{dx} = a - bf$$

where $$\frac{d\tau}{dx} = K_n \sqrt{(2t/\pi)} n.$$

The Boltzmann equation in terms of τ, the time variable, reads

$$\frac{df}{d\tau} = a - bf$$

This applies to the pseudo-shock problem.

10. Simulated Heat Transfer Runs for Incomplete Accommodations:

If the accommodation coefficient α is defined by

$$\alpha = \frac{T_i - T_r}{T_i - T_w}$$

where T_i = temperature of molecules incident to a wall, T_r = temperature of molecules reflected from the wall, and T_w = wall temperature, then it is possible to make a simulated computer run with $\alpha_s = 1$ and simulated temperature ratio $(T_2/T_1)_s$. The following expressions are needed to compute $(T_2/T_1)_s$ from given values of α and T_2/T_1.

Cold Side:

$$\frac{T_i(0)}{T_r(0)} = \frac{2m_1(0)T(0) - 1}{2m_1(0) - 1}$$

$$[T_1/T_r(0)] = T_i(0) - \left[T_i(0) - 1\right]/\alpha$$

Hot Side:

$$T_r(d)/T_r(0) = (T_2/T_1)_s$$

$$\frac{T_i(0)}{T_r(d)} = \frac{2m_1(d)[T(d)/T_r(d)] - 2\bar{m}_1(d)}{2m_1(d) - 2\bar{m}_1(d)}$$

$$\frac{T_2}{T_r(d)} = \frac{T_i(d)}{T_r(d)} - \left[\frac{T_i(d)}{T_r(d)} - 1\right]/\alpha$$

$$(T_2/T_1)_s = (T_2/T_1)\left[\frac{T_1/T_r(0)}{T_2/T_r(d)}\right]$$

11. Heat Transfer Solutions - Limiting Cases

(1) Free-Molecule:

$$T/T_1 = \sqrt{(T_2/T_1)}$$

$$n/n_1 = (1/2)\left[\sqrt{(T_1/T_2)} + 1\right]$$

$$p/\rho_1 RT_1 = (1/2)\left[1 + \sqrt{(T_2/T_1)}\right]$$

$$\frac{q}{\rho_1(2RT_1)^{3/2}/2} = \frac{1}{\sqrt{\pi}}\left[1 - (T_2/T_1)\right]$$

(2) Continuum:

$$T/T_1 = \left\{1 + \left[(T_2/T_1)^{3/2} - 1\right](x/d)\right\}^{2/3}$$

$$(n/n_1) = (T_1/T)$$

$$p/\rho RT_1 = 1$$

$$\frac{q}{\rho_1 (2RT_1)^{3/2}/2} = \frac{5(.499)}{\pi^{1/2}} \left[1-(T_2/T_1)^{3/2}\right] Kn$$

$$\tau = (T_2/T_1)^{1/2} (T_1/T)^{-1/2} (x/d)$$

III. THEORY AND EQUATIONS - AVERR Program

1. Symbol List

$\hat{B}$	BHAT[a]	
$\hat{\hat{B}}$	BHATS	
$d\hat{m}_5/d\hat{n}$	HDH/DN	
$d\hat{m}_k/d\hat{n}$	HDMK/DN	
$dn/dn\|_j$	DNDNBAR	$(n_{j+1}-n_{j-1})/2\delta n$
dt/dn	DT/DN	
$dt_\perp/dn$	DTP/DN	
dt_x/dn	DTX/DN	
$d\hat{t}/d\hat{n}$	HDT/DN	
$d\hat{t}_\perp/d\hat{n}$	HDTP/DN	
$d\hat{t}_x/d\hat{n}$	HDTX/DN	
h	HMOL	m_5/m_1
J	J	number of stations
j	JL	ordinal number of stations ($j = 0,1,\cdots(J-1)$)
k	K	(local) coefficient of heat conduction/ its upstream value
k_{rel}	KREL	$Kt^{-\frac{1}{2}}$
M	M	(local) Mach number

[a] AVERR Output Name

$\mathcal{M}_k$	MK	moment of f (Sect. II.5)
$\mathcal{M}'_k$	M*K	moment of (a-bf)/v_{xa}(Sect. II.5)
$\mathcal{M}'_{ka}$	M*KA	moment of a/v_{xa}(Sect. II.5)
$\hat{\mathcal{M}}_{10}$	HM10	
$\underline{n}$	NBAR	$1+j\delta\underline{n} = 1+j(\mathcal{M}_1^{(h)}-\mathcal{M}_1^{(c)})/(J-1)$
$\underline{n}'$	M*1	$\int(a-bf)_{MC}d\bar{v}/v_{xa}$
n'	M**1	dn/dx
$\hat{\underline{n}}$	NHAT	j/(J-1)
$\hat{\underline{n}}'$	NHAT*	$\underline{n}'/(\mathcal{M}_1^{(h)}-\mathcal{M}_1^{(c)})$
$\underline{N}$	NHMS	$\hat{n}(1-\hat{\underline{n}})$
$\mathcal{M}'_{2a}$rel	NUREL	
p		pressure
p_1		upstream pressure
p/p_1	P/P_1	
$\tilde{p}_r$	PR	$\frac{4}{3}$ of Prandtl number
$q^{(a)}$	Q	heat flux/unit mass transport rate
$2q_\perp$	2QP	
q_x	QX	
$q/(\tau/p_1)$	QP1/TAU	
$2q_\perp/(\tau/p_1)$	2QPP1/TAU	
$q_x/(\tau/p_1)$	QXP1/TAU	
S_{eq}	SEQ	negative entropy
t	T	temperature

(a) units of q are $\pi kT_1/m$

t_x	TX	
$t_\perp$	TP	
$\hat{t}$	THAT	
$\hat{t}_x$	TXHAT	
$\hat{t}_\perp$	TPHAT	
t_g	TGAS	$2\pi u^2$, (local) energy of the mean motion
$t_\ddagger$ [b]	TENTH	$\frac{3}{5}t_x+\frac{2}{5}t_\perp$, (local) enthalpy/$\gamma$
$5t_u$ [c]	TTOT	$5t+t_g$, (local) non-conductive energy transport
t'	T*	dt/dx
t'_x	TX*	
$t'_\perp$	TP*	
u	UGAS	$\mathcal{M}_2/\mathcal{M}_1$, (local) mean speed
u_m	UMOL	$t^{\frac{1}{2}}$
w	W	$2M(3+M^2)^{-\frac{1}{2}}$, (local) Crocco number

Differences

δH_1	DELH1	$\mathcal{M}_5-S_{eq}$
δH_2	DELH2	$(\mathcal{M}_{10}/u)-S_{eq}$
δH_3	DELH3	$(\mathcal{M}_{10}/u)-\mathcal{M}_5$
δt_x	DELTX	t_x-t
$\delta t_\perp$	DELTP	$t_\perp-t$

---

[b] reduced to 1 at the upstream boundary

[c] same units as q

Measures of Errors and Corrections

$\rho_j \delta_I f$	RHJDIFA	rms value of $\delta_I f$ at j^{th} station ($\delta_I f = f_I - f_{I-1}$ = increment in I^{th} iteration)
$\rho_j \overrightarrow{\delta_I f}$	RHJDIFF	
$\rho_j \overleftarrow{\delta_I f}$	RHJDIFB	
$\rho \delta_I f$	RHDIFA	rms value of $\delta_I f$ for all (internal) stations
$\rho \overrightarrow{\delta_I f}$	RHDIFF	
$\rho \overleftarrow{\delta_I f}$	RHDIFB	
$\sigma_j \delta a$	SIGCORAB	rms correction of a at j^{th} station (least squares adjustment)
$\delta \nu_{a\|j}$	CORRNUA	change in (scaled) value of $\nu_a = \int a d\bar{v}$ (to prevent negative values of a or bf)

Variables Related to Viscous Stress

σ	SIGM	(local) coefficient of viscosity/ its upstream value
σ_{rel}	SIGMREL	$\sigma t^{-\frac{1}{2}}$
τ		viscous stress
τ/p_1	TAU/P1	
τ/p	TAU/P	
$\hat{\tau}$	TAUHAT	

Subscripts

x	associated with x component of velocity
$\perp$	associated with $\perp$ component of velocity

Superscripts

$\longrightarrow$	refers to molecules for which $v_{xa} > 0$
$\longleftarrow$	refers to molecules for which $v_{xa} < 0$

2. Equations for AVERR Output.

	AVERR Output Name	Equations
Heading	J	J
	JL	j
	NHAT	$\hat{n} = j/(J-1)$
	NHMS	$\underline{N} = (1-\hat{n})\hat{n}$
	NBAR	$\underline{n} = j\Delta\underline{n} = j(\mathcal{M}_1^{(h)} - \mathcal{M}_1^{(c)})/(J-1)$
1	MK	$\mathcal{M}_k = \int \Phi_k f d\bar{v}$ $k = 1,2,\ldots 11$
2	M*K	$\mathcal{M}'_k = \int \Phi_k (a-bf) d\bar{v}/v_{xa}$ $k=1,2,\ldots 11$
3	M*KA	$\mathcal{M}'_{ka} = \int \Phi_k a d\bar{v}/v_{xa}$ $k=1,2,\ldots 11$
4	RHJDIFA	$\rho_j \delta_I f = \text{rms}_{\bar{v}}[\delta_I f]$ where $\delta_I f = f_I - f_{I-1}$
	RHJDIFF	$\rho_j \overrightarrow{\delta_I f} = \text{rms}_{\bar{v}}[\overrightarrow{\delta_I f}]_j$
	RHJDIFB	$\rho_j \overleftarrow{\delta_I f} = \text{rms}_{\bar{v}}[\overleftarrow{\delta_I f}]_j$

	RHDIFA	$\rho\delta_I f = \text{rms}_j\{\rho_j \delta_I f\}$ $j = 1,2\ldots J-2$
	RHDIFF	$\rho\delta_I \overrightarrow{f} = \text{rms}_j\{\rho_j \delta_I \overrightarrow{f}\}$
	RHDIFB	$\rho\delta_I \overleftarrow{f} = \text{rms}_j\{\rho_j \delta_I \overleftarrow{f}\}$
	SIGCORAB	$\sigma_j \delta a = (\text{rms corr. of a})\big\|_j$
	CORRNUA	$\delta\nu_a\big\|_j = (\text{change of } \nu_a \text{ in forcing all a and bf to be} \geq 0)\big\|_j$
5	UGAS	$u = \mathcal{M}_2/\mathcal{M}_1$
	UMOL	$u_m = t^{\frac{1}{2}}$
	M	$M = (6\pi/5)^{\frac{1}{2}} u t^{-\frac{1}{2}}$
	W	$W = 2M(3+M^2)^{-\frac{1}{2}}$
	NUREL	$\mathcal{M}'_{2a}\ \text{rel} = \mathcal{M}'_{2a}\ \pi/\sqrt{2t}\ \mathcal{M}_1^2$
	HMOL	$h = \mathcal{M}_5/\mathcal{M}_1$
	SEQ	$S_{eq} = \mathcal{M}_1\{\log_e(\mathcal{M}_1 t^{-3/2}) - 3/2\}$
	DELH1	$\delta H_1 = \mathcal{M}_5 - S_{eq}$
	DELH2	$\delta H_2 = (\mathcal{M}_{10}/u) - S_{eq}$
	DELH3	$\delta H_3 = (\mathcal{M}_{10}/u) - \mathcal{M}_5$
	M**1	$n' = \underline{n}'(dn/d\underline{n})$
6	DNDNBAR	$dn/d\underline{n}\big\|_j = [\mathcal{M}_1^{(j+1)} - \mathcal{M}_1^{(j-1)}]/$ $(\mathcal{M}_1^{(h)} - \mathcal{M}_1^{(c)})(\hat{n}^{j+1} - \hat{n}^{j-1})$

	NHAT*	$\hat{\underline{n}}' = \underline{n}'/(\mathcal{M}_1^{(h)} - \mathcal{M}_1^{(c)})$
	BHAT	$\hat{B} = \hat{\underline{n}}'/N$
	BHATS	$\hat{\hat{B}} = \hat{B}/\sqrt{(\mathcal{M}_1^{(h)} - \mathcal{M}_1^{(c)})}$
	HDH/DN	$d\hat{\mathcal{M}}_5/d\hat{\underline{n}}$
	HDMK/DN	$d\hat{\mathcal{M}}_k/d\hat{\underline{n}} = \mathcal{M}'_k/\hat{\underline{n}}'(\mathcal{M}_k^{(h)} - \mathcal{M}_k^{(c)})$ k=6...11
7	T	$t = \frac{1}{3} t_x + \frac{2}{3} t_\perp$
	TX	$t_x = 2\pi\{\frac{\mathcal{M}_3}{\mathcal{M}_1} - u^2\} = 2\pi \bar{v}_{xr}^2$
	TP	$t_\perp = \pi\mathcal{M}_9/\mathcal{M}_1 = \pi\bar{v}_\perp^2$
	TGAS	$t_g = 2\pi u^2$
	TENTH	$t_\ddagger = \frac{3}{5}t_x + \frac{2}{5}t_\perp$
	TTOT	$5t_u = 5t + t_g$
	DELTX	$\delta t_x = t_x - t$
	DELTP	$\delta t_\perp = t_\perp - t$
	THAT	$\hat{t} = (t - t^{(c)})/(t^{(h)} - t^{(c)})$
	TXHAT	$\hat{t}_x = (t_x - t^{(c)})/(t^{(h)} - t^{(c)})$
	TPHAT	$\hat{t}_\perp = (t_\perp - t^{(c)})/(t^{(h)} - t^{(c)})$

8	T*	$t' = \frac{1}{3}t'_x + \frac{2}{3}t'_\perp$
	TX*	$t'_x = 2\pi\{-\frac{m_3}{m_1} + 2u^2\}m'_1/m_1$
	TP*	$t'_\perp = \pi\{-\frac{m_9}{m_1}m'_1 + m'_9\}/m_1$
	DT/DN	$dt/d\underline{n} = t'/\underline{n}'$
	DTX/DN	$dt_x/d\underline{n} = t'_x/\underline{n}' = 2\pi\{\frac{-m_3}{m_1}+2u^2\}/m_1$
	DTP/DN	$dt_\perp/d\underline{n} = t'_\perp/\underline{n}'$
	HM10	$\hat{m}_{10} = (m_{10}-m_{10}^{(c)})/(m_{10}^{(h)}-m_{10}^{(c)})$
	HDT/DN	$d\hat{t}/d\underline{\hat{n}} = t'/\underline{\hat{n}}\ (t^{(h)}-t^{(c)})$
	HDTX/DN	$d\hat{t}_x/d\underline{\hat{n}} = t'_x/\underline{\hat{n}}'(t^{(h)}-t^{(c)})$
	HDTP/DN	$d\hat{t}_\perp/d\underline{\hat{n}} = t'_\perp/\underline{\hat{n}}'(t^{(h)}-t^{(c)})$
9	Q	$q = q_x+2q_\perp$
	QX	$q_x = 2\pi\frac{m_6}{m_2} - 3t_x - t_q = 2\pi\bar{v}_{xh}^3/u$
	2QP	$2q_\perp = 2\pi\frac{m_4-m_6}{m_2} - 2t_\perp = 2\pi\bar{v}_{xh}\bar{v}^2/u$
	QP1/TAU	$= q/(\tau/p_1)$
	QXP1/TAU	$= q_x/(\tau/p_1)$
	2QPP1/TAU	$= 2q_\perp/(\tau/p_1)$

10 P/P1 $p/p_1 = \mathcal{M}_1 t$

TAU/P1 $\tau/p_1 = \frac{2}{3}\mathcal{M}_1(t_\perp - t_x)$

TAU/P $\tau/p = (\tau/p_1)/(p/p_1)$

TAUHAT $\hat{\tau} = ((\frac{p}{p_1}+\frac{\tau}{p_1})-1)/(\frac{p_2}{p_1}-1)$ where

$$\frac{p_2}{p_1} = \mathcal{M}_1^{(h)} \cdot \frac{t^{(h)}}{t^{(c)}}$$

SIGM $\sigma = \mu/\mu_1 = -\frac{3}{16\times 0.499}(\frac{3\pi}{5})^{\frac{1}{2}}\mathcal{M}_1^2\tau/(\mathcal{M}_1 p_1 \underline{n}')$

SIGMREL $\sigma_{rel} = \sigma t^{-\frac{1}{2}}$

K $k = 8\sigma/(9\tilde{p}_r)$

KREL $k_{rel} = kt^{-\frac{1}{2}}$

PR $\tilde{p}_r = 3M_1^{-2}\mathcal{M}_1^2(dt/d\underline{n})(\tau/p_1 q)$

3. Additional Equations for AVERR2 (used for heat transfer problems)

DTAUDX/KN $\frac{1}{Kn}\frac{dt}{dx} = \sqrt{(2t/\pi)}\mathcal{M}_1$

DT/DX/KN $\frac{dt}{dx}\frac{1}{Kn} = (t^{(j+1)} - t^{(j-1)})(\frac{d\tau}{dx}\frac{1}{Kn})$

DLOGDX/KN $\frac{1}{Kn}\frac{d(\log t)}{dx} = \frac{1}{K_n t}\frac{dt}{dx}$

DM1DX/KN $\frac{1}{Kn}\frac{d\mathcal{M}_1}{dx} = 4(\mathcal{M}_1^{(j+1)} - \mathcal{M}_1^{(j-1)})(\frac{1}{Kn}\frac{d\tau}{dx})$

DM9DX/KN $$\frac{1}{Kn}\frac{d\mathcal{M}_9}{dx} = 4(\mathcal{M}_9^{(j+1)} - \mathcal{M}_9^{(j-1)})(\frac{1}{Kn}\frac{d\tau}{dx})$$

NUAREL $$(\mathcal{M}'_{2a})_{rel} = \mathcal{M}'_{2a}/(\frac{1}{Kn}\frac{d\tau}{dx})$$

4. AVERR3

Moment of order n = (simulated moment of order n) $\left[\frac{T_r(0)}{T_1}\right]^{n/2}$

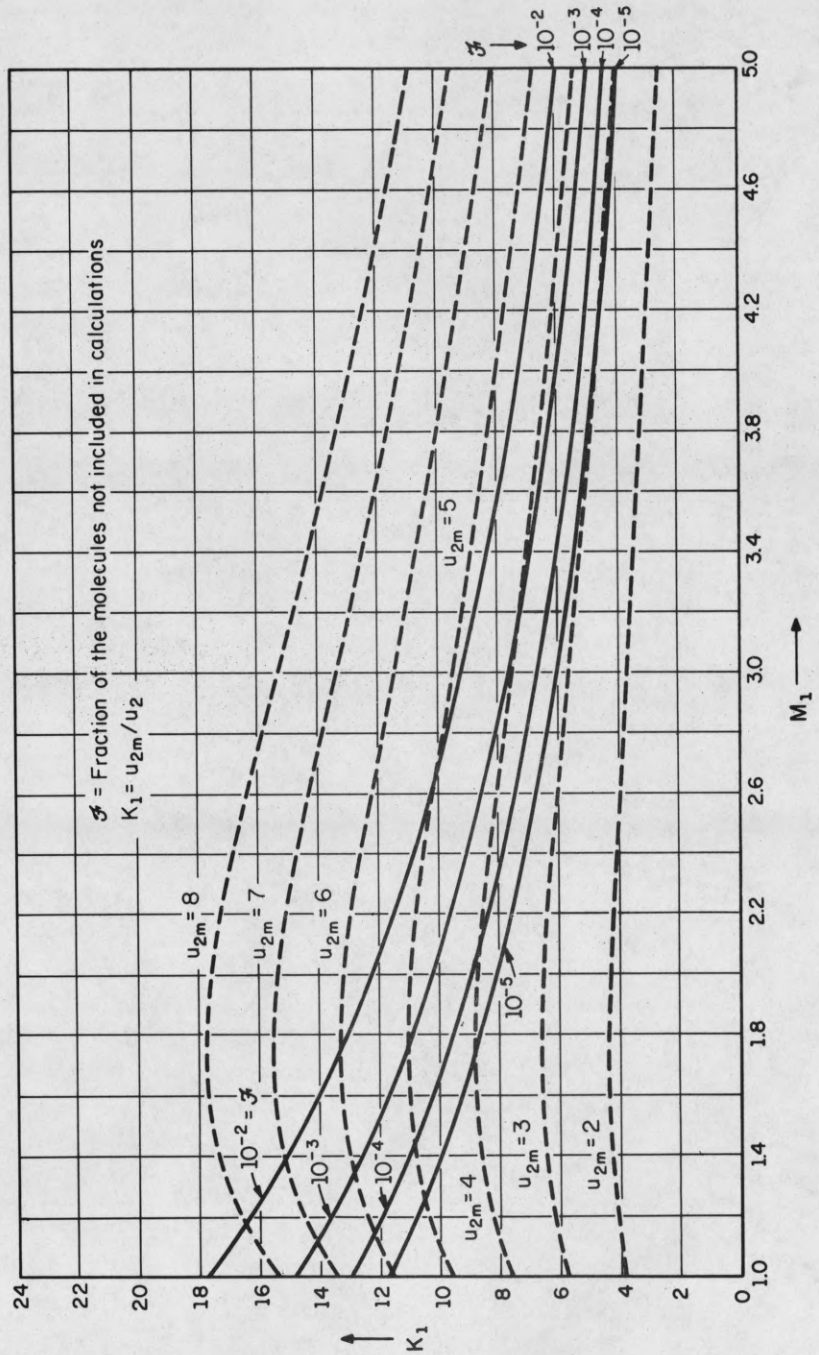

Figure 1. "Cut-off" Errors and Velocity Scaling

TABLE 1(a)

Table of Isolet Symbols and Values

Relative address (decimal)	Symbol	Values of Lower Limits for Each Symbol				
		f (1)	$(2^{N_5-N_3-N_8} v_{\perp m} K_1/A')2^{-28} a$ (2)	Ψ (3)	X_1/X_2 (4)	$\frac{X_1-X_2}{X_1}$
0	1	$1-2^{-47}$	4×10^5	$1-2^{-47}$	2^{48} or $\frac{X_1}{2}\neq0$, $\frac{X_2}{2}=0$	
1	2	0.999999	3	0.9	19	.9474
2	A	0.9	2	0.8	9	.8889
3	B	0.8	1.5	0.7	5.67	.8236
4	C	0.7	1×10^5	0.6	4.00	.7500
5	D	0.6	6×10^4	0.5	3.00	.6667
6	E	0.5	4	0.4	2.33	.5708
7	F	0.45	3	0.35	2.08	.5192
8	G	0.4	2	0.3	1.86	.4624
9	H	0.35	1.5	0.25	1.67	.4012
10	I	0.3	1×10^4	0.2	1.50	.3333
11	J	0.25	6×10^3	0.15	1.35	.2593
12	K	0.2	4	0.1	1.22	.1803
13	L	0.15	3	0.05	1.11	.0991
14	M	0.1	2	0.025	1.05	.04762
15	N	5×10^{-2}	1.5	0.01	1.02	.01961
16	O	2	1×10^3	0.005	1.01	.00990
17	P	1×10^{-2}	6×10^2	0.0025	1.005	.00498
18	Q	5×10^{-3}	4	0.001	1.002	.00200

TABLE 1(a) continued

Relative address (decimal)	Symbol	f [1]	$(2^{N_5-N_3-N_8} v_{\perp m} K_1/A')2^{-28}{}_a$ [2]	Ψ [3]	X_1/X_2 [4]	$\frac{X_1-X_2}{X_1}$
19	R	2×10^{-3}	3×10^{2}	0.0005	1.001	.00100
20	S	1×10^{-3}	2	0.00025	1.0005	.00050
21	T	5×10^{-4}	1.5	0.0001	1.0002	.00020
22	U	2	1×10^{2}	0.00005	1.0001	.00010
23	V	1×10^{-4}	60	0	1.0000	0
24	W	5×10^{-5}	40			
25	X	2	30			
26	3	1	20			
27	4	5×10^{-6}	15			
28	5	2	10			
29	6	1	6			
30	7	5×10^{-7}	4			
31	8	2×10^{-7}	3			
32	9	2×2^{-47}	2			
33	Y	1×2^{-47}	1			
34	Z	-1×2^{-47}	0			

(1) The symbols Y and Z indicate that f is exactly equal to 1 and -1 respectively.

(2) The same values are used for bf and (a-bf) (both scaled). The symbols 8, 9, 4, Z, 1 indicate that a (scaled) is exactly equal to 3, 2, 1, 0 and $1-2^{-47}$ respectively.

(3) $\Psi = \frac{X_1-X_2}{X_1+X_2}$

(4) $\frac{X_1}{X_2} = \frac{1+\Psi}{1-\Psi}$

TABLE 1(b)

Table of Isolet Symbols and Values

		Values of Lower Limits for Each Symbol[5]	
Symbol	Ψ[6]	X_1/X_2	$\frac{X_1-X_2}{X_1}$
-1	$-1+2^{-47}$	2^{-48} or $\frac{X_1}{2}=0, \frac{X_2}{2}\neq 0$	
-2	-0.9	.0526	-18.001
-A	-0.8	.1111	- 8.001
-B	-0.7	.1765	- 4.666
-C	-0.6	.2500	- 3.000
-D	-0.5	.3333	- 2.000
-E	-0.4	.4286	- 1.3333
-F	-0.35	.4815	- 1.0768
-G	-0.3	.5385	- 0.8570
-H	-0.25	.6000	- 0.6667
-I	-0.2	.6667	- 0.5000
-J	-0.15	.7391	- 0.3530
-K	-0.1	.8182	- 0.2222
-L	-0.05	.9048	- 0.1052
-M	-0.025	.9512	- 0.0513
-N	-0.01	.9802	- 0.0202

TABLE 1(b) continued

Symbol	Ψ [6]	X_1/X_2	$\frac{X_1-X_2}{X_1}$
-O	-0.005	.9900	- 0.01010
-P	-0.0025	.9950	- 0.00503
-Q	-0.001	.9980	- 0.00200
-R	-0.0005	.9990	- 0.00100
-S	-0.00025	.9995	- 0.00050
-T	-0.0001	.9998	- 0.00020
-U	-0.00005	.9999	- 0.00010
-V	-0	$\frac{X_1}{2} = \frac{X_2}{2} = 0$	- 0

[5] Values of lower limits for f and a are minus the values in Table 1(a).

[6] $\Psi \rightarrow -\Psi$ corresponds to interchange of X_1 and X_2.

TABLE 2(a)

Table of Isolet Symbols and Values

Symbol	Average Values for Each Symbol				
	f	$(2^{N_5-N_3-N_8} v_{\perp m} K_1/A')2^{-28} a$	Ψ	X_1/X_2	$\frac{X_1-X_2}{X_1}$
A	0.95	2.5×10^5	0.85	14	0.918
B	0.85	1.7	0.75	7.33	0.856
C	0.75	1.2×10^5	0.65	4.83	0.787
D	0.65	8×10^4	0.55	3.50	0.708
E	0.55	5	0.45	2.66	0.619
F	0.475	3.5	0.375	2.20	0.545
G	0.425	2.5	0.325	1.97	0.491
H	0.375	1.7	0.275	1.76	0.432
I	0.325	1.2×10^4	0.225	1.58	0.367
J	0.275	8×10^3	0.175	1.42	0.296
K	0.225	5	0.125	1.28	0.220
L	0.175	3.5	0.075	1.16	0.140
M	0.125	2.5	0.0375	1.075	0.0734
N	0.075	1.7	0.0175	1.035	0.0336
O	0.035	1.2×10^3	0.0075	1.015	0.0148
P	0.015	800	0.00375	1.0075	0.0074
Q	0.0075	500	0.00175	1.0035	0.0035
R	0.0035	350	0.00075	1.0015	0.0015
S	0.0015	250	0.000375	1.0007	0.00075

TABLE 2(a) continued

Symbol	f	$(2^{N_5-N_3-N_8}{}_{v}{}_{m}K_1/A')2^{-28}{}_{a}$	Ψ	X_1/X_2	$\frac{X_1-X_2}{X_1}$
T	7.5×10^{-4}	170	0.000175	1.00035	0.00035
U	3.5	120	0.000075	1.00015	0.00015
V	1.5	80	0.000025	1.0000	0
W	7.5×10^{-5}	50	0		
X	3.5	35			
3	1.5	25			
4	7.5×10^{-6}	17			
5	3.5	12			
6	1.5	8			
7	7.5×10^{-7}	5			
8	3.5×10^{-7}	3			
9	1×10^{-7}	2			
Y		1			
Z		0			

TABLE 2(b)

Table of Isolet Symbols and Values

Symbol	Average[7] Values for Each Symbol[8] X_1/X_2	$\frac{X_1-X_2}{X_1}$
-2	0.082	-13.001
-A	0.144	- 6.33
-B	0.213	- 3.83
-C	0.292	- 2.50
-D	0.381	- 1.67
-E	0.455	- 1.20
-F	0.510	- 0.97
-G	0.569	- 0.76
-H	0.633	- 0.58
-I	0.703	- 0.43
-J	0.779	- 0.29
-K	0.861	- 0.16
-L	0.9280	- 0.078
-M	0.9657	- 0.036
-N	0.9851	- 0.015
-O	0.9925	- 0.0076
-P	0.9965	- 0.0035
-Q	0.9985	- 0.0015
-R	0.9992	- 0.00075
-S	0.9996	- 0.00035
-T	0.9998	- 0.00015

TABLE 2(b) continued

Symbol	X_1/X_2	$\frac{X_1-X_2}{X_1}$
-U	0.9999	- 0.00005
-V	$1 - \epsilon$	- 0

(7) Algebraic lower limits are used to find averages.

(8) Average values for f, a and Ψ are minus the values in Table 2(a).

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