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THE BOLTZMANN COLLISION INTEGRALS FOR A BINARY GAS MIXTURE WITH A COMBINATION OF MAXWELLIAN DISTRIBUTION FUNCTIONS

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by

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1. Introduction

If the distribution function, F, is a linear combination of two Maxwellians with distinct temperatures, densities, average velocities, and masses, both the gain and loss terms of the collision integral in the Boltzmann equation can be evaluated analytically. A gas with such a bimodal distribution function is referred to here as a Mott-Smith gas. (Mott-Smith (1951) was the first to use this form of the distribution function to analyze the shock wave structure.)

Desphande (1969a) obtained the following closed form expression of the collision integral for a rigid sphere Mott-Smith gas:

$$J(F_{i},F_{j}) = \frac{\pi \sigma^{2}}{B_{i}B_{j}} F_{i}F_{j} \left[\frac{1}{2R} \left({}_{1}F_{1}(1;\frac{1}{2};Q+R) - {}_{1}F_{1}(1;\frac{1}{2};Q-R) \right) - \frac{2B_{i}}{B_{j}} {}_{1}F_{1} \left(2;\frac{3}{2};C_{j}^{2} \right) \right]$$
(1)

where J = the collision integral for the two Maxwellian distribution functions F_i and F_i respectively,

$$\begin{split} \mathbf{Q} &\equiv \frac{1}{2} (\mathbf{C}_{i}^{2} + \mathbf{C}_{j}^{2}) , \\ \mathbf{R}^{2} &= \frac{1}{4} (\mathbf{C}_{i}^{2} - \mathbf{C}_{j}^{2}) + \left| \vec{\mathbf{C}}_{i} \times \vec{\mathbf{C}}_{j} \right| , \\ \mathbf{F}_{i} &= \mathbf{n}_{i} \left(\frac{\mathbf{B}_{i}}{\pi} \right)^{3/2} \exp \left(-\mathbf{B}_{i} \left(\vec{\nabla} - \vec{\mathbf{U}}_{i} \right)^{2} \right) , \end{split}$$

$$\vec{C}_{j} = B_{j}^{1/2} (\vec{V} - \vec{U}_{j}),$$

$$\vec{C}_{i} = B_{i}^{1/2} (\vec{V} - \vec{U}_{i}),$$

$$d B_{i} = \frac{m_{i}}{2kT_{i}}.$$

an

In the above expressions T is the temperature; k the Boltzmann constant; \vec{U} is the average velocity; n is the number density; B is the inverse square of the most probably thermal speed; σ is the average of the rigid sphere collision diameters; $_{1}F_{1}$ denotes a confluent hypergeometric function; and the subscripts i and j refer to the two different Maxwellian gases. In equation (1), the first two terms give the gain term G_{ij} , and the last term is the loss term $F_{i}L_{i}$.

In this report, the results of Deshpande (1968, 1969a,b) and Narasimha (1968) are generalized to binary gas mixtures. Also, certain limitations on their analysis are examined. Section 1.2 presents a method by which this analysis may also be extended to electron (or ion)-neutral mixtures. The neutrals are considered to be Maxwellian and the electrons (or ions) are assumed to possess "Maxwellian type" distribution functions.

2. Evaluation of the Collision Integral for a Binary Gas Mixture

The generalization of Deshpande (1969a) to include a mixture of gases involves a reformulation of almost every step in the analysis. The necessary mathematical steps for mixtures are presented in Table 1- below. The integration formulas and identities necessary for the evaluation of the collision integral were obtained from Erdelyi (1954a,b; 1955a,b,c); Slater (1960); Rainville (1960); Whittaker (1963); and Abramowitz (1965).

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The Boltzmann collision integral for any two distribution functions, F_i and F_j may be written in terms of the gain and loss terms as

$$J(F_{i},F_{j}) = G(F_{i},F_{j}) - F_{i}L(F_{j})$$
(2)

where
$$G(F_i, F_j) \equiv G_{ij} \equiv gain term = \int F_i(\vec{V}) F_j(\vec{W}') gbdbdcD\vec{W}$$
, (3)

and $L(F_j) \equiv L_j \equiv loss term = \int F_j(\vec{w}) gbdbdcD\vec{w}$. (4)

In these equations,

and

 \vec{v} = velocity at which the integrals are being evaluated, \vec{w} = velocity of the collision partner (j is the target molecule), \vec{g} = $\vec{v} \cdot \vec{w}$ = relative velocity, b = impact parameter, ε = azimuth angle, \vec{W} = volume element in \vec{W} space.

The prime values (') denote conditions after a collision and F denotes a Maxwellian distribution function.

The subscripts i and j refer to different components of a gas mixture. (They could just as well refer to different terms in an expansion of any distribution function into a series of Maxwellians for a single gas.)

The loss term for a Maxwellian F_i, from equation (4) becomes

$$L_{j} = \int n_{j} \left(\frac{B_{j}}{\pi}\right)^{3/2} \exp\left(-B_{j} (\vec{W} - \vec{U}_{j})^{2}\right) gbdbdc D\vec{W}.$$
(5)

Now, since \vec{v} is held constant with respect to the integration over \vec{w} , \vec{w} is replaced by $\vec{v} \cdot \vec{g}$, and integrating over de from 0 to 2π , equation (2-5) becomes

$$L_{j} = n_{j} \left(\frac{B_{j}}{\pi}\right)^{3/2} \frac{2\pi}{B_{i}^{2}} \int \exp\left(-B_{ji}(g^{2}-2\vec{g}\cdot\vec{c}_{j}+c_{j}^{2})\right) gbdb \ D\vec{g}$$
(6)

where

$$\vec{c}_{j} = \vec{V} \cdot \vec{U}_{j}$$
 and $B_{ji} = \frac{B_{j}}{B_{i}}$,

and all velocity terms have been nondimensionalized with respect to $B_i^{1/2}$, consistent with Deshpande (1969a). (In Appendix B another form of non-dimensionalization is considered.)

The next step is to transform \vec{g} to a spherical polar coordinate system (g,θ,ϕ) with \vec{c}_i as the axis and write (Chapman (1964))

$$\vec{Dg} = g^2 dg \sin\theta d\theta d\phi.$$
 (7)

Thus, after integrating over $d\phi$ from 0 to 2π and evaluating the integral over $d\theta$ in terms of the hyperbolic sine function, equation ((6)) becomes

$$L_{j} = n_{j} \left(\frac{B_{j}}{\pi}\right)^{3/2} \left(\frac{2\pi}{B_{j}}\right)^{2} \frac{\exp(-B_{ji}c_{j}^{2})}{B_{ji}c_{j}} \int \exp(-B_{ji}g^{2}) \sinh(2B_{ji}gc_{j})g^{2}bdbdg.$$
(8)

So far, a general collision cross section is being considered, i.e.,

 $bdb = b(\psi,g)\frac{db}{d\psi} d\psi$

where 2ψ is the angle between the asymptotes of the relative velocity vectors before and after a collision. At this point, before integration over g, a collision interaction model must be specified since bdb may be a function of g. A rigid elastic sphere interaction model is assumed where

$$b = \sigma \sin \psi$$
$$bdb = \sigma^2 \sin \psi \cos \psi d\psi.$$

and

Thus, integrating over d ψ from 0 to $\pi/2$ and expressing the sinh in terms of exponential functions, equation (2-8) becomes,

$$L_{j} = n_{j} \left(\frac{B_{j}}{\pi}\right)^{3/2} \frac{\sigma^{2} \pi^{2} \exp(-B_{ji}c_{j}^{2})}{B_{i}^{2}B_{ji}c_{j}} \int_{0}^{\infty} (\exp(-B_{ji}g^{2} + 2B_{ji}gc_{j}))$$

- $\exp(-B_{ji}g^{2} - 2B_{ji}gc_{j}) g^{2}dg.$ (9)

The integration over g is performed using D_{-3} , a parabolic cylinder function (from Erdelyi (1955b)), and equation (9) becomes

$$L_{j} = n_{j} \left(\frac{B_{j}}{\pi}\right)^{3/2} \frac{\pi^{2} \sigma^{2} \exp(-B_{ji} c_{j}^{2})}{B_{i}^{2} B_{ji} c_{j}} \left(\frac{D_{-3}(\sqrt{2B_{ji}} c_{j})}{\sqrt{2B_{ji}} B_{ji}}\right)$$
$$\exp\left(\frac{B_{ji} c_{j}^{2}}{2}\right) - \frac{D_{-3}(\sqrt{2B_{ji}} c_{j})}{\sqrt{2B_{ji}} B_{ji}} \exp\left(\frac{B_{ji} c_{j}^{2}}{2}\right). \quad (10)$$

Then, expressing D_{-3} in terms of error functions (erf) by Erdelyi (1955b), the loss term becomes

$$L_{j} = n_{j} \left(\frac{B_{j}}{\pi}\right)^{3/2} \frac{\pi^{2} \sigma^{2}}{B_{j}^{2}} \left(\exp(-C_{j}^{2}) + \left(\frac{1+2C_{j}}{C_{j}}\right)\operatorname{erf} C_{j}\right)$$
(11)

where $C_j = \sqrt{B_{ji}} c_j$.

Equation (11) is identical to that given by Chapman (1964) or Deshpande (1969a). The calculation of the loss term is now complete. The gain term remains to be determined; its expression is

$$G_{ij} = \int F_{i}(\vec{v}')F_{j}(\vec{w}')gbdbdeD\vec{w}.$$
 (12)

The evaluation of the gain term is considerably more involved than the evaluation of the loss term. The procedure by which the gain term is determined is shown in Table 1 and the computational details are given in Appendix A. From Appendix A, the gain term, loss term, and collision integral are respectively,

$$G_{ij} = \frac{\pi^2 \sigma^2 F_i F_j}{B_i B_j^{2AR}} \left[{}_{1F_1(1;\frac{1}{2};\Delta_1 + R) - {}_{1F_1(1;\frac{1}{2};\Delta_1 - R)} \right],$$

$$F_i L_j = F_i F_j \frac{\pi^2 \sigma^2 2}{B_j^2} {}_{1F_1(2;\frac{3}{2};C_j^2)},$$

and

where

 $J(F_i,F_j) = G_{ij}-F_iL_j$

 $R^{2} = \lambda^{2} + \Delta_{2}^{2},$ $\Delta_{2} = \lambda_{2} - \lambda_{3},$ $\Delta_{1} = \lambda_{1} - \lambda_{3},$

$$A = a^{2} - 2bB_{ji} + b^{2}B_{ji} + B_{ji},$$

$$a = 2M_{i},$$

$$b = 2M_{j},$$

$$M_{i} = \frac{m_{i}}{m_{i} + m_{j}},$$

$$M_{j} = \frac{m_{j}}{m_{i} + m_{j}},$$

$$\vec{c}_{j} = \sqrt{B_{j}} \vec{c}_{j},$$

$$\vec{c}_{i} = \sqrt{B_{i}} \vec{c}_{i},$$

$$\vec{c}_{i} = \vec{\nabla} \cdot \vec{v}_{i},$$

$$A'' = \frac{a^{2}}{(a^{2} - 2bB_{ji} + b^{2}B_{ji} + B_{ji})B_{i}},$$

$$B'' = \frac{B_{i}(b - 1)^{2}}{B_{i}^{2}(a^{2} - 2bB_{ji} + b^{2}B_{ji} + B_{ji})} - \frac{1}{B_{i}},$$

$$D'' = \frac{2(b - 1)aB_{ji}}{\sqrt{B_{i}B_{j}}(a^{2} - 2bB_{ji} + b^{2}B_{ji} + B_{ji})},$$

$$E'' = \frac{2a}{B_{i}} \left(\frac{1}{a^{2} - 2bB_{ji} + b^{2}B_{ji} + B_{ji}}\right)^{1/2},$$

$$\lambda_{1} = \frac{C_{i}^{2}A'' + C_{i}^{2}B'' + 2C_{i}^{2}/B_{i}}{2}$$

$$\lambda_{2} = \frac{C_{i}^{2}A'' + C_{j}^{2}B''}{2}$$

$$\lambda_{3} = \frac{D''}{2} |\vec{c}_{i} \cdot \vec{c}_{j}|,$$

I

$$\lambda = \frac{\mathbf{E''}}{2} \left| \vec{\mathbf{C}}_{i} \times \vec{\mathbf{C}}_{j} \right|,$$

1

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$$B_{ji} = B_{j}/B_{i},$$

$$B_{i} = \frac{m_{i}}{2kT_{i}}, \quad B_{j} = \frac{m_{j}}{2kT_{j}},$$

 \vec{V} = velocity of particle j, the velocity at which the integrals are being evaluated,

 \vec{U}_i = gas velocity of particle i,

 \vec{U}_{j} = gas velocity of particle j,

$$F_{i} = n_{i} \left(\frac{B_{i}}{\pi}\right)^{3/2} \exp(-C_{i}^{2}),$$

$$F_{j} = n_{j} \left(\frac{B_{j}}{\pi}\right)^{3/2} \exp(-C_{j}^{2}),$$

n and T are the number density and temperature respectively of particles i or j, depending on the subscript used,

k = ... the Boltzmann constant, and

 $\sigma = \frac{\sigma_i + \sigma_j}{2} = \text{the collision diameter.}$

It is noted that

$$\left|\frac{c_1 \sin 2\psi}{2B_{ji} c_j \sin \alpha}\right| < 1,$$

where $\vec{c}_1 = a\vec{c}_i - b\vec{B}_j\vec{c}_j$ is required. With m_j , or the jth particle taken as the heavy species, this inequality is satisfied for all cases of interest.

In Appendix B these analytical results for the collision integral are modified to allow direct comparison with Monte Carlo calculations.

TABLE 1

CALCULATION PROCEDURE FOR THE ANALYTICAL EVALUATION OF THE COLLISION INTEGRAL FOR A RIGID SPHERE MOLECULAR MODEL AND A MOTT-SMITH BINARY GAS MIXTURE.



LOSS TERM

GAIN TERM





Rewrite the loss term in terms of confluent hypergeometric functions for consistency

> Write the closed form expression for the collision integral

3. Analytical Evaluation of the Collision Integral for Electron-Neutral Mixtures

In this section, the analysis is generalized to include the mixture of electrons (or ions) and neutrals. The distribution function of the neutrals is assumed to be Maxwellian. The electron distribution function is taken to be of the same general form as a Maxwellian gas. Chapman (1964) and Margenau (1946) employ a similar approach by considering the electron distribution function to be Maxwellian with a "temperature" considerably higher than that of the neutrals. Also, Comisar (1961); Krook (1959); Jukes (1957); and Tidman (1958) applied the Mott-Smith Ansatz to electron (or ion) -neutral mixtures. Specifically, the electron (or ion) -neutral distribution functions were taken to be a linear combination of two "modified" Maxwellian distribution functions.

Appendix C lists several theoretical electron distribution functions. Some distribution functions are appropriate for use in the analytical evaluation of the collision integral. Certain other electron distribution functions may be used in Monte Carlo calculations to check their validity, i.e., to see if they are solutions of the Boltzmann equation.

From Appendix C, an electron distribution function of the form

$$f_{e} = A \exp\left(\frac{-mv^{2}B}{2k\tau}\right) , \qquad (13)$$

in terms of the parameters A and B, is considered. A and B are taken to be constants. This form of f_e is selected as being more general than

$$f_e = A \exp[-Bv^2]$$

which is also analytically feasible.

Using equation ((13)) as representative of the electron distribution function, it remains to determine the parameters A and B. Since the parameters usually considered in electron-neutral studies are the number density and the mean energy, e.g., Allis (1956), Margenau (1948c), Morse (1935), Davydov (1935), and Chapman (1964), the following definitions of the electron number density and electron mean energy

 $n = \int f_{\rho} d\vec{v}$

and

$$\vec{v}^2 = \frac{3kT}{m} = \frac{1}{n} \int f_e v^2 d\vec{v}$$

are used to determine A and B. In this case, m is the electron mass, τ the electron temperature and \vec{v} is the electron velocity. Calculating A and B from the assumed f_e yields

$$A = n \left(\frac{3}{2\pi}\right)^{3/2} \frac{1}{\frac{1}{v^3}},$$

 $B = \frac{3}{-2} \left(\frac{k\tau}{m}\right)$

and

or

$$f_{e} = m(\frac{3}{2\pi})^{3/2} \frac{1}{\frac{1}{\sqrt{3}}} \exp\left[-\frac{3}{2} \frac{v^{2}}{\frac{1}{\sqrt{2}}}\right]. \qquad (14)$$

Alternately, the definition of the mean velocity,

$$\vec{\overline{v}} = \frac{1}{n} \int f_e \vec{v} d\vec{v}$$

could be used with that of the number density to determine A and B. However, A and B determined by either method differ only by numerical constants. The distribution functions of Druyvesteyn and Margenau, (given in Appendix C) are of the same form as equation (14). Also, Chapman (1964) gives results consistent with this equation.

These observations justify the choice of equation ((14)) to represent the electron distribution function. Of course, mathematical complications in the analytical evaluation of the collision integral precludes the use of all the proposed electron distribution functions given in Appendix C.

Mathematically, equation ((14)) is still of the same general form as a Maxwellian. The coefficient of the exponential term is constant and can be factored out of the integration. Redefining the constant B_i in the exponential then converts the results of Appendix A to an electron-neutral mixture. The gain and loss terms given in Appendix A apply to an electronneutral mixture with F_i replaced by f_e and $B_i = \frac{3}{2r^2}$.

4. Significance of the Analytical Calculations

The analytical evaluation of the collision integral for a Mott-Smith binary gas mixture is significant in two respects.

First, since Monte Carlo methods have statistical errors, comparison with analytical results are essential in establishing their accuracy. For the case of a monatomic gas such comparison has been made. Secondly, solutions of the Boltzmann transport equation on the basis of the Mott-Smith Ansatz have been found to yield accurately certain properties for strong shock waves in monatomic gases (Mott-Smith (1951, 1954); Narasimha (1969); Yen (1972)). Therefore, use of this Ansatz has been proposed to study rarefied gas flow problems in gas mixtures (Martikan (1966)).

The advantage of Mott-Smith shocks is the simplicity in their description, the validity of which can readily be studied, e.g., by using the Monte Carlo method (Hicks (1963a, 1967c, 1969a, 1970); Yen (1972)). In such studies, the detailed comparison of the collision integrals may be necessary.

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APPENDIX A

EVALUATION OF THE GAIN TERM FOR A BINARY MIXTURE

The gain term is evaluated from equation (12) by the procedure outlined in Table 1. The gain term is

$$G_{ij} = \int F_i(\vec{V}')F_j(\vec{W}')gbdbdeD\vec{W}.$$

First, the velocities after collision are related to the velocities before collision from Chapman (1964), where

$$\vec{V}' - \vec{V} = -2M_{\star} (\vec{g} \cdot \vec{k}) \vec{k},$$

and

 $\vec{W}' - \vec{W} = 2M_{i}(\vec{g} \cdot \vec{k})\vec{k},$

with

$$M_{i} = \frac{m_{i}}{m_{i}+m_{j}} \text{ and } M_{j} = \frac{m_{j}}{m_{i}+m_{j}}.$$

Now, since $\vec{g}=\vec{V}-\vec{W}$ and $\vec{g}\cdot\vec{k} = g\cos\psi$, where \vec{k} is the apse vector or the unit vector bisecting the angle between the asymptotes of \vec{g} and \vec{g}' (the angle between \vec{g} and \vec{k} or \vec{g}' and \vec{k} is ψ), the velocities after the collision become:

$$\vec{v}' = \vec{v} - 2M_i \vec{k} g \cos \psi$$

 $\vec{W}' = \vec{V} \cdot \vec{g} + 2M_j \vec{k}g\cos\psi$.

The coordinate system for the gain term is shown in Figure A-1. The vector \vec{c}_1 corresponds to the \vec{c} of Deshpande (1969a), and the components

and

of \vec{k} , k_{\parallel} and k_{\perp} , represent components parallel and perpendicular to \vec{g} , respectively.

The product $F_i(\vec{V}')F_j(\vec{W}')$, (with all velocities nondimensionalized by $B_i^{1/2}$) becomes

$$F_{i}(\vec{V}')F_{j}(\vec{W}') = F_{i}(\vec{V})F_{j}(\vec{W})exp(2gcos\psi(2\vec{k}) \cdot$$

$$(\mathbf{M}_{\mathbf{i}}\vec{\mathbf{c}}_{\mathbf{i}}-\mathbf{M}_{\mathbf{j}}\mathbf{B}_{\mathbf{j}}\mathbf{i}\vec{\mathbf{c}}_{\mathbf{j}}) + 2\mathbf{B}_{\mathbf{j}}\mathbf{i}\vec{\mathbf{c}}_{\mathbf{j}}\cdot\vec{\mathbf{g}}-\mathbf{g}^{2}(4\mathbf{M}_{\mathbf{i}}^{2}\cos^{2}\psi$$

 $\vec{c}_i = \vec{v} \cdot \vec{U}_i$

 $\vec{c}_i = \vec{v} \cdot \vec{U}_i$

 $B_{ji} = \frac{B_j}{B_j}$.

 $- 4M_{j}B_{ji}\cos^{2}\psi + 4M_{j}^{2}B_{ji}\cos^{2}\psi + B_{ji})), \qquad (A-1)$

where

and

Equation (A-1) is valid for a mixture of gases i and j.

In order to continue with the evaluation of G_{ij} , a new velocity \vec{c}_1 is defined as

 $\vec{c}_1 = 2M_i \vec{c}_i - 2M_j B_j \vec{c}_j.$ (A-2)

Next, in the integration over d ϵ , ϵ appears only in the term $\vec{k} \cdot \vec{c}_1$ of equation (A-1), (Margenau (1964), Jeans (1940)). When \vec{k} and \vec{c}_1 are resolved into components parallel and normal to \vec{g} , denoted by the subscripts || and $_{\perp}$, respectively, only the term $\vec{k} \cdot \vec{c}_1$ involves ϵ in the form of a linear combination of sin ϵ and cos ϵ . Then, in the integration over d ϵ ,



Fig. A-1 Coordinate System and Vector Geometry.

$$\int_{0}^{2\pi} d\varepsilon \exp(\vec{k} \cdot \vec{c}_{1}(2g\cos\psi)) = \exp(C_{1||}^{2g\cos^{2}\psi}) 2\pi I_{0}(gC_{1|}^{\sin^{2}\psi})$$

where I_0 is a modified Bessel function of the first kind and order zero (Abramowitz (1965)). In this integral

$$\vec{k} \cdot \vec{c}_1 = c_1 \cos \psi + c_1 \sin \psi \cos (\epsilon + \epsilon_0)$$

where ψ is defined in Figure A-1 and ε_0 is a constant.

In the integration over $D\vec{W}$, \vec{W} is replaced by the relative velocity and spherical coordinates are used with \vec{c}_1 as an axis, so

$$\overrightarrow{Dg} = g^2 \sin \xi d\xi d\phi dg$$

(see Figure A-1).

The angle ϕ appears only in the term $\exp(2B \vec{c_j} \cdot \vec{g})$ of the gain term and

$$\vec{c}_{j} \cdot \vec{g} = \left\{ c_{j} \cos \alpha g \cos \xi + c_{j} \sin \alpha \sin \xi \cos (\phi + \phi_{o}) \right\} g$$

after resolving \vec{c}_j and \vec{g} into components parallel and perpendicular to \vec{c}_1 . Here, ϕ_0 is a constant and α is the polar angle of \vec{c}_j . Then as done in the integration over de,

 $\int_{0}^{2\pi} d\phi \exp(2B_{ji}\vec{c}_{j}\cdot\vec{g}) = \exp(2B_{ji}gc_{j}\cos\alpha\cos\xi)2\pi I_{0}(2B_{ji}c_{j}gsin\alpha\sin\xi).$

Now, the integration over de and d ϕ is complete. Rewriting the product of the two modified Bessel functions in terms of the hypergeometric function ($_2F_1$), (from Erdelyi (1955b)) the gain term, equation (2-14), becomes

$$G_{ij} = 4\pi^{2} F_{i}F_{j} \int \left[\left\{ \sum_{n=0}^{\infty} \frac{(-1)^{n} (B_{ji}c_{j}gsingsin\alpha)^{2n}}{(n!)^{2}} 2^{F_{1}} - n, -n; 1; \frac{c_{1}^{2}sin^{2}2\psi}{4B_{ji}^{2}c_{j}^{2}sin^{2}\alpha} \right) \right\}$$

$$g^{3}bdbdgexp\left\{-g^{2}\left(4M_{i}^{2}cos^{2}\psi-4M_{j}^{B}_{ji}cos^{2}\psi+4M_{j}^{2}B_{ji}cos^{2}\psi+B_{ji}\right)\right\}exp\left(2gc_{1}cos\xi cos^{2}\psi\right)$$

exp(2B_{ji}gc_jcosccos5)sin5d5

Next, the integration over d5 is considered and

$$\int_{0}^{\pi} d\xi \exp(c_{1} \cos\xi 2g \cos^{2}\psi + 2B_{ji}g_{j}c_{j}\cos\alpha\cos\xi) \cdot \left[(\sin\xi)^{2n+1}\right]$$

= n! 2(gX)⁻ⁿi_n(2gX) = n! $\sqrt{\pi}$ (gX)^{-n-1/2} I_{n+1/2}(2gX)

where

$$I_{n+1/2} = a \mod ified \ Bessel \ function,$$

$$i_n = a \mod ified \ spherical \ Bessel \ function, \ and$$

$$X = c_1 \cos^2 \psi + B_{ji} c_j \cos \alpha,$$

(see Abramowitz (1965)).

Using this result, and completing the nondimensionalization of $g^3 dg$, equation (A-3) becomes

(A-3)

$$G_{ij} = \frac{8\pi^{2}F_{i}F_{j}}{B_{i}^{2}} \int \left\{ dgdbd \exp(-g^{2}\gamma^{2}) \sum_{n=0}^{\infty} \frac{(-1)^{n}(B_{ji}c_{j}sin\alpha)^{2n}}{n! x^{n}} \right\}$$

$$2^{F_{1}(-n,-n,1;\Psi)} i_{n}(2gX)g^{n+3}$$
(A-4)

where

 $\gamma^{2} = 4M_{i}^{2}\cos^{2}\psi - 4M_{j}B_{ji}\cos^{2}\psi + 4M_{j}^{2}B_{ji}\cos^{2}\psi + B_{ji}$ $\psi = \frac{c_{1}^{2}\sin^{2}2\psi}{4B_{ji}^{2}c_{j}^{2}\sin^{2}\alpha} .$

and

Next, for rigid elastic spheres,

 $bdb = \sigma^2 sin \psi cos \psi d\psi$

and equation (A-4) becomes

$$G_{ij} = \frac{4\pi^{5/2} F_{i} F_{j} \sigma^{2}}{B_{i}^{2}} \int \left\{ \sin\psi \cos\psi \, d\psi \sum_{n=0}^{\infty} \frac{(-1)^{n} (B_{ji} c_{j} \sin \alpha)^{2n}}{n! x^{n+1/2}} \right\}$$
$$2^{F_{1}(-n,-n;1;\Psi) \exp(-g^{2}\gamma^{2})} I_{n+1/2}(2gX) g^{n+5/2} dg \left\}.$$
(A-5)

From Erdelyi (1955b),

$$\int_{0}^{\infty} I_{n+1/2}(2gX) \exp(-\gamma^{2}g^{2})g^{n+5/2}dg = \frac{\gamma^{-2n-4}\Gamma(n+2)X^{n+1/2}}{2\Gamma(n+3/2)} I_{1}^{F_{1}(n+2;n+3/2;-\frac{X^{2}}{\gamma^{2}})}$$

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where $\Gamma($) denotes a gamma function. In equation (A-5), the confluent hypergeometric function ${}_2F_1$ is replaced by

$$\frac{1}{2\pi}\int_{0}^{2\pi}\mathrm{d}\theta\left(1+2\Psi^{1/2}\cos\theta+\Psi\right)^{n},$$

Erdelyi (1955a), where

$$\left|\frac{c_1 \sin 2\psi}{2B_{ji} c_j \sin 2\psi}\right| < 1$$

is required.

A similar restriction exists in the analysis by Deshpande (1969a) for $m_i = m_j$; however, it was not mentioned in his paper. Now equation (A-5) becomes

$$G_{ij} = \frac{\pi^{3/2} F_{i} F_{j} \sigma^{2}}{B_{i}^{2}} \int_{0}^{2\pi} d\theta \int_{0}^{\pi/2} d\psi \sin\psi \cos\psi \sum_{n=0}^{\infty} \frac{(B_{ji} c_{j} \sin\alpha)^{2n}}{n! \gamma^{4}} (1 + \psi^{1/2} 2\cos\theta + \psi)^{n} \frac{\Gamma(n+2)}{\Gamma(n+\frac{3}{2})} \frac{1^{F_{1}(n+2;n+3/2;\frac{X^{2}}{\gamma^{2}})}}{\gamma^{2n}} .$$
(A-6)

Replacing ${}_{1}F_{1}$ by the summation formula of Slater (1960) and Rainville (1960),

$$G_{ij} = \frac{2\pi F_{ij}F_{j\sigma}^{2}}{B_{i}^{2}} \int_{0}^{2\pi} \int_{0}^{2\pi} \int_{0}^{\pi/2} \frac{d\psi \sin\psi \cos\psi}{\gamma^{4}} {}_{1}F_{1}(2;\frac{3}{2}; \frac{X^{2} + (B_{ji}^{2}c_{j}^{2}\sin^{2}\alpha)(1 + 2\Psi^{1/2}\cos\theta + \Psi)}{\gamma^{2}})$$
(A-7)

Next, X, γ^2 , and Ψ are replaced by their full expressions; \vec{c}_1 is replaced by \vec{c}_i and \vec{c}_j and the necessary angles resulting from the vector geometry; and ψ is transformed to a new variable ζ

$$\zeta^{-1} = 1 + \frac{B_{ji}}{A} \tan^2 \psi$$

where

and

 $A = a^{2} - 2bB_{ji} + b^{2}B_{ji} + B_{ji},$ $a = 2M_{i},$ $b = 2M_{j},$ $\gamma^{2} = A\cos^{2}\psi + B_{ji}\sin^{2}\psi.$

Then equation (A-7) becomes

$$G_{ij} = \frac{\pi \sigma^{2} F_{i} F_{j}}{AB_{i} B_{j}} \int_{0}^{2\pi} d\theta \int_{0}^{1} d\zeta {}_{1} F_{1} \left[2; \frac{3}{2}; \zeta c_{i}^{2} A' + \zeta c_{j}^{2} B' + B_{ji} c_{j}^{2} - D' \zeta |\vec{c}_{i} \cdot \vec{c}_{j}| + \zeta^{1/2} (1 - \zeta)^{1/2} E' \cos \theta |\vec{c}_{i} \times \vec{c}_{j}| \right]$$
(A-8)

where A', B', D', and E' are constants involving B_i , B_j and the masses and are defined below.

At this point it is noted that for equal masses $G_{ij} = G_{ji}$ or the gain term is symmetric. However, for a mixture of gases when $m_i \neq m_j$, the gain term is not symmetric. This may be shown by interchanging the roles of i and j and nondimensionalizing with respect to $\sqrt{B_j}$ instead of $\sqrt{B_i}$.

Next, a new velocity is introduced with

 $\vec{c}_{i} = \sqrt{B_{ji}} \vec{c}_{j}$

$$\vec{c}_{j} = \sqrt{B_{j}} (\vec{v} \cdot \vec{u}_{j}) = \sqrt{B_{j}} \vec{c}_{j}$$

or

when \vec{c}_{j} is returned to dimensional form. Thus, since all velocities are already nondimensional,

$$\vec{C}_{j} = \sqrt{B_{j}} \vec{c}_{j}$$
 and $\vec{C}_{i} = \sqrt{B_{i}} \vec{c}_{i}$

are the new velocities. Now, equation (A-8) becomes

$$S_{ij} = \frac{2\pi\sigma^{2}F_{i}F_{j}}{B_{i}B_{j}^{A}} \int_{0}^{\pi} d\theta \int_{0}^{1} d\zeta {}_{1}F_{1}[2;\frac{3}{2};\zeta A''C_{i}^{2} + \zeta B''C_{j}^{2} + C_{j}^{2}/B_{i}]$$

- D''\zeta | $\vec{c}_{i} \cdot \vec{c}_{j}| + \zeta^{1/2} (1-\zeta)^{1/2} E'' \cos\theta | \vec{c}_{i} \times \vec{c}_{j}|]$
$$= \frac{\pi\sigma^{2}F_{i}F_{j}}{B_{i}B_{j}^{A}} g_{ij} \qquad (A-9)$$

where

1

$$A'' = \frac{A'}{B_{i}} = \frac{a^{2}}{(a^{2}-2bB_{ji}+b^{2}B_{ji}+B_{ji})B_{i}},$$

$$B'' = \frac{B'}{B_{j}} = \frac{B_{ji}^{2}(b-1)^{2}}{(a^{2}-2bB_{ji}+b^{2}B_{ji}+B_{ji})B_{j}} - \frac{1}{B_{i}}$$

$$D'' = \frac{D'}{\sqrt{B_{i}B_{j}}} = \frac{2(b-1)B_{ji}a}{\sqrt{B_{i}B_{j}}(a^{2}-2bB_{ji}+b^{2}B_{ji}+B_{ji})},$$

$$E'' = \frac{E'}{\sqrt{B_{i}B_{j}}} = \frac{2a}{\sqrt{B_{i}B_{j}}} \left(\frac{B_{ji}}{a^{2}-2bB_{ji}+b^{2}B_{ji}+B_{ji}}\right)^{1/2}$$

and

$$g_{ji} = 2 \int_{0}^{\pi} d\theta \int_{0}^{1} d\zeta \, {}_{1}F_{1} \left[2; \frac{3}{2}; \zeta A''C_{i}^{2} + \zeta B''C_{j}^{2} + C_{j}^{2} / B_{i} - D''\zeta |\vec{c}_{i} \cdot \vec{c}_{j}| + \zeta^{1/2} (1-\zeta)^{1/2} E'' \cos\theta |\vec{c}_{i} \cdot \vec{c}_{j}| \right].$$
(A-10)

Next, another substitution is made where

$$\begin{split} \zeta &= \cos^{2}(\frac{\tau}{2}) = \frac{1 + \cos\tau}{2}, \\ \lambda_{1} &= \frac{c_{1}^{2}A'' + B''c_{j}^{2} + 2c_{j}^{2}/B_{i}}{2}, \\ \lambda_{2} &= \frac{c_{1}^{2}A'' + c_{j}^{2}B''}{2}, \\ \lambda_{3} &= \frac{D''}{2} |\vec{c}_{i} \cdot \vec{c}_{j}|, \\ \lambda_{3} &= \frac{E''}{2} |\vec{c}_{i} \cdot \vec{c}_{j}|, \\ \lambda_{1} &= \frac{E''}{2} |\vec{c}_{i} \cdot \vec{c}_{j}|, \\ \lambda_{2} &= \lambda_{1} - \lambda_{3}, \\ \lambda_{2} &= \lambda_{2} - \lambda_{3}, \end{split}$$

and for

and

equation (A-10) becomes:

$$g_{ij} = \int_0^{\pi} d\theta \int_0^{\pi} \sin\tau d\tau \, {}_{1}F_1 \left[2; \frac{3}{2}; \Delta_1 + \Delta_2 \cos\tau + \lambda \sin\tau \cos\theta \right]. \tag{A-11}$$

Next, take $R^2 = \lambda^2 + \Delta_2^2$ and define an angle α_1 such that $\cos \alpha_1 = \frac{\Delta_2}{R}$ and $\sin \alpha_1 = \frac{\lambda}{R}$. Thus

 $\Delta_2 \cos \tau + \lambda \sin \tau \cos \theta = R \cos \alpha_1 \cos \tau + R \sin \alpha_1 \cos \theta \sin \tau = R \cos \theta$

where

$$\cos \theta = \cos \alpha_1 \cos \tau + \sin \alpha_1 \cos \theta \sin \tau$$
,

and equation (A-11) becomes,

$$g_{ij} = \int_{0}^{\pi} d\theta \int_{0}^{\pi} {}_{1}F_{1}\left[2;\frac{3}{2};\Delta_{1}+R\cos\Theta\right]\sin\tau d\tau. \qquad (A-12)$$

From Erdelyi (1955a) the confluent hypergeometric function $_{1}F_{1}$ is replaced by a contour integral and equation (A-12) becomes

$$g_{ij} = \frac{\Gamma(\frac{3}{2})\Gamma(\frac{3}{2})}{2\pi i \Gamma(2)} \int_{\mathcal{B}} dt \int_{0}^{\pi} d\theta \int_{0}^{\pi} \sin\tau d\tau \exp\left\{\left(\Delta_{1} + \operatorname{Rcos}_{\Theta}\right)t\right\} t(t-1)^{-3/2}$$
(A-13)

where i is an imaginary number and & is a contour in the form of a loop starting and ending at t = 0 and encircling one once in the positive sense.

Then, from Erdelyi (1955a,b)

$$\exp(\operatorname{Rtcos}^{\otimes}) = \sum_{n=0}^{\infty} (2n+1) \operatorname{P}_{n}(\cos^{\otimes}) \operatorname{i}_{n}(\operatorname{Rt})$$

where $P_n($) is a Legendre polynomial. Also,

$$\int_{0}^{\pi} \sin \tau \, d\tau \int_{0}^{\pi} \exp(\operatorname{Rtcos}_{\Theta}) \, d\theta = \pi \int_{0}^{\pi} \sin \tau \, d\tau \, i_{o}(\operatorname{Rt}),$$

since $\cos\theta = \cos\alpha_1 \cos\tau + \sin\alpha_1 \cos\theta \sin\tau$, and from Erdelyi (1955b),

$$\int_{0}^{\pi} \exp(\operatorname{Rtcos}\theta) d\theta = \pi i_{0}(\operatorname{Rt}) + \pi \left[\sum_{n=1}^{\infty} (2n+1) i_{n}(\operatorname{Rt}) P_{n}(\cos \alpha_{1}) P_{n}(\cos \tau)\right]$$

 $\int_0^{\pi} P_n(\cos\tau) \sin\tau d\tau = 0.$

and

Now, using the above results for the integration over τ and θ in equation (A-13), and replacing i by exponential functions (Abramowitz (1965)), equation (A-13) becomes

$$g_{ij} = \frac{\pi}{R} \left(\frac{\Gamma(\frac{3}{2})\Gamma(\frac{3}{2})}{2\pi i \Gamma(2)} \right) \left[\int_{\mathscr{Q}} dt \exp(t\Delta_1) (t-1)^{-3/2} \exp(Rt) - \int_{\mathscr{Q}} dt \exp(t\Delta_1) (t-1)^{-3/2} \exp(-Rt) \right].$$
(A-14)

Previously, the confluent hypergeometric function was replaced by the contour integral over ¢. Now the contour integral in equation (A-14) is rewritten in terms of a confluent hypergeometric function (Erdelyi 1955a)) and equation (A-14) becomes,

$$g_{ij} = \frac{\pi}{2R} \left[{}_{1}F_{1}(1;\frac{1}{2};\Delta_{1}+R) - {}_{1}F_{1}(1;\frac{1}{2};\Delta_{1}-R) \right], \qquad (A-15)$$

and from equation (A-9),

$$G_{ij} = \frac{\pi^2 \sigma^2 F_{i} F_{j}}{B_{i} B_{j}^{2} A R} \Big[{}_{1}F_{1}(1; \frac{1}{2}; \Delta_{1} + R) - {}_{1}F_{1}(1; \frac{1}{2}; \Delta_{1} - R) \Big].$$
(A-16)

Also $G_{ij} \neq G_{ji}$ except for the special case where the masses of the two gases of equal. In either case $L_{ij} \neq L_{ji}$, so the loss term is never symmetric.

Equation (A-16) is the final closed form expression for the gain term. Now equation ((11)) for the loss term will be converted into a form similar to the gain term. From equation (11), using the expression for F_i , the loss term becomes,

$$F_{i}L_{j} = F_{i}F_{j}\left(\frac{\pi}{B_{j}}\right)^{2}\sigma^{2}\left[1 + \left(\frac{1+2C_{j}^{2}}{C_{j}}\right)erfC_{j}expC_{j}^{2}\right].$$
(A-17)

From Erdelyi (1955a,b), the exponential and error functions may be expressed in terms of confluent hypergeometric functions, in which case equation (A-17) becomes

$$F_{i}L_{j} = F_{i}F_{j}(\frac{\pi}{B_{j}})^{2}\sigma^{2}2_{1}F_{1}(2;\frac{3}{2};C_{j}^{2}).$$
 (A-18)

The collision integral, J, is

$$J(F_{i},F_{j}) = G_{ij}-F_{i}L_{j} = \frac{\pi^{2}\sigma^{2}F_{i}F_{j}}{B_{i}B_{j}}\left[\frac{1}{2AR}\left\{_{1}F_{1}(1;\frac{1}{2};\Delta_{1}+R)-_{1}F_{1}(1;\frac{1}{2};\Delta_{1}-R)\right\} - \frac{2B_{i}}{B_{j}}\left\{_{1}F_{1}(2;\frac{3}{2};c_{j}^{2})\right\}\right], \qquad (A-19)$$

from equations (A-16) and (A-18). Recall that $\left|\frac{c_1 \sin 2\psi}{2B_{ji}c_j \sin \alpha}\right| < 1$ is required, where $\vec{c}_1 = 2M_i \vec{c}_i - 2M_j B_{ji} \vec{c}_j$.

APPENDIX B

COMPARISON OF THE COLLISION INTEGRALS FOR A BINARY GAS MIXTURE

An analytical expression for the collision integral for a Mott-Smith gas mixture and a rigid elastic sphere collision model has been derived in section 1 and Appendix A. In this appendix, a means by which the analytical values of the collision integral may be compared with Monte Carlo calculations is given.

From equation (A-19), the confluent hypergeometric functions appearing in the collision integral, may be expanded by Kummer's series,

$$_{1}F_{1}(a;b;Z) = 1 + \frac{aZ}{b} + \frac{(a)_{2}Z^{2}}{(b)_{2}Z^{2}} + \dots + \frac{(a)_{n}Z^{n}}{(b)_{n}n!} + \dots$$

where (a) = a(a+1)(a+2)...(a+n-1),

and (a) = 1.

The function ${}_{1}F_{1}$ represents one independent solution of

$$Z \frac{d^2 W}{dz^2} + (b-Z)\frac{dW}{dZ} - aW = 0,$$

and the series for ${}_{1}F_{1}$ is convergent for all finite Z when b is neither zero nor a negative integer. (See Abramowitz (1965); Whittaker (1963); and Rainville (1960)).

Next, to compare the analytical values of the collision integral with the Monte Carlo calculations, it is first necessary to establish a consistent set of nondimensionalization parameters. Toward this end, the analytical collision integral is converted into Hicks units, following Hicks (1963b); Nordsieck (1966), and Reilly (1969), where (denoting nondimensional terms by a bar) Hicks defines:

$$\bar{\mathbf{x}} = \frac{\mathbf{x}\sqrt{2}}{1},$$

and l_c , the reference mean free path is

1

$$1_{c} = \frac{1}{\sqrt{2} \pi n_{i} \sigma^{2}}$$

 n_{i_c} is a reference density (on the cold side of a shock wave), and

$$\begin{aligned} \overline{\overline{v}}_{i} &= \overline{v}_{i} \left(\frac{m_{i}}{2\pi kT_{c}}\right)^{1/2}, \\ \overline{\overline{v}}_{j} &= \overline{v}_{j} \left(\frac{m_{i}}{2\pi kT_{c}}\right)^{1/2}, \\ T_{i_{c}} &= T_{j_{c}} = T_{c} \\ \overline{F}_{i} &= \frac{F_{i}}{n_{c_{i}}} \left(\frac{2\pi kT_{c}}{m_{i}}\right)^{3/2}, \\ \overline{F}_{j} &= \frac{F_{j}}{n_{c_{j}}} \left(\frac{2\pi kT_{c}}{m_{i}}\right)^{3/2}, \\ \overline{n}_{j} &= \frac{n_{j}}{n_{c_{j}}}, \\ \overline{n}_{i} &= \frac{n_{i}}{n_{c_{i}}}, \\ \overline{T}_{i} &= \frac{T_{i}}{T}, \end{aligned}$$

$$\bar{T}_{i} = \frac{I_{i}}{T_{c}},$$

$$\alpha = \frac{m_{i}}{m_{i}},$$

i,j = 1,2.

and

where

-

Then converting the loss term from equation (A-18) to Hicks units yields

$$\bar{\mathbf{F}}_{i}\bar{\mathbf{L}}_{j} = \left\{\bar{\mathbf{n}}_{j}\left(\frac{\bar{\mathbf{T}}_{j}}{\alpha}\right)^{1/2}\left(\exp(-\bar{\mathbf{C}}_{2}^{2}) + \left(\frac{1+2\bar{\mathbf{C}}_{2}^{2}}{\bar{\mathbf{C}}_{2}}\right)\exp(\bar{\mathbf{C}}_{2}\right)\right\} \left\{\bar{\mathbf{n}}_{i}(\bar{\mathbf{T}}_{i})^{-3/2}\exp(\frac{-\pi\bar{\mathbf{C}}_{3}^{2}}{\bar{\mathbf{T}}_{i}})\right\} \quad (B-1)$$

where

$$\begin{split} \overline{\vec{c}}_{2} &= \left(\frac{\alpha\pi}{\overline{T}_{j}}\right)^{1/2} \overline{\vec{c}}_{1}, \\ \overline{\vec{c}}_{1} &= \overline{\vec{v}}_{i} - \overline{\vec{v}}_{j}, \\ \overline{\vec{c}}_{3} &= \overline{\vec{v}}_{i} - \overline{\vec{v}}_{i}, \\ \overline{\vec{c}}_{3} &= \overline{\vec{v}}_{i} - \overline{\vec{v}}_{i}, \\ \overline{\vec{L}}_{j} &= \frac{L_{j}}{\sigma^{2}n_{c}} \left(\frac{m_{i}}{2\pi kT_{c}}\right)^{1/2}. \end{split}$$

and

Similarly, the gain term (equation (A-16)) in Hicks units becomes

$$\overline{G}_{ij} = \frac{\pi^2 \overline{F}_{i} \overline{F}_{j}}{2ARB} j \left[{}_{1}F_1(1; \frac{1}{2}; \Delta_1 + R) - {}_{1}F_1(1; \frac{1}{2}; \Delta_1 - R) \right]$$
(B-2)

where

$$\begin{split} & \Delta_{1} = \lambda_{1} - \lambda_{3}, \\ & \Delta_{2} = \lambda_{2} - \lambda_{3}, \\ & R^{2} = \lambda^{2} + \Delta_{2}^{2}, \\ & \lambda_{1} = \frac{\bar{c}_{1}^{2}A^{\prime\prime} + \bar{c}_{1}^{2}B^{\prime\prime} + 2B\bar{c}_{1}^{2}}{2} , \\ & \lambda_{2} = \frac{\bar{c}_{1}^{2}A^{\prime\prime} + B^{\prime\prime}\bar{c}_{1}^{2}}{2} , \\ & \lambda_{3} = \frac{D^{\prime\prime}}{2} |\bar{\vec{c}}_{1} \cdot \bar{\vec{c}}_{j}|, \\ & \lambda_{3} = \frac{D^{\prime\prime}}{2} |\bar{\vec{c}}_{1} \cdot \bar{\vec{c}}_{j}|, \\ & \lambda_{4} = \frac{E^{\prime\prime}}{2} |\bar{\vec{c}}_{1} \cdot \bar{\vec{c}}_{j}|, \\ & A = \left[\frac{4M_{2}^{2}\pi}{\bar{T}_{1}} + \frac{4M_{1}^{2}\pi\alpha}{\bar{T}_{j}} - \frac{4M_{1}\alpha\pi}{\bar{T}_{j}} + B\right] \\ & B = \frac{\pi\alpha}{\bar{T}_{j}}, \\ & \alpha_{4} = \frac{m_{1}}{\bar{T}_{j}}, \\ & \alpha_{7} = \frac{m_{1}}{\bar{m}_{1}}, \\ & \bar{\vec{c}}_{1} = \bar{\vec{v}}_{1} - \bar{\vec{v}}_{1}, \\ & \bar{\vec{c}}_{j} = \bar{\vec{v}}_{1} - \bar{\vec{v}}_{j}, \\ & M_{1} = \frac{1}{1+\alpha}, \\ & M_{j} = \frac{\alpha_{1}}{\sigma^{2}} \left(\frac{m_{1}}{2\pi kT_{c}}\right)^{2}, \\ \end{split}$$

,

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 $a = \frac{2M_{j}\pi}{\bar{T}_{i}},$ $b = 2M_{i},$ $A'' = \frac{a^{2}}{A},$ $B'' = \frac{B^{2}}{A}(b-1)^{2}-B,$

$$D'' = \frac{2(b-1)aB}{A}$$

 $E'' = 2(\frac{B}{A})^{1/2}a$.

and

The collision integral becomes,

$$\bar{J}(F_{i},F_{j}) = \bar{G}_{ij} - \bar{F}_{i}\bar{L}_{j}$$
 (B-3)

Utilization of Hicks units allows direct comparison with the binary mixture Monte Carlo program recently developed by Yen (1972b).

APPENDIX C

ELECTRON DISTRIBUTION FUNCTIONS

For electrons diffusing through a neutral gas, several distribution functions have been proposed and compared with available experimental data. In this appendix, the proposed electron distribution functions are reviewed for their suitability for theoretical treatment.

For the purpose of discussion, the electron distribution functions are grouped as follows:

 <u>Druyvesteyn distribution</u>: (from Druyvesteyn (1936); Allis (1956);
 Loeb (1960); and Chapman (1964)). The Boltzmann equation is considered in the form,

$$\vec{F}_2 \cdot \frac{\partial f_e}{\partial \vec{c}_2} = J = \text{collision integral}$$

where \vec{F}_2 = the constant external force = $\frac{e_2\vec{E}}{m_2}$,

e = the electron charge,

m = the electron mass,

 \vec{E} = the external electric field,

 $f_e =$ the electron distribution function,

and \vec{C} = the velocity.

The subscript 1 refers to neutrals and the subscript 2 designates electrons. An approximate solution of this equation yields and

$$f_{e}^{(1)} = \left(\frac{m_{2}C_{2}\lambda}{kTC_{2}^{2} + \frac{m_{1}F_{2}^{2}\lambda^{2}}{3}}\right) f_{e}^{(0)} \qquad (C-1)$$

(see Chapman (1964)). In equation (C-1),

 λ = the electron mean free path,

 $f_{e}^{(0)} = A \exp \left[-\int_{0}^{C_{2}} \frac{m_{2}C_{2}dC_{2}}{kT + \frac{m_{1}F_{2}^{2}\lambda^{2}}{kT + \frac{m_{1}F_{2}^{2}\lambda^{2}}{kT + \frac{m_{2}C_{2}}{kT + \frac{m_{2}C$

T = the gas temperature or the temperature of the electron-neutral mixture,

k = the Boltzmann constant,

A = a constant dependent on the number density of the electrons.

Since

and

$$n = 4\pi \int_0^\infty f_e v^2 dv,$$

A can be determined in terms of n with f_e given by equation (C-1). In equation (C-1), the superscript 0 represents a zeroth order approximation and the superscript 1 represents the first order approximation and

$$f_e = f_e^{(0)} + \vec{F}_2 \cdot \vec{C}_2 f_e^{(1)}$$

becomes the final electron distribution function.

Here, several assumptions have been made; some terms of order m_2/m_1 have been discarded; and it is assumed that

$$C_1 = C'_1,$$

 $C_2 = C'_2 = g,$
 $C_2 - C'_2 = C_2(1 - \cos \psi)$

where a prime denotes velocity after a collision,

g = the relative velocity,

and ψ = the deflection angle.

Consider three special cases of equation (C-1):

Case 1: When F_2 is small, f_e approximates the Lorentz expression for a slightly ionized gas (Chapman (1964)), and $f_e^{(0)}$ is Maxwellian. Case 2: For F_2 large, when the mean energy of an electron is large compared with $\frac{3}{2}$ kT, equation (C-1) may be approximated by

$$f_{e}^{(0)} = A \exp \left[-\int_{0}^{C_{2}} \frac{3m_{2}C_{2}^{3}dC_{2}}{m_{1}F_{2}^{2}\lambda^{2}} \right],$$

$$f_{e}^{(1)} = \frac{3m_{2}C_{2}}{m_{1}F_{2}^{2}\lambda} f_{e}^{(0)}, \qquad (C-2)$$

$$m_{2}F_{2}^{2}\lambda^{2}$$

and

for kT $\ll \frac{m_1 r_2^{\Lambda}}{3c_2^2}$ in the range of C_2 for which $f_e^{(0)}$ is appreciable.

Since $m_2 c_2^2 > 3kT$ when this is true, this condition implies that the mean value of $e_2 E\lambda$ (where $F_2 = \frac{e_2 E}{m_2}$) must be large compared to $3kT(\frac{m_2}{m_1})^{1/2}$. Case 3: If the molecules are rigid elastic spheres, so that the mean free path is independent of C_2 , equation (C-2) becomes

$$f_{e}^{(0)} = A \exp \left(-\frac{3m_{2}C_{2}^{4}}{4m_{1}F_{2}^{2}\lambda^{2}} \right)$$

$$f_{e}^{(1)} = \left(\frac{3m_{2}C_{2}}{m_{1}F_{2}^{2}\lambda} \right) f_{e}^{(0)}$$
(C-3)

which is Druyvesteyn's result (1936). It indicates that the number of electrons with energies large compared with the mean energy is much smaller than in a Maxwellian distribution with the same mean energy. Using this result, it follows that A is connected with the number density n_2 by the relation

$$m_2 = \pi A \left(\frac{4m_1F_2^2\lambda^2}{3m_2}\right)^{3/4} \Gamma(\frac{3}{4}),$$

and the mean energy of an electron is

$$\frac{1}{2}m_2\overline{c_2^2} = 0.427(m_1m_2)^{1/2}F_2\lambda.$$

2) <u>Distribution functions proposed by Margenau and associates</u>:
 Case 1: Consider the Boltzmann equation in the form (Margenau (1958))

$$\frac{e_2 E}{m_2} \frac{\partial f_e}{\partial v_y} + \frac{\partial f_e}{\partial t} = J, \qquad (C-4)$$

$$f_{e}(\vec{v}) = f_{0}(\vec{v}) + \frac{e_{2}E}{m_{2}} v_{x}f_{1}(\vec{v})$$

where the frequency of the E field is assumed zero, (d.c. case), \vec{v} is the electron velocity (v is its x component), t is the time and E = E₀, a constant. Also,

$$f_0 = \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(-\frac{mv^2}{2kT}\right),$$

and f₁ is defined below.

Case 2: Margenau (1946) also obtained

$$\ln f_0 = -\int_0^{v^2} \frac{(\frac{m_2}{2}) dv^2}{kT + \frac{m_1 \gamma^2 \lambda^2}{6 v^2}}$$
(C-5)

where $\gamma = \frac{e_2 E_0}{m_2}$.

A

For small γ , f_o is Maxwellian. For small kT, f_o is Druyvesteyn (see equation (C-3)).

In general, from equation (C-5)

$$f_0 = A \exp\left(-\frac{\epsilon}{kT}\right) \left[1 + \frac{\epsilon/kT}{\alpha}\right]^{\alpha}$$
(C-6)

where $\epsilon = \frac{m_2 v^2}{2}$,

and

 $\alpha = \frac{m_1}{12m_2} \left(\frac{\varepsilon_2}{kT}\right)^2 .$

 $\varepsilon_2 = e E_0 \lambda$,

A is determined from

$$m_2 = 2\pi \left(\frac{2kT}{m_2}\right)^{3/2} A \int_0^\infty e^{-x} \left(1 + \frac{x}{\alpha}\right)^\alpha x^{1/2} dx, \qquad (C-7)$$

where $x = \epsilon/kT$.

Expanding the term in brackets in equation (C-6), f_0 becomes a Druyvesteyn distribution, when only the dominant term is considered. For the alternating current (a.c.) case, the dominant term becomes Maxwellian with a "temperature"

$$T' = T(1 + \frac{\alpha 2kT}{m_2 w^2 \lambda^2})$$

(Margenau (1946)), where w is the frequency of the \vec{E} field. Also,

$$f_{1} = 2A(\frac{m_{2}}{2kT})^{3/2} \lambda \frac{(x+x_{1}+\alpha)^{\alpha-1}}{(x_{1}+\alpha)^{\alpha}} e^{-x_{x}^{1/2}}, \qquad (C-8)$$

and

$$f_{e}(\vec{v}) = f_{o}(\vec{v}) + \gamma v_{x} f_{1}(\vec{v})$$

where $x_1 = \frac{m_2(w\lambda)^2}{2kT}$ and w is zero for the d.c. case. Case 3: Both a.c. and d.c. electric fields were considered by Margenau (1948a). For the d.c. case,

$$f = f^{(0)} + \alpha f^{(1)},$$

$$f^{(1)} = \text{the Maxwellian distribution,}$$

$$\alpha = \frac{x}{v} ,$$

$$f^{(0)} = A \exp\left(\frac{-3m_2v^4}{4m_1\gamma^2\lambda^2}\right), \qquad (C-9)$$

and

which is the Druyvesteyn distribution. In this case w=0 and T=0.

The a.c. case is not considered here, since the time dependent distribution functions are not of interest. In all the cases given above the initial velocity was related to the final velocity by

$$v_i = (1 + \frac{m_2}{m_1})v_f$$

The neutral gas molecules were assumed to be at rest and the cosine of the deflection angle was taken much less than one. Also, distinct electron and neutral temperatures were not considered.

3) Distribution functions of the Druyvesteyn form :

Morse (1935), Holstein (1946), and Bowe (1963) all obtained forms similar to the Druyvesteyn distribution although different assumptions were made by each author (see Loeb (1960)).

4) Distribution functions proposed by Davydoy:

Davydov (1935) assumed

$$f = f_0(v) + f_1(v)\cos\psi \qquad (C-10)$$

where ψ is the deflection angle, and considered two cases:

Case 1: For
$$e_2 E\lambda \sqrt{m_1/m_2} \ll kT$$
,
 $f_o = v^{\frac{1}{3}} \frac{m_2}{m_1} (\frac{e_2 E\lambda}{kT})^2 \exp(-\frac{m_2 v^2}{2kT})$,
and $f_1 = \frac{e_2 E\lambda}{kT} f_o$. (C-11)

Case 2:

For
$$e_2 E \lambda \sqrt{m_1/m_2} \gg kT$$
,
 $f_0 = \exp\left\{-\frac{3}{4} \frac{m_2}{m_1} \left(\frac{m_2 v^2}{e_2 E \lambda}\right)^2\right\}$,
 $f_1 = 3\frac{m_2}{m_1} \left(\frac{m_2 v^2}{e_2 E \lambda}\right) f_0$. (C-12)

and

5) Other theoretical distribution functions :

Theoretical distribution functions were given by Morrone (1967, 1968a,b); Johnston (1960,1966) and Carpenter (1961). The distribution function was expanded in terms of Legendre Polynomials where

$$f(v,\theta,\phi) = \sum_{\ell=0}^{\infty} \sum_{n=-1}^{n=+1} f^{\ell}, n(v) P_{\ell}^{n}(\cos\theta) e^{in\phi},$$

 θ and ϕ being polar angles of v. Zero speed neutrals were assumed and the collision cross section was taken to be kv^n , k, n being constants. To the first order, a Maxwellian f was obtained for n=0 and Druyvesteyn's distribution was obtained for n=1.

Some of the proposed electron distribution functions given above are either Maxwellian or of the Maxwellian form. For example, Margenau, Davydov (case 1), and Morrone give distribution functions of this type. In general, these electron distributions may be written as

$$f_e = A \exp(-BC_2^2),$$
 (C-13)

$$f_e = A \exp(\frac{-m_2 C_2^2 B}{2kT})$$
 (C-14)

or

where τ is the electron temperature, and A and B are constants to be determined from the moments of f_e, i.e., from the number density, n; the average velocity, \bar{C}_2 ; or the mean energy $\frac{1}{2}m\bar{C}_2^2$. Two moment equations are needed to determine the two constants, A and B.

Equations (C-13) and (C-14) represent electron distribution functions whose collision integrals can be evaluated analytically by the methods given in this report.

Any of the distribution functions proposed in this appendix may be used to evaluate the collision integral by the Monte Carlo method. Also the molecular collision is not limited to that of rigid spheres.

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