

Interspecies transfer of momentum and energy in disparate-mass gas mixtures

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(Received 29 January 1986; accepted 18 September 1986)

The collision integrals describing the rate of exchange of momentum and tensorial energy between the components in a binary mixture of neutral gases with very different atomic masses are determined for arbitrary values of their two temperatures and velocities, for realistic intermolecular potentials, and allowing for large departures of the heavy gas from equilibrium conditions. In the range of interest where the system is perturbed within times of the order of the slow relaxation time characterizing the transfer of energy between unlike molecules, the light gas distribution function is Maxwellian to lowest order, with corrections given asymptotically in powers of the small parameter m/m_p formed with the ratio of the species molecular masses. Also, provided that the ratio T_p/T between the temperatures of the two gases remains much smaller than m_p/m , the desired collision integrals may be evaluated asymptotically in powers of m/m_p in all generality. The computation is carried out in detail for the case when the interaction between atoms is described by a Lennard-Jones potential. A combination of numerical computations with optimal matching of analytical expressions valid for large and small slip velocities leads to a set of compact formulas which hold for the limits of high and low temperatures and to a general approximate expression for all temperatures.

I. INTRODUCTION

The relative inefficiency of the interchange of kinetic energy in collisions between gaseous molecules of very different masses makes it often necessary to describe their dynamical behavior in terms of two-fluid theories rather than by means of the ordinary equations of hydrodynamics. One important feature of two-fluid theories is the existence of a transfer of momentum and energy between the two species, so that these moments are not conserved for each gas, but only for the mixture as a whole. The form of the coupling terms measuring the rates of momentum and energy transfer has been discussed in the literature in a diversity of works concerned about such topics as free jet expansions,^{1,2} aerodynamic separation of species,³ reactive crossed molecular beam experiments,⁴ etc. A general treatment for the case when the two gases are under near-equilibrium conditions is given by Burgers.⁵

The set of two-fluid governing laws may be obtained straightforwardly by taking moments in the Boltzmann equations describing the evolution of the velocity distribution functions f and f_p for the light and heavy gas, respectively. The following equations are obtained for the heavy species:

$$\partial_t \rho_p + \nabla \cdot (\rho_p \mathbf{U}_p) = 0, \quad (1)$$

$$\partial_t (\rho_p \mathbf{U}_p) + \nabla \cdot (\mathbf{P}_p + \rho_p \mathbf{U}_p \mathbf{U}_p) = -\rho_p \mathbf{b}, \quad (2)$$

$$\partial_t \mathbf{P}_p + \nabla \cdot (2\mathbf{Q}_p + \mathbf{U}_p \mathbf{P}_p) + (\mathbf{P}_p \cdot \nabla) \mathbf{U}_p + [(\mathbf{P}_p \cdot \nabla) \mathbf{U}_p]^T = -\rho_p (\mathbf{E} + \mathbf{E}_{\text{self}}), \quad (3)$$

where the superscript T denotes the transposed tensor ($A_{ij}^T \equiv A_{ji}$) and the hydrodynamic magnitudes, density, mean velocity and pressure tensor $\rho_p, \mathbf{U}_p, \mathbf{P}_p$ are defined based on the mean speed of each individual species rather than the mean mixture velocity:

$$\rho_p = \int m_p f_p d^3 \mathbf{u}_p, \quad (4)$$

$$\rho_p \mathbf{U}_p = \int m_p \mathbf{u}_p f_p d^3 \mathbf{u}_p, \quad (5)$$

$$\mathbf{P}_p = \int m_p (\mathbf{u}_p - \mathbf{U}_p)(\mathbf{u}_p - \mathbf{U}_p) f_p d^3 \mathbf{u}_p, \quad (6)$$

$$\mathbf{Q}_p = \frac{1}{2} \int m_p (\mathbf{u}_p - \mathbf{U}_p)(\mathbf{u}_p - \mathbf{U}_p)(\mathbf{u}_p - \mathbf{U}_p) f_p d^3 \mathbf{u}_p. \quad (7)$$

The same definitions, without subscript, apply to the light gas. Following Burgers,⁵ the coupling terms \mathbf{b} and \mathbf{E} can be written as

$$\rho_p \mathbf{b} = \int m_p f_p (\mathbf{u}_p) d^3 \mathbf{u}_p \mathbf{B}, \quad (8)$$

$$-\rho_p \mathbf{E} = \int m_p f_p (\mathbf{u}_p) d^3 \mathbf{u}_p (\mathbf{\Pi} - (\mathbf{u}_p - \mathbf{U}_p) \mathbf{B} - \mathbf{B}(\mathbf{u}_p - \mathbf{U}_p)), \quad (9)$$

where

$$\mathbf{B}(\mathbf{u}_p) = M \int d^3 \mathbf{g} g g Q_1 f(\mathbf{u}_p - \mathbf{g}), \quad (10)$$

$$\mathbf{\Pi}(\mathbf{u}_p) = M^2 \int d^3 \mathbf{g} g \left(\frac{1}{2} (g^2 \mathbf{I} - 3\mathbf{g}\mathbf{g}) Q_2 + 2\mathbf{g}\mathbf{g} Q_1 \right) f(\mathbf{u}_p - \mathbf{g}), \quad (11)$$

Q_1 and Q_2 are the usual collision cross sections given in terms of the differential scattering cross section $\sigma(\vartheta, g)$ for the heavy-light collisions,

$$Q_i = 2\pi \int \sigma(\vartheta, g) (1 - \cos^i \vartheta) \sin \vartheta d\vartheta, \quad (12)$$

\mathbf{g} is the relative molecular velocity $\mathbf{u}_p - \mathbf{u}$, and M is the small

parameter formed with the masses m and m_p of the light and heavy gas,

$$M \equiv m/(m + m_p).$$

Notice that we have written Eq. (3) for all the components of the stress tensor of the heavy gas. Contracting it with the unit tensor would yield the conservation equation for the thermal energy e , free from the term \mathbf{E}_{self} measuring the rate of change of \mathbf{P}_p caused by heavy-heavy collisions. Only the trace of \mathbf{E} would be of interest in standard two-fluid theories. However, here we will evaluate the full tensor \mathbf{E} because of its importance in the case where the heavy gas is dilute and departs substantially from equilibrium.

As can be seen from Eqs. (8)–(11), the evaluation of \mathbf{b} and \mathbf{E} requires the specification of both velocity distribution functions, as well as the interaction potential between heavy and light molecules, needed to determine the differential scattering cross section.

Different choices for the interaction potential have been used in the literature for neutral gases. Inverse fourth order attractive potentials (i.e., Maxwellian molecules) have been used in a number of works, because the resulting Q_i vary as g^{-1} making expressions (8) and (9) independent of the velocity distribution functions. This assumption, however, leads to an unrealistic description of the transfer terms. A long range *repulsive* interaction decreasing as the inverse sixth power of the distance has been used^{3,6} in an attempt to give a simpler description of the behavior at low temperatures, dominated by the long range *attractive* part of the interaction. A full Lennard–Jones potential has been used by Patch⁴ among others.

When both species are close to equilibrium, the velocity distribution functions can be described by means of the Maxwellian expression to lowest order,⁷ or by the Chapman–Enskog solution to the Boltzmann equation to include first-order corrections in the gradients of the hydrodynamical quantities. Some of these corrections are discussed by Burgers,⁵ using Grad’s 13 moment method. A common procedure to describe nonequilibrium effects is to use an “ellipsoidal Maxwellian” function, which allows for different parallel and perpendicular temperatures.^{2,6} This function is suggested by experimental measurements of the parallel and perpendicular components of molecular speeds of pure gases or mixtures expanding into a vacuum.⁸ Since there is no theoretical foundation for the ellipsoidal function (though it may be produced for the heavy gas on the basis of the present work), the range of validity cannot be assessed. Other approximate fitting expressions for the velocity distribution, such as the drifting Maxwellian or the Hermite polynomial expansion model, are discussed by Patch.⁴

Even when the distribution functions f and f_p are assigned, some other hypotheses can help to simplify the task of performing the coupling integrals. The one adopted most widely consists in linearizing,^{2,6} assuming small mean velocity or temperature differences between the two species; most of the published results are subject to this restriction. In free jet expansions, when ellipsoidal Maxwellian distribution functions are used, the large parallel to transversal temperature ratio can provide further simplifications.⁴ Schwartz and Andres³ relaxed the small slip velocity assumption obtaining

an interpolation formula for the momentum coupling term for the case of an inverse sixth attractive potential [see discussion following Eq. (56)]. Burgers⁵ reports the momentum and energy (scalar) collision integrals for unrestricted velocity differences and unrestricted temperatures in the case of hard elastic spheres and Maxwellian distribution functions.

The present work is motivated by the conditions of our own experimental research and those of many situations of potential industrial interest involving disparate-mass gas mixtures. Typically the light gas is close to equilibrium, while the heavy gas is characterized by a narrow but far from Maxwellian distribution function. Furthermore, the slip velocity is not necessarily small, and the temperatures are such that both the repulsive and the attractive parts of the interaction potential may be important. We shall therefore use the Lennard–Jones interaction potential and will abstain from linearizing in the velocity slip. The standard near-equilibrium road will be used for the assignment of the distribution function f only, while f_p will be described following Bernstein⁹ and Fernandez de la Mora¹⁰ in taking advantage of the large disparity in the masses m and m_p between the two species to develop a systematic perturbation theory in powers of the small parameter m/m_p . Our final expression for the integrals (8) and (9) will be valid to lowest order in m/m_p , although the procedure to incorporate higher-order corrections is sketched. Our results will be limited by the condition that the molar fraction of the heavy gas does not exceed order unity ($n_p \lesssim n$); but such a constraint is satisfied in most situations in which disparate-mass mixtures are of practical relevance.

II. EXPRESSIONS FOR THE INTERSPECIES MOMENTUM AND ENERGY TRANSFER

One of the objectives of this work is to give easily used closed form expressions for the interspecies momentum and energy transfer terms shown in Eqs. (2) and (3). The expressions given in Eqs. (8)–(11) are completely general. Following Bernstein,⁹ the large mass ratio can now be exploited by noticing that, in the particular case where $m \ll m_p$, the characteristic range of values of the heavy gas thermal speed $\mathbf{u}'_p \equiv \mathbf{u}_p - \mathbf{U}_p$ is smaller than that of the light gas $\mathbf{u}' \equiv \mathbf{u} - \mathbf{U}$ by a factor $|T_p m/Tm_p|^{1/2}$, which is much smaller than unity provided that the heavy species temperature does not become much larger than T . As a result, the integration of Eqs. (8) and (9) over the \mathbf{u}_p variable is straightforward: f_p is so narrowly centered at $\mathbf{u}_p = \mathbf{U}_p$ (nearly a Delta function) that \mathbf{B} and $\mathbf{\Pi}$ can only contribute to the integrals (8) and (9) in a small neighborhood of $\mathbf{u}_p = \mathbf{U}_p$. We may thus approximate these functions within the integrand by their Taylor expansion about $\mathbf{u}'_p = 0$ (see Refs. 9 and 10):

$$\mathbf{B}(\mathbf{u}_p) = (1 + \mathbf{u}'_p \cdot \nabla_{\mathbf{u}_p} + \frac{1}{2} \mathbf{u}'_p \mathbf{u}'_p : \nabla_{\mathbf{u}_p} \nabla_{\mathbf{u}_p} + \dots) \mathbf{B}(\mathbf{U}_p), \quad (13)$$

and analogously for $\mathbf{\Pi}(\mathbf{u}_p)$. The integration over \mathbf{u}_p can now be easily performed:

$$\rho_p \mathbf{b} = (\rho_p + \frac{1}{2} \mathbf{P}_p : \nabla_{\mathbf{u}_p} \nabla_{\mathbf{u}_p} + \dots) \mathbf{B}, \quad (14a)$$

$$-\rho_p \mathbf{E} = (\rho_p + \frac{1}{2} \mathbf{P}_p : \nabla_{\mathbf{u}_p} \nabla_{\mathbf{u}_p} + \dots) \mathbf{\Pi} - (\mathbf{P}_p \cdot \nabla_{\mathbf{u}_p} \mathbf{B})^+, \quad (14b)$$

where for a general square mixture the notation $\mathbf{A}^+ \equiv \mathbf{A} + \mathbf{A}^T$ is followed, and the right-hand side terms are evaluated at $\mathbf{u}_p = \mathbf{U}_p$. As we see, f_p enters into Eqs. (14) only through its moments $\rho_p, \mathbf{U}_p, \mathbf{P}_p, \dots$. To first order in \mathbf{u}'_p , Eq. (13) is equivalent to the assumption that the heavy gas distribution function is so narrow that it can be considered a delta function centered in \mathbf{U}_p . In this approximation, \mathbf{u}_p is simply substituted by \mathbf{U}_p in Eqs. (10) and (11). The first correction, proportional to \mathbf{P}_p , takes into account the finite width of f_p and is proportional to the curvature of the \mathbf{B} and Π functions at $\mathbf{u}_p = \mathbf{U}_p$.

A specification of f is now necessary to proceed. Remarkably enough, within the range of parameters of interest, it is possible to determine f by a rigorous expansion in powers of the small quantity m/m_p (see Ref. 10),

$$f = f_0 [1 + O(m/m_p)], \quad (15)$$

where f_0 is the Maxwellian distribution with number density $n = \rho/m$, mean velocity \mathbf{U} , and temperature T . Equation (15) results from the fact that the departures of f from Maxwellian are of the order of the Knudsen number Kn , defined as the ratio between τ_1 (self-collision relaxation time given by the ratio μ/p between its viscosity component and partial pressure) and t_f (fluid dynamic deceleration time $\sim |\mathbf{U}|/|D\mathbf{U}/Dt|$). Furthermore, if τ is the slow relaxation time characteristic of the transfer of energy between two gases, by purely mechanical considerations one has that

$$\tau/\tau_1 \sim m_p/m, \quad (16)$$

in the range where n_p/n is up to order 1. In other words, the relative heavy molecule change of momentum or energy per collision with a light molecule is only a small fraction m/m_p of the relative change in a light gas self-collision.

The point of interest here is that the peculiar relaxation phenomena that make disparate-mass mixtures so interesting do set in when the system is perturbed within a characteristic macroscopic time t_f of the order of the slow relaxation time τ . Defining therefore the interspecies Knudsen number

$$S \equiv \tau/t_f, \quad (17)$$

which is analogous to the Stokes number arising in aerosol dynamics, it results that S will take values of order 1 in the problems that occupy our attention. This same condition,

$$S \sim 1, \quad (18)$$

is what makes two-fluid theories really necessary, since ordinary hydrodynamics would be perfectly adequate to describe the region where $S \ll 1$. Combining now Eqs. (17) and (18) we conclude that

$$\text{Kn} \sim mS/m_p \sim m/m_p \ll 1. \quad (19)$$

Equation (16) is thus confirmed and the light gas distribution function can be considered Maxwellian with errors of the order m/m_p :

$$f(\mathbf{u}) = n(m/2\pi kT)^{3/2} \exp(-|\mathbf{u} - \mathbf{U}|^2/2kT) \times [1 + O(m/m_p)]. \quad (20)$$

Higher-order corrections to Eq. (20) can be carried out systematically in the whole range of concentrations, and will be considered elsewhere.

Using the Maxwellian approximation (20), the differentiation with respect to \mathbf{U}_p in (13) becomes equivalent to a

differentiation with respect to $\xi = \mathbf{U}_p - \mathbf{U}$. At the same time we notice that \mathbf{B} , Π_1 , and Π_2 (where Π_1 and Π_2 are the contributions of Q_1 and Q_2 to Π) are not independent:

$$\Pi_1 = 2M[(kT/m)\nabla_\xi \mathbf{B} + \xi \mathbf{B}], \quad (21)$$

although Eq. (21) is no longer true when higher-order corrections are incorporated in Eq. (20) for f . The ensuing expressions are therefore only valid for the first approximation which takes f to be Maxwellian.

In order to determine \mathbf{B} , Π_1 , and Π_2 , the interaction potential between light and heavy molecules has to be specified. Our choice is the Lennard-Jones potential

$$\varphi(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6], \quad (22)$$

where ϵ and σ are the depth and radial location of the potential well. These two parameters are used to define the following dimensionless variables:

$$T^* = kTM_p/\epsilon, \quad (23)$$

$$\mathbf{T}_p^* = k\mathbf{T}_p/\epsilon, \quad (24)$$

$$\mathbf{v} = \xi/(2kT/m)^{1/2}, \quad (25)$$

$$x = g/(2kT/m)^{1/2}, \quad (26)$$

where $M_p = m_p/m_0$, $m_0 = m + m_p$, and \mathbf{T}_p is the tensor of temperatures $\mathbf{T}_p \equiv m_p \mathbf{P}_p / k\rho_p$. Notice a slight variation in the normalization of T^* with respect to the expression $T^* = kT/\epsilon$ given by Hirschfelder *et al.*¹¹ The difference results from the product of two Maxwellian functions (one for each component) present in their treatment, whereas only one Maxwellian function is involved here because f_p is introduced by perturbation around a Delta rather than a Gaussian function. If terms of order m/m_p are neglected, the difference between the two normalizations disappears, but definition (23) must be used in a higher order theory. Before substituting the normalized variables, the integration in Eqs. (10) and (11) can be carried out over all the \mathbf{g} directions by choosing the polar axis in the direction of ξ , that is, $\mathbf{e}_3 = \xi/\xi$. Then

$$d^3\mathbf{g} = g^2 dg d\Omega_g,$$

where $d\Omega_g$ is the solid angle differential. Integrating by parts over $d\Omega_g$ leads to the following normalized expressions which depend only on three scalar functions:

$$\Pi_1^* = [I_B(\mathbf{e}_1\mathbf{e}_1 + \mathbf{e}_2\mathbf{e}_2)/2v + I_{\pi_1}\mathbf{e}_3\mathbf{e}_3]T^{*3/2}, \quad (27)$$

$$\Pi_2^* = (\mathbf{I} - 3\mathbf{e}_3\mathbf{e}_3)I_{\Pi_2}T^{*3/2}, \quad (28)$$

$$\mathbf{B}^* = T^*I_B\mathbf{e}_3, \quad (29)$$

where $\Pi_i^* = \Pi_i/K_{\Pi}$ and $\mathbf{B}^* = \mathbf{B}/K_B$, with $K_B = 8n\pi^{1/2}\sigma^2\epsilon/m_p$, $K_{\Pi} = 2(2\epsilon mm_0^{-1}m_p^{-1})^{1/2}K_B$, (30)

and the following integrals have been introduced:

$$I_B = \int_0^\infty x^4 e^{-(x^2+v^2)} Q_1^*(xT^{*1/2}) \left(\frac{\cosh \alpha}{\alpha} - \frac{\sinh \alpha}{\alpha^2} \right) dx, \quad (31)$$

$$I_{\Pi_2} = \int_0^\infty x^5 e^{-(x^2+v^2)} Q_2^*(xT^{*1/2}) \times \left(\frac{\sinh \alpha}{\alpha} - \frac{3 \cosh \alpha}{\alpha^2} + \frac{3 \sinh \alpha}{\alpha^3} \right) dx, \quad (32)$$

$$I_{\Pi_1} = \frac{1}{2} \frac{\partial I_B}{\partial v} + v I_B, \quad (33)$$

and $\alpha = 2vx$. Expression (33) giving I_{Π_1} as a function of I_B is only convenient when using the analytic approximate limits of the I integrals determined below. When a numerical approach is adopted, it is better to use the full expression of I_{Π_1} as an integral over x to avoid numerical differentiation.

Substituting these results into Eqs. (14), (15) and defining $\mathbf{b}^* = \mathbf{b}/K_B$ and $\mathbf{E}^* = \mathbf{E}/K_{\Pi}$, we obtain

$$\mathbf{b}^* = (1 + \frac{1}{4} M T^{*-1} T_p : \nabla_v \nabla_v + \dots) \mathbf{B}^*, \quad (34)$$

$$-\mathbf{E}^* = (1 + \frac{1}{4} M T^{*-1} T_p : \nabla_v \nabla_v + \dots) (\Pi_1^* + \Pi_2^*) - \frac{1}{4} [T^{*-1/2} (\mathbf{T}_p^* \cdot \nabla_v) \mathbf{B}^*]^+. \quad (35)$$

Two alternative forms for \mathbf{E}^* can be deduced from the dimensionless form of Eq. (21),

$$\Pi_1^* = T^{*1/2} (v \mathbf{B}^* + \frac{1}{2} \nabla_v \mathbf{B}^*), \quad (36)$$

leading to the expressions

$$-\mathbf{E}^* = \frac{1}{2} T^{*-1/2} (T^{*-1/2} \Pi_1^* \cdot (T^* \mathbf{I} - \mathbf{T}_p^*) + \mathbf{T}_p^* \cdot v \mathbf{B}^*)^+ + \Pi_2^*, \quad (37a)$$

or

$$-\mathbf{E}^* = \frac{1}{4} T^{*-1/2} ((T^* \mathbf{I} - \mathbf{T}_p^*) \cdot \nabla_v \mathbf{B}^*) + T^{*1/2} v \mathbf{B}^* + \Pi_2^*, \quad (37b)$$

and

$$\mathbf{b}^* = \mathbf{B}^*, \quad (38)$$

valid to first order in M . As will be seen later, the last two terms in both expressions for \mathbf{E}^* are quadratic in v and would not enter in a theory linear in v . Conversely, these terms become dominant for large values of the slip velocity v . Notice that although the term \mathbf{E}^* has a complicated dependence on \mathbf{v} , its dependence on \mathbf{T}_p^* is linear. The second terms in Eqs. (37) are always positive, heating up the gas indefinitely in the direction of motion as soon as $v \neq 0$. This effect is counterbalanced by the first term, which tends to bring light and heavy gas temperatures closer. The term Π_2^* is traceless and gives no contribution to the total internal energy, leaving the average heavy temperature $T_p \equiv \text{Trace}(\mathbf{T}_p)/3$ unaffected. Here Π_2^* is proportional to $v^2 \mathbf{I} - 3v\mathbf{v}$, thus tending to extract heat from the direction of motion to put it into the transverse direction. The influence of the different terms will be illustrated in an example (Sec. V.).

III. ASYMPTOTIC FORMS OF THE TRANSFER INTEGRALS

The integrals (31)–(33) can be approximated analytically for the limiting cases $v \ll 1$ or $1 \ll v$, when the slip velocity $U_p - U$ is much smaller or much larger than the light gas thermal speed $(2kT/m)^{1/2}$. In the first case ($v \ll 1$), $\cosh 2vx$, $\sinh 2vx$, and $\exp(-v^2)$ can be expanded in a Taylor series about $v = 0$, with the following results in terms of the Ω^* integrals of Hirschfelder *et al.*¹¹:

$$\Omega_{lm}^*(T^*) = \frac{2}{(m+1)!} \int_0^\infty x^{2m+3} e^{-x^2} Q_l^*(x T^{*1/2}) dx, \quad (39)$$

$$I_B = v \left[\frac{4}{3} \Omega_{11}^* + (-\frac{4}{3} \Omega_{11}^* + \frac{4}{3} \Omega_{12}^*) v^2 + (\frac{4}{3} \Omega_{11}^* - \frac{4}{3} \Omega_{12}^* + \frac{16}{33} \Omega_{13}^*) v^4 + \dots \right], \quad (40)$$

$$I_{\Pi_2} = v^2 \left[\frac{4}{3} \Omega_{22}^* + (-\frac{4}{3} \Omega_{22}^* + \frac{32}{33} \Omega_{23}^*) v^2 + (\frac{2}{5} \Omega_{22}^* - \frac{32}{35} \Omega_{23}^* + \frac{32}{63} \Omega_{24}^*) v^4 + \dots \right], \quad (41)$$

from which I_{Π_1} follows immediately.

For most values $v < 1$ the first term gives a very good approximation (Fig. 1). For instance, for $v = 1$, $T^* = 1$, the errors in I_B and I_{Π_2} taking only the first term are, respectively, 2% and 0.4%. For the same temperature, using the three first terms of the expansion, I_B and I_{Π_2} can be evaluated for v as large as 2 with errors below 5%.

For large values of v the integrals (31)–(33) can be rearranged into the form

$$I = \int_{-v}^\infty e^{-t^2} f_1(t, v) dt + \int_v^\infty e^{-t^2} f_2(t, v) dt. \quad (42)$$

A Hermite quadrature gives a good approximation. If $\{(t_k, w_k)\}$ is the set of abscissas and weight factors for Hermite integration, tabulated in Abramowitz *et al.*,¹² the integral sum (42) can be expressed as

$$I \simeq \sum_{t_k > -v} f_1(t_k) w_k + \sum_{t_k' > v} f_2(t_k') w_k. \quad (43)$$

This series gives a very accurate result for moderate to large v . As shown in Fig. 1, the domains (where the small and large v approximations are accurate to 5%) do overlap, so that the numerical integration is only required when a greater accuracy is necessary.

For very large v , the Laplace method,¹³ equivalent to the infinite sum of the Hermite series, yields the following approximations:

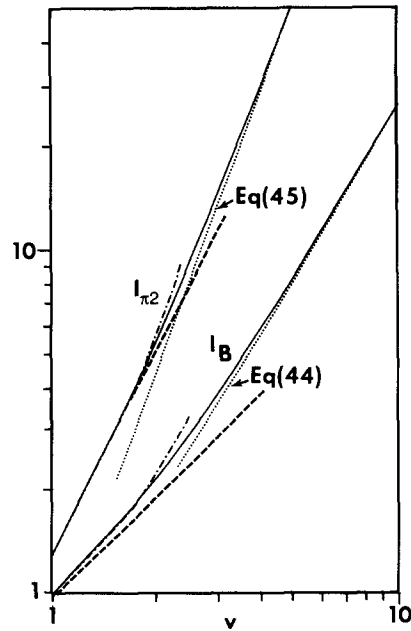


FIG. 1. Integrals I_B and I_{Π_2} as a function of v for $T^* = 1$: — numerical computation from Eqs. (31) and (32); - - - first term from expansions (40) and (41); - · - · - three first terms of expansions (40) and (41); ····· high velocity slip limit, Eqs. (44) and (45). The results from Hermite integration only differ noticeably from the numerical computation for low velocities and are thus invisible here.

$$I_B = \frac{1}{4}\pi^{1/2}v^2Q_1^*(vT^{*1/2}), \quad (44)$$

$$I_{\Pi_2} = \frac{1}{4}\pi^{1/2}v^3Q_2^*(vT^{*1/2}), \quad (45)$$

$$I_{\Pi_1} = vI_B, \quad (46)$$

which are very accurate for $v > 10$.

A further simplification can be made by assuming that T^* is very large or very small, which has the physical meaning of making repulsive or attractive forces dominant in the Lennard-Jones potential.

For $1 \ll T^*$, the molecules behave as point centers of repulsion and the approximation given by Hirschfelder *et al.*¹⁴ for the collision cross sections can be applied:

$$Q_i = 2\pi(\delta d / (\mu g^2/2))^{2/\delta} A_i(\delta), \quad (47)$$

where $\delta = 12$, $\mu = m_p M$, and the coefficients A_i are given by Hirschfelder *et al.*¹⁴ and $d = 4\epsilon\sigma^{12}$. The resulting limiting forms for Q_i^* and Ω_{ij}^* can be substituted in the lower order approximations for I_B and I_{Π_2} at $1 \ll v$ and $v \ll 1$.

For the opposite limit $T^* \ll 1$, long range attraction prevails over repulsive forces. However, a strictly attractive inverse-sixth potential is inconsistent because low energy collisions would result in molecules merging. The repulsive part has to be retained in a portion of the g range. But, since the main contribution is a result of the attractive sixth power law, a formula similar to Eq. (47) is to be expected:

$$Q_i' = 2\pi(\delta d' / (\mu g^2/2))^{2/\delta} A_i'(\delta), \quad (48)$$

where $\delta = 6$ and $d' = 4\epsilon\sigma^6$. This $A_i'(\delta)$ may be estimated from the asymptotic behavior at small values of g and T^* ,

respectively, of the functions Q_i^* and Ω_{is}^* tabulated in the literature for the Lennard-Jones potential. Our estimated values, based on the tabulation of Ferziger *et al.*¹⁵ for the Ω_{is}^* at low T^* and the curves representing Q_i^* for low g in Hirschfelder *et al.*,¹¹ are $A_1'(6) = 0.429$, $A_2'(6) = 0.328$, while the asymptotic trend of these computations agrees well with Eq. (48) particularized with $\delta = 6$. This fitting approach yields analytic expressions for Q_i^* and Ω_{is}^* , which can be inserted in Eqs. (40), (41), (44), and (45). Some references^{3,6} incorrectly adopt for $A_i'(\delta)$ the values given by Hirschfelder *et al.*¹¹ for the inverse-sixth interaction of point centers of repulsion [$A_1(6) = 0.306$, $A_2(12) = 0.283$], even though attraction prevails at low temperatures. Their choice leads to important differences with our results (compare Eqs. (50b) and (56)). An alternative approach in the low temperature region would be to use the Sutherland model which represents the molecules as rigid spheres surrounded by an inverse sixth attractive potential.

A. Interpolation formulas for I and Π

For each case ($T^* \ll 1$ or $1 \ll T^*$) we have obtained interpolation formulas covering the full range of values of v with expressions of the type

$$I = I_0[1 + (I_\infty/I_0)^\alpha]^{1/\alpha}, \quad (49)$$

where $I_0 = I(v \ll 1)$ and $I_\infty = I(1 \ll v)$, while α can be determined by minimizing the error relative to the numerical solution. In this way, the following high and low temperature fitting expressions are obtained:

$$I_B = \begin{cases} 0.7573 v T^{*-1/6} (1 + 0.4596 v^2)^{1/3}, & 1 \ll T^* \text{ or } 1 \ll v T^{*1/2}, \\ 1.2467 v T^{*-1/3} (1 + 0.4760 v^2)^{1/6}, & T^* \ll 1 \text{ and } v T^{*1/2} \ll 1, \end{cases} \quad (50a)$$

$$I_{\Pi_2} = \begin{cases} 1.040 v^2 T^{*-1/6} (1 + 0.312 v^2)^{1/3}, & 1 \ll T^* \text{ or } 1 \ll v T^{*1/2}, \\ 1.504 v^2 T^{*-1/3} (1 + 0.322 v^2)^{1/6}, & T^* \ll 1 \text{ and } v T^{*1/2} \ll 1. \end{cases} \quad (51a)$$

$$I_{\Pi_1} = \begin{cases} 0.7573 v T^{*-1/6} (1 + 0.4596 v^2)^{1/3}, & 1 \ll T^* \text{ or } 1 \ll v T^{*1/2}, \\ 1.2467 v T^{*-1/3} (1 + 0.4760 v^2)^{1/6}, & T^* \ll 1 \text{ and } v T^{*1/2} \ll 1. \end{cases} \quad (51b)$$

A similar expression for I_{Π_1} follows from Eq. (33). Upon direct substitution in Eqs. (27)–(29), analytical expressions of Π_i^* and \mathbf{B}_i^* are obtained. A plot of I_B and I_{Π_2} in the low and high temperature limits is presented in Figs. 2

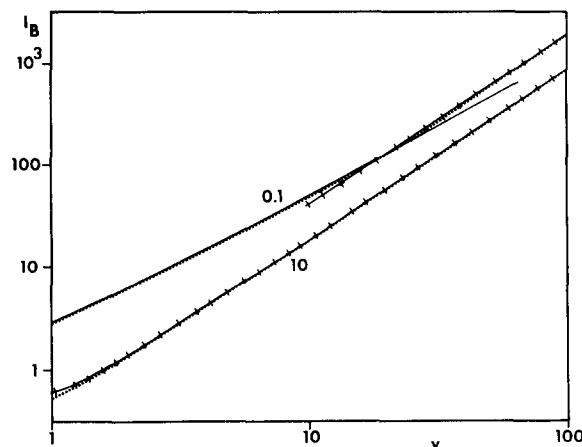


FIG. 2. I_B as a function of v for high ($T^* = 10$) and low ($T^* = 0.1$) temperatures: numerical computation from Eq. (31); + + + Eq. (50a); — Eq. (50b).

and 3 where the numerical computation is seen to be practically indistinguishable from the correlations (50) and (51).

The similarity of the terms within parentheses in Eqs. (50a) and (50b) and in Eqs. (51a) and (51b) is not accidental. In effect, using the asymptotic expressions given by Hirschfelder *et al.*¹⁴ for the Ω_{is}^* integrals, a recurrence formula can be obtained:

$$\frac{\Omega_{is+1}^*}{\Omega_{is}^*} = \frac{\Gamma(s+3-2/\delta)(s+1)!}{\Gamma(s+2-2/\delta)(s+2)!} = 1 - \frac{2}{\delta(s+2)},$$

where δ is the order of the interaction potential, which according to previous considerations can be taken to be 6 at low temperatures and 12 in the opposite limit. This permits us to write expansions (40) and (41) in a simplified fashion for these two limits:

$$\frac{I_B}{I_{B_0}} = \begin{cases} 1 + \frac{2}{15}v^2 - \frac{4}{315}v^4 + \cdots, & \delta = 12, \\ 1 + \frac{1}{15}v^2 - \frac{1}{126}v^4 + \cdots, & \delta = 6, \end{cases} \quad (52a)$$

$$\frac{I_{\Pi_2}}{I_{\Pi_2_0}} = \begin{cases} 1 + \frac{2}{21}v^2 - \frac{4}{567}v^4 + \cdots, & \delta = 12, \\ 1 + \frac{1}{21}v^2 - \frac{5}{1134}v^4 + \cdots, & \delta = 6, \end{cases} \quad (52b)$$

$$\frac{I_{\Pi_1}}{I_{\Pi_1_0}} = \begin{cases} 1 + \frac{2}{21}v^2 - \frac{4}{567}v^4 + \cdots, & \delta = 12, \\ 1 + \frac{1}{21}v^2 - \frac{5}{1134}v^4 + \cdots, & \delta = 6, \end{cases} \quad (53a)$$

$$\frac{I_{\Pi_2}}{I_{\Pi_2_0}} = \begin{cases} 1 + \frac{2}{21}v^2 - \frac{4}{567}v^4 + \cdots, & \delta = 12, \\ 1 + \frac{1}{21}v^2 - \frac{5}{1134}v^4 + \cdots, & \delta = 6, \end{cases} \quad (53b)$$

where I_{B_0} and $I_{\Pi_2_0}$ are the first terms of expansions (40) and (41). Similar expressions can be obtained by binomial ex-

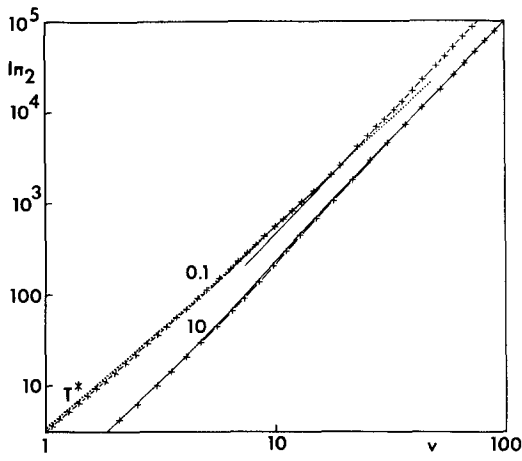


FIG. 3. I_{II_2} as a function of v for high ($T^* = 10$) and low ($T^* = 0.1$) temperatures: — x — x — numerical computation from Eq. (32); Eq. (51a); — Eq. (51b).

pansion of the fitting equations (50) and (51):

$$\frac{I_B}{I_{B_0}} = \begin{cases} 1 + 0.1532 v^2 + \dots, & 1 \ll T^* \text{ or } 1 \ll v T^{*1/2}, \\ 1 + 0.0793 v^2 + \dots, & T^* \ll 1 \text{ and } v T^{*1/2} \ll 1, \end{cases}$$

$$\frac{I_{II_2}}{I_{II_2_0}} = \begin{cases} 1 + 0.104 v^2 + \dots, & 1 \ll T^* \text{ or } 1 \ll v T^{*1/2}, \\ 1 + 0.0537 v^2 + \dots, & T^* \ll 1 \text{ and } v T^{*1/2} \ll 1, \end{cases}$$

whose coefficients differ from those of Eqs. (52) and (53) in a range of 9% to 16%. This shows that if the fitting formulas were perfectly accurate in the low v region, the terms within parentheses in Eq. (50a) and (50b) and in Eq. (51a) and (51b) would be exactly coincident. In any case, the similarity between the terms within parentheses observed in Eqs. (50) and (51) permits us to rewrite these expressions in the approximate form:

$$T^* I_B = \begin{cases} 0.7573 w x^{1/3}, & x \gg 1, \\ 1.2467 w x^{1/6}, & x \ll 1, \end{cases}$$

$$T^{*3/2} I_{II_2} = \begin{cases} 1.040 w^2 y^{1/3}, & y \gg 1, \\ 1.504 w^2 y^{1/6}, & y \ll 1, \end{cases}$$

where $w = v T^{*1/2}$, $x = T^* + 0.4678 w^2$, and $y = T^* + 0.3165 w^2$. The definition of x and y is obtained by averaging the parenthesis terms in Eqs. (50) and (51). The former expressions suggest writing I_B and I_{II_2} in the following form:

$$T^* I_B = 1.2467 w x^{1/6} f(x), \quad (54a)$$

$$T^{*3/2} I_{II_2} = 1.504 w^2 y^{1/6} g(y), \quad (54b)$$

where f and g are undetermined functions subject to the conditions

$$f \rightarrow 1 \text{ for } x \rightarrow 0 \quad \text{and} \quad g \rightarrow 1 \text{ for } y \rightarrow 0,$$

$$f \rightarrow 0.6074 x^{1/6} \text{ for } x \rightarrow \infty \quad \text{and} \quad g \rightarrow 0.6915 y^{1/6} \text{ for } y \rightarrow \infty.$$

Numerical computation confirms that indeed, the functions f and g are approximately independent of the variable w . In Figs. 4 and 5, $T^* I_B / (1.2467 w x^{1/6})$ and $T^{*3/2} I_{II_2} / (1.504 w^2 y^{1/6})$ are represented as functions of x and y , respectively, for different values of v . It can be seen that, provided v does not become too large, the curves fall together. Functions f and g can be fitted from numerical results by using an interpolation formula of the type

$$[1 - A(1 - e^{-cx^2})x^a + Bx^b]^{1/(6b)}.$$

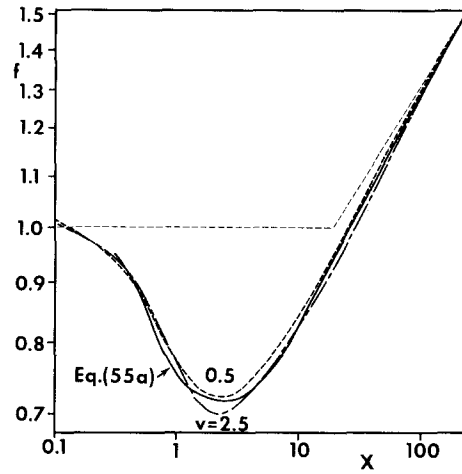


FIG. 4. $T^* I_B / (1.2467 w x^{1/6})$ as a function of $x = T^* + 0.4678 w^2$ for different values of v . Results are approximately independent of v so that a single curve can be fitted [Eq. (55a)].

In this expression, only B is given (from the conditions at infinity), so that the four parameters A, a, b and c are unknown. This multiple degree of freedom optimization problem can be easily addressed with the particular expression chosen, because the search for a solution can be done in two stages: first, the fitting function is forced to go through the minimum point of the numerically obtained curves in Figs. 4 and 5. In these points, the factor $1 - e^{-cx^2}$ can be approximated by unity, so that the relation dependence between A , a , and b can be explicitly derived, provided that b is chosen to be the free parameter. Once that a and A are known as a function of b , b is chosen so as to fit the large x region of the curve, where c can be ignored. Next, the convenient c , to match with the rest of the curve, is selected.

Our results for f and g are

$$f(x) = [1 - 0.8794(1 - e^{-4.25x^2})x^{0.1271} + 0.0502x]^{1/6}, \quad (55a)$$

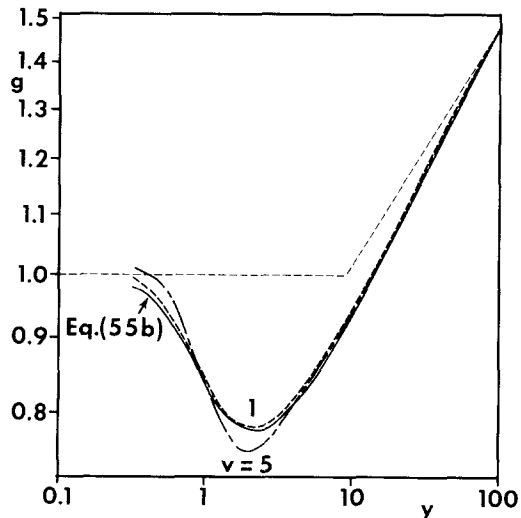


FIG. 5. $T^{*3/2} I_{II_2} / (1.504 w^2 y^{1/6})$ as a function of $y = T^* + 0.3165 w^2$ for $v = 1$ and $v = 5$. A single curve, given in Eq. (55b), is fitted as an approximation for general w .

$$g(y) = [1 - 0.8414(1 - e^{-2.5y^2})y^{0.2255} + 0.0876y^{1.1}]^{1/6.6}. \quad (55b)$$

Equations (54) and (55), represented in Figs. 4 and 5, provide a general expression of the transfer integrals for unrestricted T^* and v . Notice, however, that the approximation becomes poorer in the vicinity of the minimum point for large v ; in such cases, Eqs. (44) and (46) can be more convenient. However, in most physical problems, v does not exceed the value $[\gamma/(\gamma - 1)]^{1/2} \sim 1.5$, so that Eqs. (55a) and (55b) are very suitable.

B. Comparison with previous work

A correlation similar to (50b) has been used by Schwartz and Andres³ for I_B in the case $T^* \ll 1$, $vT^{*1/2} \ll 1$. In our notation their expression reads

$$I'_B = 0.8848 vT^{*-1/3} (1 + 0.4744 v^2)^{1/6}, \quad (56)$$

which differs from Eq. (50b) only in the value of the leading coefficient. The difference (40%) is caused by their use of the repulsive inverse-sixth constant $A_1(6)$ to account for the long range attractive interaction constant which has been called $A'_1(6)$ in the present work.

The low temperature expression (51) for I_B can also be compared to Burgers'⁵ calculation of the momentum transfer integral for unrestricted velocity differences, performed under the assumption of hard elastic spheres. This model can roughly describe low-medium temperature range systems. In our notation,

$$I'_B = (2v/3) [(3\pi^{1/2}/8)(v + v^{-1} - v^{-3}/4) \times \operatorname{erf} v + \frac{3}{8}(1 + v^{-2}/2)e^{-v^2}], \quad (57)$$

which for the limiting cases $v \ll 1$ and $v \gg 1$, respectively, becomes

$$I'_{B_0} = 2v/3, \quad I'_{B_\infty} = \pi^{1/2}v^2/4. \quad (58)$$

Our own results are

$$I_{B_0} = (2v/3)\Omega_{11}^*(T^*), \quad I_{B_\infty} = (\pi^{1/2}v^2/4)Q_1^*(T^{*1/2}v). \quad (59)$$

This is consistent with the normalization adopted following Hirschfelder *et al.*,¹¹ which reduces Ω_{ii} and Q_i by dividing them by the corresponding rigid sphere values. Consequently, Eq. (58) can be derived from Eq. (59) by simply setting $\Omega_{11}^* = Q_1^* = 1$.

We can compare Burgers' energy transfer term (scalar) with our resulting energy transfer tensor by setting $\mathbf{T}_p^* = T_p^*\mathbf{I}$ and considering the trace of Eq. (37),

$$-E^* \equiv -\operatorname{Trace}(\mathbf{E}^*)/3 = (T^{*1/2}/3) \times [(I_B/v + (\partial I_B/\partial v)/2)(T^* - T_p^*) + vI_B T^*]. \quad (60)$$

The corresponding expression in Burgers' equation (15.15) is

$$-E^{*'} = (T^{*1/2}/3) [(\pi^{1/2}(v + v^{-1}/2)\operatorname{erf} v + e^{-v^2}) \times (T^* - T_p^*)/2 + vI'_B T^*], \quad (61)$$

where I'_B is given by Eq. (57). Low and high velocity limits for Burgers' expression can again be obtained by setting Ω_{11}^* and Q_1^* equal to 1 in our results. For $v \ll 1$,

$$-E_0^* = T^{*1/2}\Omega_{11}^*(T^*)(T^* - T_p^*)/3. \quad (62)$$

For $1 \ll v$, the second term in (60), which represents the dissipation of energy connected with the resistance or drag force caused by the transfer of momentum from the light to the heavy species [$T^{*1/2}v\mathbf{B}^*$ in Eq. (37b)], prevails over the term proportional to the difference of temperatures:

$$-E_\infty^* = \pi^{1/2}v^3T^{*3/2}Q_1^*(vT^{*1/2})/12. \quad (63)$$

As it was pointed out, Eqs. (60)–(63) were obtained assuming $\mathbf{T}_p^* = T_p^*\mathbf{I}$. This condition is quite restrictive, since according to our temperature tensor equations, large differences in the parallel and perpendicular components of temperature are to be expected when $1 \ll v$. Therefore, for unrestricted v , \mathbf{T}_p^* should be allowed to be a general tensor. The corresponding expression for E^* is obtained by contracting Eq. (37a) and dividing by 3:

$$-E^* = \frac{1}{3}[T^{*-1}\Pi_{11}:(T^*\mathbf{I} - \mathbf{T}_p^*) + T^{*-1/2}\mathbf{T}_p^*:v\mathbf{B}^*]. \quad (64)$$

In the particular limit $v \ll 1$ Eq. (62) remains valid even when the heavy gas is far from equilibrium, provided that we define $T_p^* = \operatorname{Trace}(\mathbf{T}_p^*)/3$. For v of order unity or larger Eqs. (60) and (64) differ considerably because E^* depends separately on the components of the heavy species temperature tensor, \mathbf{T}_p^* :

$$-E^* = (T^{*1/2}/3)[I_B(2T^* - T_{p_1}^* - T_{p_2}^*)/(2v) + I_{\Pi_1}(T^* - T_{p_1}^*) + T_{p_1}^*I_B v]. \quad (65)$$

For large v , the first term in the right-hand side becomes negligible and given that $I_{\Pi_1} \rightarrow vI_B$ as $v \rightarrow \infty$, the same limiting form given in (63) is formally recovered. However, this cancellation of $I_B v$ and I_{Π_1} is unrealistic because for large v , $T_{p_1}^*$ (the component of \mathbf{T}_p^* along the slip direction) will become very large and amplify the small difference $(I_B v - I_{\Pi_1})$ making it as important as the other terms. Therefore the expressions involving an average heavy gas temperature can only be used in the low slip velocity limit.

IV. HIGHER-ORDER CORRECTIONS AND RANGE OF VALIDITY

The expansion in powers of $\mathbf{u}_p - \mathbf{U}_p$, which gave rise to the series in (14) and (15) or, in dimensionless form, in (34) and (35), becomes poorer as the ratio of the widths of the two distribution functions ceases to be large. Inspection of the dimensionless expansion provides a criterion for the convergence of the series:

$$T_p^* \ll T^*/M. \quad (66)$$

For large values of v , the range of convergence is even broader, as can be seen from the order of magnitude of $\mathbf{P}_p \cdot \nabla_v \nabla_v$:

$$T_p^* \ll v^2 T^*/M. \quad (67)$$

As T_p^* grows closer to the limit value given in (66) and (67), the importance of the next-order correction in M becomes greater. This additional term can easily be introduced by carrying out the direct differentiation indicated in Eqs. (34) and (35), which is straightforward given the simple form of correlations (50). In this way, analytic expressions for the

high and low temperature ranges are obtained; they will not be included here because of their complexity. Notice however that a systematic theory including first-order corrections in M must incorporate our modification in the definition of T^* [Eq. (23)]. It also has to account for the departure of the distribution function f from a Maxwellian resulting from the nonhomogeneity of the velocity and temperature fields.

Under the assumption of number density dilution, $n_p \ll n$, the kinetic influence of the heavy gas on the light gas distribution function f can be neglected, so that f can be described in terms of the pure gas Chapman-Enskog solution.¹⁶ If we also approximate the solutions of the integral equations appearing in the theory by the first term in their Sonine polynomial expansion, we may write

$$f(\mathbf{u}) = n(2\pi kT/m)^{-3/2} e^{-c^2} [1 - \epsilon \cdot \mathbf{c}(c^2 - \frac{5}{2}) - \mathbf{K} : \mathbf{c}\mathbf{c}], \quad (68)$$

where $\mathbf{c} = (\mathbf{u} - \mathbf{U})/(2kT/m)^{1/2}$, ϵ is the dimensionless temperature gradient,

$$\epsilon = (3\mu/2p)(2kT/m)^{1/2} \nabla \ln T, \quad (69)$$

and \mathbf{K} is the dimensionless, symmetrized, and traceless velocity gradient tensor,

$$\mathbf{K} = (\mu/p)[\nabla \mathbf{U} + (\nabla \mathbf{U})^T - 2/3 \mathbf{I}(\nabla \cdot \mathbf{U})]. \quad (70)$$

Using the expression for the cross collision operator given by Fernandez de la Mora and Mercer¹⁷ for the limit of small v , we obtain the following expressions, valid to first order in M and v :

$$\mathbf{B}^* = (T^*/3) [2v \cdot \{\Omega_{11}^* \mathbf{I} - \frac{2}{3} (3\Omega_{12}^* - \frac{5}{2} \Omega_{11}^*) \mathbf{K}\} + \epsilon (3\Omega_{12}^* - \frac{5}{2} \Omega_{11}^*)], \quad (71)$$

$$- \mathbf{E}^* = (T^{*1/2}/3) (\Omega_{11}^* \mathbf{I} - \frac{6}{5} \Omega_{12}^* \mathbf{K}) \cdot (T^* \mathbf{I} - T_p^*) + T^{*1/2} (-\frac{1}{3} \Omega_{11}^* \mathbf{T}_p^* + \frac{2}{3} \Omega_{22}^* T^* \mathbf{I}) \cdot \mathbf{K}, \quad (72)$$

while the full nonlinear v dependence of \mathbf{B}^* and \mathbf{E}^* on the new \mathbf{K} and ϵ terms could be evaluated similarly as done before. We note that even in the absence of velocity slip there is an acceleration \mathbf{B}^* leading to the drift of heavy molecules down temperature gradients caused by the term proportional to ϵ in Eq. (71). This thermal force degenerates into the thermal diffusion effect under near equilibrium conditions. In these conditions, the \mathbf{K} term does not contribute to the net force, but it does make a contribution to the energy transfer term \mathbf{E}^* . The order of magnitude of this contribution is only a fraction M of that of the analogous compression heating terms $\mathbf{P}_p \cdot (\nabla \cdot \mathbf{U}_p)$, $(\mathbf{P}_p \cdot \nabla) \mathbf{U}_p$ in the left-hand side of Eq. (3).

V. HEAVY GAS PENETRATION INTO A LIGHT GAS AT REST

In this section, the expressions obtained previously will be applied to the study of heavy molecules penetrating into a stagnant light gas. The impingement of fast heavy molecules on a target gas at rest is an approximate model for different phenomena occurring in gas mixture flows. For instance, the shock layer that develops in front of a probe or any other obstacle immersed in a supersonic field can roughly be considered a light gas stagnation zone through which the heavy

molecules keep a large fraction of their former speed, while their temperatures may overshoot significantly above the gas temperature.

The starting point is Eqs. (1)–(3), where two assumptions are introduced: first, the flow is assumed to be unidirectional, along the z direction; and, second, the pressure tensor is neglected in the momentum equation and the heat flux in the energy equation. For \mathbf{P} and \mathbf{Q} to be negligible, respectively, in Eqs. (2) and (3), it is necessary that

$$kT_p \ll m_p U_p^2, \quad (73)$$

which turns out to be a hypersonic condition stating that the Mach number of the heavy species has to be much larger than unity. For simplicity's sake the constraint $\rho \ll \rho_p$ (small heavy gas mass loading) is added, so that the self-collision energy tensor transfer term [\mathbf{E}_{self} in Eq. (3)] can be neglected.

With these restrictions Eqs. (1)–(3) become

$$U_p U_{pz} = b, \quad (74)$$

$$(k/m_p) U_p T_{\parallel pz} = E_{\parallel} - 2T_{\parallel p} k U_{pz}/m_p, \quad (75)$$

$$(k/m_p) U_p T_{\perp pz} = E_{\perp}, \quad (76)$$

where $b = |\mathbf{b}|$, and $T_{\parallel p}$, E_{\parallel} and $T_{\perp p}$, E_{\perp} , are, respectively, the components along the z direction and in any perpendicular direction of the temperature and energy transfer terms. Equations (74)–(76) can be normalized by defining

$$v = U/U_0, \quad \tau = t/t_0, \quad x = z/L_0, \quad (77)$$

where $U_0 = (2\epsilon T^*/\mu)^{1/2}$, so that the definition of v agrees with that given in Eq. (25), $t_0 = U_0/K_B$, and $L_0 = t_0 U_0$. The variable τ will be used later. Notice how the deceleration scale is determined by the interaction potential. Denoting $d/dx = '$, Eqs. (74)–(76) become

$$vv' = B^*, \quad (78)$$

$$vT_{\parallel p}' + 2T_{\parallel p}^* v' = -4T^{*-1/2} E_{\parallel}^*, \quad (79)$$

$$vT_{\perp p}' = -4T^{*-1/2} E_{\perp}^*, \quad (80)$$

where B^* is given by (29) and

$$-E_{\parallel}^* = [I_{\parallel 1} (T^* - T_{\parallel p}^*) + vT_{\parallel p}^* I_B - T^* I_{\parallel 2}/3] T^{*1/2}, \quad (81)$$

$$-E_{\perp}^* = [(I_B/2v)(T^* - T_{\perp p}^*) + I_{\perp 2} T^*/6] T^{*1/2}. \quad (82)$$

This system is to be solved given initial conditions for the impinging heavy gas:

$$v = v_0, \quad T_{\perp p}^* = T_{\perp p0}^*, \quad T_{\parallel p}^* = T_{\parallel p0}^*, \quad \text{at } x = 0. \quad (83)$$

A. Limit $v_0 \ll 1$

If v_0 is small enough, the approximations (40) and (41) hold and we are left with

$$v' = -2\Omega_{11}^* T^*/3, \quad (84)$$

$$T_{\parallel p}^{*'} = 4T^{*2} \Omega_{11}^*/(3v), \quad (85)$$

$$T_{\perp p}^{*'} = 4T^* \Omega_{11}^* (T^* - T_{\perp p}^*)/(3v), \quad (86)$$

which can easily be solved to yield

$$V = 1 - x/(S'v_0), \quad (87)$$

$$T_{\parallel p}^* = T_{\parallel p0}^* - 2T^* \ln V, \quad (88)$$

$$T_{\perp p}^* = T^* + (T_{\perp p0}^* - T^*) V^2, \quad (89)$$

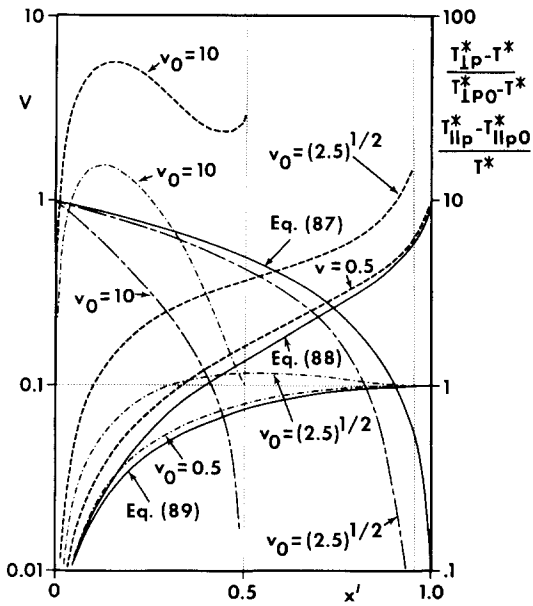


FIG. 6. Velocity and temperature tensor evolution as a function of x' [depth normalized with the linear theory stopping distance $x/(S'v_0)$] for $T^* = 10$ and different initial velocities v_0 . The limiting solution for small v , given by Eqs. (87)–(89), is shown in continuous line. The rest of the curves are obtained using numerically evaluated transfer terms: — — — — — V ; — — — — — $(T_{lp}^* - T_{lp0}^*)/T^*$; — · — · — $(T_{lp}^* - T^*)/(T_{lp0}^* - T^*)$.

where $V = v/v_0$ and $S' = (2\Omega_{11}^* T^*/3)^{-1}$. A stopping distance $x_s = S'v_0$ is thus predicted. At this point, Eq. (88) becomes singular and T_{lp}^* has a vertical asymptote while T_{lp}^* tends monotonically to T^* . Of course, close to the singular point, the solution for T_{lp}^* is no longer valid since the hypersonic condition $T_{lp}^* \ll v^2 T^*/M$ fails to be true. Notice that for small v , the hypersonic condition is more stringent than the condition for the expandability in powers of M given in (66). Expressions (87)–(89) are represented in Fig. 6 as a function of $x' \equiv x/(S'v_0)$.

In the same figure, the results of integrating Eqs. (78)–(80) with transfer terms E^* and B^* numerically evaluated by direct integration of Eqs. (31)–(33) is shown for different v_0 . As can be seen, the agreement with the linearized solution (87)–(89) is good even in the case $v_0 = 0.5$. The case $v_0 = [\gamma/(\gamma - 1)]^{1/2}$, corresponding to the strong shock wave limit when the light gas is assumed to be fully decelerated after the shock while the heavy gas conserves its initial speed, is also included. The differences with respect to the linearized solution increase as v_0 grows. In the case $v_0 = 10$, an overshoot in both T_{lp}^* and T_{lp}^* is seen to occur, while the behavior close to the singular point is the same as in the small- v solution: vertical asymptote for T_{lp}^* and convergence to T^* for T_{lp}^* . Obviously the different behavior observed in the \perp and \parallel directions results from the compression heating term $-2T_{lp} k U_{pz}/m_p$, which acts only along the deceleration path. Notice as well that for large v_0 , an overshoot occurs in the transversal temperature. As was discussed at the end of Sec. III, this behavior is caused by the redistribution term $\Pi_2[I_{11}]$ in Eq. (82), which extracts heat from the parallel direction to put it into the perpendicular direction.

B. Limit $1 \ll v_0$

For large v_0 a new limit for Eqs. (77)–(79) is reached. Substituting expressions (44)–(46), the following set of equations is obtained:

$$v' = -T^* Q_1^* \pi^{1/2} v/4, \quad (90)$$

$$v T_{lp}^{*'} + 2T_{lp}^* v' = T^{*2} \pi^{1/2} v^3 (Q_1^* - Q_2^*/3), \quad (91)$$

$$v T_{lp}^{*'} = [2(T^* - T_{lp}^*) Q_1^* v + 2T^* Q_2^* v^3/3] \pi^{1/2} T^*/4. \quad (92)$$

Provided that $v^{-2} \ll T^*$, which is a condition very easily met because $1 \ll v$, Q_1^* and Q_2^* can be written as

$$Q_1^* = 1.319 v^{-1/3} T^{*-1/6}, \quad (93)$$

$$Q_2^* = 1.210 Q_1^*. \quad (94)$$

In this limit, the following solution is obtained:

$$V = (1 - x''/3)^3, \quad (95)$$

$$\theta_{lp}^* - \theta_{lp0}^* = C(1 - V^4)/V^2, \quad (96)$$

$$\theta_{lp}^* - \theta_{lp0}^* = -DV^2 \ln V, \quad (97)$$

where

$$V = v/v_0, \quad \theta_p^* = T_p^*/(T^* v_0^2),$$

$$x'' = \pi^{1/2} Q_{10}^* T^* x, \quad Q_{10}^* = Q_1^*(T^*, v_0),$$

$$C = 0.59676, \quad D = 0.80647.$$

These expressions are restricted again by the condition $\theta_p^* \ll V^2/M$. Figure 7 shows the predicted shape of V , θ_{lp}^* , and θ_{lp}^* as a function of x'' , together with the results for numerically computed transfer terms: as can be seen, V and θ_{lp}^* are accurately predicted by formulas (95) and (97), but Eq. (96) only agrees with the computed θ_{lp}^* in the first stages of the deceleration. The same discussion made about Eq. (65) applies here: The otherwise negligible difference $I_{11} - vI_B = (\partial I_B/\partial v)/2$ is amplified through the factor T_{lp}^* becoming as important as the other terms. This causes T_{lp}^* to reach a peak and then decrease.

C. Stopping distance

The hypersonic assumption decouples the momentum from the energy equation, so that the problem can be independently solved for the velocity in a simple way. A single curve giving the stopping distance $x_s^* \equiv x_s/S'$ as a function of the initial velocity is obtained for each temperature (Fig.

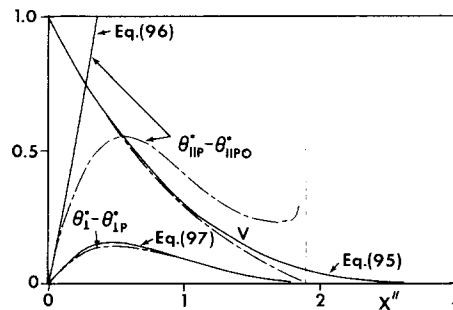


FIG. 7. V , $\theta_{lp}^* - \theta_{lp0}^*$ and $\theta_{lp}^* - \theta_{lp0}^*$ as a function of x'' in the high initial velocity case with $T^* = 10$: — — — — — Eqs. (95)–(97); — — — — — numerically computed transfer terms, in the case $v_0 = 10$.

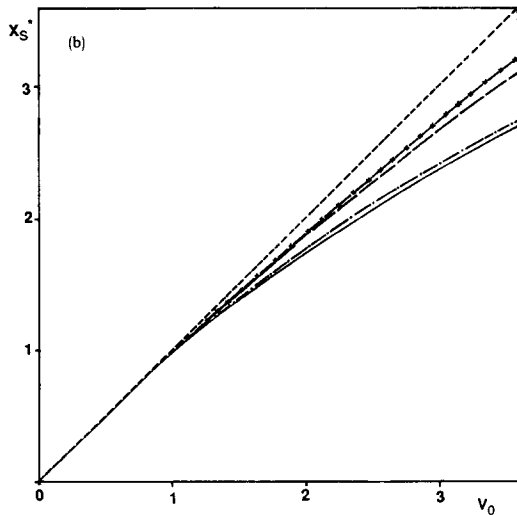
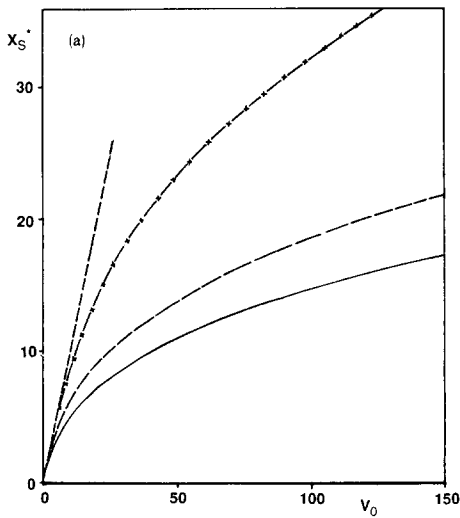


FIG. 8. Stopping distance x_s^* as a function of initial velocity v_0 . Figure 8(b) is an expanded Fig. 8(a) for moderate values of v_0 : — High temperature limit, obtained by integration of Eq. (50a); - - - low v_0 limit; — × — $T^* = 0.1$; — — — $T^* = 1$; — · — · — $T^* = 10$.

8). The low v_0 limit given by Eq. (84), $x_s^* = v_0$, is also indicated. For high temperature cases, expression (50a) for I_B can be substituted in (78) to give a general stopping distance curve valid for $1 \ll T^*$. This condition is not very stringent because in most mixtures ϵ/k is a small temperature.

In order to compare our results with those of Anderson,¹⁸ who used a Monte Carlo method to simulate the deceleration of fast molecules penetrating through a gas at rest, Eq. (78) is rewritten in a time frame:

$$\frac{dv}{d\tau} = -B^*, \quad \frac{dx}{d\tau} = v. \quad (98)$$

In Fig. 9, $x' \equiv x/(S'v_0)$ is plotted as a function of $\tau' = \tau/S'$. Anderson's data for a repulsive inverse-12th potential can be compared with our own results for high T^* , since at high temperature the repulsive part of the Lennard-Jones potential prevails. In the case $v_0 = 4/\pi$, corresponding to Anderson's $Q = 1$, the agreement is good. For low v_0 the curves $x'(\tau')$ are close to the small- v limit, $x' = 1 - e^{-\tau'}$.

For large values of v_0 , Anderson presents an analytical

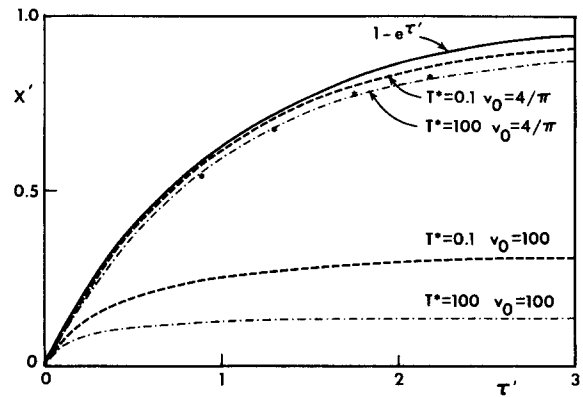


FIG. 9. Penetration depth as a function of time for different values of v_0 and T^* . * Anderson's results using Monte Carlo simulation for $M = 100$ and inverse-12th repulsive potential.

expression obtained by averaging the velocity change of the impinging molecules as they collide with target molecules at rest. The effect of the target molecules motion is estimated by using an approximate expression for the collision rate. His results are thus more accurate when the stagnant gas molecules have a thermal speed much smaller than the mean velocity of the incident molecules, that is, $1 \ll v_0$. His results for the 12th potential can be written as

$$\frac{dv}{d\tau} = -0.471 v^{5/3} T^{*5/6} \left(1 + \frac{4}{\pi v^2}\right)^{1/2}, \quad (99)$$

while our expression for $1 \ll T^*$ [Eqs. (50) and (74)] can be rewritten as

$$\frac{dv}{d\tau} = -0.584 v^{5/3} T^{*5/6} \left(1 + \frac{2.175}{v^2}\right)^{1/3}. \quad (100)$$

A difference of about 20% is observed. The terms within the parentheses, when expanded in v^{-1} , respectively become $(1 + 0.6366/v^2 + \dots)$ and $(1 + 0.7252/v^2 + \dots)$. Differences probably arise from the approximate expression for the collision rate used by Anderson.

VI. CONCLUSIONS AND LIMITATIONS OF RESULTS

In this paper, simple formulas are given for the cross-collision integrals describing the light-heavy momentum and energy (tensor) transfer in a binary disparate-mass gas mixture. Our results, to lowest order in m/m_p , are subject to the constraint that the molar fraction of the heavy gas be moderately small ($n_p/n \leq 1$) so that the distribution function of the light gas can be considered unaffected by the presence of the heavy molecules. However, this is not a severe restriction in disparate-mass mixtures, since large heavy gas mass fractions are compatible with $n_p \leq n$. Furthermore, the complementary situation can easily be handled by using an equilibrium two-fluid approach,⁵ which describes both species distribution functions as Maxwellians. Only to go one step further in our perturbation technique in powers of m/m_p is one forced to impose the more restrictive condition $n_p \ll n$ so that f can be described in terms of the first-order pure gas Chapman-Enskog solution. Our equations are also subject to the restriction that the relation S between the interspecies relaxation time and the characteristic macroscopic time be at most of order unity. This constraint precludes

extreme nonequilibrium conditions, in which the light gas distribution also departs considerably from the Maxwellian distribution.

On the other hand, this work is only concerned with the cross-collision integral terms, \mathbf{b} and \mathbf{E} in Eqs. (2) and (3). Given that the self-collision integral terms become important as soon as the mass fractions are comparable ($\rho \sim \rho_p$), some model for the heavy gas distribution functions is required in order to compute the self-collision integral tensorial energy transfer term \mathbf{E}_{self} . In Sec. V the heavy gas temperature tensor was determined without a model for \mathbf{E}_{self} thanks to the assumption $\rho \ll \rho_p$.

The expressions for the interspecies transfer are based on the disparity of thermal speeds between the two species, which requires T_p to be much smaller than $m_p T/m$. Under extreme circumstances (i.e., a hot beam encountering a cool light gas) this assumption is not fulfilled, but in practically all relevant situations T_p and T are of the same order, thus ensuring the legitimacy of our expansion. This condition should not be confused with the hypersonic requirement which was added for simplicity in the example of Sec. V.

Finally, the normalization and the resulting correlations are based on the Lennard-Jones interaction model, which provides a simple and realistic representation for spherical nonpolar molecules at a wide range of temperatures. The extension of these results to other interaction potentials is straightforward.

ACKNOWLEDGMENTS

The present work has been supported by a cooperative research grant from Schmitt Technologies Associates and

the State of Connecticut (number 885-176). P. Riesco-Chueca is sponsored by the U.S.-Spanish Joint Committee for Cultural and Educational Cooperation.

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