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R. G. Lord



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Some extensions to the Cercignani-Lampis gas-surface scattering kernel

R. G. Lord

Department of Engineering Science, Oxford University, Parks Road, Oxford OX1 3PJ, England

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The Cercignani-Lampis gas-surface scattering kernel is extended to include two important cases not covered by the basic model. These are (a) diffuse scattering with partial energy accommodation, and (b) accommodation of vibrational energy of a diatomic molecule with equally spaced energy levels. Both extensions are easily implemented in direct simulation Monte Carlo (DSMC) calculations. The results of some test calculations are presented.

I. INTRODUCTION

The direct simulation Monte Carlo (DSMC) method has become an important means of analysis of rarefied gas flows, on account of its ability to handle complex flow geometries and such phenomena as energy exchange in elastic intermolecular collisions, dissociation, ionization, and chemical reactions.¹ Much effort has been devoted toward developing realistic models of intermolecular collision processes.²⁻⁵ By comparison, the equally important problems of accurate simulation of interactions between the gas molecules and the solid boundaries of the flow have been largely neglected; most DSMC calculations to date have either assumed completely diffuse reflection of gas molecules from solid surfaces with complete energy accommodation, or else have adopted the Maxwell model of a fraction of specularly reflected molecules with the remainder being completely accommodated. However, molecular beam studies show that neither of these models is realistic; in general, reemitted molecules show a lobular distribution in direction and a continuous spread of energies.

Of the phenomenological models that have been proposed to describe gas-surface interactions, that of Cercignani and Lampis⁶ (the C-L model), while not entirely satisfactory, appears to be the most useful. It satisfies detailed balance (reciprocity), produces physically reasonable distributions of direction and energy of reemitted molecules, and provides a continuous spectrum of behavior from specular reflection at one end to diffuse reflection with complete energy accommodation at the other. The C-L model has not yet been incorporated into direct simulation Monte Carlo calculations; although Lord⁷ has shown that it is ideally suited for this purpose and can easily be adapted to account for classical internal degrees of freedom of the gas molecule, which were not considered in the original formulation of the model.

The most serious shortcomings of the C-L model are that it does not include the important case of diffuse reflection with incomplete energy accommodation and that, being purely classical, it cannot be used to describe discrete internal quantum states of the molecule. The latter is not too serious in the case of rotational degrees of freedom, except at very low temperatures, but it precludes a realistic description of vibrational states. We begin with a brief description of the basic C-L model and then go on to discuss

some simple extensions which go some way toward overcoming the above deficiencies in the model.

II. THE CERCIGNANI-LAMPIS MODEL

In the C-L model, the transformations of the normal and tangential components of velocity of the molecule on collision with the surface are mutually independent, and the scattering kernel, or probability density function of the reflected state per unit volume of phase space, therefore consists of a product of three terms, one for each component. For isotropic surfaces, however, the two tangential velocity components v and w must behave identically so that two of the terms are exactly similar in form. The part of the scattering kernel for a tangential velocity component v is

$$P(v' \rightarrow v) = \{1/[\pi\sigma(2-\sigma)]^{1/2}\} \times \exp - \{[v - (1-\sigma)v']^2/\sigma(2-\sigma)\}, \quad (1)$$

with a similar expression for w . This satisfies the reciprocity or detailed balance relation

$$\exp - v'^2 P(v' \rightarrow v) = \exp - v^2 P(-v \rightarrow -v') \quad (2)$$

and the normalization condition

$$\int_{-\infty}^{+\infty} P(v' \rightarrow v) dv = 1. \quad (3)$$

In the above equations, v' and v are the incident and reflected velocity components measured in units of $(2RT_w)^{1/2}$, where T_w is the wall temperature. The parameter σ is the accommodation coefficient for the tangential momentum of the molecule and is called α_t by Cercignani and Lampis. However, in the interests of consistency with the treatment of the normal component of velocity, we shall use the symbol α , for $\sigma(2-\sigma)$, which is the accommodation coefficient for the kinetic energy v^2 (in units of kT_w , where k is Boltzmann's constant) associated with this component of velocity.

The part of the scattering kernel relating to the normal component of velocity u satisfies a different reciprocity relation from that of v or w because the velocity distribution of colliding molecules is biased toward those with a high velocity component toward the wall. The relation is

$$|u'| \exp -u'^2 P(u' \rightarrow u) = u \exp -u^2 P(-u \rightarrow -u'), \quad (4)$$

where velocities away from the wall are regarded as positive. Moreover, the kernel also has to be normalized differently, as u is always positive, with the normalization condition now being

$$\int_0^\infty P(u' \rightarrow u) du = 1. \quad (5)$$

The resultant magnitude of two orthogonal velocity components, each obeying the scattering kernel given by Eq. (1), satisfies Eqs. (4) and (5) and is used in the C-L model to describe the behavior of the normal velocity component. This leads to the expression

$$P(u' \rightarrow u) = \frac{2u}{\alpha_n} I_0 \frac{2(1 - \alpha_n)^{1/2} u u'}{\alpha_n} \times \exp - \frac{u^2 + (1 - \alpha_n) u'^2}{\alpha_n} \quad (6)$$

for this part of the scattering kernel, where α_n is the accommodation coefficient for the kinetic energy u^2 . It follows that the probability density function of the magnitude of the tangential component of velocity $V [(v^2 + w^2)^{1/2}]$ is also given by the expression in (6), with appropriate changes of variable.

For the particular case of a distribution of incident molecules which is Maxwellian but at a temperature different from that of the surface, the model yields a distribution of reemitted molecules in the form of a two-temperature Maxwellian, having different characteristic temperatures in the normal and tangential directions. The accommodation coefficients for the normal and tangential temperatures are α_n and α_p , respectively, and that for the kinetic energy of translation of the molecule is $(\alpha_n + \alpha_p)/2$.

The model was originally applied only to the velocity components of the gas molecule, with no reference being made to any internal degrees of freedom; however, the scattering kernel for the tangential velocity components, Eq. (1), can also be used for the angular velocity components of a polyatomic gas, hence describing the change of rotational kinetic energy of the molecule in the collision with the surface.⁷

The basic C-L transformation is thus the same for the normal component of velocity, the tangential components of velocity, or two components of angular velocity. This is illustrated in Fig. 1, where molecular states are represented by points on the diagram, either with radial distance from the origin representing the magnitude of the normal velocity component or with Cartesian coordinates representing components of tangential or angular velocity.

Point P represents the state of the incident molecule and is taken for simplicity to lie on one axis, since the transformation is invariant with respect to rotation of axes. Thus the distance OP can represent any one of $-u'$, v' , or ω' . Point Q represents the average state of the reemitted molecules and is situated on OP such that OQ/OP = $(1 - \alpha)^{1/2}$, where α is the appropriate "energy" ac-

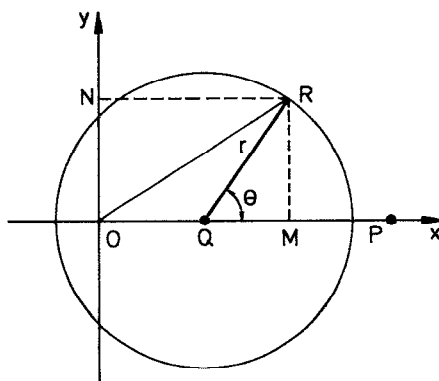


FIG. 1. Geometrical representation of the Cercignani-Lampis model.

commodation coefficient (i.e., α_n , α_p , or α_r). Point R represents the actual state of a reemitted molecule, the probability of this state being distributed according to a two-dimensional Gaussian distribution centered on Q, such that the probability that it lies in an element of area dA at the point r, θ is $(1/\pi\alpha) \exp -r^2/\alpha dA$ and is independent of θ . Here r is the distance QR, and θ the angle PQR. The distance OR now represents u , $(v^2 + w^2)^{1/2}$, or ω , whereas the projections OM and ON onto the axes represent either v and w or ω_1 and ω_2 . A numerical algorithm for selecting the point R according to the correct probability distribution is given by Lord.⁷

III. DIFFUSE SCATTERING WITH INCOMPLETE ENERGY ACCOMMODATION

The principle of the extension of the model to diffuse reflection can be illustrated by considering first the tangential velocity components only. Writing $\mathbf{V} = v\mathbf{j} + w\mathbf{k}$, where $v = V \cos \phi$ and $w = V \sin \phi$ and ϕ is the azimuth angle, the reciprocity relation for \mathbf{V} is

$$\exp -V'^2 P(\mathbf{V}' \rightarrow \mathbf{V}) = \exp -V^2 P(-\mathbf{V} \rightarrow -\mathbf{V}'), \quad (7)$$

where, if $\mathbf{V} = (V, \phi)$ in plane polar coordinates, then $-\mathbf{V} = (V, \phi + \pi)$. The normalization condition becomes

$$\int_0^{2\pi} \int_0^\infty P(\mathbf{V}' \rightarrow \mathbf{V}) V dV d\phi = 1. \quad (8)$$

By inspection, these relations can be seen to be satisfied by the kernel

$$P(\mathbf{V}' \rightarrow \mathbf{V}) = \frac{1}{\pi\alpha_t} I_0 \frac{2(1 - \alpha_t)^{1/2} V V'}{\alpha_t} \times \exp - \frac{V^2 + (1 - \alpha_t) V'^2}{\alpha_t}. \quad (9)$$

Since this kernel is independent of ϕ (and ϕ') the reflected molecules will be distributed uniformly in the azimuthal direction, irrespective of the incident direction, giving a tangential momentum accommodation coefficient, σ , of unity. However, the distribution of tangential speed V , given by

$$f(V) dV = 2\pi V dV P(\mathbf{V}' \rightarrow \mathbf{V}) \quad (10)$$

is the same as for the C-L kernel, and hence the accommodation coefficient for the kinetic energy V^2 is still α_r . It is clear that the kernel can be implemented in DSMC calculations simply by proceeding as for the C-L kernel to calculate V and then reselecting the azimuth angle of the reflected molecule according to the required uniform distribution.

The above kernel still does not include the case of diffuse elastic reflection, as the normal and tangential velocity components are still independent of each other. To construct a kernel that does include this case, it is first necessary to calculate the distribution of resultant speed c $[=(u^2 + v^2 + w^2)^{1/2}]$ of reflected molecules for the C-L kernel for the particular case when $\alpha_n = \alpha_t = \alpha$. This requires integration over all directions in four-dimensional polar coordinates, the result being, after some manipulation

$$f(c)dc = \frac{2c^2 dc}{c'\alpha(1-\alpha)^{1/2}} I_1 \frac{2(1-\alpha)^{1/2}cc'}{\alpha} \times \exp - \frac{c^2 + (1-\alpha)c'^2}{\alpha} \quad (11)$$

The corresponding kinetic energy distribution is given by

$$f(E)dE = \frac{E^{1/2} dE}{\alpha[(1-\alpha)E]^{1/2}} I_1 \frac{2[(1-\alpha)EE']^{1/2}}{\alpha} \times \exp - \frac{E + (1-\alpha)E'}{\alpha} \quad (12)$$

The scattering kernel which gives the same speed and energy distributions but completely diffuse relection (i.e., uniform azimuth angle ϕ and cosine polar angle θ distributions), is

$$P(c' \rightarrow c) = \frac{2 \cos \theta}{\pi c' \alpha (1-\alpha)^{1/2}} I_1 \frac{2(1-\alpha)^{1/2}cc'}{\alpha} \times \exp - \frac{c^2 + (1-\alpha)c'^2}{\alpha}, \quad (13)$$

which satisfies the appropriate reciprocity condition

$$c' |\cos \theta'| \exp - c'^2 P(c' \rightarrow c) = c \cos \theta \exp - c^2 P(c \rightarrow c'), \quad (14)$$

where, if \mathbf{c} equals (c, θ, ϕ) in polar coordinates, then $-\mathbf{c} = (c, \pi - \theta, \pi + \phi)$. Normalization is also satisfied, since

$$\int_0^\infty \int_0^{2\pi} \int_0^{\pi/2} P(c' \rightarrow c) \sin \theta d\theta d\phi c^2 dc = \int_0^\infty f(c)dc = 1. \quad (15)$$

In the case $\alpha = 0$ the above kernel reduces to the diffuse elastic scattering kernel, whereas $\alpha = 1$ corresponds to complete accommodation. Again, the kernel is easily implemented in DSMC calculations by proceeding as for the C-L kernel, calculating the resultant speed c , and then reselecting the polar and azimuth angles of the reflected

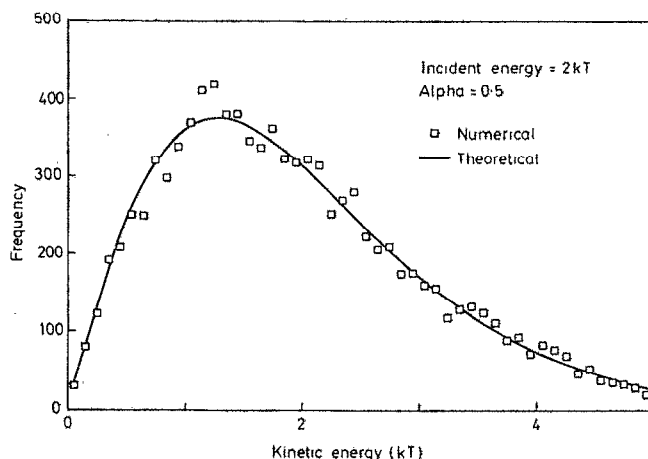


FIG. 2. Energy distribution for four degrees of freedom.

molecule according to the required diffuse distribution, as for complete accommodation.

Figure 2 shows the results of Monte Carlo calculations of the energy distribution of an initially monoenergetic sample of 10 000 molecules after reflection from the surface for the particular values $E' = 2$, $\alpha = 0.5$. The results are compared with calculated values of the energy distribution using Eq. (12) and the agreement is seen to be excellent.

The scattering kernels represented by Eqs. (9) and (13) both produce complete accommodation of tangential momentum ($\sigma = 1$). No kernel has yet been proposed which provides a continuous variation in σ from unity to the C-L value given by $\sigma(2 - \sigma) = \alpha_r$. A linear combination of either of the above with the C-L kernel, in the manner of the Maxwell model, would do this, but the resulting angular distributions of the reflected molecules might not be very realistic, especially for small values of α_r .

IV. INTERNAL DEGREES OF FREEDOM

As stated previously, Lord⁷ has shown that the C-L model can be used without modification to describe classical (i.e., continuous) internal degrees of freedom. The classical approximation would be expected to apply to rotational degrees of freedom at moderate and high temperatures but the separation of vibrational energy levels is generally much greater. In order to be applied to vibration, therefore, modification of the model is required.

We consider only the case of a diatomic molecule regarded as a rigid rotator and harmonic oscillator. Classically, the vibration of such a molecule behaves like any other two-degree-of-freedom system, with possible states uniformly and continuously distributed in phase space, and, therefore, possible energy levels also continuously and uniformly distributed (i.e., having the same statistical weighting for equal energy ranges). Quantum mechanically, allowed energy levels are still uniformly distributed but are now discrete, being restricted to the values $(n + \frac{1}{2})h\nu$ where h is Planck's constant and ν the natural frequency of the oscillator.

In order to describe vibration, therefore, it is necessary to construct a scattering kernel $P(m' \rightarrow n)$, giving the probability of a transition from an initial vibrational state m' , of energy $E' = (m' + \frac{1}{2})E_0$, to a final state n of energy $E = (n + \frac{1}{2})E_0$, where E_0 is the (constant) separation of the energy levels $h\nu$, and m', n are integral quantum numbers. The kernel must satisfy the reciprocity and normalization conditions appropriate to discrete vibrational states, which are

$$\begin{aligned} \exp - (m' + \tfrac{1}{2})E_0 P(m' \rightarrow n) \\ = \exp - (n + \tfrac{1}{2})E_0 P(n \rightarrow m') \end{aligned} \quad (16)$$

and

$$\sum_{n=0}^{\infty} P(m' \rightarrow n) = 1. \quad (17)$$

For two degrees of freedom, the energy distribution of the molecules reemitted from a surface is, according to the C-L model, given by⁷

$$\begin{aligned} f(E)dE = \frac{1}{\alpha} I_0 \frac{2[(1-\alpha)EE']^{1/2}}{\alpha} \\ \times \exp - \frac{E + (1-\alpha)E'}{\alpha}. \end{aligned} \quad (18)$$

Since E' , the vibrational energy of the incident molecule, will automatically be discrete, it would appear reasonable, as a first attempt, simply to discretize the variable E in (18), associating all energy in the range nE_0 to $(n+1)E_0$ with the n th quantum state. This yields the scattering kernel

$$\begin{aligned} P(m' \rightarrow n) = \frac{1}{\alpha} \int_{nE_0}^{(n+1)E_0} I_0 \frac{2[(1-\alpha)EE']^{1/2}}{\alpha} \\ \times \exp - \frac{E + (1-\alpha)E'}{\alpha} dE, \end{aligned} \quad (19)$$

where $E' = (m' + \frac{1}{2})E_0$, which satisfies the normalization condition (17) but, unfortunately, not the reciprocity condition (16). Equation (16) can, however, be satisfied if the initially discrete variable E' is first converted into a continuous variable by the addition of a suitably distributed random component between $+E_0/2$ and $-E_0/2$. The "suitable distribution" turns out to be exponential, as can be seen from the following.

Consider the scattering kernel $P(m' \rightarrow n)$ given by

$$\begin{aligned} (1 - \exp - E_0) \exp - m'E_0 P(m' \rightarrow n) \\ = \frac{1}{\alpha} \int_{m'E_0}^{(m'+1)E_0} \exp - E' \\ \times \int_{nE_0}^{(n+1)E_0} I_0 \frac{2[(1-\alpha)EE']^{1/2}}{\alpha} \\ \times \exp - \frac{E + (1-\alpha)E'}{\alpha} dE dE'. \end{aligned} \quad (20)$$

This satisfies reciprocity condition (16), as can be seen by writing

$$\begin{aligned} (1 - \exp - E_0) \exp - \left(m' + \tfrac{1}{2}\right) E_0 P(m' \rightarrow n) \\ = \frac{1}{\alpha} \int_{m'E_0}^{(m'+1)E_0} \int_{nE_0}^{(n+1)E_0} I_0 \frac{2[(1-\alpha)EE']^{1/2}}{\alpha} \\ \times \exp - \frac{E + E' + \frac{1}{2}\alpha E_0}{\alpha} dE dE' \\ = (1 - \exp - E_0) \exp - \left(n + \tfrac{1}{2}\right) E_0 P(n \rightarrow m'). \end{aligned} \quad (21)$$

It also satisfies normalization condition (17) since

$$\frac{1}{\alpha} \int_0^{\infty} I_0 \frac{2[(1-\alpha)EE']^{1/2}}{\alpha} \exp - \frac{E + (1-\alpha)E'}{\alpha} dE = 1 \quad (22)$$

and

$$\begin{aligned} \int_{m'E_0}^{(m'+1)E_0} \exp - E' dE' \\ = (1 - \exp - E_0) \exp - m'E_0. \end{aligned} \quad (23)$$

Equation (20) can be implemented in DSMC calculations as follows.

(a) Replace $E' = (m' + \frac{1}{2})E_0$ by $m'E_0 + E^*$, where E^* has an exponential probability density function between 0 and E_0 , i.e., if X is a random number uniformly distributed between 0 and 1, put X equal to the cumulative distribution function of E^* , giving

$$X = [1 - \exp(-E^*)]/[1 - \exp(-E_0)] \quad (24)$$

or

$$E^* = -\log(1 - X + X \exp - E_0). \quad (25)$$

(b) Calculate E by the same method as in the classical case, i.e., by putting $E^{1/2} = u'$, selecting u , and putting $u'^2 = E$.

(c) Finally, put $n = \text{INT}(E/E_0)$ (where INT means the integral part of), so that all energies between nE_0 and $(n+1)E_0$ are associated with quantum state n .

Table I shows the results of some sample calculations using the above algorithm for the case $\alpha = 0.5$ and $E_0 = 1$ for $m' = 0, 1$, and 2. The fraction of reemitted molecules in each of the first 11 vibrational states is shown, with no molecules being scattered outside this range. Also shown are the calculated values of $P(m' \rightarrow n)$, which satisfy the reciprocity condition (16) exactly, these having been obtained by numerical integration of the double integral in (20) using Simpson's rule. Again the agreement is excellent although, in order to obtain the degree of convergence shown, it proved necessary to use a larger sample size of 100 000 molecules.

A shortcoming of the above discrete kernel is that the actual accommodation coefficient α_Q for the quantized energy is, in general, not equal to α , as in the continuous case, but depends also on m' and E_0 . Calculated values of α_Q for

TABLE I. Results of sample calculations of vibrational energy exchange for $E_0 = 1$ and $\alpha = 0.5$.

n	$m' = 0$		$m' = 1$		$m' = 2$	
	Monte	Calculated	Monte	Calculated	Monte	Calculated
0	0.754 02	0.753 755	0.515 32	0.513 326	0.328 93	0.329 323
1	0.188 60	0.188 842	0.302 94	0.304 060	0.335 81	0.334 846
2	0.044 14	0.044 569	0.122 30	0.123 184	0.194 58	0.195 025
3	0.010 33	0.010 058	0.042 13	0.041 811	0.089 20	0.088 487
4	0.002 24	0.002 191	0.012 58	0.012 735	0.033 74	0.034 526
5	0.000 53	0.000 464	0.003 31	0.003 598	0.012 27	0.012 141
6	0.000 13	0.000 096	0.001 04	0.000 961	0.003 78	0.003 951
7	0.0	0.000 019	0.000 31	0.000 246	0.001 28	0.001 211
8	0.000 01	0.000 004	0.000 07	0.000 060	0.000 34	0.000 353
9	0.0	0.000 001	0.0	0.000 014	0.000 06	0.000 099
10	0.0	0.000 000	0.0	0.000 003	0.0	0.000 027
α_Q	0.550 43	0.549 83	0.598 60	0.591 08	0.547 39	0.546 29

the cases covered in Table I are some 10% to 20% greater than α , as shown. It is not clear at present how this problem could be overcome.

V. DISCUSSION

The C-L model appears to be ideally suited to incorporation into DSMC calculations of rarefied gas flows, but a serious shortcoming of the model is its inability to in-

clude the case of completely diffuse scattering with partial or zero energy accommodation. Also, the model is purely classical and thus cannot realistically describe energy exchange to and from vibrational states, where the separation of energy levels is typically of the same order as, or larger than, kT_w . The present work goes some way toward removing these restrictions. The algorithms described satisfy the necessary detailed balance (reciprocity) conditions and are easily incorporated into DSMC calculations. Further work remains to be done to devise extensions of the model which, in the case of velocity components, will allow independent partial accommodation of both tangential momentum and kinetic energy and, in the case of vibration, will remove the restriction to the equally spaced energy levels of a purely harmonic oscillator.

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