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Statistical Collision Model for Monte Carlo Simulation of Polyatomic Gas Mixture

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A formal derivation of the direct simulation technique of solution to the Boltzmann equation for a mixture of polyatomic gases is presented. A phenomenological model for binary collisions in a gas mixture having continuous internal energy is then developed. The model is based on the relaxation concept applied to individual collisions and interpreted statistically in a manner suitable to Monte Carlo simulation of rarefied flows. The model has a high degree of flexibility and requires little more computing time per collision than the hard-sphere model of monatomic gas. Sample calculations of a rotationally relaxing gas are compared to loaded-sphere and rough-sphere results.

1. INTRODUCTION

Owing to the complexity of the Boltzmann collision integral for diatomic or polyatomic gases, only simple problems of nonequilibrium kinetic theory have been treated. The collisional processes are not well understood and only calculations with appeal to classical mechanical models such as rough-spheres, loaded-spheres and various *C*-bodies, or special intermolecular potentials have been practicable.

The need for more tractable analytical methods which may be applied to a variety of rarefied flows has lead to the development of model equations such as those proposed by Morse [1], Holway [2], and Brau [3]. Essentially these relaxation models are based on the local equilibrium concept for postcollision ensemble averages paired with an appropriate evaluation of collision frequencies. Such model equations may be viewed as extensions of the BGKW-approximation of monatomic gas by Bhatnagar, Gross, and Krook [4] and Welander [5]. Further refinements and generalizations include the anisotropic source term proposed by Holway [2], application to mixtures of monatomic gases by Hammel [6], mixtures of diatomic gases by Haas, Arpaci, and Springer [7], and diatomic gas-radiation interaction by Phillips, Arpaci, and Larsen [8] and Phillips and Arpaci [9].

Unlike analytical methods the numerical methods based on Monte Carlo schemes (see, for example, Haviland [10]; Bird [11, 12]) for simulating individual collisions in principle demand no simplifications of the collision integral. Given an appropriate description of the kinematics, dynamics, and energetics of collisions, steady and unsteady rarefied flows may be simulated. In practice, however, the computational task becomes almost prohibitive, even for simple one-dimensional flow problems, say of diatomic gas. Rough-sphere and loaded-sphere calculations by Bird [12] and Melville [13], respectively, appear to be manageable for one-dimensional problems, although time consuming. On the other hand, use of the Parker potential [14] as discussed by Macpherson [15] requires elaborate computations of particle trajectories, severely limiting the practical use of the approach.

To meet the need for a more tractable, although approximate, numerical method for the calculation of rarefied flows the present study introduces a statistical model for individual binary collisions of a polyatomic gas mixture. The model is similar in form to the analytical relaxation models for ensemble averages. However, the relaxation concept is applied to individual collisions and interpreted statistically in a manner suitable to a Monte Carlo simulation scheme. Typically, the model formulation specifies the number of internal degrees of freedom, the collision probability and a postcollision probability, such as the angular distribution of relative velocity. In the simple case of monatomic gas, these details are sufficient for the simulation to become identical to a hard-sphere calculation provided the collision probability is made proportional to relative velocity and postcollision relative velocity is uniformly distributed over the full solid angle.

For a preliminary study the model is applied to a rotationally relaxing one-component gas. Results for the case of adiabatic, isotropic relaxation are compared to the loaded-sphere calculations of Melville [13], and results for the one-dimensional flow associated with steady spherical expansion are compared to rough-sphere calculations by Bird [12]. For application of the model, in a modified version, to two-dimensional hypersonic leading edge flow of diatomic gas we refer to the already published work of Pullin, Harvey, and Bienkowski [16].

2. SIMULATION OF THE BOLTZMANN EQUATION

Considering a gas mixture of polyatomic molecules possessing internal energy a rarefied flow is described mathematically by the solution to the Boltzmann equations (ignoring body forces),

$$\frac{\partial n_a f_{al}}{\partial t} + \mathbf{u}_a \cdot \boldsymbol{\nabla}(n_a f_{al}) = \frac{\partial_e n_a f_{al}}{\partial t}, \tag{2.1}$$

subject to appropriate initial and boundary conditions. The number density of species a is denoted by $n_a(\mathbf{x}, t)$ and the distribution function f_{al} is defined so that $f_{al}(\mathbf{u}, E_l\,; \mathbf{x}, t)$ gives the probability that a molecule of species a with internal energy E_l (where l stands for all quantum numbers of the internal states) has velocity and position at time t within the volume $[\mathbf{u}, \mathbf{u} + d\mathbf{u}]$ and $[\mathbf{x}, \mathbf{x} + d\mathbf{x}]$.

To solve Eq. (2.1) physical space is first divided into a finite number of cells in which the particles, simulating molecules, are located according to the initial conditions. Velocity, internal energy, and position coordinates are stored in the computer for each particle. The number of real molecules represented by each particle is the same large number throughout the flow, $n_{ao}V_o/N_{ao} = n_{aj}V_j/N_{aj}$, where V_j denotes cell volume and N_{aj} number of particles of species a in cell j, and subscript o denotes a reference cell at some equilibrium state.

Equation (2.1) is solved successively over a basic time increment Δt by a finite difference scheme in which motion and collisions are decoupled yielding two partial differential equations. Collisional contributions are evaluated within each cell separately ignoring both the distribution in space within the cell and the presence of other cells. Conversely, during motion, collisions are ignored and particles are moved according to their instantaneous velocities.

Then, for cell j, the change in f_{al} due to collision is

$$\left(\frac{\partial n_a f_{al}}{\partial t}\right)_j = \left(\frac{\partial_e n_a f_{al}}{\partial t}\right)_j; \qquad t_o \leqslant t \leqslant t_o + \Delta t, \tag{2.2}$$

subject to the initial condition $f_{al} = f_{al}(t_o)_j$. The differential equation governing the motion is that of collisionless flow,

$$\frac{\partial n_a f_{al}}{\partial t} + \mathbf{u}_a \cdot \nabla(n_a f_{al}) = 0, \tag{2.3}$$

having the solution

$$\begin{aligned} &n_a(\mathbf{x}, t_o + \Delta t) f_{al}(\mathbf{u}, E_l\,; \mathbf{x}, t_o + \Delta t) \\ &\qquad = n_a(\mathbf{x} - \mathbf{u}\,\Delta t, t_o) f_{al}(\mathbf{u}, E_l\,; \mathbf{x} - \mathbf{u}_a\,\Delta t, t_o). \end{aligned} \tag{2.4}$$

Replacing the right-hand side of Eq. (2.4) by the solution of Eq. (2.2) gives the final solution at time $t_o + \Delta t$, which also serves as the initial condition to Eq. (2.2) for the subsequent time step. Solving in this way Eqs. (2.2) and (2.3) successively in time increments Δt gives an approximate solution of an unsteady problem. The foregoing procedure is expected to lead to the exact solution of Eq. (2.1) as cell size and time increment decrease and particle number increases. No stability criterion for this procedure can be explicitly stated, however, due to the strong nonlinearity of Eq. (2.1).

Whereas the solution to Eq. (2.3) is exact and is readily obtained the collision term needs elaboration. Following Morse [1], starting from the Wang Chang and

Uhlenbeck [17] semiquantum mechanical formulation, Eq. (2.2) is rewritten for a mixture of C components (see Chapman and Cowling [18]) as the sum of the elastic and inelastic collision integrals. The contribution to class (a, l) in cell j is then

$$\left(\frac{\partial_e n_a f_{al}}{\partial t}\right)_j = \sum_{b=1}^{C} \left\{ \sum_{m,r,s} \int_{\mathbf{u}_b} \int_{\mathbf{k}} n_{aj} n_{bj} g_{ab}\, {}^{lm}_{rs}I_{ab}(\mathbf{k}, \mathbf{g}_{ab}) [f'_{ar} f'_{bs} - f_{al} f_{bm}]_j \, d\mathbf{k}\, d\mathbf{u}_b \right\}, \quad (2.5)$$

where g_{ab} denotes relative velocity, $\mathbf{k}$ a general symbol for all appropriate collision parameters, and by the usual assumption $g_{ab}I = g'_{ab}I'$, a prime signifying post-collision parameters. Elastic and inelastic contributions can be separated by introducing the collisional cross sections

$${}^{lm}_{lm}I_{ab}(\mathbf{k}, \mathbf{g}_{ab}) = [(Z_{ab} - 1)/Z_{ab}]\, I_{\mathrm{TOT},ab}(\mathbf{k}, \mathbf{g}_{ab}), \quad (2.6)$$

$${}^{lm}_{rs}I_{ab}(\mathbf{k}, \mathbf{g}_{ab}) = (1/Z_{ab})\, I_{\mathrm{TOT},ab}(\mathbf{k}, \mathbf{g}_{ab}) \qquad (r, s) \neq (l, m), \quad (2.7)$$

where $I_{\mathrm{TOT},ab}(\mathbf{k}, \mathbf{g}_{ab})$ denotes the total cross section and Z_{ab} the inelastic collision number, the ratio of inelastic to total collision time.

Equation (2.5) represents a sum over collisions so the integrand is proportional to the probability of a specific collision. To evaluate Eq. (2.5) by a Monte Carlo technique we compute collisions according to these probability densities. Dropping summations and integrals, we rewrite the integrand for elastic and inelastic collisions in terms of collision frequencies and probabilities as

$$\begin{aligned}\delta \left(\frac{\partial_e n_a f_{al}}{\partial t}\right)_j &= n_{aj} \nu_{ab,el} [p(a_l', b_m') - p(a_l, b_m)]_j\, p(\mathbf{k}_{el})\, p(\mathrm{coll})_{ab} \\ &\quad + n_{aj} \nu_{ab,in} [p(a_r', b_s') - p(a_l, b_m)]_j\, p(\mathbf{k}_{in})\, p(\mathrm{coll})_{ab}, \quad (2.8)\end{aligned}$$

where $\nu_{ab,el}$ and $\nu_{ab,in}$ correspond to Eqs. (2.6) and (2.7), respectively, giving $\nu_{ab,el} = \nu_{\mathrm{TOT},ab}(Z_{ab} - 1)/Z_{ab}$ and $\nu_{ab,in} = \nu_{\mathrm{TOT},ab}/Z_{ab}$. Here $\nu_{\mathrm{TOT},ab}$ is the total collision frequency for cell j.

Note that sink and source terms in Eqs. (2.5) and (2.8) can be written in the same form,

$$h_{ab} n_a \nu_{\mathrm{TOT},ab}\, p(a, b)\, p(\mathbf{k})\, p(\mathrm{coll})_{ab}, \quad (2.9)$$

where h_{ab} equals $(Z_{ab} - 1)/Z_{ab}$ or $1/Z_{ab}$ for elastic or inelastic collision, respectively. The definition of f implies $p(a_l, b_m) = f_{al} f_{bm}$, and comparing Eqs. (2.9) and (2.5),

$$p(\mathbf{k})\, p(\mathrm{coll})_{ab} \sim g_{ab} I_{\mathrm{TOT},ab}(\mathbf{k}, \mathbf{g}_{ab}), \quad (2.10)$$

which with Eqs. (2.6) and (2.7) applies to both elastic and inelastic collisions, hence

$$p(\mathrm{coll})_{ab} \sim \int_{\mathbf{k}} g_{ab} I_{\mathrm{TOT},ab}(\mathbf{k}, \mathbf{g}_{ab})\, d\mathbf{k}. \tag{2.11}$$

Once a collision model has been chosen, the probabilities in Eq. (2.10) can be specified.

While other details of Monte Carlo schemes may be found elsewhere [10, 11, 12] the time variable needs elaboration. To ensure that the correct collision frequency for elastic or inelastic collisions between pairs a_l, b_m is maintained, a time-counter for each type of collision in each cell controls the number of collisions computed. Since Eq. (2.9) gives the collision frequency for collisions of class $(a_l, b_m, \mathbf{k})$ we find the total number of collisions per unit time in cell j for class (a_l, b_m) by integrating over V_j and $\mathbf{k}$,

$$\left(\frac{\Delta n_{\mathrm{coll},ab}}{\Delta t}\right)_j = h_{ab} V_j n_{aj} n_{bj} f_{al} f_{bm} \int_{\mathbf{k}} g_{ab} I_{\mathrm{TOT},ab}(\mathbf{k}, \mathbf{g}_{ab})\, d\mathbf{k}. \tag{2.12}$$

To obtain a time-counter for each type of collision rather than employ one for each class, Eq. (2.12) is normalized with $f_{al} f_{bm}$. Recalling that a b_m, a_l collision is identical to an a_l, b_m collision, the appropriate time increment δt for one collision ($\Delta n_{\mathrm{coll},ab} = 1$) becomes

$$\delta t_{ab,j} = \frac{1 + \delta_{ab}}{h_{ab}} \left\{ V_j n_{aj} n_{bj} \int_{\mathbf{k}} g_{ab} I_{\mathrm{TOT},ab}(\mathbf{k}, \mathbf{g}_{ab})\, d\mathbf{k} \right\}^{-1}, \tag{2.13}$$

where δ_{ab} is the Kronecker delta.

The calculation of collisions in a given cell proceeds by selecting type of collision according to whichever of the $C(1 + C)$ time-counters shows the smaller value. The appropriate time-counter is then incremented until all counters have been augmented by at least the nominal value Δt. In the case of continuous internal energy the summation in Eq. (2.5) is replaced by an integral and the collisional cross section becomes a differential cross section with respect to internal energy Taking these collision parameters to be included in the general symbol $\mathbf{k}$, the foregoing expressions are unchanged.

For the purpose of illustration, consider a single-component gas obeying the central force inverse power law. In terms of the usual notation, see, for example, Chapman and Cowling [18], the collision parameters are ϵ and $v_o = b(mg^2/2\kappa)^{1/(1-\nu)}$. Writing

$$I_{\mathrm{TOT}}(\mathbf{k}, \mathbf{g})\, d\mathbf{k} = b\, db\, d\epsilon,$$

Eq. (2.10) becomes

$$p(\mathbf{k})\, p(\mathrm{coll}) = p(v_o)\, p(\epsilon)\, p(\mathrm{coll}) \sim (2v_o/[v_o]^2_{\max})\, g^{(\nu-5)/(\nu-1)}, \tag{2.14}$$

implying the probabilities

$$p(\text{coll}) = g^{(\nu-5)/(\nu-1)}/[g^{(\nu-5)/(\nu-1)}]_{\max}\,; \quad p(\epsilon) = 1/2\pi; \quad p(v_o) = 2v_o/[v_o]^2_{\max}\,. \qquad (2.15)$$

Substituting Eq. (2.14) into Eq. (2.13) we obtain for the time increment

$$\delta t_j = 2\{V_j n_{aj}^2 \pi (2\kappa/m)^{2/(\nu-1)}\, g^{(\nu-5)/(\nu-1)} [v_o]^2_{\max}\}^{-1}. \qquad (2.16)$$

3. STATISTICAL COLLISION MODEL WITH UNRESTRICTED ENERGY EXCHANGE

Below we develop a simple statistical model for individual elastic and inelastic binary collisions between molecules having continuous internal energy. The model is particularly suitable to particle simulation methods.

Recall first the characteristics of the BGKW-approximation [4, 5] and its extensions to polyatomic gases [1, 2] and mixtures [6, 7]. These models approximate the collision integral with a relaxation of ensemble averages toward equilibrium based on one or more relaxation times. While sink terms are proportional to instantaneous distribution functions, source terms are proportional to local equilibrium distributions that are isotropic with respect to the ensemble mass center.

Adopting the foregoing characteristics for individual binary collisions implies that postcollision parameters are isotropic with respect to pair mass center and are determined by local equilibrium distributions for, respectively, translational and internal energies corresponding to pair energy in the center of mass system. Momentum and energy are explicitly conserved in the collision and pre- and postcollision parameters are otherwise uncorrelated.

For an inelastic collision between molecules 1 and 2 of masses m_1 and m_2, internal energies e_{i1} and e_{i2}, relative velocity $\mathbf{g}$ and center of mass velocity $\mathbf{G}$, the conservation of momentum and energy is

$$\mathbf{G}' = \mathbf{G} = (m_1\mathbf{u}_1 + m_2\mathbf{u}_2)/(m_1 + m_2); \qquad e = e_t' + e_i' = e_t + e_i\,, \qquad (3.1)$$

where $e_t = \frac{1}{2}\mu g^2$ and $e_i = e_{i1} + e_{i2}$ denote pair energies and μ the reduced mass $m_1 m_2/(m_1 + m_2)$. Assuming now that postcollision parameters are distributed according to equilibrium and internal energies are independent of translational energy, the source term, expressed by probabilities, becomes

$$\begin{aligned} p(1', 2' \mid e, \text{coll}) &= p(e_t', e_{i1}', e_{i2}' \mid e, \text{coll}) \\ &= f^0_{t,\text{coll}}(e_t') f_i^0(e_{i1}') f_i^0(e - e_t' - e_{i1}'), \end{aligned} \qquad (3.2)$$

where $f^0_{t,\text{coll}}(e_t')$ denotes the equilibrium distribution of relative kinetic energy of collision pairs and $f_i^0(e'_{i1})$ the equilibrium distribution of continuous internal energy for a polyatomic gas with χ degrees of freedom,

$$f^0_{t,\mathrm{coll}}(\tilde{e}_t') = p_{\mathrm{coll}}(\tilde{e}_t')\, 2(\tilde{e}_t'/\pi)^{1/2} \exp(-\tilde{e}_t'), \tag{3.3}$$

$$f_i^0(\tilde{e}'_{i1}) = [(\chi/2)/\Gamma(\chi/2+1)]\, \tilde{e}'^{\chi/2-1}_{i1} \exp(-\tilde{e}'_{i1}). \tag{3.4}$$

Here, $\tilde{e}_t' = e_t'/kT$, $\tilde{e}'_{i1} = e'_{i1}/kT$ and T denotes the equilibrium temperature defined by e of Eq. (3.1). For an explicit deduction of Eq. (3.3) see, for example, Chapman and Cowling [18] (the case $p_{\mathrm{coll}}(\tilde{e}_t') \sim g$) and of Eq. (3.4) Vincenti and Kruger [19] or Phillips *et al.* [8]. In Eq. (3.3) the probability $p(\mathrm{coll})_{12}$ of Eq. (2.11) has been transformed to $p_{\mathrm{coll}}(\tilde{e}_t')$ for later convenience and it may be noted that Eq. (3.2) incorporates the conservation of pair energy.

For a practical approach suitable to Monte Carlo calculations Eq. (3.2) is not in a convenient form since it involves two independent variables e_t' and e'_{i1}. Rather, adding the internal energies $\tilde{e}'_{i1}$ and $\tilde{e}'_{i2} = \tilde{e} - \tilde{e}_t' - \tilde{e}'_{i1}$ to form $\tilde{e}_i' = \tilde{e}'_{i1} + \tilde{e}'_{i2} = \tilde{e} - \tilde{e}_t'$ by integrating Eq. (3.2) over $\tilde{e}'_{i1}$ from zero to $e_i' = e - e_t'$ gives the desired probability distribution for dividing pair energy into translational and internal energy,

$$p(\tilde{e}_t' \mid \tilde{e}_i' = \tilde{e} - \tilde{e}_t') = f^0_{t,\mathrm{coll}}(\tilde{e}_t')\, f^0_{2i}(\tilde{e} - \tilde{e}_t'), \tag{3.5}$$

where

$$f^0_{2i}(\tilde{e}_i') = [\chi/\Gamma(\chi+1)]\, \tilde{e}'^{\chi-1}_i \exp(-\tilde{e}_i'). \tag{3.6}$$

Once $\tilde{e}_t'$ is selected from Eq. (3.5), and thereby $\tilde{e}_i' = \tilde{e} - \tilde{e}_t'$, $\tilde{e}_i'$ is divided into $\tilde{e}'_{i1}$ and $\tilde{e}'_{i2} = \tilde{e}_i' - \tilde{e}'_{i1}$ according to Eq. (3.2) integrated over $\tilde{e}_t'$. This gives the product of $f_i^0(\tilde{e}'_{i1})$ and $f_i^0(\tilde{e}'_{i2} = \tilde{e}_i' - \tilde{e}'_{i1})$, which is normalized to

$$p(\tilde{e}'_{i1} \mid \tilde{e}'_{i2} = \tilde{e}_i' - \tilde{e}'_{i1}) = \frac{\Gamma(\chi)}{\Gamma(\chi/2)^2}\, \frac{1}{\tilde{e}_i'} \left[\frac{\tilde{e}'_{i1}}{\tilde{e}_i'}\left(1 - \frac{\tilde{e}'_{i1}}{\tilde{e}_i'}\right)\right]^{\chi/2-1}. \tag{3.7}$$

Given postcollisional energies according to Eq. (3.5) and Eq. (3.7), the relative velocity after collision is determined from $\tilde{e}_t'$ and the isotropy condition. Introducing a random unit vector $\mathbf{n}'$ of rectangular distribution over the 4π solid angle we have

$$\mathbf{g}' = |\, \mathbf{g}' \,|\, \mathbf{n}'; \qquad |\, \mathbf{g}' \,|^2 = 2e_t'/\mu, \tag{3.8}$$

and velocities $\mathbf{u}_1'$ and $\mathbf{u}_2'$ are

$$\mathbf{u}_1' = \mathbf{G} - (\mu/m_1)\, \mathbf{g}'; \qquad \mathbf{u}_2' = \mathbf{G} + (\mu/m_2)\, \mathbf{g}'. \tag{3.9}$$

Clearly, for an elastic collision, $e'_{i1} = e_{i1}$, $e'_{i2} = e_{i2}$, and $e_t' = e_t$, only Eqs. (3.8) and (3.9) are applied.

In the particular case of a rigid rotor $\chi = 2$, employing furthermore the central force inverse power law, the pair energy $\tilde{e}$ in an inelastic collision is divided according to Eq. (3.5) as

$$p(\tilde{e}_t' \mid \tilde{e}_i' = \tilde{e} - \tilde{e}_t') = \frac{(\eta + 1)(\eta + 2)}{\tilde{e}} \left(\frac{\tilde{e}_t'}{\tilde{e}}\right)^{\eta} \left(1 - \frac{\tilde{e}_t'}{\tilde{e}}\right), \tag{3.10}$$

where $\eta = (\nu - 3)/(\nu - 1)$, and from Eq. (3.7) the internal energy of each molecule becomes rectangularly distributed,

$$p(\tilde{e}_{i1}' \mid \tilde{e}_{i2}' = \tilde{e}_i' - \tilde{e}_{i1}') = 1/\tilde{e}_i'. \tag{3.11}$$

For a summary of the computational steps of a collision, see Appendix A.

4. ISOTROPIC RELAXATION

To study the rate of energy exchange between translational and internal modes the statistical model is applied to the case of isotropic relaxation of a single-component gas from a constant-speed and constant-internal energy state of different characteristic temperatures. The specific case $\chi = 2$, $\eta = 1$, for which Eqs. (3.10) and (3.11) apply, is chosen for comparison with the calculations of Melville [13] based on the loaded-sphere model having an equivalent inelastic collision number of 5.

The simulation starts by setting up an ensemble of particles with the same speed and same internal energy according to the initial temperatures $T_t/T_o = 7/6$ and

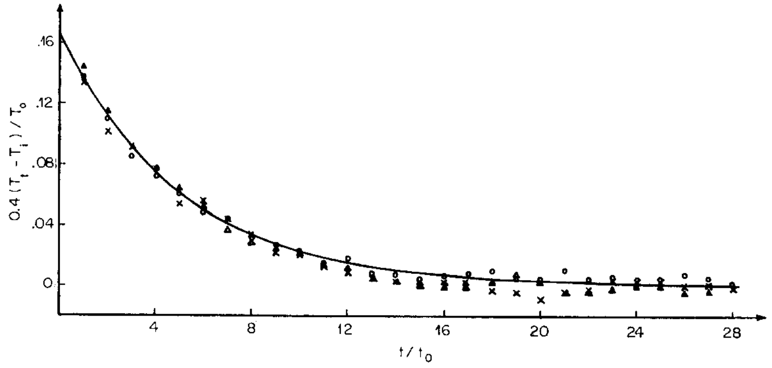

FIG. 1. Isotropic adiabatic relaxation of constant-speed constant-internal energy gas, initially at $T_t/T_o = 7/6$ and $T_i/T_o = 3/4$. ——, Jean's theory [20]; ×, loaded-sphere model by Melville [13]; △, hard-sphere statistical model $\chi = 2$, $\eta = 1$, $Z = 4.3$; ○, hard-sphere statistical model with restricted energy exchange, $\chi = 2$, $\eta = 1$, $\varphi = 0.3$.

$T_i/T_o = 3/4$, where T_o is the reference temperature. At zero time the calculation of collision begins by solving Eq. (2.2). Periodically in time, moments of the ensemble are calculated, until the ensemble approaches the equilibrium state with $T_t/T_o = T_i/T_o = 1$ and the proper distributions for velocity and rotational energy.

Figure 1 shows the energy relaxation calculated from 10 statistically independent simulations with 500-particle ensembles compared to the results of Melville [13] and the theory of Jeans [20]. As shown, the statistical model can reproduce the loaded-sphere temperature moments to within a few percentage points for $Z = 4.3$. Although this value is close to that employed by Melville the two collision numbers cannot be directly compared owing to differences in their definitions.

5. SPHERICAL SOURCE FLOW

To study the statistical collision model for a spatially nonuniform problem we consider the one-dimensional case of spherical source flow which was treated by Bird [12] for the cases of hard-sphere, Maxwell, and rough-sphere molecules, respectively.

The steady flow between two fixed radii, $R_1/R_* = 1.3$ and $R_2/R_* = 6$, where R_* denotes the throat radius, is simulated by 2,000 particles, placed in 90 cells of equal radial width. The reference Knudsen number is $Kn = \lambda_o/R_* = 0.002$, where λ_o denotes the mean free path in the stagnation state.

The flow is started as isentropic equilibrium flow with appropriate radial distributions of density, velocity, and temperature. Because of the low Mach-number at the upstream boundary the particle flux supplied there is that of isentropic flow. The probability density (normalized to its maximum value) of the radial velocity component, $\tilde{u}_x = u_x/(2kT_b/m)^{1/2}$, is

$$\mathscr{P}_{\tilde{u}_x} = \frac{2\tilde{u}_x}{\tilde{v}_x + (\tilde{v}_x^2 + 2)^{1/2}} \exp\{\tfrac{1}{2} - \tilde{u}_x^2 - \tfrac{1}{2}\tilde{v}_x[\tilde{v}_x - 4\tilde{u}_x + (\tilde{v}_x^2 + 2)^{1/2}]\},$$

where $\tilde{v}_x = v_x/(2kT_b/m)^{1/2}$ is the macroscopic radial velocity and T_b the temperature at the boundary. The probability distribution of the normal velocity component, $\tilde{u}_n = u_n/(2kT_b/m)^{1/2}$ is proportional to $\tilde{u}_n \exp(-\tilde{u}_n^2)$, which may be inverted to $\tilde{u}_n = (-\ln \mathscr{R})^{1/2}$. Because of the high Mach-number at the downstream boundary, on the other hand, no particle flux need be supplied there.

Once steady state is established the flow is sampled for temperature moments of axial $T_x/T_o = 2(\langle\tilde{u}_x^2\rangle - \langle\tilde{u}_x\rangle^2)$, normal $T_n/T_o = \langle\tilde{u}^2\rangle - \langle\tilde{u}_x^2\rangle$, translational $T_t/T_o = \frac{2}{3}(\langle\tilde{u}^2\rangle - \langle\tilde{u}_x\rangle^2)$, internal $T_i/T_o = (2/\chi)\langle\tilde{e}_i\rangle$ and total temperature $T/T_o = [3(T_t/T_o) + \chi(T_i/T_o)]/(3 + \chi)$, where $\tilde{u} = u/(2kT_o/m)^{1/2}$ and $\tilde{e}_i = e_i/kT_o$.

The sample size is about 5,000 particles at each cell location, attained by sampling an appropriate number of times while computation proceeds at steady state. The time between samples is such that samples are statistically independent.

Figure 2 shows sample calculations for the simulation of spherical source flow employing the statistical collision model. The internal energy represents rotation with three degrees of freedom ($\chi = 3$) and collision dynamics is that of hard-sphere particles ($\eta = 1$). The results for three values on inelastic collision number Z are shown in the figure. Also shown, as smooth curves for case $Z = 1.2$, are the simulation data of Bird [12] for rough-sphere particles. It appears that the present statistical model can reproduce the rough-sphere temperature moments of source flow to within a few percentage points when $Z = 1.2$. This result confirms the well-known fact that the rough-sphere model exaggerates the coupling between translation and rotation to an extent evidenced by few gases. Similar calculations employing pseudo-Maxwell collision dynamics ($\eta = \frac{1}{2}$), as shown in Fig. 3, predict less departure from equilibrium than the hard-sphere dynamics for the same value of Z due to the collision frequency's independence of temperature.

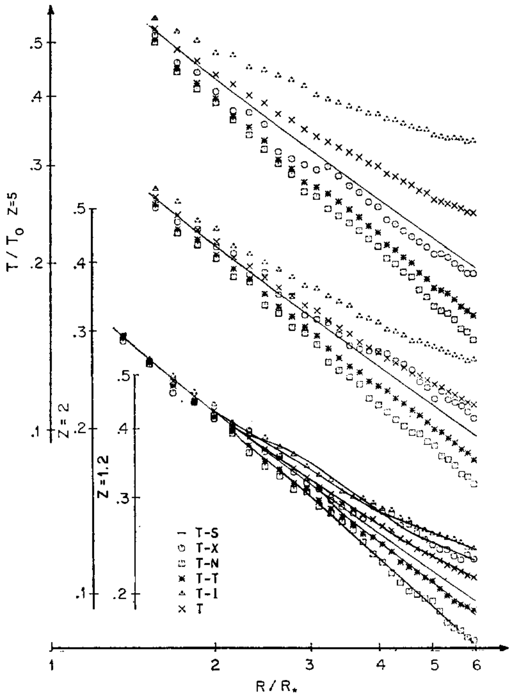

FIG. 2. Steady spherical source flow of rotationally relaxing gas. Hard-sphere statistical model. $\eta = 1$, $\chi = 3$, and $Kn = 0.002$.

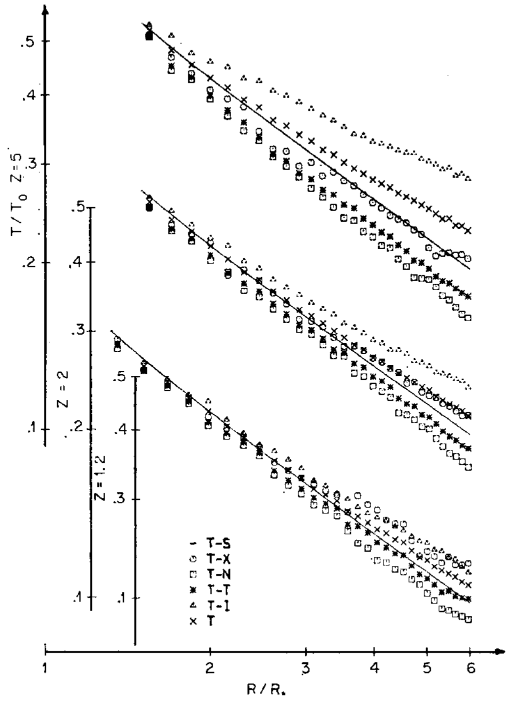

FIG. 3. Steady spherical source flow of rotationally relaxing gas. Pseudo-Maxwell statistical model. $\eta = \frac{1}{2}$, $\chi = 3$, and $Kn = 0.002$.

6. DISCUSSION

By deriving the simulation technique of Bird from the semiquantum mechanical formulation of the collision integral the method has been extended to gas mixtures and to include internal energy. The derivation shows how arbitrary collision models may be applied and how time counters should be kept.

The proposed statistical model constitutes an alternative phenomenological model to the classical models that include internal energy. From its formulation it is clear that the source term satisfies the principle of detailed balance at equilibrium. Also, the Boltzmann *H*-theorem is satisfied, a fact that has been demonstrated by simulations for isotropic relaxation. The model has been described in terms of a single class of inelastic exchanges, a collision probability depending only on relative velocity raised to some power and postcollision isotropy in the center of mass system. However, the model may readily be generalized to include several classes of exchange and less restrictive probability distributions.

One modification, leading to a statistical collision model with restricted energy exchange, has already been reported [21]. Applied to a one-component gas having continuous internal energy this model treats all collisions as being inelastic with the restriction that a given constant fraction φ $(0 \leqslant \varphi \leqslant 1)$ of pair internal and translational energies is made available for statistical exchange during a collision. The parameter φ may be viewed as a pseudosteric factor and the condition of retention of precollision energy is interpreted as a reduction in the number of active pair energy modes. Supposing, furthermore, that energy modes are independent and conform to Boltzmann statistics, the model is obtained from the present one for $Z = 1$ by replacing e with Δe, χ with $\varphi\chi$, and η with $\varphi(1 + \eta) - 1$. Postcollisional pair energies are computed from

$$e_t' = (1 - \varphi)\, e_t + \Delta e_t'; \qquad e_i' = (1 - \varphi)\, e_i + \Delta e_i',$$

while postcollision velocities and internal energies are in turn computed as before.

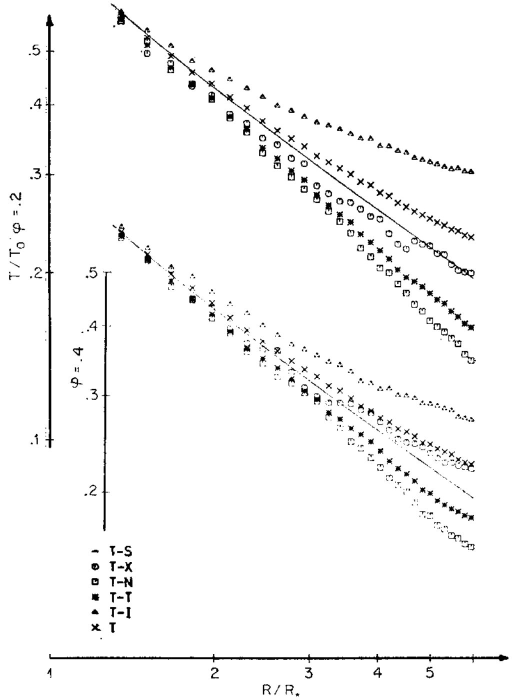

FIG. 4. Steady spherical source flow of rotationally relaxing gas. Hard-sphere statistical model with limited energy exchange. $\eta = 1$, $\chi = 3$, and $Kn = 0.002$.

Calculations with this model for $\varphi = 0.3$ in the case of isotropic relaxation is shown in Fig. 1, and for the spherical source flow with $\varphi = 0.2$ and $\varphi = 0.4$, in Fig. 4. These and other simulations with varying Z and φ show that the relation between Z and φ of the two models is not significantly affected by the type of problem. At equilibrium both models give the correct Boltzmann distributions for velocities and internal energy with a tendency toward more scatter for the model with restricted energy exchange.

TABLE I

Typical CPU-Times (IBM 370/165) in Seconds
for Spherical Source Flow

	Per 1,000 collisions	Total job time
Monatomic gas models:		
Hard-sphere	1.7	150
Maxwell	1.0	130
Diatomic gas models:		
Hard-sphere statistical ($ZR = 1.2$)	1.8	200
Pseudo-Maxwell statistical ($ZR = 1.2$)	1.1	180
Hard-sphere statistical with restricted energy exchange ($\varphi = 1.0$–0.2)	1.8–3	200–350

The proposed statistical model for inelastic collisions is found generally to be economical for computer simulation. Table I shows typical CPU-times (IBM 370/165) for 1,000 collisions and total job times for various cases of the spherical source flow described in Section 5, including some monatomic cases for reference. The times include evaluation of moments, statistics on these, and the necessary bookkeeping, but, nevertheless, they do not exceed 10%–20% of the smallest times indicated. Total Fortran program size is 128 k bytes for spherical source flow compared to 58 k for isotropic relaxation. It is found that CPU-times depend to a large extent on the values of parameters entering the probability distributions sampled by the implicit method (see Appendix A, Eqs. (A2), (A5), and (A7)). Distributions thus become unbounded for $\varphi < 0.5$ and $\chi = 2$ in the model with restricted energy exchange leading to a two- to threefold increase in time per collision depending on the accuracy requested. On the other hand, the model with unrestricted energy exchange, employing an inelastic collision number, is seen to require little more CPU-time per collision than the hard-sphere collision model for monatomic gas and is therefore generally recommended.

APPENDIX A

To clarify the application of the collision model the computational steps for one collision are summarized.

Collision type is selected by $\min(t_{ab,j})$ in cell j, say, an inelastic a, b collision. Having random numbers $\mathscr{R}_1, \mathscr{R}_2, \ldots$, rectangular distributed in [0; 1], and the molecules ordered in numbers from one to N_{aj} and N_{bj}, respectively, two particles are selected by

$$N(a) = \mathscr{R}_1 N_{aj} + 1; \qquad N(b) = \mathscr{R}_2 N_{bj} + 1. \tag{A1}$$

From the stored velocities $\mathbf{u}_a$ and $\mathbf{u}_b$, the relative velocity $\mathbf{g}_{ab} = \mathbf{u}_b - \mathbf{u}_a$ is calculated and the criterion $p(\text{coll})$ of Eq. (2.11) is applied, say, in terms of Eq. (2.15), for the purpose of illustration. Given a predetermined cutoff value $[g^{(\nu-5)/(\nu-1)}]_{\max}$ collision between a and b occurs provided

$$g_{ab}^{(\nu-5)/(\nu-1)} / [g^{(\nu-5)/(\nu-1)}]_{\max} \geqslant \mathscr{R}_3 . \tag{A2}$$

Otherwise a new pair a, b is selected by Eq. (A1). Given collision and the pair energy e by Eq. (3.1), $\tilde{e}_t'$ is determined according to Eq. (3.5) with the use of Eq. (2.15) in Eq. (3.3) for this case. Explicit selection by inversion of

$$\int_0^{\tilde{e}_t'} p(x \mid \tilde{e}_i' = \tilde{e} - x)\, dx = \mathscr{R}_4 \tag{A3}$$

is usually not possible and we employ instead the implicit method. Normalizing Eq. (3.5) with respect to its maximum value gives

$$\begin{aligned} \mathscr{P}_{e_t'} &= \frac{p(\tilde{e}_t' \mid \tilde{e}_i' = \tilde{e} - \tilde{e}_t')}{[p(\tilde{e}_t' \mid \tilde{e}_i' = \tilde{e} - \tilde{e}_t')]_{\max}} \\ &= \left(\frac{\chi + \eta - 1}{\eta}\right)^{\eta} \left(\frac{\chi + \eta - 1}{\chi - 1}\right)^{\chi - 1} \left(\frac{\tilde{e}_t'}{\tilde{e}}\right)^{\eta} \left(1 - \frac{\tilde{e}_t'}{\tilde{e}}\right)^{\chi - 1}, \end{aligned} \tag{A4}$$

and sets of two random numbers are drawn till the inequality

$$\mathscr{P}_{e_t'}\{\tilde{e}_t' = \mathscr{R}_5 \tilde{e}\} \geqslant \mathscr{R}_6 \tag{A5}$$

is satisfied. Now having $\tilde{e}_t{}' = \mathscr{R}_5\tilde{e}$ and $\tilde{e}_i{}' = (1 - \mathscr{R}_5)\tilde{e}$, we divide $\tilde{e}_i{}'$ according to Eq. (3.7), which, normalized to unit maximum value, is

$$\mathscr{P}_{e'_{i1}} = 2^{\chi-2}\left[\frac{\tilde{e}'_{i1}}{\tilde{e}_i}\left(1 - \frac{\tilde{e}'_{i1}}{\tilde{e}_i}\right)\right]^{\chi/2-1}, \tag{A6}$$

and $\tilde{e}'_{i1}$ and $\tilde{e}'_{i2} = (1 - \mathscr{R}_7)\,\tilde{e}_i{}'$ are accepted, provided

$$\mathscr{P}_{e'_{i1}}\{\tilde{e}'_{i1} = \mathscr{R}_7\tilde{e}_i{}'\} \geqslant \mathscr{R}_8\,. \tag{A7}$$

Finally, the postcollision velocities are computed from Eqs. (3.8) and (3.9), with

$$\mathbf{n}' = (\cos\theta, \sin\theta\cos\epsilon, \sin\theta\sin\epsilon),$$

where

$$\cos\theta = 1 - 2\mathscr{R}_9\,; \qquad \epsilon = 2\pi\mathscr{R}_{10}\,.$$

The appropriate time-counter is then incremented with

$$\delta t = \frac{1 + \delta_{ab}}{h_{ab}}\,[V_j n_{aj} n_{bj} \pi\sigma_\nu{}^2 g^{(\nu-5)/(\nu-1)}]^{-1}, \tag{A8}$$

where $\pi\sigma_\nu{}^2$ is the molecular cross section. Note that the special case $\nu \to \infty$ ($\eta = 1$) coincides with the hard-sphere model and $\nu = 5$ ($\eta = \frac{1}{2}$) with the pseudo-Maxwell model.

Whenever symmetry conditions exist the number of stored coordinates for $\mathbf{u}$ and $\mathbf{x}$ may be reduced. Random directions are accordingly assigned for $\mathbf{u}$ whenever needed to evaluate precollision parameters.

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