Monte Carlo Simulation of Hypersonic Rarefied Gas Flow using Rotationally and Vibrationally Inelastic Cross Section Models

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Abstract. The rotational collision number, vibrational relaxation time, and transport coefficients of real gases were used to determine key functions for molecular collision models. The functions determined were the characteristic function for rotationally inelastic collision cross section in the statistical inelastic cross section (SICS) model, parameters for the transient probability density function in the vibrationally inelastic collision cross section (VICS) model, and the probability density function of the deflection angle for these diatomic models. The validity of the present models was investigated by applying a Monte Carlo simulation of hypersonic rarefied gas flow around a flat plate and comparing the results with experimental data. The modeled profiles of rotational temperature and rotational energy distribution near the plate were in reasonable agreement with those found by experiment.

Keywords: Direct Simulation Monte Carlo, Rotationally Inelastic Collision, Vibrationally Inelastic Collision, Hypersonic, Flat Plate.

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INTRODUCTION

The direct simulation Monte Carlo (DSMC) method is an efficient tool for the prediction of non-equilibrium phenomena in rarefied gas flow. Realistic and effective molecular collision models are required in order to apply the DSMC method to rarefied gas flow problems. For elastic molecular collisions, accurate and realistic calculation techniques based on scattering theory as well as simple scattering models based on kinetic theory have been developed and applied to various rarefied gas flow problems. For a rotationally and vibrationally inelastic molecular collision, a simple model is more practical for engineering; because inelastic collision phenomena are quite complicated; enormous calculation time may be required for an accurate approach. Some attractive models have been developed, including the dynamic molecular collision (DMC) model, the phenomenological model formulated by Borgnakke and Larsen (the BL model), the statistical inelastic cross section (SICS) model for rotationally inelastic collisions, and the BL model and the vibrationally inelastic cross section (VICS) model for vibrationally inelastic collisions.

These diatomic collision models require the probability density function for deflection angle, the probability density function for inelastic collision and energy transition, or the cross sections for inelastic collisions and energy transition, in order to express the transport coefficients and the inelastic collision number or relaxation time of real gases. In the present study, the function for the rotationally inelastic collision cross section of the SICS model, parameters for the vibrationally inelastic collision probability of the VICS model, and the probability density function for deflection angle were defined from transport coefficients, rotational collision number, and vibrational relaxation time of nitrogen gas. The validity of the present cross section model was examined by applying it to the simulation of hypersonic rarefied gas flow around a flat plate and comparing the results with experimental data.
BASIC EQUATION AND MOLECULAR COLLISION MODELS

Generalized Boltzmann Equation

The motion of a diatomic molecule with continuous translational and rotational energy and discrete vibrational energy is described by the generalized Boltzmann equation as

\[
\frac{\partial (nf)}{\partial t} + c \frac{\partial (nf)}{\partial r} = n^2 \sum_{i,j} \int \left[ f_i \left( \mathbf{e}, \xi, E_i \right) f_j \left( \mathbf{e}', \xi', E_j \right) g_{i,j} \right] d\xi' d\xi \sin \chi d\chi dcd\xi dc,
\]

(1)

\[
f_i = f \left( \mathbf{e}, \xi, E_i \right), \quad f_i' = f \left( \mathbf{e}', \xi', E_j \right),
\]

(2)

where \( t \) is time, \( r \) is the physical space coordinate, \( n \) is the number density, \( f \) is the distribution function for velocity class \( c \), rotational energy class \( \xi \) and vibrational energy of quantum level \( i \), \( \max \) is the maximum vibrational level, and \( I_{\xi,\xi'}^{i,j} \) is the differential cross section. Variables with a prime (') refer to the post-collision state. In this study, the differential cross section is reduced to the following form by assuming that molecular collision is limited to elastic, rotationally inelastic, and vibrationally inelastic collisions.

\[
I_{\xi,\xi'}^{i,j} d\xi' d\xi = \int \sin \chi d\chi dc,
\]

(4)

where \( p_c \) and \( p_r \) are the probability density functions for deflection and azimuth angles, respectively. The terms \( \sigma_i \), \( \sigma_v \), \( s_{\xi,\xi'} \), \( s_{\xi,\xi'} \) are respectively the total cross section, the probability density function for elastic, rotational and vibrational collisions, and the rotational and vibrational transition probabilities. They are defined as

\[
\sigma_i = \sigma_d + \sigma_r + \sigma_v, \quad p_c = \frac{\sigma_d}{\sigma_i}, \quad p_r = \frac{\sigma_r}{\sigma_i}, \quad p_v = \frac{\sigma_v}{\sigma_i},
\]

(5)

\[
\sigma_d = \int I \sin \chi d\chi dc,
\]

(6)

\[
\sigma_r = \int s_{\xi,\xi'} d\xi' d\xi, \quad s_{\xi,\xi'} = \int I_{\xi,\xi'}^{i,j} d\xi' d\xi,
\]

(7)

\[
\sigma_{v,i,j} = \sum_{i',j'} s_{i',j'}^{i,j}, \quad s_{i',j'}^{i,j} = \int I_{i',j'}^{i,j} d\xi' d\xi,
\]

(8)

respectively, where \( \sigma_d \) is the elastic collision cross section, \( \sigma_r \) the rotational collision cross section, \( \sigma_v \) the vibrational collision cross section, \( s_{\xi,\xi'} \) the rotational transition cross section, and \( s_{i',j'}^{i,j} \) the vibrational transition cross section. The DSMC method requires \( p_c \), \( p_r \), and a set of cross sections \( (\sigma_d, s_{\xi,\xi'}, \sigma_v) \) or \( \sigma_i \) and a set of collision probabilities \( (p_d, p_r, p_v, p_{\xi,\xi'}) \).

Molecular Collision Models

a. Elastic Collision Model

The VSS model for a Lennard-Jones potential is applied here for elastic collisions. The cross section \( \sigma_d \) is defined as

\[
\sigma_d = \frac{Q^{(2)}}{2} \left[ \frac{2Q^{(1)} + Q^{(2)}}{2Q^{(2)} - Q^{(1)}} \right],
\]

(9)

where \( Q^{(1)} \) and \( Q^{(2)} \) are cross sections for diffusion and viscosity, respectively; the definitions for these terms are found in Ref.13 and numerical values are listed in Refs.4 and 6.
b. Rotationally Inelastic Collision Model

For rotationally inelastic collisions, the SICS model is used. The rotational collision cross section \( \sigma_R \) and the transient probability \( p_{\xi;\xi'} \) is defined as

\[
\sigma_R = \sigma_0 Z(E),
\]

\[
p_{\xi;\xi'} = \frac{\left[ E - \xi - \xi' \right] \sigma_0(\xi)}{\max\left( \left[ E - \xi - \xi' \right] \sigma_0(\xi) \right)},
\]

where \( E \) is the translational energy and \( \xi \) is a characteristic function for the rotationally inelastic collision cross section. In this study, the function \( Z \) is assumed to be of the following form.

\[
Z = \sum_{i=0}^{2} a_i E_i^{1/2}, \quad E < E_{th},
\]

\[
E > E_{th},
\]

where \( E_{th} \) is the threshold energy taken to be \( 6k\theta_r \) with the characteristic rotational temperature \( \theta_r \), \( \xi \) is the depth of the potential well of the Lennard-Jones potential are fitting parameters defined from the rotational collision number \( Z_R \) of a rigid rotor model. Parameters \( a_0=0.1009, a_1=0.6093 \) and \( a_2=-0.1586 \) are obtained with \( c_{\xi} / k = 91.5 \) K (k is the Boltzmann constant), and \( \theta_r=2.863 \) K for nitrogen from the rotational collision number \( Z_R \) of the rigid rotor model as shown in Fig.1a.

c. Vibrationally Inelastic Collision Model

For vibrationally inelastic collisions, the VICS model is introduced. The vibrational transition cross section \( s_{ij;j'} \) is defined as

\[
s_{ij;j'} = \eta_i p_{ij;j'}(E_{ij}) \left( 1 - \frac{\Delta E_{ij;j'}}{E_{ij}} \right),
\]

where \( E_{ij} \) is the vibrational energy of quantum level \( i \), \( \eta_i \) is the vibrational steric factor, and \( p_{ij} \) is the vibrational transition probability defined as

\[
p_{ij;j'} = \frac{\left( \frac{1}{I} \right)^{1/2} \exp(-q\left[ L_{ij}^{-1}(q) \right]^2),}{\sqrt{\frac{J_{ij}^{1/2}}{2}}}.
\]

\[
q = 2 \left( \frac{\pi}{\alpha_v} \right) \cosh \left( \frac{k\theta_v}{L_v} \right)^{1/2}, \quad \alpha_v = \frac{h}{2\pi L_v (mk\theta_v)},
\]

where \( L_{ij}^n(x) \) is the associated Laguerre polynomial, \( I = \min(i,j) \), \( J = \max(j,j') \), \( L_v \) is the steepness parameter, \( \theta_v \) is the characteristic vibrational temperature, and \( h \) is Planck’s constant. For one-quantum transitions \( i \to i \pm 1 \) and \( j \to j \pm 1 \), the vibrational transition probability \( p_{ij;j'} \) is also defined as

\[
p_{ij;j'} = \sin^2 \frac{\left( \frac{1}{I} \right)^{1/2}}{2\omega_i \omega_j} g, \quad \omega_v = \frac{2\pi k\theta_v}{h},
\]
The vibrational steric factor $\eta_v$ and the steepness parameter $L_v$ are determined from the Millikan-White formula. Using a Landau-Teller plot of vibrational relaxation obtained by the Millikan-White formula, as shown in Fig.1b, and setting $\theta_v = 3393$ K for nitrogen, we obtain $L_v = 0.25$ Å and $\eta_v = 1.2$.

**d. Probability density function of deflection angle and azimuth angle**

The probability density functions for azimuth angle $p_\chi$ and deflection angle $p_\chi$ for elastic, rotationally inelastic, and vibrationally inelastic collisions are defined as

$$p_\chi = \frac{1}{2\pi}, \quad (19)$$

$$p_\chi = \begin{cases} \alpha \cos^2 \left( \frac{\chi}{2} \right) \sin \left( \frac{\chi}{2} \right) & b_r \leq b_{el}, \text{and} \\ \delta(\chi = 0) & b_r > b_{el} \end{cases}, \quad (20)$$

$$\alpha = \frac{2(Q_1^{(1)} - Q_2^{(1)})}{2Q_1^{(1)} + Q_2^{(2)}}, \quad (21)$$

respectively, where $\delta$ is the Dirac delta function, $b_r$ is the reduced impact parameter which is introduced so as to describe the transport coefficients of real gases, and $b_{el}$ is the impact parameter for elastic collisions. The reduced and elastic impact parameters are defined as

$$b_r = \sqrt{R_{nd}}, \quad b_{el} = \sqrt{\sigma_{el}/\pi}, \quad (22)$$

respectively, where $R_{nd}$ is an uniform random number in the range $[0,1]$, and $b_{max}$ is the maximum value of the reduced impact parameter defined as

$$b_{max} = \sqrt{(\sigma_{el} + \sigma_R + \sigma_{i,i})/\pi}. \quad (23)$$

**CALCULATION OF HYPERSONIC FLOW AROUND A FLAT PLATE AND DISCUSSION**

A set of inelastic cross section models (SICS-VICS model) presented in this study was applied to the simulation of hypersonic flow around a flat plate and compared with the experimental results. The computational domain was taken as $-0.25 \leq x/L \leq 1.25, -0.8 \leq y/L \leq 0.7$ and divided into collision and data cells $\Delta x/L = \Delta y/L = 0.0025$, where $L$ is the length of the flat plate. The flat plate had a thickness $d/L = 3/26$ and the leading edge angle $30^\circ$ and was set to $0 \leq x/L \leq 1$ and $-3/26 \leq y/L \leq 0.0$. The upstream boundary conditions at $x/L = -0.25$ and $y/L = -0.8, 0.7$ were set to the equilibrium uniform flow, and the downstream boundary condition at $x/L = 1.25$ was set to be $(\partial n_f)/\partial x = 0$. The surface of the plate was set to the diffuse reflection with the temperature $T_w$. Initially, the computational domain was set to be an upstream equilibrium condition. Influx molecules across the upstream boundary were assigned an equilibrium Maxwellian distribution by upstream boundary conditions. The time evolution of the position and velocity of each molecule was simulated using the same algorithm used in reference 1, except for the treatment of estimating molecular collisions.

In this paper, collision sampling was conducted using the null-collision technique. After the steady state was established, flow properties were calculated and averaged until statistical fluctuations became sufficiently small. Figures 2(a) and 2(b) show comparisons of the rotational temperature profiles obtained with the SICS-VICS model and experimental data near the flat plate surface ($x=1$ mm), and perpendicular to the plate surface. The experimental conditions were as follows: upstream Mach number $M=4.89$, upstream temperature $T_w=119$ K, surface temperature of the flat plate $T_w=300$ K, and upstream Knudsen number $Kn = l_0/L = 0.02$, where $l_0$ is the mean free path in the upstream equilibrium state. As shown in Fig. 2(a), the rotational temperature profile near the flat plate surface obtained by the SICS-VICS models agrees reasonably with experimentally measured values. On the other hand, some discrepancies are observed in the rotational temperature profiles perpendicular to the plate, and these discrepancies increase with increasing $x$ and $y$ as shown in Fig.2(b). The relative rotational energy distributions of the SICS-VICS model are in reasonable agreement with those of experiment for the position $x=5$ mm, however discrepancies increase with increasing $x$ and $y$ as shown in Figs.3(a) and (b) which is similar to the rotational temperature distribution in Fig.2(b).
Figure 4 shows the vibrational temperature distribution around the flat plate. Some of the molecules were excited to the vibrational energy level from the ground state \( i=0 \) to \( i=1 \) by interacting with the flat plate, and traveled down stream with very little vibrationally inelastic collision probability as shown in Fig.4; this indicates that the flow field was not affected by the vibrationally inelastic collisions in this study. The results of this study suggest that the characteristic function or parameters for rotationally inelastic collision model require some appropriate optimization.

**FIGURE 1.** (a) Comparison of rotational collision number given by the SICS-VISC and rigid rotor models, (b) Comparison of the Landau-Teller plot of vibrational relaxation obtained by the SICS-VICS model and the Millikan-White formula

**FIGURE 2.** Comparison between calculation results and experimental data. (a) Rotational temperature profile near the flat plate surface \( (y=1\text{mm}) \), (b) Rotational temperature profiles perpendicular to the plate.

**FIGURE 3.** Comparison of relative rotational energy distributions given by the SICS-VICS model and experimental data at (a) \( x=5\text{mm} \), (b) \( x=20\text{mm} \).
CONCLUDING REMARKS

The rotational collision number, vibrational relaxation time, and transport coefficients of a real gas were used to determine the parameters of the characteristic function for the rotationally inelastic collision cross section in the SICS model, the fitting parameters for vibrationally inelastic transient probability in the VICS model, and the probability density function of deflection angle for diatomic molecular collision models. The validity of the present model was tested by applying it to the simulation of hypersonic flow around a flat plate and comparing the results with the experimental data. The rotational temperature profile near the flat plate surface and the relative rotational energy distribution given by the SICS-VICS models agree reasonably with those obtained by experiment. However, discrepancies between the simulation and experiment increased with increasing distance from the flat plate. This study shows that the characteristic function or parameters for the rotationally inelastic collision model require some appropriate optimization.

REFERENCES