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

Hiroaki Matsumoto[a]

[a]*Division of systems research, Yokohama National University*
79-5 Tokiwadai Hodogaya Yokohama 240-8501 Japan

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, Hyper Sonic, Flat Plate.
PACS: 47.45.-n

INTRODUCTION

The direct simulation Monte Carlo (DSMC) method[1] 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[2,3,4,5,6] 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[7], the phenomenological model formulated by Borgnakke and Larsen (the BL model[8]), the statistical inelastic cross section (SICS) model[9] for rotationally inelastic collisions, and the BL model[10] and the vibrationally inelastic cross section (VICS) model[11] 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[12].

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

$$\frac{\partial(nf_i)}{\partial t} + \mathbf{c}\frac{\partial(nf_i)}{\partial \mathbf{r}} = n^2 \sum_{j}^{l_{\max}} \sum_{i',j'}^{l_{\max}} \int \left[f'_{i'} f'_{1,j'} - f_i f_{1,j} \right] g\, I^{ij,i'j'}_{\xi\xi_1,\xi'\xi'_1} d\xi' d\xi'_1 \sin\chi d\chi d\epsilon d\xi_1 d\mathbf{c}_1 \tag{1}$$

$$f_i = f(\mathbf{c}, \xi, E_i),\ f_{1j} = f(\mathbf{c}_1, \xi_1, E_j) \text{ and} \tag{2}$$

$$f'_{i'} = f(\mathbf{c}', \xi', E_{i'}),\ f_{1j'}' = f(\mathbf{c}'_1, \xi'_1, E_{j'}), \tag{3}$$

where t is time, r is *the* physical space coordinate, n is the number density, χ is the deflection angle, ϵ is the azimuth angle, g is the relative velocity, f is the distribution function for velocity class c, rotational energy class ξ and vibrational energy of quantum level i, $l_{\max}$ is the maximum vibrational level, and $I^{ij,i'j'}_{\xi\xi_1,\xi'\xi'_1}$ 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.

$$\begin{aligned} I^{ij,i'j'}_{\xi\xi_1,\xi'\xi'_1} d\xi' d\xi'_1 \sin\chi d\chi d\epsilon &= \left[I \sin\chi d\chi d\epsilon \right]_{el} + \left[I_{\xi\xi_1,\xi'\xi'_1} d\xi' d\xi'_1 \sin\chi d\chi d\epsilon \right]_R + \left[I_{ij,i'j'} \sin\chi d\chi d\epsilon \right]_v \\ &= \sigma_t \left[p_{el} \left(p_\chi d\chi p_\epsilon d\epsilon \right) + p_R \left\{ \left(p_{\xi'\xi'_1} d\xi' d\xi'_1 \right) \left(p_\chi d\chi p_\epsilon d\epsilon \right) \right\} + p_v \left\{ \left(p_{i'j'} \right) \left(p_\chi d\chi p_\epsilon d\epsilon \right) \right\} \right] \end{aligned}, \tag{4}$$

where p_χ and p_ϵ are the probability density functions for deflection and azimuth angles, respectively. The terms σ_t p_{el}, p_R, p_v, $p_{\xi'\xi 1'}$, $p_{i'j'}$ 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

$$\sigma_t = \sigma_{el} + \sigma_R + \sigma_{ij},\ p_{el} = \frac{\sigma_{el}}{\sigma_t},\ p_R = \frac{\sigma_R}{\sigma_t},\ p_v = \frac{\sigma_v}{\sigma_t}, \tag{5}$$

$$\sigma_{el} = \int I \sin\chi d\chi d\epsilon, \tag{6}$$

$$\sigma_R = \int s_{\xi\xi_1,\xi'\xi'_1} d\xi' d\xi'_1,\ \ s_{\xi\xi_1,\xi'\xi'_1} = \int I_{\xi\xi_1,\xi'\xi'_1} \sin\chi d\chi d\epsilon,\ p_{\xi'\xi'_1} = \frac{s_{\xi\xi_1,\xi'\xi'_1}}{\sigma_R}, \text{ and} \tag{7}$$

$$\sigma_{i,j} = \sum_{i'\neq i, j'\neq j}^{l_{\max}} s_{ij,i'j'},\ s_{ij,i'j'} = \int I_{ij,i'j'} \sin\chi d\chi d\epsilon,\ p_{i'j'} = \frac{s_{ij,i'j'}}{\sigma_{i,j}}, \tag{8}$$

respectively , where σ_{el} is the elastic collision cross section, σ_R the rotational collision cross section, σ_{ij} the vibrational collision cross section, $s_{\xi\xi 1,\xi'\xi 1}$ the rotational transition cross section , and $s_{ij,i'j'}$ the vibrational transition cross section. The DSMC method requires p_χ , p_ϵ , and a set of cross sections (σ_{el}, $s_{\xi\xi 1,\xi'\xi 1}$, and $s_{ij,i'j'}$) or σ_t and a set of collision probabilities (p_{el}, p_R, p_v, $p_{\xi'\xi 1'}$, $p_{i'j'}$).

Molecular Collision Models

a. Elastic Collision Model

The VSS model for a Lennard-Jones potential[4] is applied here for elastic collisions. The cross section σ_{el} is defined as

$$\sigma_{el} = \frac{Q^{(2)}}{2} \frac{2Q^{(1)} + Q^{(2)}}{2Q^{(2)} - Q^{(1)}}, \tag{9}$$

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[9] is used. The rotational collision cross section σ_R and the transient probability $p_{\xi'\xi_1'}$ is defined as

$$\sigma_R = \sigma_{el} Z\left(E\right), \text{ and} \tag{10}$$

$$p_{\xi',\xi_1'} \sim \frac{\left[E-\xi'-\xi'_1\right]\sigma_{el}(E-\xi'-\xi'_1)}{\max\left\{\left[E-\xi'-\xi'_1\right]\sigma_{el}(E-\xi'-\xi'_1)\right\}}, \tag{11}$$

$$E = E_{tr} + \xi + \xi_1 = E'_{tr} + \xi' + \xi'_1, \tag{12}$$

where E_{tr} is the translational energy and Z 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.

$$Z = \begin{cases} \sum_{i=0}^{2} a_i \left(\frac{E}{\varepsilon_{LJ}}\right)^{-i/2} & E \geq E_{th} \\ 0 & E < E_{th} \end{cases}, \tag{13}$$

where E_{th} is the threshold energy taken to be $6k\theta r$ with the characteristic rotational temperature θr, ε_{LJ} 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 ε_{LJ} / k =91.5 K (k is the Boltzmann constant), and θr=2.863 K for nitrogen from the rotational collision number Z_R of the rigid rotor model[14] as shown in Fig.1a.

c. Vibrationally Inelastic Collision Model

For vibrationally inelastic collisions, the VICS model[11] is introduced. The vibrational transition cross section $s_{ij,i'j'}$ is defined as

$$s_{ij,i'j'} = \begin{cases} \eta_v \sigma_{el}\left(\left\langle E_{tr}\right\rangle\right)\left(1-\frac{\Delta E_{ij,i'j'}}{E_{tr}}\right) p_{ij,i'j'}(E_{tr}) & E_{tr} \geq \Delta E_{ij,i'j'}, \quad \Delta E_{ij,i'j'} > 0 \\ 0 & E_{tr} < \Delta E_{ij,i'j'}, \quad \Delta E_{ij,i'j'} > 0 \\ \eta_v \sigma_{el}\left(\left\langle E_{tr}\right\rangle\right) p_{ij,i'j'}(E_{tr}) & \Delta E_{ij,i'j'} \leq 0 \end{cases}, \tag{14}$$

$$\Delta E_{ij,i'j'} = E_{i'} + E_{j'} - E_i - E_j, \ \left\langle E_{tr}\right\rangle^{1/2} = \frac{\sqrt{E_{tr}} + \sqrt{E'_{tr}}}{2}, \tag{15}$$

where E_i *i*s the vibrational energy of quantum level i, η_v is the vibrational steric factor, and p_{ij} is the vibrational transition probability defined as

$$p_{ij,i'j'} = p_{ij} p_{i'j'}, \quad p_{ij} = \left(\frac{I!}{J!}\right) q^{J-I} \exp(-q)\left[L_I^{J-1}(q)\right]^2, \text{ and} \tag{16}$$

$$q = 2\left\{\frac{1}{6}\left(\frac{\pi}{\alpha_v}\right)\text{cosech}\left[\frac{1}{4}\left(\frac{\pi}{\alpha_v}\right)\left(\frac{k\theta_v}{\left\langle E_{tr}\right\rangle}\right)^{1/2}\right]\right\}^2, \alpha_v = \frac{h}{2\pi L_v\left(mk\theta_v\right)}, \tag{17}$$

where $L_n^{(\alpha)}(x)$ is the associated Laguerre polynomial, I = min(i,i'), J = max(j,j'), L_v is the steepness parameter, θ_v is the characteristic vibrational temperature, and h is Plank's constant. For one-quantum transitions $i \rightarrow i \pm 1$ and $j \rightarrow j \pm 1$, the vibrational transition probability p_{ij} is also defined as

$$p_{ij,i'j'} = \sin^2\left[\frac{(IJ)^{1/2}}{2\omega_v L_v} g\right], \ \omega_v = \frac{2\pi k\theta_v}{h}, \tag{18}$$

The vibrational steric factor η_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 θ_v = 3393 K for nitrogen, we obtain L_v = 0.25 Å and η_v = 1.2.

d. Probability density function of deflection angle and azimuth angle

The probability density functions for azimuth angle p_ϵ and deflection angle p_χ for elastic, rotationally inelastic, and vibrationally inelastic collisions are defined as

$$p_\epsilon = \frac{1}{2\pi}, \tag{19}$$

$$p_\chi = \begin{cases} \alpha \cos^{2\alpha-1}\left(\frac{\chi}{2}\right)\sin\left(\frac{\chi}{2}\right) & b_r \le b_{el} \\ \delta(\chi = 0) & b_r > b_{el} \end{cases} \text{,and} \tag{20}$$

$$\alpha = \frac{2Q^{(1)} - Q^{(2)}}{2Q^{(1)} + Q^{(2)}}, \tag{21}$$

respectively, where δ is the Dirac delta function, b_r is the reduced impact parameter[15] 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

$$b_r = b_{r\max}\sqrt{R_{nd}}\ ,\ b_{el} = \sqrt{\sigma_{el}/\pi}\ , \tag{22}$$

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

$$b_{r\max} = \sqrt{\left(\sigma_{el} + \sigma_R + \sigma_{i,j}\right)/\pi}\ . \tag{23}$$

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 $-0.25 \le x/L \le 1.25$, $-0.8 \le y/L \le 0.7$ 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°and was set to $0 \le x/L \le 1$ and $-3/26 \le y/L \le 0.0$. 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 down stream boundary condition at x/L=1.25 was set to be $\partial(nf_i)/\partial x = 0$. 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[16]. 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 (y=1mm), and perpendicular to the plate surface. The experimental conditions were as follows: upstream Mach number M=4.89, upstream temperature T_∞=119K, surface temperature of the flat plate T_w=300K, 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.

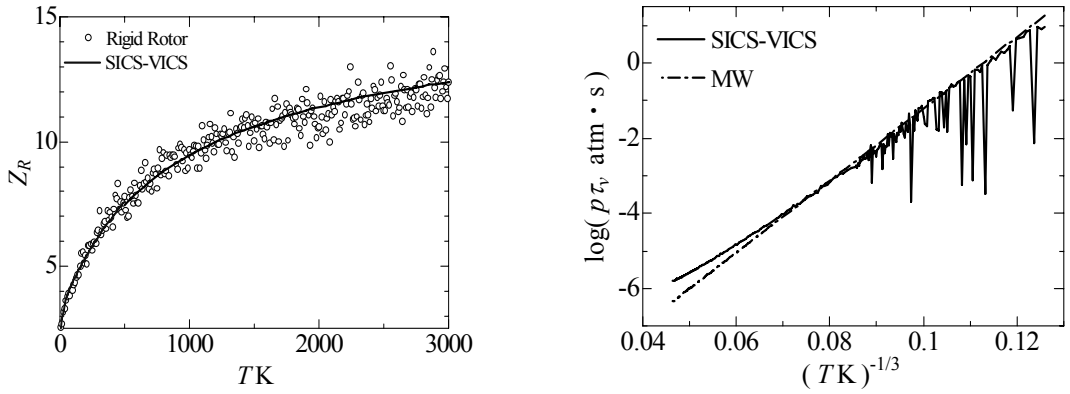

FIGURE 1. (a) Comparison of rotational collision number given by the SICS-VISC and rigid rotor models, (b) Comparison of the Landau-Teller plot of vibrational relaxation obtained by the SICS-VICS model and the Millikan-White formula

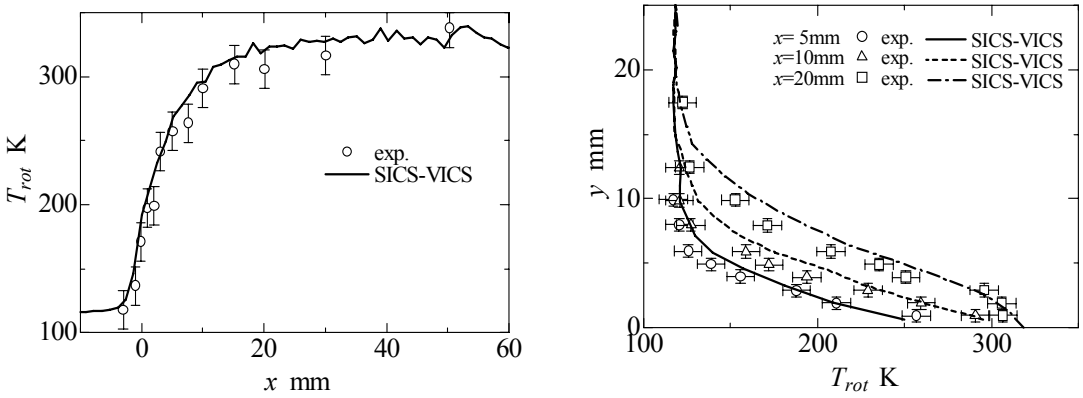

FIGURE 2. Comparison between calculation results and experimental data. (a) Rotational temperature profile near the flat plate surface (y=1mm), (b) Rotational temperature profiles perpendicular to the plate.

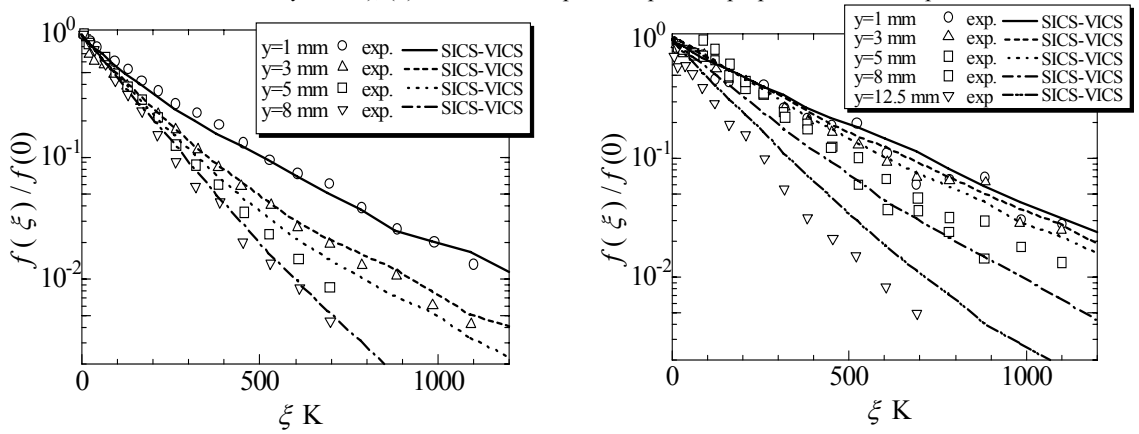

FIGURE 3. Comparison of relative rotational energy distributions **g**iven by the SICS-VICS model and experimental data at (a) x=5mm, (b) x=20mm.

FIGURE 4. Profile of non-dimensional vibrational temperature T_v/T_∞ around the flat plate.

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

1. G. A. Bird, Molecular Gas Dynamics and the Direct Simulation of Gas Flow (Clarendon press, Oxford, 1994).
2. G. A. Bird, "Monte Carlo Simulation in an Engineering Context," Prog. Astronaut. Aeronaut. AIAA 74, 239 (1981).
3. G. A. Bird, "Definition of Mean Free Path for Real Gases," Phys. Fluids 26, 3222 (1983).
4. K. Koura and H. Matsumoto, "Variable Soft Sphere Molecular Model for Inverse-Power-Law and Lennard-Jones Potentials," Phys. Fluids A3, 2459 (1991)
5. K. Koura and H. Matsumoto, "Variable Soft Sphere Molecular Model for Air Species," Phys. Fluids A4, 1083 (1992).
6. H. Matsumoto, "Variable sphere molecular model for inverse power law and Lennard-Jones potentials in Monte Carlo simulations," Phys. Fluids 14, 4256 (2002).
7. Tokumasu, T. and Matsumoto, Y., Dynamic molecular collision (DMC) model for rarefied gas flow simulations by the DSMC method, Phys. Fluids, 11,1907(1999).
8. Borgnakke, C. and Larsen, P. S., Statistical collision model for Monte Carlo simulation of polyatomic gas mixture, J. Comput. Phys.,18 ,405(1975).
9. Koura, K., Statistical inelastic cross-section model for the Monte Carlo simulation of molecules with continuous internal energy, Phys. Fluids, A5, 778(1993).
10. Boyd, I.," Relaxation of discrete rotational energy distributions using a Monte Carlo method," Phys. Fluids A**5** 2278 (1993).
11. Koura, K., "Improved Null-Collision Technique in the Direct Simulation Monte Carlo Method," Computers Math. Applic, 35(1998), 139-154.
12. N.Tsuboi and Y.Matsumoto, "Interaction between Shock Wave and Boundary Layer in Nonequilibrium Nypersonic Rarefied Flow," JSME International Jouanal, B49, 771(2006).
13. S. Chapman and T. G. Cowling, The Mathematical Theory of Non-Uniform Gases (Cambridge Univ. Press, 1976: 3rd edition, 1939: 1st edition).
14. H.Matsumoto.,"Rotational Collision Number nad Rotationally Collision Cross Section of Inelastic Collision Model for Nitrogen Molecule in the Direct Simulation Monte Carlo Method," Trans,. Japan Society of Mech. Eng., 73, 2193 (2007).
15. H.Matsumoto.,"Transport Coefficients of Inelastic Collision model in the Direct Simulation Monte Carlo Method," Trans,. Japan Society of Mech. Eng., 70, 1927 (2004).
16. Koura, K., "Null-Collision Technique in the Direct Simulation Monte Carlo Method," Phys. of Fluids 29,3509-3511 (1986).