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Effects of Gas-surface Interaction Models on Spacecraft Aerodynamics

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Abstract

The influence of boundary condition of the bodies with gas flows is one of the most important problems in high-altitude aerodynamics. In this paper presents the results of the calculation of aerodynamic characteristics of aerospace vehicle using Monte-Carlo method based on three different gas-surface interaction models – Maxwell model, Cercignani-Lampis-Lord (CLL) model and Lennard-Jones (LJ) potential. These models are very sensitive for force and moment coefficients of aerospace vehicle in the hypersonic free molecular flow. The models, method and results can be used for new generation aerospace vehicle design.

Key words: Gas-surface interaction models, DSMC, Spacecraft technology, DSMC, Maxwell, CLL, Lennard-Jones potential, High-altitude aerodynamics.

1. Introduction

The development of aerospace and high-altitude aviation technologies requires to obtain correct data on the aerodynamic characteristics in all ranges of flow regimes, i.e., from free-molecular flow regime to continuum flow regime. The difficulty in the development of hypersonic flows research is caused by quite number of problems, for example, modeling full-scale flight conditions in the wind tunnels. It's impossible to reproduce the heat regime of flow over a vehicle, i.e., the model heating in the wind tunnel leads to a high value of temperature factor, while the temperature of the vehicle surface in full-scale conditions is significantly lower than the total temperature of the flow. Therefore, it's required the involvement of the calculation at the initial stage of aircraft vehicle design.

While the aircrafts are moving in an upper atmosphere where it's necessary to take into account the molecular structure of gas, kinematic models are applied (such as the Boltzmann equation and corresponding numerical simulation methods). In the case of high-altitude (such as free molecular flow regime) the integral of collisions in the Boltzmann equation becomes zero and its general solution is a function of distribution, which remains constant along the paths of particles. The basic quantitative tool for the study of rarefied gas flow is direct simulation Monte Carlo method (DSMC). In order to determine the forces and heat exchange of the gas on the body, it's sufficient to know local exchanges of coefficients of impulse and energy.

In kinetic theory, the gas-surface interaction is a main form of a boundary condition between the gas molecules and solid surface. Although various gas-surface interaction models have been proposed over the last century, the validity of these models remains an important fact in rarefied gas dynamics.

The aim of this paper is to predict aerodynamic characteristics of aerospace vehicles using Direct Simulation Monte Carlo (DSMC) method by taking into account various gas-surface interaction models.

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2. Description of Monte Carlo Method

The Boltzmann integro-differential kinetic equation in rarefied gas dynamics is

$$\frac{\partial f}{\partial t}+\xi\nabla f=\int(f'f_1'-ff_1)\mathbf{g}bdbd\varepsilon d\xi_1 \quad (1)$$

where, $f=f(t, x, y, z, \xi_x, \xi_y, \xi_z)$ is the distribution function and f, f_1, f', f_1', correspond to the molecules with the velocities before ξ, ξ_1 and after ξ', ξ_1' collisions, **g** is the relative velocity of the molecules in binary collisions $\mathbf{g}=|\mathbf{g}|=|\xi_1-\xi|$, and b - the impact parameter and ε is the azimuth angle for the binary collisions [1, 2].

From the above equation, we easily can obtain all the macroscopic parameters from the definition of the function f. For example, the number of molecules in a unit volume of the gas is

$$n(t,\mathbf{r})=\int f(t,\mathbf{r},\xi)d\xi \quad (2)$$

The mean velocity of the molecules, the tensor, and the energy flux is determined by as below

$$\mathbf{v}(t,\mathbf{r})=\frac{1}{n}\int\xi f(t,\mathbf{r},\xi)d\xi \quad (3)$$

$$P_{ij}=m\int c_i c_j f(t,\mathbf{r},\xi)d\xi \quad (4)$$

$$q_i=\frac{m}{2}\int c^2 c_i f(t,\mathbf{r},\xi)d\xi \quad (5)$$

here $c = \boldsymbol{\xi} - V$ is the thermal velocity of the molecules.

The mean energy of the heat flux of molecules can be described in terms of the temperature

$$\frac{3}{2}kT=\frac{1}{n}\int\frac{mc^2}{2}f(t,\mathbf{r},\xi)d\xi \quad (6)$$

The expressions for the components of the thermal velocity can be obtained by simulating the normally distributed random variable

$$\xi_x=\sqrt{\frac{2k_BT}{m}}\sqrt{-\ln\alpha_1}\cos(2\pi\alpha_2) \quad (7)$$

$$\xi_y=\sqrt{\frac{2k_BT}{m}}\sqrt{-\ln\alpha_1}\sin(2\pi\alpha_2) \quad (8)$$

$$\xi_z=\sqrt{\frac{2k_BT}{m}}\sqrt{-\ln\alpha_3}\cos(2\pi\alpha_4) \quad (9)$$

here, α_k is independent random numbers that are uniformly distributed on the interval 0 and 1.

The algorithm of the Monte Carlo method is as follows:

1. Constant data entry.
2. Defining the boundaries of entry of the molecule in the computational domain.
3. Calculating the coordinates of the point of entry and the velocities of molecules.
4. Calculating the coordinates of an intersection of the trajectory of the molecule with the surface of the body and calculating the momentum transfer.
5. Calculating the rate of the reflected molecules and calculating the reactive pulse.
6. Implementation of steps 4-5 to escape molecule from computational domain.
7. Data Averaging.

The velocities of the particles after the collision are chosen according to the molecular interaction models. Although the efficiency of the method depends on many parameters of the computation scheme (relaxation, splitting with respect to time, stabilization, time step, space grid, and so on), the main studies devoted to the improvement of the method focus on the improvement of the collision procedure and on reducing the statistical error because this is the main instrument that makes it possible to reduce the number of particles in the cells and thus decrease the computation time and the requirements for computer memory. One of the features of the method proposed appears to be the fact, that due to the computer memory in the number of molecules are 10^6 in the cell. At this stage it is considered necessary to carry out the transformation of the velocities.

3. The description of gas-surface interaction models

The problem of interaction of gases with surfaces occupies an important role in aerodynamics. Diffuse reflection with complete momentum and energy accommodation is most frequently used in DSMC method. In a diffuse reflection, the molecules are reflected equally in all directions usually with a complete thermal accommodation. The problem of gas-surface interaction takes an essential role in aerodynamics. The role of laws of molecular interaction with surfaces is shown more strongly than more gas is rarefied [3].

The boundary conditions for Boltzmann equation are the conditions relating the distribution function of incident and reflected molecules. The most popular gas-surface interaction model for kinetic theory is specular and diffuse reflection model developed by Maxwell (1879). This model is based on the assumption that the portion $(1 - \sigma_t)$ of molecules reflected specularly from the surface, and the rest

part σ_τ of the molecule diffusely. The density of distribution of reflected molecules is set as follows:

$$f_r(\mathbf{x}_w,\xi_r) = (1-\sigma_\tau) f_i\left(\mathbf{x}_w,\xi_r - 2(\xi_r\cdot\mathbf{n})\mathbf{n}\right) + \sigma_\tau n_r \pi^{-3/2} h_r^{3/2} \exp\left(-h_r\xi_r^2\right),\ (\xi_r\cdot\mathbf{n})>0 \quad (10)$$

and the scattering kernel has form

$$K(\xi_i\to\xi_r) = (1-\sigma_\tau)\delta\left[\xi_i - 2(\xi_r\cdot\mathbf{n})\mathbf{n}\right] - \sigma_\tau \frac{2h_r^2}{\pi}\exp\left[-h_r\xi_r^2\right]\cdot(\xi_i\cdot\mathbf{n}),\ h_r = \frac{m}{2kT_r} \quad (11)$$

Here, ξ_r –velocity vector of the reflected molecules, δ – Dirac delta-function, n –outward unit normal to the surface x_w, h_r - most probable velocity of molecules at a temperature T_w. Indexes i and r denote the quantities for the incident and reflected fluxes, and an index w - the value corresponding to diffuse reflection at temperature of wall T_w. Parameter $0 \le \sigma_\tau \le 1$ in Maxwell model defines accommodation coefficient for the tangential momentum. For complete specular reflection $\sigma_\tau = 0$ and for complete diffuse reflections $\sigma_\tau = 1$.

$$\sigma_\tau = \frac{p_{i\tau} - p_{r\tau}}{p_{i\tau}} \quad (12)$$

Popularity of Maxwell model is due to its simplicity and with the fact that it satisfies the principle of detailed balance. Maxwell's model is suitable for low speed experiments and low rarefaction environments.

The velocity vector components at diffuse reflection are modelled on a local spherical coordinate system which axis is directed along outward unit normal to the surface, by means of expressions [4]

$$|\xi_r| = h_r^{-1/2}\sqrt{-\ln(\alpha_1\alpha_2)},\ \cos\theta = \sqrt{\alpha_3},\ \varphi = 2\pi\alpha_4 \quad (13)$$

Here, α_1, α_2, α_3, α_4 - the independent random numbers. The accommodation coefficient of kinetic energy is defined in terms of incident and reflected fluxes as follows

$$\sigma_E = \frac{E_i - E_r}{E_i - E_w} = \frac{\xi_i^2 - \xi_r^2}{\xi_i^2 - h_w^{-1}} \quad (14)$$

Here E_w - energy of reflected molecules.

If $\sigma_E \neq 0$, expression for the velocity of the reflected molecule looks like

$$|\xi_r| = k h_r^{-1/2}\sqrt{-\ln(\alpha_1\alpha_2)} \quad (15)$$

where,

$$k = \sqrt{(1-\sigma_E)\xi_i^2 h_r + \sigma_E} \quad (16)$$

At work [5] described the gas-surface interaction model of Cercignani-Lampis (CL) which has been improved from Maxwell models [3]. The model is based on the introduction of two parameters which represent accommodation coefficient of kinetic energy connected with normal momentum $\sigma_n = \sigma_{En}$, and tangential momentum accommodation coefficient σ_τ, respectively.

Model CL well corresponds to the results of laboratory researches with high-speed molecular beams. Later, there were modification of scattering kernel of CL model; however, they give a slight improvement in comparison with laboratory experiments. Generally the interaction model has some arbitrary physical parameters that allow achieving the reasonable agreement with results of laboratory researches in a range of conditions. In this case, CL model is suitable for theoretical and numerical research.

In CL model, the diffusion kernel of velocity of surface normal has the following form

$$K(\xi_{ni}\to\xi_{nr}) = \frac{2\xi_{nr}}{\sigma_n} I_0\left(2\sqrt{1-\sigma_n}\frac{|\xi_{ni}|\xi_{nr}}{\sigma_n}\right)\exp\left[-\frac{\xi_{nr}^2 + (1-\sigma_n)\xi_{ni}^2}{\sigma_n}\right] \quad (17)$$

$$I_0(x) = \frac{1}{2\pi}\int_0^{2\pi}\exp(x\cos\phi)d\phi \quad (18)$$

Here I_0 –first type Bessel function, ξ_{ni}, ξ_{nr} – molecular velocities of surface normal for the incident and reflected molecules. A scattering kernel is written as follows

$$K(\xi_{\tau i}\to\xi_{\tau r}) = \frac{1}{\sqrt{\pi\sigma_\tau(2-\sigma_\tau)}}\exp\left[-\frac{\left(\xi_{\tau r} - (1-\sigma_\tau)\xi_{\tau i}\right)^2}{\sigma_\tau(2-\sigma_\tau)}\right] \quad (19)$$

here $\xi_{\tau i}$, $\xi_{\tau r}$ – molecular velocities of tangent to surface for the incident and reflected molecules. Twenty years after the creation CL model, the modification of CL model called Cercignani-Lampis-Lord model (CLL) have been published [6, 7]. Usage of CL model transformation expands to account for rotational energy exchange between gas and surface. Then, updating CLL model in the form of [8] is to account for vibrational energy exchange of the reflected molecules.

In Fig. 2, we can see that the agreement is quite good for all

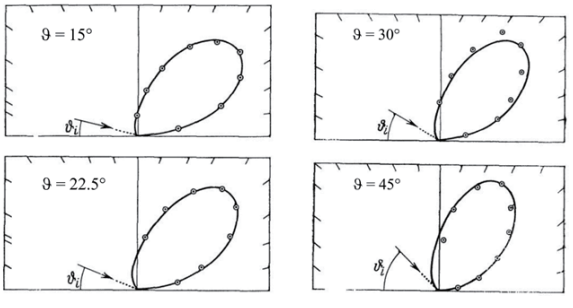

Fig. 1. Comparison between the experimental data [9] and the calculation results by using $\sigma_\tau = 0.1$, $\sigma_n = 0.3$ [10] ($\sigma_n = 0.3$, $\sigma_\tau = 0.1$, $\theta = 15^o, 22.5^o, 30^o$ and 45^o)

incident angles with the same values of the accommodation coefficients σ_τ = 0.1 and σ_n = 0.3 [9, 10]. Data taken from the experiment with a beam of argon at 295 K, and in the platinum at 1081 K. Four polar diagrams related to four different angles of incidence, and represented the inclination of the scattered molecules in the plane of incidence. The circles correspond to the experimental data, and the curves were calculated using the scattering kernel.

Let's see an expression to find the velocity components of the reflected molecules. Let α_i - independent random numbers uniformly distributed on (0, 1). For the normal component of the velocity

$$r = h_w^{-1/2}\sqrt{-\sigma_n \ln \alpha_1}, \quad \theta = 2\pi\alpha_2, \; \xi_{nm} = \sqrt{1-\sigma_n}\,|\,\xi_{ni}\,| \tag{20}$$

$$\xi_{nr} = \sqrt{r^2 + \xi_{nm}^2 + 2r\xi_{nm}\cos\theta} \tag{21}$$

For tangential velocity components.

$$r = h_w^{-1/2}\sqrt{-\sigma_\tau(2-\sigma_\tau)\ln\alpha_3}, \quad = \\ \theta = 2\pi\alpha_4, \; \xi_{\tau 1m} = \sqrt{1-\sigma_\tau(2-\sigma_\tau)}\;\xi_{\tau 1i}, \tag{22}$$

$$\xi_{\tau 1r} = \xi_{\tau 1m} + r\cos\theta, \tag{23}$$

$$r = h_w^{-1/2}\sqrt{-\sigma_\tau(2-\sigma_\tau)\ln\alpha_5}, \quad \theta = 2\pi\alpha_6, \tag{24}$$

$$\xi_{\tau 2r} = r\sin\theta. \tag{25}$$

In order to simulate the partial surface accommodation, the CLL model was implemented into this DSMC calculation. The CLL model is derived assuming momentum components. The two adjustable parameters appearing in the CLL model are the normal component of translational energy α_n and the tangential component of momentum σ_τ. However, in the implementation of the CLL model in the DSMC method, Bird has shown that it is equivalent to specify the normal α_n and tangential σ_τ components of translational energy, since α_τ=σ_τ(2–σ_τ), and thus σ_τ<α_τ, assuming that σ_τ lies between 0 and 1. For molecular velocity distributions, the Maxwell and CLL models gave similar ξ_x distributions, but distinct ξ_y distributions, at partial levels of gas-surface accommodation. Moreover, while the Maxwell scattering distributions experienced abrupt changes with increasing accommodation and position, the CLL distributions varied smoothly. For no significant additional cost, the CLL model gave more realistic scattering distributions [11]. CLL model is widely recognized examples of its application are presented in multiple works [11-28].

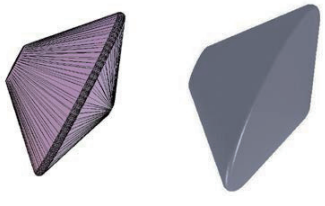

Fig. 2. Geometrical view of reentry vehicle

At the molecular level, it is necessary to consider interaction potentials, using electron-nuclear representations. Empirical potential dependences reflect the fact, that attractive forces at large distance and repulsive forces at short distances. This feature is reflected most simply with Lennard-Jones potential. The sixth power is the attractive potential. The twelfth-power is repulsive potential.

$$U(r) = 4\varepsilon\left[\left(\frac{d}{r}\right)^{12} - \left(\frac{d}{r}\right)^{6}\right] \tag{26}$$

when $\pi r^2 = d$ the potential is equal to zero. The value ε characterizes potential of the depth. It's shown that this model qualitatively correctly described the behavior of aerodynamic characteristics [3, 23].

4. Results and discussions

The calculation has been carried out through the method described in the previous section within the range of angles of attack α from -90° to +90° with an angle step 5°. The parameters of the problem are the following: ratio of heat capacities γ = 1.4; temperature factor $t_w = T_w/T_0$ = 0.04; velocity ratio M∞ = 20, energy accommodation coefficient σ_n = 0.5, 0.75, 1; momentum accommodation coefficient σ_τ = 0.5, 0.75, 1.

The body surface of geometry is reorganized into the format Stereo Lithography (STL). It was carried out with the help of engineering software program SolidWorks. The format STL proves to be sufficiently simple and supports the property of a solid body.

In the Fig. 3 presented the results of the calculation of the coefficients of drag force C_x, lift force C_y with the value of angle of attack α from 0° to 30° for reentry vehicle (Fig. 2) by using the DSMC method with the use of two gas-surface interaction models (Maxwell, Cercignani-Lampic-Lord). The parameters of the reentry vehicle: half cone angle: 60°; nose bluntness ratio (radius of nose/ radius of base): 0.25.

In the Fig. 5 presented the results of the calculation of the coefficients of drag force C_x, lift force C_y with the value of angle of attack α from -90° to +90° for aerospace vehicle (Fig.

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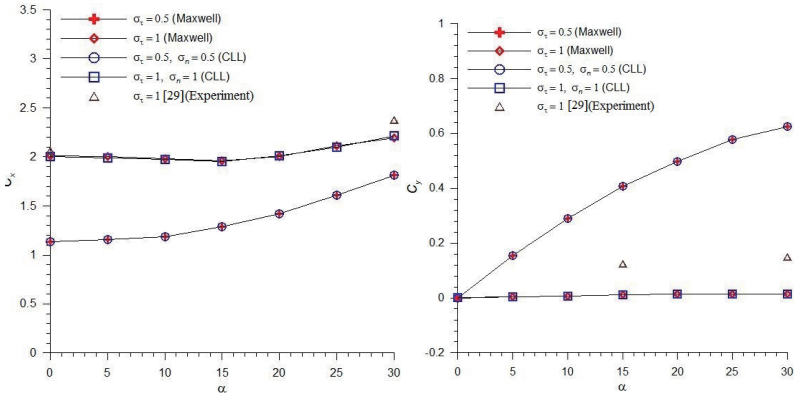

Fig. 3. Dependencies of C_x (α) and C_y (α) for reentry vehicle

Fig. 4. Geometrical view of aerospace vehicle

4) by using the DSMC method with the use of two gas-surface interaction models. From these results we can explain that the values of coefficients of drag force and lift force by CLL model are less than by Maxwell model. The values are the same when the accommodation coefficients are equal to zero or one. In fact that for $\alpha_\tau = 1$ in Maxwell model and $\alpha_\tau = \alpha_n = 1$ in the CLL model, the two models give precisely the same results. Otherwise, the CLL model gives higher aerodynamic forces than the Maxwell model respectively at different accommodation coefficients.

Figure 6 shows the dependence of $C_x(\alpha)$ with the use of various molecular interactions with surfaces. Coefficient C_x increases with the rise of the angle of attack. Multiple reflections are not considered, for a given body, they are unimportant at angle of attack. From these graphs, it is clear that the values of the coefficients are sensible different at various gas-surface interaction models.

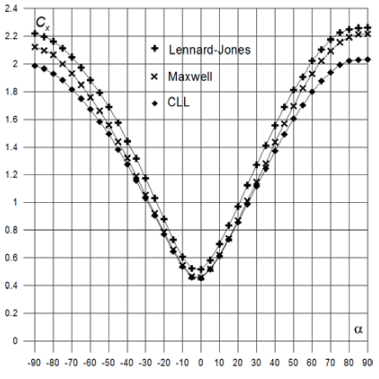

Fig. 6. Dependencies of C_x(α) for aerospace vehicle with various gas-surface interaction models

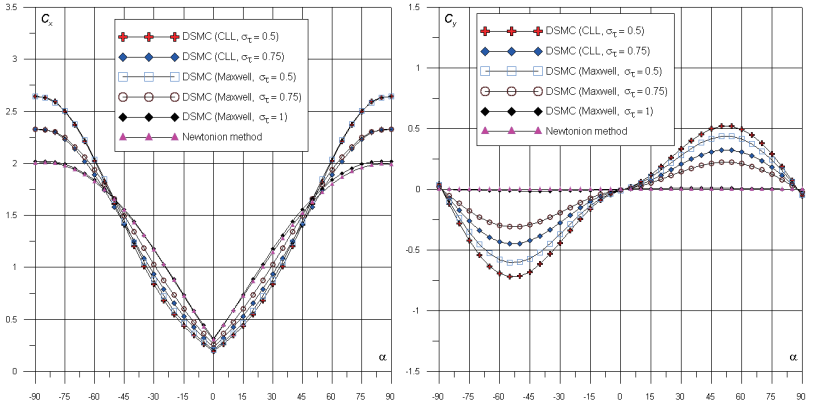

Fig. 5. Dependencies of C_x (α) and C_y (α) for aerospace vehicle

5. Conclusions

The Maxwell model and the Cercignani-Lampis-Lord (CLL) model have fundamental differences and they give similar predictions of aerodynamic forces on various vehicle designs. The interaction potential (Lennard-Jones) for aerodynamics calculation is proposed. The coefficients of forces and moments are sensitive not only to variations accommodate properties of the surface, but also in the details of the distribution of velocities of the molecules reflected normally at the same accommodation coefficient of tangential momentum. The impact of these factors is comparable and should be considered together. CLL model gives the coefficients of forces and moments, lying closely to the case of completely diffuse reflection. The calculations with different accommodation coefficients provide more sensitive for the aerothermodynamics quantities of aerospace vehicles.

The investigation provides better understanding of the effects of gas-surface interaction models in high-altitude aerodynamics and ultimately a better understanding of the accommodation coefficients of materials and gas flows for orbital conditions.

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