Probability of Inelastic Collisions for the Larsen-Borgnakke Model to the Monte Carlo Simulation Method

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Nomenclature

c_p = specific heat at constant pressure
h = distance between two walls
k = Boltzmann constant
Kn = Knudsen number
Pr = Prandtl number
q = heat flux
R = gas constant
T = temperature
u = flow velocity
U = wall velocity
γ = specific heat ratio
ϑ_v = characteristic temperature for vibration
λ = mean free path
μ = viscosity
ρ_0 = average density
τ = shear stress

Subscripts
w = hot wall
∞ = cold wall

Introduction

THE Larsen-Borgnakke (LB) model[1] has become a standard for calculating inelastic collisions in the Monte Carlo direct simulation method.[2] The essential assumption of the LB model is that the postcollision state of a collision pair is subject to a temporal equilibrium. The model is not a collision-dynamical one but a statistical one. The problem in using the model is how to assign the probabilities of inelastic events in collision. Owing to the very nature of the model, the probabilities of inelastic collisions have no direct connection with measured probabilities or relaxation times, which are of course the outcome of collision dynamics of real molecules. In this Note, the probabilities of inelastic collisions for the LB model are determined in such a way that the difference between the Monte Carlo solution for a very small Knudsen number and the Navier-Stokes solution takes a minimum.

Preliminaries

We consider a hypersonic Couette flow with the following conditions. The hot wall at $y = 0$ with temperature T_w is at rest and the cold wall at $y = h$ with temperature T_∞ is moving with a constant speed U. We choose

$$T_w = 1500 \text{ K}, \qquad T_\infty = 300 \text{ K}, \qquad U = 7 \text{ km/s} \tag{1}$$

Roughly, this is a re-entry condition. The gas is pure oxygen, and the viscosity μ is assumed to be proportional to the gas temperature T, i.e., the molecular model is Maxwellian. Molecular collisions in the Monte Carlo method are treated by the collision-number scheme.[3] The Knudsen number Kn is defined by λ/h, where $\lambda = (\mu_w/\rho_0)\sqrt{\pi/2RT_w}$.

Table 1 Shear stress $\tilde{\tau}_w$ and heat flux to shear-stress ratio $\tilde{q}_w$

	$\tilde{\tau}_w$		$\tilde{q}_w$	
Kn	Exact	VHS	Exact	VHS
0.10	11.94	12.05	0.4756	0.4783
0.07	14.05	14.08	0.4749	0.4772
0.05	15.75	15.60	0.4749	0.4759
0.03	17.04	17.02	0.4743	0.4764
0.02	17.41	17.55	0.4743	0.4747
0.01	17.40	17.42	0.4762	0.4808

First, the accuracy of the Monte Carlo method itself is examined for a monatomic gas. The solutions are obtained by use of the exact scattering law for the following computational parameters: the time step is less than half of the mean free time, the cell size is 0.2λ, and the average number of simulator molecules in a cell is 30. The column Exact in Table 1 shows the shear stress $\tilde{\tau}_w(=\tau_w h/\mu_\infty U)$ and heat flux to shear-stress ratio $\tilde{q}_w(=q_w/\tau_w U)$. The number of molecules incident on the hot wall during the sampling time is greater than a half million. It is seen that $\tilde{q}_w$ hardly depends on Kn and $\tilde{\tau}_w$ is constant for $Kn \le 0.02$. We can regard the value of $\tilde{\tau}_w$ at $Kn = 0.01$ as the continuum limit. The exact solution of the Navier-Stokes equation is[4]

$$(\tilde{q}_w)_{\rm NS} = \frac{c_p(T_r - T_w)}{PrU^2} \tag{2}$$

$$(\tilde{\tau}_w)_{\rm NS} = 1 - A(\tilde{q}_w)_{\rm NS} + \tfrac{2}{3}A \tag{3}$$

where $T_r/T_\infty = 1 + A$, $A = Pr(\gamma - 1)M_\infty^2/2$, and $M_\infty = U\sqrt{\gamma R T_\infty}$. Eucken's relation $Pr = 4\gamma/(9\gamma - 5)$ is used for the Prandtl number. For a monatomic gas, $(\tilde{\tau}_\infty)_{\rm NS} = 16.97$ and $(\tilde{q}_w)_{\rm NS} = 0.4761$. We see that the latter agrees with the Monte Carlo solution. We have tried in vain to find the reason of the 2% difference between $\tilde{\tau}_w$ and $(\tilde{\tau}_w)_{\rm NS}$ by halving the cell size, by using a much smaller time step, or by doubling the number of simulators. It has been concluded that this small difference should be ascribable to the Monte Carlo method itself when it is used for computation of hypersonic flows.

Next, we checked the accuracy of the variable hard sphere (VHS) model[5] because it is usually used together with the LB model. Table 1 shows that the use of the VHS model causes no significant errors. Hereafter, the LB model is employed together with the VHS model.

T-R Energy Transfer

Here we consider only the translational-rotational (T-R) energy transfer. How to divide the total collision energy into the translational and internal energies is omitted since it is in Ref. 1. Our concern is in the magnitude of the probability $P_{\rm TR}$ of inelastic collision. The probability of elastic collision is $(1 - P_{\rm TR})$. The Monte Carlo solutions $\tilde{\tau}_w$ and $\tilde{q}_w$ at $Kn = 0.01$ are obtained for various values of $P_{\rm TR}$. The solution of the Navier-Stokes equation is given by Eqs. (2) and (3), in which γ is now 7/5. Figure 1 shows the differences $\Delta\tilde{\tau}_w$ and $\Delta\tilde{q}_w$ as a function of $P_{\rm TR}$. Here $\Delta\tilde{\tau}_w = [\tilde{\tau}_w - (\tilde{\tau}_w)_{\rm NS}]/(\tilde{\tau}_w)_{\rm NS}$, $\Delta\tilde{q}_w$ being similarly defined. It is seen that $\Delta\tilde{\tau}_w$ takes a minimum at $P_{\rm TR} = 0.05$. We recommend that $P_{\rm TR}$ be between 0.03 and 0.08. Then $\Delta\tilde{\tau}_w$ is nearly 4% and $\Delta\tilde{q}_w$ is within 1%.

T-R-V Energy Transfer

In hypersonic flows, heat is generated by viscous dissipation and the highest temperature in flowfields is far beyond the characteristic temperature for vibration. The LB model is extended so as to implement the vibrational energy transfer.[6] Before employing the extended LB model, we must assign the

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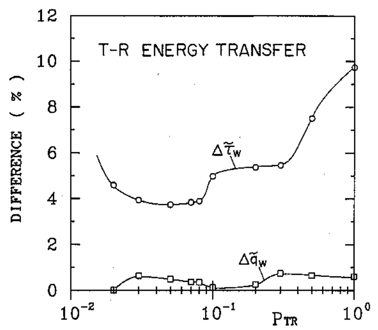

Fig. 1 Difference between the Monte Carlo solution ($Kn = 0.01$) and the Navier-Stokes solution (T-R energy transfer).

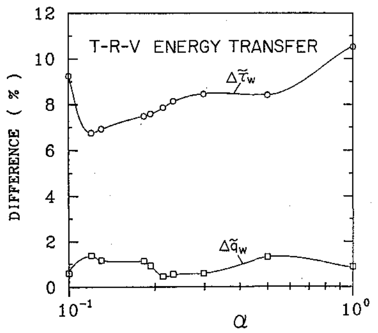

Fig. 2 Difference between the Monte Carlo solution ($Kn = 0.01$) and the Navier-Stokes solution (T-R-V energy transfer).

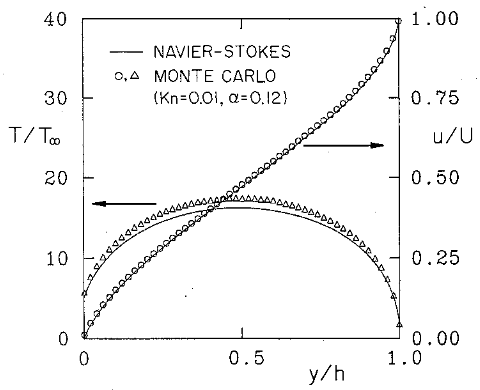

Fig. 3 Comparison of the Monte Carlo solution ($Kn = 0.01$, $\alpha = 0.12$) with the Navier-Stokes solution (T-R-V energy transfer).

probability of elastic collision P_{EL}, the probability of translational-rotational (T-R) energy transfer P_{TR}, and the probability of translational-rotational-vibrational (T-R-V) energy transfer P_{TRV}. Of course, we have

$$P_{EL} + P_{TR} + P_{TRV} = 1 \tag{4}$$

Here we propose a model for P_{TR} and P_{TRV}. In using the LB model, the collision temperature T_c is first determined from

$$\frac{7}{2} kT_c + \frac{2k\vartheta_v}{\exp(\vartheta_v/T_c) - 1} = E \tag{5}$$

where E is the sum of the translational energy of relative motion and the total internal energy of a collision pair. Note that Eq. (5) holds for Maxwellian molecules whereas the corresponding equation in Ref. 6 holds for hard-sphere molecules. The temperature T_c increases with E. The probability P_{TRV} is expected to be small for low T_c. Our model, which is of a statistical nature, is

$$P_{TR} = \alpha(2/\zeta), \qquad P_{TRV} = \alpha(\zeta_v/\zeta) \tag{6}$$

where α is a free parameter, $\zeta(=5+\zeta_v)$ is the total degree of freedom, and ζ_v is the apparent vibrational degree of freedom defined by $\zeta_v = 2(\vartheta_v/T_c)/[\exp(\vartheta_v/T_c) - 1]$. When T_c is low, P_{TRV} is small as it should be. Equation (6) means that probability of an inelastic collision is proportional to the corresponding internal energy. From Eq. (4), we have $P_{EL} = 1 - \alpha(2+\zeta_v)/\zeta$; the magnitude of P_{EL} can be adjusted by α.

The Monte Carlo solutions $\tilde{\tau}_w$ and $\tilde{q}_w$ at $Kn = 0.01$ are obtained for various values of α. The Navier-Stokes solution is

$$(\tilde{q}_w)_{NS} = \frac{1}{2} - \frac{R\vartheta_v}{2PrU^2}\left[F(\eta_w) - F(\eta_\infty)\right] \tag{7}$$

where $F(\eta) = 7/2\eta + \coth\eta$, $\eta_w = \vartheta_v/2T_w$, and $\eta_\infty = \vartheta_v/2T_\infty$. The shear stress is

$$(\tilde{\tau}_w)_{NS} = \eta_\infty \int_0^1 d\xi/\eta(\xi) \tag{8}$$

The function $\eta(\xi)$ is given in the implicit form

$$\frac{1}{2}\xi^2 - (\tilde{q}_w)_{NS}\xi = \frac{R\vartheta_v}{2PrU^2}\left[F(\eta_w) - F(\eta)\right] \tag{9}$$

Eucken's relation is used with $\gamma = 7/5$ since Pr is known to be unchanged even at high temperature. The differences $\Delta\tilde{\tau}_w$ and $\Delta\tilde{q}_w$ are shown in Fig. 2. We see that $\Delta\tilde{\tau}_w$ takes a minimum at $\alpha = 0.12$. For this value of α, Eq. (6) would give $P_{TR} = 0.048$ if ζ_v were zero. The value 0.048 is close to that which yields a minimum also in Fig. 1. We recommend that α be between 0.12 and 0.22. Then $\Delta\tilde{\tau}_w$ is 7–8% and $\Delta\tilde{q}_w$ is about 1%. Figure 3 shows the profiles of temperature and velocity for $\alpha = 0.12$. As to the velocity, the Monte Carlo solution agrees well with the Navier-Stokes solution. However, there is a slight difference between the two temperatures.

Conclusions

When the Larsen-Borgnakke model is used in the Monte Carlo simulation method, the following choice is recommendable to the probabilities of inelastic events in collision. If the inelastic event is only rotational energy transfer, the probability of inelastic collision is 0.03–0.08. If not only rotational but also vibrational energy transfer is possible in collision, the probabilities of the inelastic events are given by Eq. (6) having α of 0.12–0.22.

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