ACTA MECHANICA SINICA (English Series), Vol.16, No.2, May 2000 ISSN 0567-7718
The Chinese Society of Theoretical and Applied Mechanics
Chinese Journal of Mechanics Press, Beijing, China
Allerton Press, INC., New York, U.S.A.

DIRECT NUMERICAL TEST OF THE B-G-K MODEL EQUATION BY THE DSMC METHOD*

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ABSTRACT: In the present paper the rarefied gas flow caused by the sudden change of the wall temperature and the Rayleigh problem are simulated by the DSMC method which has been validated by experiments both in global flow field and velocity distribution function level. The comparison of the simulated results with the accurate numerical solutions of the B-G-K model equation shows that near equilibrium the B-G-K equation with corrected collision frequency can give accurate result but as farther away from equilibrium the B-G-K equation is not accurate. This is for the first time that the error caused by the B-G-K model equation has been revealed.

KEY WORDS: BGK model equation, DSMC method, rarefied gas flow, Rayleigh problem

1 INTRODUCTION

The basic equation of the kinetic theory, i.e. the Boltzmann equation

$$\frac{\partial}{\partial t}(nf) + \boldsymbol{c}\cdot\frac{\partial}{\partial \boldsymbol{r}}(nf) + \boldsymbol{F}\cdot\frac{\partial}{\partial \boldsymbol{c}}(nf) = \int_{-\infty}^{\infty}\int_{0}^{4\pi} n^2(f^*f_1^* - ff_1)c_r\sigma \mathrm{d}\Omega \mathrm{d}c_1 \tag{1}$$

is difficult to be solved because of its complicated right hand side collision term. P.L.Bhatnagar, E. P. Gross, and M. Krook[1] put forward the following equation

$$\frac{\partial}{\partial t}(nf) + \boldsymbol{c}\cdot\frac{\partial}{\partial \boldsymbol{r}}(nf) + \boldsymbol{F}\cdot\frac{\partial}{\partial \boldsymbol{c}}(nf) = n\nu(f_0 - f) \tag{2}$$

to replace the Boltzmann equation. Here f is the velocity distribution function, f_0 is the equilibrium or the Maxwellian distribution function, ν is the collision frequency, $\boldsymbol{r}$ is the space coordinate, $\boldsymbol{c}$ is the molecular velocity, $\boldsymbol{c}_1$ is the velocity of another molecule of the colliding pair, $\boldsymbol{F}$ is the external force per unit mass, f_1 is the distribution function of c_1, f^* is the distribution function of post-collision velocities. This equation (2) is the so called BGK (Bhatnagar-Grass-Krook) equation, and it is also named as Krook equation or BKW (Boltzmann-Krook-Welander[2]) equation. It is widely used in place of the Boltzmann equation to solve the molecular gas dynamics problems in transition regime. There are a lot of papers and chapters and sections of textbooks discussing the mathematical and numerical solutions of this model equation. But the error caused by replacing a physically realistic

Received 16 June 1999, revised 27 March 2000
* The project supported by the National Natural Science Foundation of China (19772059, 19889209)

collision operator with an approximate term is unknown and is not predictable generally. Recently the Direct Simulation Monte Carlo (DSMC) method has been developed (see [3,4]) to solve molecular gas dynamics problem in the transition regime. And the DSMC method has been validated by the strict experimental tests both in the aspects of the global flow field and of the fine structure including the molecular velocity distribution function (see [5]). In this paper, we use the Direct Simulation Monte Carlo (DSMC) method to evaluate the BGK model by calculating the flow circumstances deviated far away from the equilibrium, and reveal the error of BGK model. To be specific, the rarefied gas flow caused by the sudden change of the wall temperature and the Rayleigh problem are chosen and the results obtained by Direct Simulation Monte Carlo method are compared with those by BGK equation to exam the error caused by the BGK equation in solving the flow cases deviated far from equilibrium.

2 RAREFIED GAS FLOW CAUSED BY THE SUDDEN CHANGE OF THE WALL TEMPERATURE

Aoki et al.[6] calculated the one-dimension rarefied gas flow caused by the sudden change of the wall temperature by using the accurate numerical solution of the BGK model equation (2) and presented the gas temperature and pressure distribution normal to the wall in the following instants after the sudden rise of the wall temperature to twice the initial temperature T_0

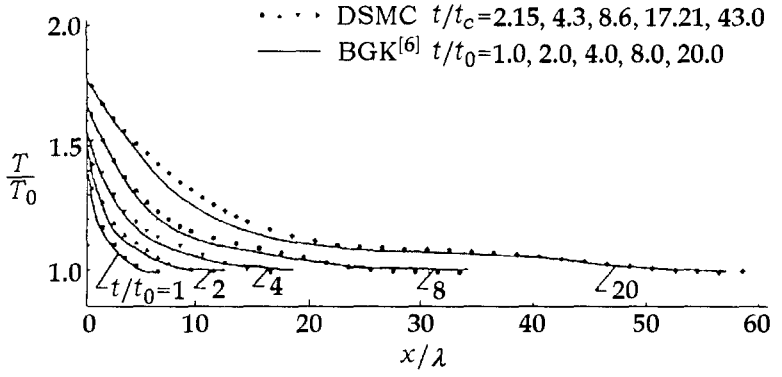
$$t/t_0 = 1.0, 2.0, 4.0, 8.0, 20.0 \tag{3}$$

where $t_0 = \sqrt{\pi} t_c/2$ is the time factor introduced by Aoki et al. that is proportional to the collision time, $t_c = \lambda/\bar{c}$ is the collision time, $\bar{c}$ is the average thermal speed at the initial temperature, λ is the molecular mean free path. In order to compare with the result in the time instants (3) in [6] , our DSMC simulation gives the gas temperature and pressure (see Fig.1) in the following time instants after the sudden temperature rise

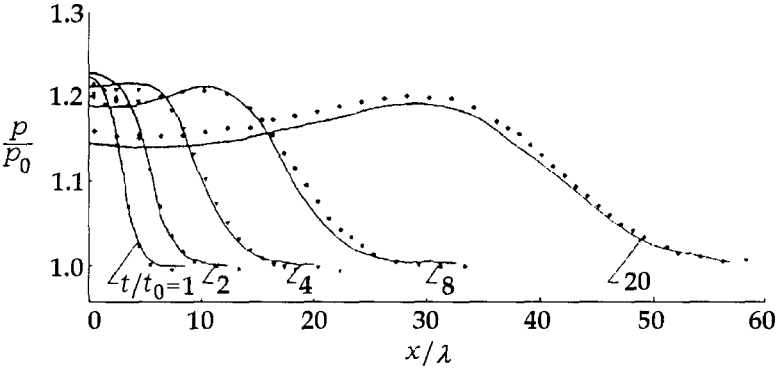
$$t/t_c = 2.15, 4.3, 8.6, 17.21, 43.0 \tag{4}$$

The reason that we select these time instants is that the BGK model can reflect the physical reality only after the adjustment of the collision frequency ν. Then (3) and (4) are completely corresponding to each other and are the same physical instants (see the explanation in the next paragraph). T_0, p_0 in Fig.1 are the temperature and pressure at the initial time instant $t = 0$ (cf. our previous paper [7]).

In our DSMC simulation the wall is completely diffusely reflecting as in [6]. At the same time, we use the VHS molecular model[4] with $\eta = 5$ — namely, the Maxwell molecular model, because it is consistent with the assumption of the BGK model that collision frequency is independent of the molecular velocity (in this case the second terms of the right hand sides of (1) and (2) are exactly equal). And it is well known that one needs to adjust the collision frequency ν in Eq.(2) in concrete problems in order that the BGK model reflects physical reality and that the heat exchange coefficient K or the viscosity coefficient μ has the correct expression. In this problem the heat transfer is essential, so the collision frequency in the BGK equation is to be modified as



(a)



(b)

Fig.1 The result of direct numerical test of the BGK model equation by the DSMC method. The gas temperature (a) and pressure (b) curves at different time instants after the sudden temperature rise to twice its initial temperature. The dot lines are the simulation results of DSMC and the solid lines are the numerical results of the BGK model.

$$\nu = (\pi/5.988)\frac{\bar{c}}{\lambda} \tag{5}$$

ensuring the K have the correct expression (see [8])

$$K = \frac{15}{4}\frac{k}{m}(0.499\rho\bar{c}\lambda) \tag{6}$$

Here k is the Boltzmann constant, m is the molecular mass. Thus the result obtained by Aoki et al.[6] must be modified and this is why we have selected the instants (4) to correspond with the time instants (3) for presenting the results in [6]. In fact, the values of (3) have been multiplied by $5.988/\pi$ for modifying ν, and then multiplied by $2/\sqrt{\pi}$ for changing the normalization magnitude from t_0 to t_c to reach the values of (4). And for the same reason, we have stretched $1.906(= 5.988/\pi)$ times the x coordinates in [6]. We can see that after modifying the time and x coordinates, the accurate numerical results of the BGK model in [6] are in good agreement with our DSMC simulation results after short time intervals, but after large time intervals, their difference becomes more and more distinguishable.

Aoki et al. also gave the numerical result for the reduced distribution function of molecular velocity $\zeta = c_1/(2RT_0)^{1/2}$ in the above problem by using BGK model equation

$$g(x,t,\zeta) = (2RT_0)^{1/2} n_0^{-1} \iint_{-\infty}^{\infty} f(X_1,t,c_i)\mathrm{d}c_2\mathrm{d}c_3 \tag{7}$$

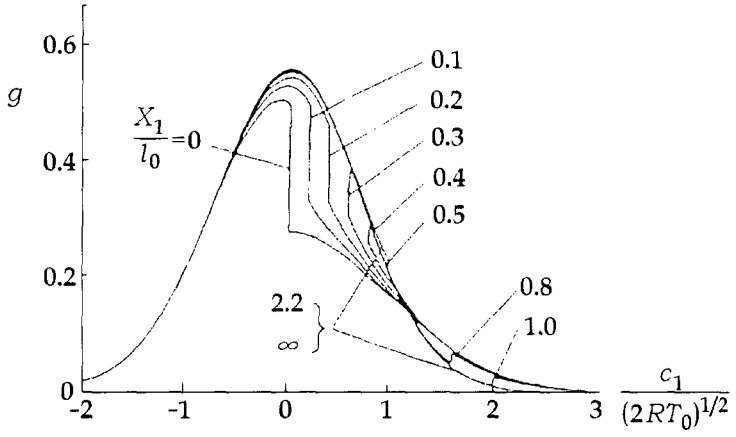
in the following time instants and spatial coordinates

$$t/t_0 = 0.5 \quad X_1/l_0 = 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.8, 1, 2.2 \tag{8}$$

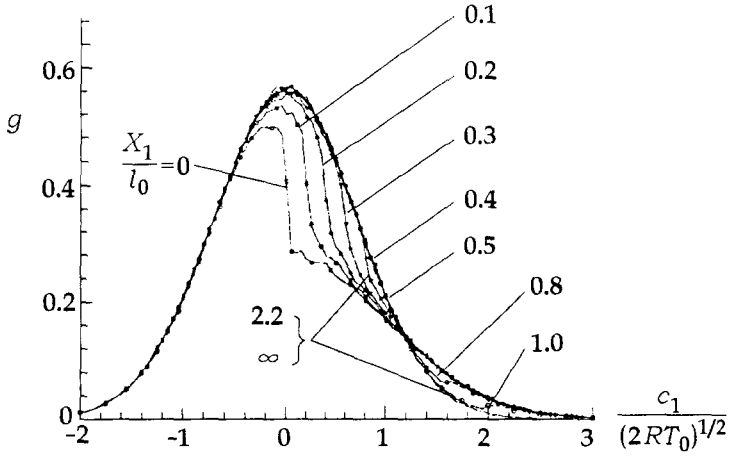
$$t/t_0 = 2.0 \quad X_1/l_0 = 0, 0.5, 1, 1.5, 2, 8.2 \tag{9}$$

where l_0 is the mean free path defined in [6].

In order to compare the result presented in [6], we calculated the reduced velocity distribution function by DSMC method in the following time instants (those in (8) and (9) multiplied by $5.988 \times 2/\pi^{3/2}$) and spatial coordinates (those in (8) and (9) multiplied by $5.988/\pi$) (see Fig.2)



(a) Result from the BGK model equation[6]



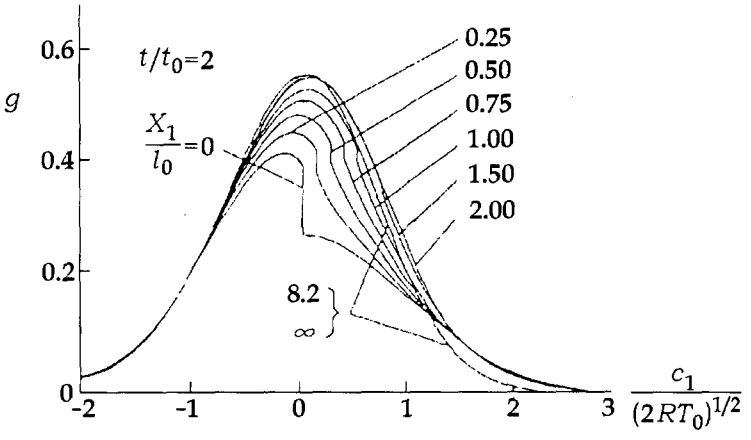
(b) Result from the DSMC method

Fig.2 Comparison between the results of the reduced velocity distribution function at time instant $t/t_0 = 0.5(t/t_c = 1.08)$

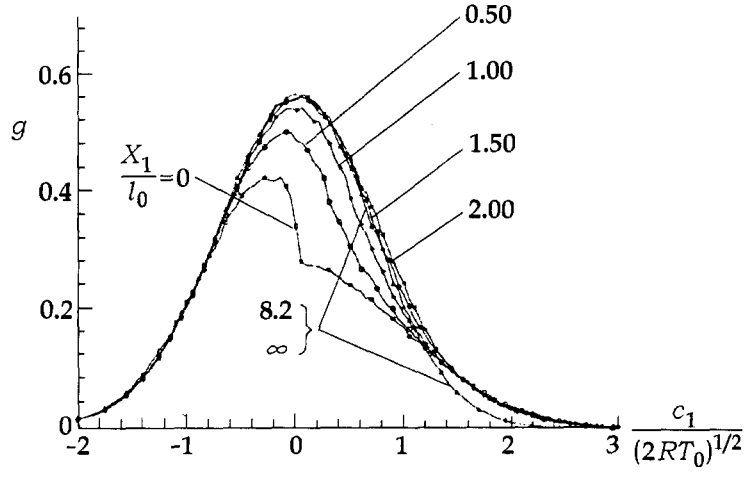
$$t/t_c = 1.08 \quad X_1/\lambda = 0, 0.19, 0.38, 0.57, 0.76, 0.95, 1.53, 1.91, 4.19 \tag{10}$$

$$t/t_c = 4.30 \quad X_1/\lambda = 0, 0.95, 1.91, 2.86, 3.81, 15.63 \tag{11}$$

We can see that the reduced velocity distribution functions in space coordinates obtained by the two different methods are close to each other within one collision time, but after four average collision times comparably large difference occurs (see Fig.3).



(a) Result from the BGK model equation[6]



(b) Result from the DSMC method

Fig.3 Comparison between the results of the reduced velocity distribution function at time instant $t/t_0 = 2.0(t/t_c = 4.30)$

All these results show clearly that in both the macroscopic value level (temperature, pressure) and the microscopic level (molecular velocity distribution function) the BGK model equation after the modification of the collision frequency can yield accurate results for flow cases not far from equilibrium (within 1~2 collision times), but for flow situation far from equilibrium BGK model is incorrect.

3 RAYLEIGH PROBLEM

Rayleigh problem studies the gas flow in one side of a flat plate caused by its sudden sliding in its own plane. Chu solved numerically the Rayleigh problem using the BGK model equation for higher Mach number[9]. In his paper he gives the flow field numerical result at the time instant $t/t_c = 10.0$ when the start-up velocity u_w of the plate is twice the initial equilibrium most probably speed ξ_0 and the wall temperature T_w is the gas static temperature T_0 at the initial equilibrium instant.

In our DSMC simulation for testing the BGK model equation, the wall reflecting model is again the diffuse reflection model and the VHS model with $\eta = 5$ is used. Because in the Rayleigh problem the transfer of momentum is essential, the collision frequency in the BGK equation is modified as

$$\nu = \frac{\pi}{3.992}\frac{\bar{c}}{\lambda} \tag{12}$$

to ensure the viscous coefficient μ have the correct expression (see [8])

$$\mu = 0.499\rho\bar{c}\lambda \tag{13}$$

and this means that Chu's result should be modified. The $t/t_c = 10.0$ in his paper really should be $t/t_c = 12.7$, i.e. should be multiplied by $3.992/\pi$ to take into account the modification of ν.

Meanwhile, in order to compare with the curves in [9], the x coordinates in the result of DSMC have been shrunken $1.27(= 3.992/\pi)$ times. After the transformation, comparison of the BGK model[9] result and our DSMC simulation result shows that these two methods have distinct diversity (see Fig.4) after a long time interval (12.7 collision times).

4 DISCUSSION

BGK model equation has been widely used in simulating the transition regime problems in rarefied gas dynamics. But it is actually only an approximation of the physically realistic Boltzmann equation, and the academic community gave too much attention to the BGK model. DSMC method's accuracy has been validated by the macro- and microscopic examination. The results obtained by the DSMC method in simulating the gas flow caused by the sudden rise of the wall temperature and the Rayleigh problem show that the BGK model equation yields rather exact results in the time range of the order of one collision time but yields results in the subsequent time interval more and more deviated from the results by the DSMC method. This should be taken into account when using the results obtained by the BGK model equation as well as the BGK equation as the basis of investigation.

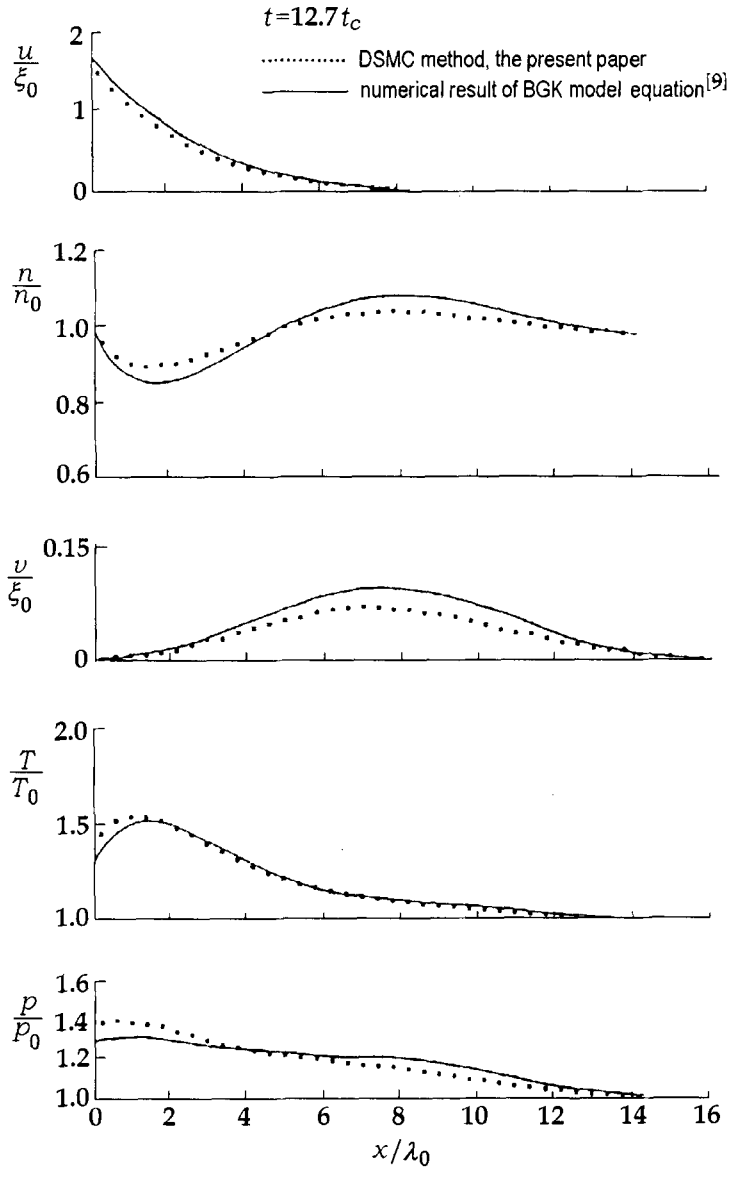


Fig.4 Comparison between the numerical test results of BGK model and those of the DSMC method. From the top down the figure gives the comparison of tangential velocity, number density, normal velocity, temperature and pressure for the Rayleigh problem at time instant $t = 12.7t_c$; The plate velocity is $u_w = 2\xi_0$, the wall temperature is $T_w = T_0$

REFERENCES

1 Bhatnagar PL, Gross EP, Krook M. A model for collision processes in gases. *Physical Review*, 1954, 94: 511~525

2 Welander P. On the temperature jump in a rarefied gas. *Ark Fys*, 1954, 7: 507~553

3 Bird GA. Molecular Gas Dynamics. Oxford: Clarendon Press, 1976

4 Bird GA. Molecular Gas Dynamics and the Direct Simulation of Gas Flows. Oxford: Clarendon Press, 1994
5 Shen C. DSMC method and the calculation of rarefied gas flow. *Advances in Mechanics*, 1996, 26(1): 1~13 (in Chinese)
6 Aoki K, Sone Y, Nishino K, Sugimoto H. Numerical analysis of motion of rarefied gas caused by sudden change of wall temperature. In: Beylich AE ed. Proceedings of the 17th International Symposium on Rarefied Gas Dynamics. VCH, Weinheims, 1991. 222~231
7 Shen C, Xu X, Hu Z, Wu W. Transient motion of rarefied gas caused by heat addition simulated by the direct simulation Monte Carlo method. Progress in Astro. and Aeronautics, 1994, 159: 234~242
8 Vincenti WG, C H Jr, Kruger. Introduction to Physical Gas Dynamics. John Wiley, 1965
9 Chu CK. The high Mach number Rayleigh problem according to the Krook model. In: Brundin ed. Rarefied Gas Dynamics. New York: Academic Press, 1967. 589~605