Chinese Science Bulletin
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Springer

Kinetic study of the Rayleigh-Bénard flows

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The present paper employs the direct simulation Monte Carlo (DSMC) method to study the Rayleigh-Bénard flows, where the temperature ratio of the upper to lower plate is fixed to 0.1. For a Knudsen number (*Kn*) of 0.01, as the Rayleigh number (*Ra*) increases, the flow changes from the thermal conductive state to the convective state at about *Ra*=1700, and the calculated relation of heat flux through the lower plate versus *Ra* is in good agreement with classical experimental and theoretical results. For *Kn*=0.05, the thermal conductive state remains stable, and the increase of *Ra* cannot trigger thermal instability.

Rayleigh-Bénard flows, thermal convection, critical Rayleigh number, rarefied gas effect, DSMC

Thermal convective motions occur in nature under many circumstances. In 1900, Bénard performed the first systematic investigation of thermal convection in a shallow fluid layer[1], which was heated from below and the upper surface was free. Bénard found that when the temperature of the lower plate exceeded a certain value, the thermal instability would occur, and then the fluid layer resolved itself into a number of cells. The theoretical foundations for a correct interpretation of the thermal convection were laid down by Rayleigh in 1916[1]. Based on linear instability analysis of the N-S equations, Rayleigh showed that what decided the instability was a non-dimensional parameter, namely the Rayleigh number (*Ra*)

$$Ra=\frac{\alpha g \Delta T d^3}{\nu\kappa}, \quad (1)$$

where α, ν, κ are the coefficients of volume expansion, kinetic viscosity and thermal diffusivity, respectively; g is the gravity acceleration, $\Delta T = T_h - T_c$, T_h and T_c are the temperatures of the lower and upper plates, respectively, and d is the height of the fluid layer. The thermal instability will take place when *Ra* exceeds a certain critical value. When the flow of heat across the fluid layer is transported entirely by conduction, the heat flux will increase linearly with ΔT. This linear relation breaks down at the onset of thermal instability because other modes of heat transport become operative. Therefore, as proposed by Schmidt and Milvertonl[1], we can detect whether the flow is in the conductive or convective state by examining the heat flux through the lower plate. Using the Rayleigh and Schmidt-Milverton's methods, the Rayleigh-Bénard (R-B) flows have been widely investigated[2]. The classical work includes the theoretical analysis of Schlüter et al.[3], which presented formulas for the initial slope of the convective heat transport, and the experimental result of Koschmieder and Pallas[4], which precisely measured the relationship of heat transport versus *Ra*.

The dissipative structure theory[5] and synergetics[6], also called the self-organization theory, have made great contributions to the mechanism research of the R-B convection. The dissipative structure theory was coined by Belgian scientist Prigogine, who proposed that the R-B system was a dissipative structure. When *Ra* reaches its critical value, the random small fluctuations will be strengthened to generate "giant fluctuations" due to coherence effects, and then the system changes

Received June 13, 2008; accepted August 28, 2008
doi: 10.1007/s11434-008-0546-4
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Supported by the National Natural Science Foundation of China (Grant Nos. 90205024, 10502051 and 10621202)

from an unstable state to a stable and orderly state. According to the synergetics found by German physicist Haken, the R-B system can be regarded as a synergy system, in which the order parameter dominates other state parameters and determines the system's behavior when the system is close to a certain critical point.

Based on the understanding of R-B flows and the self-organization theory, we decide to study the R-B flows from the kinetic theory, and expect to find out quantitative evidence of the self-organization theory; more generally, we want to investigate microscopic origin of the hydrodynamic instability. In order to achieve the goal, the first step is to verify that the direct simulation Monte Carlo (DSMC) method[7,8] is reliable for simulating R-B flows. The DSMC method uses a large number of the simulated molecules to represent the real gas molecules, where the molecular motions and the intermolecular collisions are assumed uncoupled within small time intervals. The molecular collision models are determined according to the Chapman-Enskog theory and phenomenological method, such as hard sphere (HS) model[7], variable hard sphere (VHS) model[7], and generalized soft sphere (GSS) model[9]. The results of Garcia[10,11], Golshtein and Elperin[12], Watanabe et al.[13], Stefanov et al.[14,15] and Chen et al.[16] showed that the DSMC method could simulate the R-B convection, and Chen et al.[17] studied the unsteady processes of R-B flows at large Rayleigh numbers. However, all of these results have not yet been compared with the experimental data[4] and the classical theory[3]. In this paper, the DSMC method is employed to simulate R-B flows. For a Knudsen number *Kn*=0.01, the flow state is observed to change from thermal conduction to convection, and the calculated relation of heat flux through the lower plate versus *Ra* is compared with the experimental and theoretical results. We also study the R-B flows for a relatively large Knudsen number (*Kn*=0.05), and explain why the conductive state is stable in this situation.

1 Computational parameters

In this paper we consider two-dimensional R-B flows, where L is length and d is height, with the aspect ratio $\Gamma = L/d$ and the temperature ratio $r = T_c/T_h$, and the gravity acceleration g is acting on each gas molecule.

Based on the state equation of the perfect gas, we have

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p = \frac{1}{T}. \tag{2}$$

According to the Chapman-Enskog theory, for a hard-sphere gas, the viscosity coefficient ν and thermal diffusivity coefficient κ can be expressed as

$$\nu = \frac{5\sqrt{\pi}}{16}\lambda c_m, \quad \kappa = \frac{15\sqrt{\pi}}{32}\lambda c_m, \tag{3}$$

where λ is the molecular mean free path, and $c_m = \sqrt{2kT/m}$ is the most probable thermal speed. Considering the temperature difference between the two plates, we use the average temperature in eqs. (2) and (3)[12].

Substitution of eqs. (2) and (3) into eq. (1) yields

$$Ra = \frac{2048}{75\pi} \times \frac{1-r}{(1+r)^2 Kn^2 Fr}, \tag{4}$$

where $Kn = \lambda/d$, $Fr = V_{th}^2/gd$, and $V_{th} = \sqrt{2kT_h/m}$.

It is obvious from eq. (4) that *Ra* depends on *Fr* and *Kn* for a fixed temperature ratio *r*, which is fixed as 0.1 in the present simulation. Adjusting the gravity acceleration *g*, we can change *Fr* and *Ra* conveniently. Each simulation case starts from a uniform state of gas with temperature T_h. Diffusive reflections are assumed at the upper and lower plates, while periodic boundary conditions are assumed on both sides. The hard sphere (HS) model is used to describe interactions between gaseous molecules, and the sampling is taken at the final steady state after a transient period. The space coordinates, temperature and density in flow fields are normalized by the plate distance *d*, temperature T_h and density at the initial state, respectively.

2 Transition from thermal conduction to convection for *Kn*=0.01

Schlüter et al.'s theoretical analysis[3], together with Koschmieder and Pallas's experiment[4] was obtained in the continuum regime. In order to compare with these two classical results, we first consider the R-B flows at *Kn*=0.01. The computational domain is divided into 64×32 sampling cells, and each sampling cell contains a group of 4×4 sub-cells to correctly calculate the molecular collisions. The total number of simulated molecules in the computational domain is about 1 million.

Figure 1 presents the temperature distribution for *Ra*=1159. There is no temperature gradient in the *x* direction; the temperature along the y direction deviates slightly from the linear distribution because of compressibility effect, but the flow field is in a conductive state without macroscopic motion.

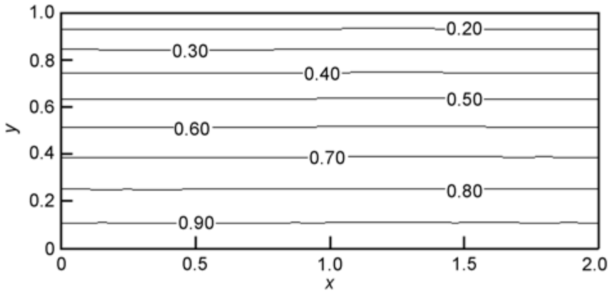

Figure 1 Temperature distribution for *Ra*=1159.

Temperature and velocity vector distributions for *Ra*=2900 are shown in Figure 2. It can be seen that the temperature is no longer uniform in the x direction and there is a pair of counter-rotating vortices, and thus the flow is in a steady convective state.

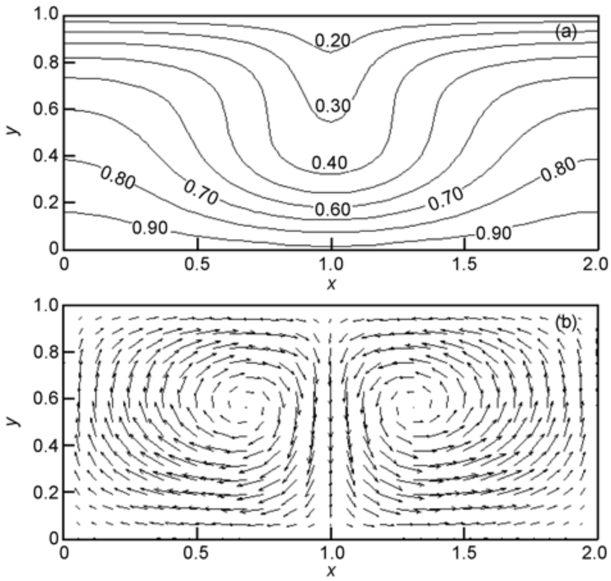

Figure 2 Temperature (a) and velocity vector (b) distributions for *Ra*=2900.

Density distributions along the y direction at the middle of the x direction for various Rayleigh numbers are given in Figure 3, which shows slight changes with increasing *Ra*. The density close to the lower plate is always the minimum, which is the basic condition of the R-B instability.

Figure 4 compares the dimensionless heat flux distributions through the lower plate for *Ra*=1159 and *Ra*=2900, where the dimensionless parameter q_{ave} is equal to the mean value over the whole lower plate. In the conductive state (*Ra*=1159), q/q_{ave} uniformly equals 1.0, whereas it becomes non-uniform in the convective state (*Ra*=2900). Because the temperature of the lower plate is fixed, the heat flux through it is determined by the gas temperature distributions in its neighborhood, though the density also has a litter influence.

Figure 5 compares the relation of the total heat flux through the lower plate versus *Ra* calculated by DSMC method with the classical theory and experiment. The Nusselt number (*Nu*) is defined as the ratio of the total heat flux to the heat flux in the conductive state, i.e.

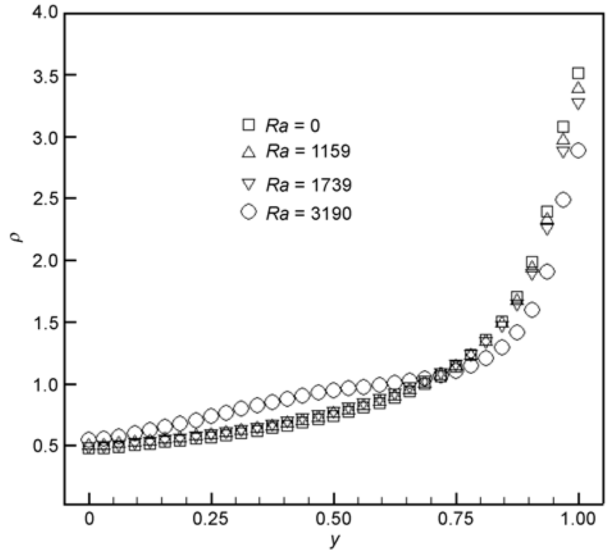

Figure 3 Density distributions along the y direction at the middle of the x direction for *Kn*=0.01.

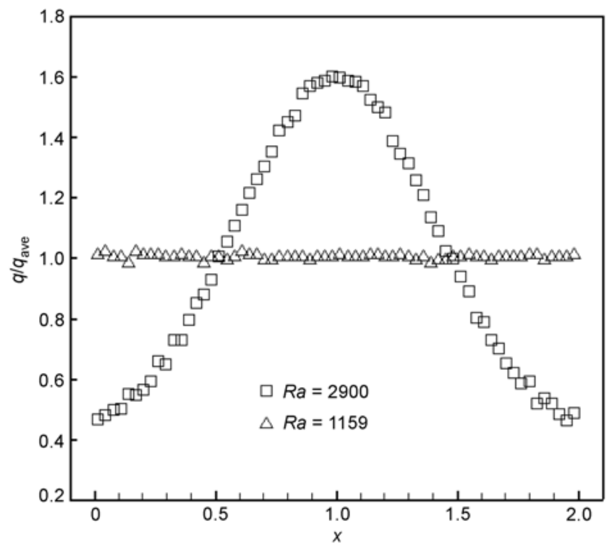

Figure 4 Comparison of heat flux distributions along the lower plate for the conductive and convective states.

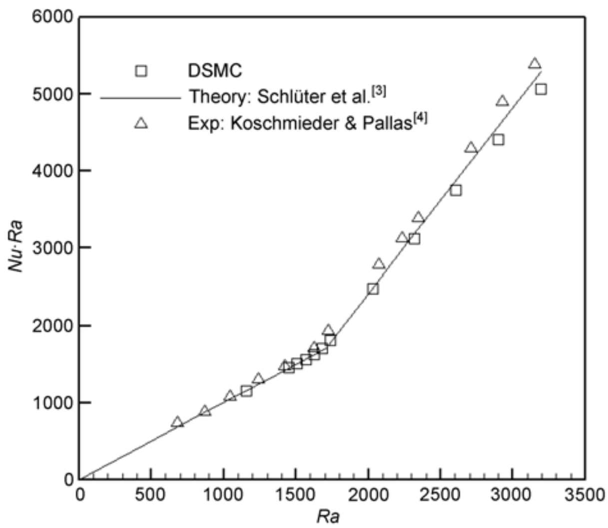

Figure 5 Relation of the total heat flux through the lower plate to *Ra*.

$$\mathrm{Nu} = q_t / q_c \,. \tag{5}$$

The theory curve came from Schlüter et al.[3] for the gas with the Prandtl number of 0.71,

$$Nu \cdot Ra \cong 2.41 Ra - 1.41 Ra_c \,, \tag{6}$$

where the critical Rayleigh number $Ra_c \cong 1708$. The experimental date given by Koschmieder and Pallas[4] showed that $Ra_c \cong 1675$ and the slope of the curve was about 2.43 after the onset of convection.

The calculated result by DSMC shows that a critical Rayleigh number is around 1700 (Figure 5). When *Ra* is below 1700, the DSMC results lie on a line with the slope of 1.0, and thus the flow is definitely in a thermal conductive state. As *Ra* increases, the slope shifts to about 2.27 at $Ra_c \cong 1700$ that is corresponding to the onset of a thermal convection. In general, the DSMC results are in good agreement with the classical theory and experiment. When *Ra* is over 1700, the curve slope of DSMC is a little smaller than those of the theory and experiment. The reason is that the temperature difference between the two plates in our simulation is relatively large, and thus the gas compressibility makes the calculated condition depart from the Boussinesq's approximation on which the theory and experiment were carried out[3,4].

3 The stable conductive mechanism for *Kn* = 0.05

When *Kn*>0.01, the compressibility, slip velocity and temperature jump at the plate boundaries have a significant effect. Using the DSMC method and the numerical calculations of compressible N-S equations associated with slip boundary conditions, Stefanov et al.[15] obtained the R-B instability zone with respect to two independent parameters *Kn* and *Fr*. The zone of the convection regime was verified by Manela and Frankel[18], who employed the linear stability analysis to the compressible N-S equations. In the following, we calculate the R-B flows for *Kn*=0.05, and analyze the physical mechanism underlying the stable conductive state.

The temperature distributions for *Ra*=1160 and *Ra*=2900 are shown in Figure 6, which are uniform in the *x* direction for both cases. The latter differs from the corresponding case at *Kn*=0.01 (Figure 2), where the flow is in a steady convective state.

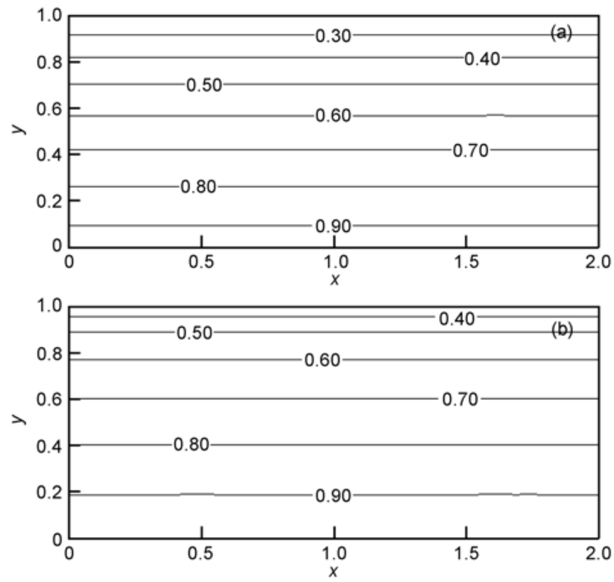

Figure 6 Temperature distributions for *Ra*=1160 (a) and *Ra*=2900 (b).

Figure 7 gives density distributions along the *y* direction at the middle of the *x* direction for various Rayleigh numbers. When *Ra*<928, the density increases monotonically along with *y*, but the buoyancy cannot overcome the thermal diffusivity and viscous dissipation to generate macroscopic convective velocity for such small Rayleigh numbers. When *Ra*>928, essentially different from the cases at *Kn*=0.01 (Figure 3), the density does not increase monotonically along with *y*: for *Ra*=1160, the density first decreases and then increases; for *Ra*=2320 and *Ra*=2900, the density decreases monotonically with increasing *y*. They mean that, for *Kn*=0.05, when *Ra* exceeds a certain value, the density gradient direction will be the same as the gravity direction. This is beneficial to the fluid stability and explains why no thermal convection occurs with increasing *Ra* for *Kn*=0.05.

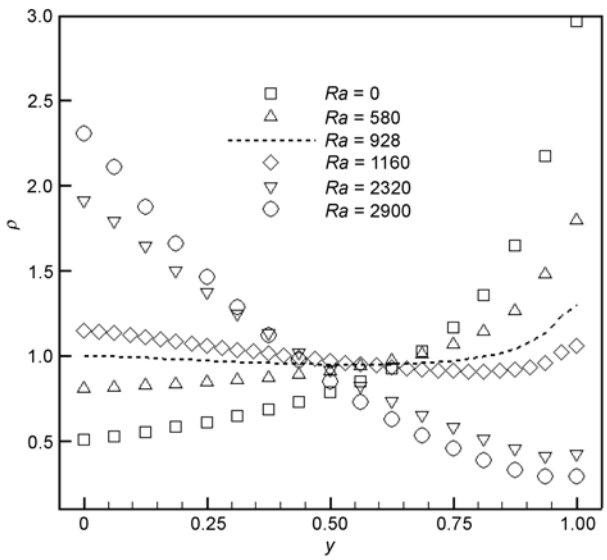

Figure 7 Density distributions along the *y* direction at the middle of the *x* direction for *Kn*=0.05.

The relation of the total heat flux through the lower plate q_t versus *Ra* for *Kn*=0.05 is also different from that for *Kn*=0.01. q_t is related to the number flux of incident molecules Γ_n, the average energy of incident molecules $\overline{E}_i$ and the average energy of reflected molecules $\overline{E}_r$ as follows:

$$q_t = \Gamma_n \cdot (\overline{E}_r - \overline{E}_i). \tag{7}$$

Because $\overline{E}_r$ equals a constant of $2kT_h$ due to the diffuse reflection at the lower plate, q_t depends on Γ_n and $\overline{E}_i$ only. The values of Γ_n and $\overline{E}_i$ given by our DSMC calculations increase along with *Ra* (Table 1), which makes q_t arrive at its maximum at *Ra*=928.

Table 1 Total heat flux, number flux and average energy of incident molecules to the lower plate for *Kn*=0.05

Ra	q_t×10^{-3} (J·m^{-2}·s^{-1})	Γ_n ×10^{-24} (m^{-2}·s^{-1})	$\overline{E}_i$ ×10^{21} (J)
0	1.84	1.10	6.61
116	1.87	1.22	6.75
580	1.95	1.79	7.19
696	1.96	1.94	7.27
928	1.97	2.26	7.41
1160	1.96	2.60	7.53
2320	1.77	4.45	7.88
2900	1.60	5.42	7.98

4 Conclusions

This paper investigates the R-B flows using the DSMC method. For *Kn*=0.01, a transition from thermal conduction to convection has been observed as *Ra* increases, and the relation of *Nu* to *Ra* given by DSMC is in good agreement with the results of the classical experiment and theory. For *Kn*=0.05, the thermal conductive state remains stable; when *Ra* exceeds a certain value, the density gradient direction will be the same as the gravity direction, which is beneficial to the fluid stability. The present work verifies the feasibility for the DSMC method to analyze the R-B instability and lays the foundation for further kinetic studies on the microscopic mechanism of hydrodynamic instability.

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