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MONTE CARLO SIMULATION OF THE BENARD INSTABILITY IN A RAREFIED GAS MIXTURE*

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The existence of the Benard instability in a rectangular 2D domain of a rarefied gas, heated from below and under the action of a constant external force (gravity), is numerically investigated by using the Direct Simulation Monte Carlo method.

1. Introduction. The Benard instability is a well-known phenomenon in the fluid dynamics. The earliest experiments with a horizontal fluid layer heated from below were made by Benard himself [1]. Rayleigh [4] analyzed the stability of the pure conduction solution of the Navier-Stokes equations in the Boussinesq approximation and introduced a nondimensional parameter (the Rayleigh number).

It seems that the corresponding problem for rarefied gas governed by the Boltzmann equation has not been studied. Here we attack the problem by using the Direct Simulation Monte Carlo (DSMC) method. Since the method is based on a system of a finite number of particles with stochastic dynamics, it is shown that it exhibits the Benard instability corresponding to the ability of a stochastic system to organize itself into a pattern of vortices.

The numerical results clearly show a formation of vortices in the studied area when the gas is composed of one component. When the gas is composed of two components and the particles of the second component are with larger volume and mass than the first component the vortex intensity vanishes.

2. Formulation of the problem. Let us consider a binary gas mixture between two parallel planes with different temperatures T_h at $x = 0$ and T_c at $x = L$ ($T_h > T_c$). An external constant force $F = mg$, directed along the axis y (gravity), acts on each molecule of the gas at each point (see Figure 1). We study the macrocharacteristics of the flow, where we fix the number density of the first component (basic one), and the concentration of the second component (additional one) varies from 0% to 4%. The masses and the diameters of the additional component are respectively M and D times greater than the ones of the basic component.

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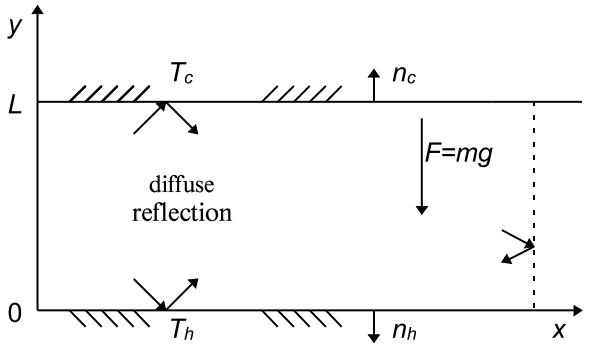

Fig. 1

Now, we are ready to construct a mathematical model describing the gas mixture motion. In accordance with the kinetic approach, the gas mixture flow is described by a system of non-linear Boltzman equations for the single-particle velocity distribution function $f_l(t, x, \underline{\xi}_l)$ around velocity vector $\underline{\xi}_l \in R^3$ and coordinate point $x \in G \subset R^3$, $t \in [0, T]$ for each of the components

$$\frac{d}{dt} f_l = \sum_{m=1}^{2} \int (f_l^* f_m^* - f_l f_m) g_{m,l} \sigma(g_{m,l}, \Omega) d\Omega d\underline{\xi}_l, \quad l = 1, 2. \tag{2.1}$$

The collision integrals on the right-hand of equation (2.1) are written in the generally accepted forms: $f_l^* = f_l(t, x, \underline{\xi}_l^*)$, $\underline{\xi}_l^*$ – post collision molecular velocity; $g_{m,l} = \left|\underline{\xi}_l - \underline{\xi}_{ml}\right|$ – relative velocity; $\sigma(g_{m,l}, \Omega) d\Omega$ – differential cross-section of the particle scatter within the solid angle $d\Omega$. We assume hard sphere molecules for both components, where $\sigma(g_{m,l}, \Omega) = \left(\frac{d_l + d_m}{2}\right)^2 g_{m,l} \sin\theta \cos\theta$, d_1 and d_2 are the molecular diameters.

From this statement of the problem for one component gas we can obtain three nondimensional parameters: the Knudsen number based on the mean free path $\lambda_0 = (\sqrt{2}\pi\sigma^2 n_0)^{-1}$ (n_0 – the mean number density), the Froude number based on the thermal speed $v_h = \sqrt{2RT_h}$, and the temperature ratio:

$$Kn = \frac{\lambda_0}{L}, \quad Fr = \frac{v_h^2}{gL}, \quad r = \frac{T_c}{T_h}. \tag{2.2}$$

We should make a note that for the binary gas mixture the mean free path is calculated by the formula:

$$\lambda_0 = \sum_{i=1}^{2} \left\{ \frac{n_i}{n} \left[\sum_{j=1}^{2} \pi n_j \left(\frac{d_i + d_j}{2} \right)^2 \left(1 + \frac{m_i}{m_j} \right)^{\frac{1}{2}} \right]^{-1} \right\}, \tag{2.3}$$

where d_i, m_i, n_i are respectively the diameters, the masses and the number densities of the molecules from the i-th component. We include three nondimensional parameters – the ratios of the masses, the diameters and the number densities when we study a binary gas mixture:

$$M = \frac{m_1}{m_2}, \qquad D = \frac{d_1}{d_2}, \qquad K = \frac{n_1}{n_2} \tag{2.4}$$

We complete our formulation assuming the following boundary conditions:

(a) a diffuse reflection of the molecules at the planes;

(b) the solution possesses a periodic structure along axis x [5].

3. Method of solution. When we solve the problem by DSMC method we don't have to solve the Boltzmann equation. To minimize the time of solution and the computer memory, as the solution is kept real, we can use a period $2L$ along axis x, where L is the distance between the planes. The simulation has been devised to be consistent with the formulation in Section 2. The basic steps of the simulation are as follows:

(a) the time interval $[0, T]$ on which the solution has been found, is subdivided into subintervals with stepΔt;

(b) the space domain is subdivided into cells with sides $\Delta x, \Delta y$;

(c) the gas molecules are simulated in the gap G using a stochastic system of N points (particles) having positions $x_i(t), y_i(t)$ and velocities $\underline{\xi}_i(t) = (\xi_1(t), \xi_2(t), \xi_3(t))$;

(d) at any given time there are $N_m(i)$ particles from the i-th component in the m-th cell; this number is varied by computing its evolution in the following two stages:

Stage 1. The binary collisions in each cell are calculated without moving the particles.

Stage 2. The particles are moved with the new initial velocities acquired after collision as if they were acted upon only by gravity. We allow no collisions in this stage.

(e) Stages 1 and 2 are repeated until $t = T$;

(f) The important moments of the distribution function are calculated by time averaging after a suitable regime has been reached.

Let us now describe the two stages of the calculation in some details:

Stage 1. We use Bird's "no time counter" scheme [2], which involves the following two steps:

1.1. To compute the maximum number of binary collisions, we use the formula:

$$N_{c\max} = \frac{N_m(p) N_m(p-1)}{2V_{cell}} \left\langle \pi\sigma^2 \left|\xi_i - \xi_j\right|_{\max} \right\rangle \Delta t \tag{3.1}$$

$$N_{c\max} = \frac{N_m(p) N_m(q)}{2V_{cell}} \left\langle \pi\sigma^2 \left|\xi_i - \xi_j\right|_{\max} \right\rangle \Delta t, \tag{3.2}$$

where $1 \le p < q \le 2$ and $V_{cell} = \Delta x \Delta y$ is the volume of the cell. We use formula (3.1) when we calculate collisions between molecules from one component and (3.2) between molecules of different components.

1.2. The pairs (i, j) of particles are chosen randomly with probability $\left|\underline{\xi_i} - \underline{\xi_j}\right| / \left(\left|\underline{\xi_i} - \underline{\xi_j}\right|\right)_{\max}$. If the collision event occurs, the velocities after collision are calculated in the following way:

$$\underline{\xi_i^+} = \frac{1}{2}\left(\underline{\xi_i} + \underline{\xi_j} + \underline{k}\left|\underline{\xi_i} - \underline{\xi_j}\right|\right), \tag{3.3}$$

$$\underline{\xi_j^+} = \frac{1}{2}\left(\underline{\xi_i} + \underline{\xi_j} - \underline{k}\left|\underline{\xi_i} - \underline{\xi_j}\right|\right), \tag{3.4}$$

where $\underline{k}$ is vector randomly distributed on the unit sphere. Otherwise the velocities are left unchanged.

Stage 2. We compute the new positions and velocities of the particles using the equations:

$$x_i^+ = x_i + \xi_{1i}\Delta t,$$

$$y_i^+ = y_i + \xi_{2i}\Delta t - \frac{g\Delta t^2}{2}, \tag{3.5}$$

$$\underline{\xi_i^+} = \underline{\xi_i} - \underline{g}\Delta t,$$

as the particles with $y_i^+ \leq 0$ or $y_i^+ \geq L$ are diffusely reflected and the particles with $x_i^+ \leq 0$ or $x_i^+ \geq 2L$ are mirror reflected.

4. Numerical results. The simulations are made with 2 000 000 modeling particles. The case of one-component gas is studied with two generators of random numbers. The first generator is based on the remainder from the division of the two high numbers – residual method [9]. The second generator based on the data encryption standard [8]. The velocity and density difference between the two cases is less than 0.2%. This means that the flow macrocharacteristics do not depended on the random number generator.

All magnitudes which we use are nondimensional so that the mean free path in the gas mixture in equilibrium state is equal to 1. In this problem the nondimensional parameters are six – Kn, Fr, r, M, D and K. For convenience we use g instead of Fr, which are mutually replaceable. When we study one component gas, the effect of the instability appears for certain values of the parameters Kn, g, r, [5, 7]. Here the instability means destruction of the stationary distribution macrocharacteristics typical for a simple heat flux between two parallel planes and creation of a new stability convectional flow which possesses a form of two vortices. Figure 3 shows the vector field of the velocity when the gas is of one component and $Kn = 0.02$, $g = 0.08$, $r = 0.1$. When the gas is binary mixture, the above three parameters are the same and M=0.2, D=0.2, K=0.03, the vortex is distracted and the gas is in a state of stability – Figure 2

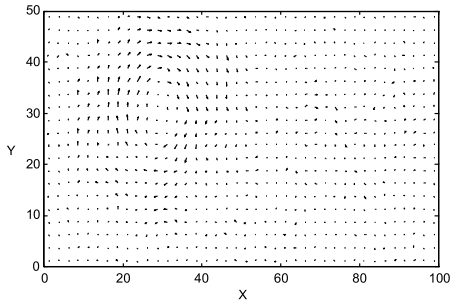

Fig. 2

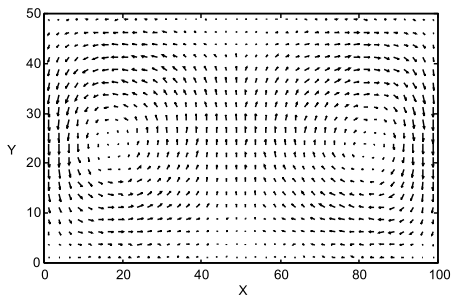

Fig. 3

The purpose of this study is to establish the influence of the concentration of the additional component over the stability of the flow. The natural way to establish the

stability or the instability of the flow is the using of the circulation of the vortex. The magnitude of the circulation is a measure for the intensity of the vortex. When the rates of the circulation vanish, the flow is stable. Otherwise, the flow is not stable. At the concrete results the rates of the circulation are of the same degree as the level of the fluctuations obtained from the finite number of particles model of the gas. That is why we use the projection of the velocity along axis x and the density. Figures 4 and 5 show the variation of the maximal, minimal and average rates of the velocity projection along axis x and respectively the density of the basic component when $y = 1.25$ and K varies from 0 to 0.04 with step 0.005. The numerical results show that $K = 0.015$ is a critical rate for the existence of the vortex flow. This means that the vortex flow in this case is in instability and when we make a small change of the concentration of the additional component the flow is transported into a no vortex stable state.

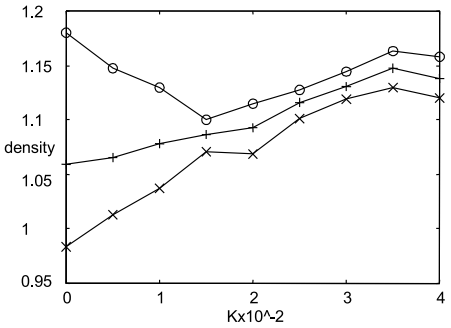

Fig. 4

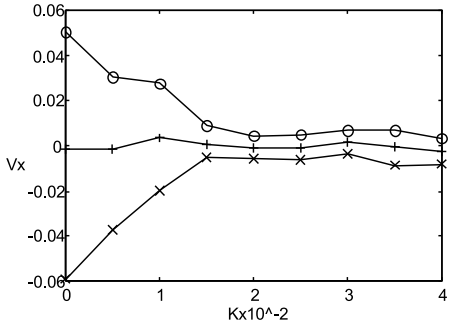

Fig. 5

In conclusion we denote that the question: how the macrocharacteristics (mostly the density) vary when the concentration of the additional component increase leaves open. This is a purpose of the further studies.

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МОНТЕ-КАРЛО СИМУЛАЦИЯ НА НЕУСТОЙЧИВОСТ НА БЕНАР В СМЕС ОТ РАЗРЕДЕНИ ГАЗОВЕ

Добри Й. Данков, Владимир М. Русинов

Числено изследване на съществуване на неустойчивост на Бенар в правоъгълна 2D област от разреден газ, нагрят отдолу и на който действа външна константна сила (гравитация), чрез използване на пряко статистическо моделиране.