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THE DYNAMICS OF A SMALL DROP IN A THERMAL DIFFUSION CHAMBER†

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The solution of the problem of the motion of a drop, whose size is small compared with the mean free path of the molecules of the gas surrounding the drop, in temperature and concentration fields is presented. The approach proposed earlier [1, 2] is used, supplemented by taking into account the phase transition on the drop surface. © 2004 Elsevier Ltd. All rights reserved.

Up to recently, the problem of the motion of aerosol drops in a thermal diffusion chamber under the action of thermal diffusiophoresis and the gravity force, taking into account phase transitions on the drop surface, has been solved either in the case of a continuum [3, 4] or in the case of free-molecular flow [5]. The model used in [3, 4] gave the best qualitative agreement with experiment [5] compared with the earlier approach used in [1, 2, 6]. Some quantitative disagreement was regarded as being due to imperfections in the model and certain simplifications employed when carrying out the calculations. In particular, no account was taken of the fact that, due to condensation growth of the drop, a transition occurs from one mode to another. In other words, the continuum model, employed in [3, 4], inadequately describes the dynamics of the drop at the initial stage of its evolution from the instant when it is formed to when it reaches its size, when the Knudsen number becomes comparable with unity. It is logical to supplement the model by a separate consideration of the initial stage and subsequent matching of the solution with the results [3, 4]. In this paper, when considering the drop motion at the initial stage it is more convenient not to use the "dusty gas" model, but to carry out a direct calculation of the momentum transferred to the drop by the gas molecules [2].

1. FORMULATION OF THE PROBLEM

An investigation of the dynamics of a small drop in a thermal diffusion chamber requires, in principle, the same approach as in the case of a large drop, considered previously [3, 4]. The equation of motion retains its previous form (everywhere henceforth, unless otherwise stated, summation is carried out over the subscript j)

$$\frac{d(m\mathbf{v})}{dt} - \mathbf{v}_{St}\frac{\sum n_j m_j}{n_1 m_1}\frac{dm}{dt} = \mathbf{F} - m\mathbf{g}$$

where n_j and m_j are the density and mass of the molecules of sort j, $\mathbf{v}$ is the drop velocity in a laboratory system, and $\mathbf{v}_{St}$ is the velocity of Stefan flow of the gas mixture. However, the expressions for the rate of change of the mass m of the drop and the force F acting on it, which occur in the equation, change. We will consider both of these characteristics in succession.

2. THE CHANGE IN THE MASS AND THE RADIUS R OF THE DROP DURING A PHASE TRANSITION

We will first calculate the balance of the number of particles which undergo a phase transition on the drop surface. The part played by the molecules of the neutral gas-carrier can be ignored in this case, since they take no direct part in the change in the drop size (although they play a decisive role in the heat balance, which indirectly affects the growth rate). We will use the well-known gas-kinetic expression for the number of gas molecules which collide the drop surface,

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$$N_j^{(i)} = n_j \langle \boldsymbol{v}_j(T_i) \rangle \pi R^2 \tag{2.1}$$

The subscript $j = 1$ corresponds to the vapour, $j = 2$ corresponds to the inert gas (air), $\langle \boldsymbol{v}_j(T_i) \rangle = \sqrt{8kT/(\pi m_j)}$ is the mean velocity of molecules of sort j, k is Boltzmann's constant and T_i is the gas temperature. We can also similarly write the number of gas molecules which evaporate from the drop surface by replacing the density of the vapour in the surrounding gas by the density n_{1s} of the saturated vapour at the drop temperature T_e.

We have the following expression for the number of reflected molecules of the inert gas

$$N_2^{(e)} = n_2 \langle v_2(T_e) \rangle \pi R^2 \tag{2.2}$$

The density of the saturated vapour is connected with its pressure p_{1s} by the relation

$$n_{1s}(T_e) = p_{1s}(T_e)/(kT_e) \tag{2.3}$$

In addition to the temperature, the pressure p_{1s} also depends on the radius of curvature of the drop surface

$$p_{1s}(T_e) = p_{1s}^{(0)}(T_e) + \alpha(T_e)/R \tag{2.4}$$

where $p_{1s}^{(0)}$ (T_e) is the pressure of the saturated vapour above a plane surface and $\alpha(T_e)$ is the surface (interphase) tension.

Bearing in mind the fact that the drop is small, we will assume the temperature to be the same over the whole volume of the drop. We then have the following equation for the change in the mass of the drop

$$\frac{dm}{dt} = m_1(N_1^{(i)} - N_1^{(e)}) = \frac{8R^2}{\langle v_1(T_i) \rangle} \left\{ p_1(T_i) - p_{1s}(T_e) \frac{\sqrt{T_i}}{\sqrt{T_e}} \right\} \tag{2.5}$$

Hence we also obtain an equation for the change in the drop radius

$$\frac{dR}{dt} = \frac{2}{\pi \rho_e \langle v_1(T_i) \rangle} \left\{ p_1(T_i) - p_{1s}(T_i) \frac{\sqrt{T_i}}{\sqrt{T_e}} \right\} \tag{2.6}$$

where ρ_e is the drop density.

3. CALCULATION OF THE QUASI-EQUILIBRIUM TEMPERATURE OF THE DROP

To find the drop temperature we will calculate the heat balance on the drop due to collisions of molecules of the surrounding gas with it. We will use the well-known gas-kinetic expression for the energy flux on the drop surface

$$W_1^{(i)}(T_i) = 2kT_i N_1^{(i)}(T_i) \tag{3.1}$$

The expression for the energy transferred to the drop by neutral molecules has a similar form (with the subscript 1 replaced by the subscript 2). Hence, we must add the energy which is released as a result of the phase transition of the vapour on the drop surface. As a result, we have the following expression for the energy flux on the drop

$$\sum W_j^{(i)}(T_i) + m_1 N_1^{(i)}(T_i) L \tag{3.2}$$

Correspondingly, for the outflow of energy when gas molecules evaporate (are reflected) from the drop surface we have an expression which differs from (3.2) by having the subscript i replaced by e. Here we have assumed the condition of complete accommodation, i.e. the temperature of the evaporated (reflected) molecules is assumed to be equal to the drop temperature. We will neglect the dependence of the specific heat of the phase transition L on the temperature.

The heat balance equation, taking Eq. (2.5) into account, therefore has the following form

$$L\frac{dm}{dt} + \sum[W_j^{(i)}(T_i) - W_j^{(e)}(T_e)] = 0 \tag{3.3}$$

or, after substituting the above expressions,

$$L\frac{8R^2}{\langle v_1(T_i)\rangle}\left[p_1(T_i) - p_{1s}(T_e)\frac{\sqrt{T_i}}{\sqrt{T_e}}\right] + 2kT_i[N_1^{(i)}(T_i) + N_2^{(i)}(T_i)]$$

$$-2kT_e[N_1^{(e)}(T_e) + N_2^{(e)}(T_e)] = 0 \tag{3.4}$$

The system of equations (2.6), (3.4), taking expression (2.4) into account, determines the change in the size and quasi-equilibrium temperature of the drop during a phase transition at a specified gas temperature T_i. This system can be solved by numerical methods without difficulty.

4. CALCULATION OF THE FORCE ACTING ON THE DROP

As before, we will assume the drop temperature to be the same over the whole volume. In this case evaporation of the volatile component, like the reflection of the non-volatile component (in the case of complete accommodation), occurs uniformly over the whole drop surface. This in turn means that the integral recoil momentum of the reflected and evaporated molecules is equal to zero. Hence, when calculating the force acting on the drop from the side of the gas, one need only take into account the momentum of the molecules which collide with its surface.

A gas-kinetic calculation [7] gives the following expression for the momentum which the gas molecules, which collide with its surface, transfer to the drop in unit time

$$\mathbf{F} = \sum n_j m_j \langle v_j\rangle^2\left(\frac{1}{3}\mathbf{X}_j - \mathbf{Z}_j\right)\pi\sqrt{\pi}R^2 \tag{4.1}$$

Here

$$\mathbf{X}_j = \frac{4}{\sqrt{\pi}\langle v_j\rangle}\left[\mathbf{u} + (-1)^j\frac{n_2 m_2}{n_j m_j}\boldsymbol{v}_{St}\right] + \frac{5}{2}\mathbf{Z}_i, \quad \mathbf{Z}_j = d_j n \,\mathrm{grad}\, n_{10} + a_j \,\mathrm{grad}\ln T$$

$$\boldsymbol{v}_{St} = -\frac{n_1 m_1}{\sum n_j m_j}\frac{n^2}{n_1 n_2}D_{12}(\mathrm{grad}\, n_{10} + k_T \,\mathrm{grad}\ln T), \quad n = \sum n_j, \quad n_{10} = \frac{n_1}{n}$$

u is the velocity of the centre of mass of the gas mixture with respect to the drop, k_T is the thermal diffusion coefficient of the mixture and D_{12} is the diffusion coefficient.

5. CALCULATION OF THE PARAMETERS d_j AND a_j

When calculating the parameters d_j and a_j we will retain the scheme described above, and also the notation employed previously [8]. We will therefore denote the parameters d_j and a_j, referred to the second component of the gas mixture, by d_{-1} and a_{-1}. The required parameters are found by solving the following two independent systems of equations

$$\sum_{s=-1}^{s=+1} a_s a_{rs} = \alpha_r, \quad \sum_{s=-1}^{s=+1} d_s a_{rs} = \delta_r; \quad r = -1, 0, +1 \tag{5.1}$$

The right-hand sides of these equations are equal to zero, with the exception of

$$\alpha_1 = -\frac{15\sqrt{\pi}}{8n_2}\langle v_1(T_i)\rangle, \quad \alpha_{-1} = -\frac{15\sqrt{\pi}}{8n_1}\langle v_2(T_i)\rangle, \quad \delta_0 = \frac{3\sqrt{2kT_i}}{2n_1 n_2} \tag{5.2}$$

The coefficients a_{rs} of systems (5.1) are found using the following relations

$$a_{00} = \frac{m_0kT}{E}, \quad a_{01} = -5(C-1)\sqrt{m_0}\frac{M_2kT}{2\sqrt{M_1}E}, \quad a_{0-1} = 5(C-1)\sqrt{m_0}\frac{M_1kT}{2\sqrt{M_2}E}$$

$$a_{1-1} = -\sqrt{M_1M_2}\frac{kT}{E}\left(\frac{11}{4} - B - 2A\right)$$

$$a_{11} = \frac{5kT}{M_1E}\left\{\frac{1}{4}(6M_1^2 + 5M_2^2) - M_2^2B + 2M_1M_2A\right\} + \frac{5kTn_1}{2\mu_1n_2} \qquad (5.3)$$

$$a_{-1-1} = \frac{5kT}{M_2E}\left\{\frac{1}{4}(6M_2^2 + 5M_1^2) - M_1^2B + 2M_1M_2A\right\} + \frac{5kTn_2}{2\mu_2n_1}$$

$$m_0 = \sum m_j, \quad M_j = \frac{m_j}{m_0}, \quad E = \frac{2}{3}nm_0D_{12}$$

(μ_j is the viscosity of the jth component of the gas).

These expression apply to any type of spherically symmetric molecules, possessing only energy of translational motion. For rigid elastic spherical molecules the coefficients A, B and C take a particularly simple form: $A = 2/5$, $B = 3/5$ and $C = 6/5$.

6. CONCLUSION

The expressions obtained for the force acting on the drop (4.1) and for the rate of change of its mass (2.5) must be substituted into the equation of motion of the drop. A calculation (generally numerical) for specific conditions (pressure, temperature and composition of the gas mixture, and the properties of the aerosol nucleus), carried out at the initial stage of evolution of the drop, and subsequent matching with the result obtained in [3, 4], in our opinion eliminates some of the quantitative disagreement with the results of measurements which remain at the present time.

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