TIME DEPENDENT ANALYSIS OF THE EVOLUTION OF THE DISTRIBUTION OF DROP SIZES OF LIQUID DROPLETS IN A FREE-MOLECULE STREAM

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Abstract—This paper deals with the study of the time-evolution of the distribution of drop sizes, velocities and temperatures of a cloud of droplets shot, with a given initial velocity and temperature and a given distribution of drop sizes, into a gas volume at fixed thermodynamical conditions. The mean free path of the gas molecules was large compared with the mean diameter of a droplet. The study is based on a phase-transition physical model, proposed by Bellomo (1974), which takes into account the kinetic theory of liquids and gases and the physics of gas–surface interaction. This model has proved suitable for time-dependent non equilibrium phenomena and has given theoretical results very close to experimental ones.

1. INTRODUCTION

The phenomenon of phase-change of small liquid droplets has been dealt with by several authors (see for example Rose & Glicksman 1973 and Ford & Lekik 1973), by means of the continuum mechanics equations. In particular Nix & Fukuta (1973) have proposed a nonsteady state theory in order to predict time-dependent evolutions. In rarefied gas conditions the boundary conditions at the interface, which require consideration at a molecular scale, (see Cipolla, Lang & Loyalka 1974), assume a great deal of importance. The problem of vaporization of droplets in the above mentioned physical conditions has been dealt with by Brock (1964) in a general form without defining the boundary conditions, whereas Lang & Kusher (1974) have discussed the boundary conditions by means of a phenomenological theory without a quantitative definition of the transport properties at the liquid–vapour interface.

Recently Bellomo (1974) has proposed a phase-change physical model, described in detail in the next paragraph, in order to analyse the non-equilibrium time-evolutions of small droplets in rarefied gas conditions. The theoretical results given by this model have been successfully compared (Bellomo 1974), with the experimental results by Kurzius & Raab (1969) and Mills & Seban (1967).

The present paper deals with the study of the time evolution of the distribution of drop sizes, velocities and temperatures of a multi-droplet system shot into a gas–vapour volume at fixed thermodynamical conditions. The phenomenon is time-dependent; in fact, in non-equilibrium conditions the droplets have strong initial variations of temperature (cooling or heating according to the gas conditions), with consequent variation of the vaporization rate. The rates of variation of the diameters, temperatures and velocities of the droplets (the velocity being reduced by the aerodynamic drag) depend upon the size of the droplet (see also Rose & Glicksman 1973; Bellomo 1973). Therefore a time-dependent evolution of the distribution of sizes, temperatures and velocities of the droplets occurs, which is studied herein.

Numerical calculations relating to the vaporization of water droplets have been realized and visualize the obtained results.

2. MATHEMATICAL DESCRIPTION OF THE PROBLEM AND OF THE PHASE-CHANGE PHYSICAL MODEL

Let us take into account a multi-droplet system shot into a gas–vapour medium; all droplets with an initial temperature T_0 and a one-directional velocity U_0, and with their diameters

distributed according to a probability density $P_D(D; t = 0)$. The dimensions of the gas–vapour volume being large enough to keep its thermodynamical conditions unchanged during the evolution and the mean free path of the gas–vapour molecules being large compared with the mean size of a droplet. The aims of our research were to find:

(a) The time-evolution of $D(t)$, $T(t)$ and $U(t)$ of a single droplet moving in a gas–vapour system in the above said physical conditions.

(b) The time evolution of the probability densities $P_T(T; t)$, $P_D(D; t)$ and $P_U(U; t)$ characterizing the state of the multidroplet system; the initial conditions as given above.

In this paper we shall study the phase-transition at the liquid surface by means of the above said physical model recently proposed by Bellomo (1974) and we relate to that paper for more detailed descriptions and comparisons between theoretical and experimental results. According to the model a statistical velocity probability density of the type:

$$P(V) = (4/\sqrt{\pi})(V/c)^2 \exp(-V^2/c^2); \quad c^2(T) = \left(2\frac{k}{m}T\right) \qquad [1]$$

is assumed both for surface vapour- and liquid-molecules, with condensation of vapour molecules with translational velocity lower than a condensation velocity $V_c(T)$ corresponding to a trapping energy, and with vaporization of the molecules of the liquid surface with translational velocity higher than a vaporization velocity $V_e(T)$ corresponding to the energy which is necessary to overcome the bonding forces of the surrounding molecules. Both $V_c(T)$ and $V_e(T)$ are assumed, for a given liquid–vapour system, to be function only of the surface temperature.

According to the said model, the vaporizing and condensing molecules unit number fluxes, respectively N^+ and N^- are given by the following equations:

$$N^+ = \frac{1}{2\sqrt{\pi}} n_L c_L f^+(T); \qquad N^- = \frac{\alpha}{2\sqrt{\pi}} n_\infty c_V \kappa(s_V, \psi) f^-(T); \qquad \alpha = n_V/n_\infty, \qquad [2]$$

$$f^+(T) = \frac{1 + (V_e/c_L)^2}{\exp(V_e^2/c_L^2)}; \qquad f^-(T) = \frac{(\exp(V_c^2/c_L^2) - 1 - V_c^2/c_L^2)}{\exp(V_c^2/c_L^2)}, \qquad [3]$$

$$\chi(s_V, \psi) = \exp(-s_V^2 \cos^2 \psi) + \sqrt{\pi} s_V \cos \omega [(1 + \text{erf}(s_V \cos \psi)], \qquad [4]$$

$$s_V = U/c_V; \qquad c_V = \left(2\frac{k}{m_V}T_\infty\right)^{1/2}; \qquad c_L = \left(2\frac{k}{m_V}T\right)^{1/2}; \qquad c_G = \left(2\frac{k}{m_G}T_\infty\right)^{1/2}, \qquad [5]$$

where the subscripts L, V, G indicate respectively liquid, vapour and gas; n is the number density, and the product $(\alpha n_\infty \chi)$ evaluate, by means of known equations of the kinetic theory, see Shidlovskiy (1967), the wall number density which is increased by the velocity U. See also figure 1.

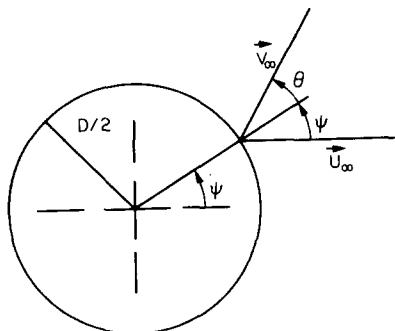The condensation and vaporization limit velocities $V_c(T)$ and $V_e(T)$ can be evaluated, for a

Figure 1. Geometry of the spherical droplet.

given liquid–vapour system, with the two equations which relate, by means of surface tension σ, the vaporization translational energy to the energy required to divide a liquid volume into single one-molecule droplets (see Merte 1973), and which state that, at equilibrium conditions and $U = 0$, N^+ must equal N^-:

$$\frac{1}{2}m_L V_e^2(T) = \sigma(T;D)\left[8\pi\left(\frac{3}{4\pi n_1}\right)^{2/3} - \frac{12}{D \cdot n_1}\right]; \qquad \sigma(T;D) = \frac{(T;D = \infty)}{(1 + \delta/D)}, \qquad [6]$$

$$n_1 f^+(T) = n_{v,eq}(T;D) \cdot f^-(T); \qquad n_{v,eq}(T \cdot D) = n_{v,eq}(T;D = \infty)\exp\left(-\frac{\sigma(T;D)}{n_L k \cdot T \cdot D}\right). \qquad [7]$$

See also Reid & Sherwood (1966) and Levich (1971) for the correlation of the surface tension and the equilibrium number density to the droplet's diameter. In [6], δ is a length, depending on the liquid, of the same order of the intermolecular distances.

In this paper we do not discuss the model, but indicate that by using[4] it has been generalized, with respect to the paper by Bellomo (1974) relating to steady drops, to the more general problem of moving droplets.

3. ANALYSIS OF THE TIME-EVOLUTION OF THE DROPLETS

The time-evolution of a liquid droplet is described by the variation, in function of t, of $D(t)$, $T(t)$ and $U(t)$. In particular the reduction rate of the diameter can be calculated equalling the variation of the mass of the droplet to the total mass-flux through the outer surface of the spherical droplet:

$$\frac{d}{dt}\left(\frac{\pi}{6}D^3 m_L n_L\right) = \int_A m_L(N^+ - N^-)\,dA; \qquad dA = \frac{\pi}{2}D^2\sin\psi\,d\psi \qquad [8]$$

and taking into account [2–5], the following equation is obtained:

$$\frac{dD}{dt} = -(1/\sqrt{\pi})[c_L f^+(T) - \alpha c_V(n/n_L)f^-(T)I_1(s_V)]$$

$$I_1(s_V) = \int_{x'\geq 0}\frac{1}{2}\chi(s_V,\psi)\sin\psi\,d\psi. \qquad [9]$$

The variation rate of $T(t)$ can be obtained by means of the energy balance of each droplet, equaling the total translational energy flux through the droplet's surface to the variation rate of the translational energy on the molecules of the liquid phase:

$$\int_A (E^- - E^+)\,dA = \frac{d}{dt}\left(\frac{\pi}{4}kTn_L D^3\right) = \frac{\pi}{4}n_L kD^2\left(3T\frac{dD}{dt} + D\frac{dT}{dt}\right), \qquad [10]$$

where E^- is the unit flux of translational energy transferred from the gas–vapour volume to the drop and E^+ is the one of vaporizing molecules. We assume, according to Kurzius & Raab (1969), accommodation of the translational degrees of freedom of the incident molecules at the temperature of the liquid surface. In this assumption E^- is given by a known result of kinetic theory and E^+ by the expression evaluated in the paper by Bellomo (1974):

$$E^- = (n_\infty c_\infty/\sqrt{\pi})kT[(T_\infty/T) \cdot \omega(s,\psi) - 2\chi(s,\psi) + \alpha(m_\infty/m_V)^{1/2} \cdot 2\chi(s_V,\psi)f^-(T)]$$

$$s = (U/c_\infty); \qquad c = \left(2\frac{k}{m_\infty}T_\infty\right)^{1/2}; \qquad m_\infty = m_V + (1 - \alpha)m_G \qquad [11]$$

$$E^+ = \frac{1}{2\sqrt{\pi}}n_L c_L kTg(T); \qquad g(T) = [2 + 2(V_e/c_L)^2 + (V_e/c_L)^4]/\exp(V_e^2/c_L^2). \qquad [12]$$

In conclusion the law of evolution of U can be deduced by the momentum equation of the motion of the drop, whose kinetic energy is reduced by the aerodynamic drag:

$$\frac{1}{2}m_\infty n_\infty U^2 C_D\left(\frac{\pi}{4}D^2\right) = -m_L n_L \frac{\pi}{6} D^3 (dU/dt) \qquad [13]$$

where C_D is the drag coefficient referred to the cross sectional area, which in the above mentioned hypotheses on the behaviour of the incident molecules, is given (see Shidlovskiy 1967) by:

$$C_D(s, T; T_\infty) = (2s^2 + 1)/(\exp(-s^2)s^3) + \text{erf}(s)(2 + 2/s^2 - 1/(2s^4)V - (2/3)(\pi T/T_\infty)^{1/2}.$$

The algebrical manipulation of [9–13] gives the following set of non-linear differential equations, of the first order, which describe, at given initial conditions, the time-evolution of each droplet:

$$\frac{dX_i}{dt} = \left(\frac{2}{\pi}\frac{k}{m_L}T_0\right)^{1/2} F_i(X_1, X_2, X_3; \alpha, (n_\infty/n_L), m_\infty, T_\infty, T_0, m_V) \qquad [15]$$

$$i = 1, 2, 3; \qquad X_1 = D; \qquad X_2 = T; \qquad X_3 = s$$

$$F_1 = \alpha(n_\infty/n_L)(T_\infty/T_0)^{1/2}f^-(T)I_1(s_V) - (T/T_0)^{1/2}f^+(T)$$

$$F_2 = (4T/D)\{(n_\infty/n_L)(m_L/m_\infty)^{1/2}(T_\infty/T_0)^{1/2}[(T_\infty/T)I_2(s) - 2I_1(s)$$

$$+ \alpha(m_\infty/m_L)^{1/2}f^-(T)I_1(s_V)] - (3/4)F_1 - g(T)(T/T_0)^{1/2}\}$$

$$F_2 = (3/4)(\pi m_\infty/m_L)^{1/2}(n_\infty/n_L)(T_\infty/T_0)^{1/2}(1/D)C_D(T, s; T_\infty)$$

where:

$$I_1(s) = \int_{\chi \geq 0} \frac{1}{2}\chi(s, \psi) \sin \psi \, d\psi; \qquad I_2(s) = \int_{\omega \geq 0} \frac{1}{2}\omega(s, \psi) \sin \psi \, d\psi. \qquad [15]$$

The numerical integration of [15], joined to the initial conditions on T, s and $P_D(D; t = 0)$, can, at fixed ambient thermodynamical conditions, fully describe the time evolution of the multi-droplet system according to aim (b) of this paper.

4. NUMERICAL CALCULATIONS AND DISCUSSION

Numerical calculations relating to the vaporization of small water droplets in a rarefied stream have been realized. The evaluation of surface tension has been based on the correlation suggested by Reid & Sherwood (1967). In particular figures 2, 3 and 4 respectively, show T,
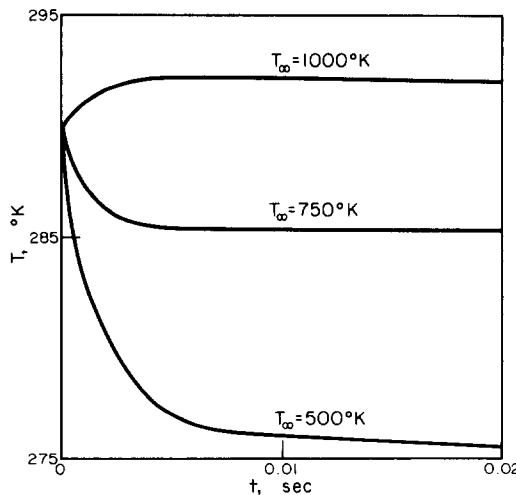

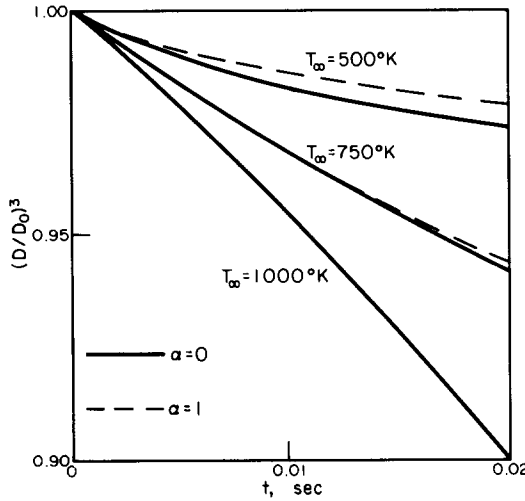Figure 2. Temperature of the droplet versus time.
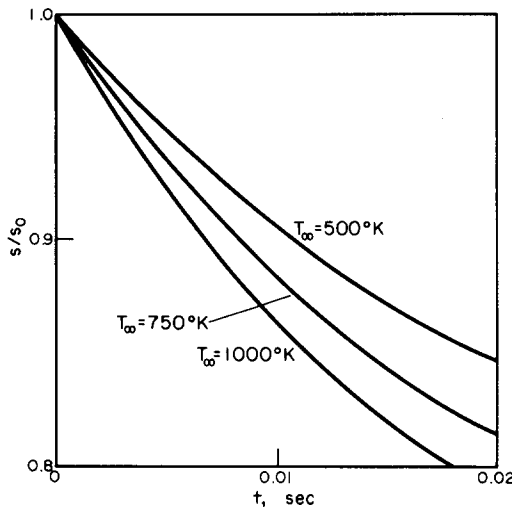
Figure 3. $(D/D_0)^3$ versus time.

Figure 4. s/s_0 versus time.

$(D/D_0)^3$ and s/s_0 versus t in the following initial and ambient conditions:

$$D_0 = 0.1 \text{ mm}; \qquad T_0 = 290°K; \qquad s_0 = 0.5; \qquad n_\infty/n_L = 10^{-6}. \qquad [17]$$

Figure 2 shows that the droplet can have an initial vaporization with cooling or heating, according to the ambient conditions. $T(t)$, however, does not reach an asymptotic value; in fact, s is reduced by the aerodynamic drag, and, therefore, the heating effect due to s is also reduced. Thus the temperature of the drop can have a continuous decreasing slope (as also experimentally observed by Danhehe et al. 1972) or an initial fast heating followed by a slow cooling until complete vaporization. Of course if U were kept constant, e.g. by means of a pressure jump along the trajectory of the motion, T would reach an asymptotic value as indicated on the previous paper on the same subject. Figure 3, in particular, points out that the influence of the presence of vapour is not negligible at low gas temperatures, whereas this effect is practically negligible in strong non-equilibrium conditions (low density or high temperature gas). These figures, besides physical considerations, visualize that large drops cool and loose velocity more slowly than small drops. Thus if N-drops start at a condition (D_0, T_0, s_0), the same number reach the condition $D(t; D_0, T_0, s_0)$, $T(t; D_0, T_0, s_0)$, $s(t; D_0, T_0, s_0)$. This behaviour makes it possible to calculate the probability densities at given initial distribution on D.

Of course, if T and s were initially distributed at $t = 0$, the mathematical background of this stochastic process would be improved, and we aim to do this in future. On the other hand the condition of initial distribution on D and s, T equal for all droplets is a realistic one and includes a large class of physical problems.

In our calculations the following initial and ambient conditions have been assumed:

$$P_D(D/D_0; t = 0) = (27/2)^{1/2}(D/D_0)^3 \exp\left(-\frac{3}{2}(D/D_0)^2\right); \qquad D_0 = 0.1 \text{ mm};$$

$$T(t = 0) = T_0 = 290°\text{K}; \qquad s(t = 0) = s_0 = 0.5; \qquad (n_\infty/n_L) = 10^{-6}; \qquad \alpha = 0. \qquad [18]$$

Figures 5 and 6 respectively, show $P_T(T/T_0; t)$ and $P_s(s/s_0; t)$ computed according to the above mentioned analysis.

Thus, this paper, by means of an experimentally confirmed physical model, has given a detailed description of the time dependent non-equilibrium evolution of a multi-droplet system in a gas–vapour stream showing both the influence of the gas conditions and of the initial conditions on the evolution. This work should also be a basis for further experimental investigation, which, in this class of problems, must not neglect the influence of all the physical parameters, as indicated in the paper, both on the initial strongly non-steady evolution and on the asymptotic behaviour at almost constant vaporization rate.
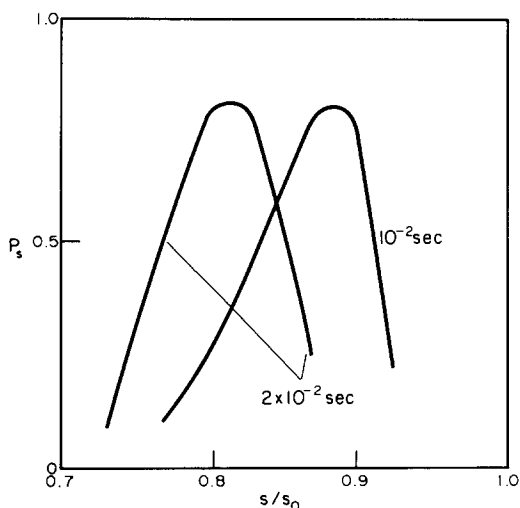
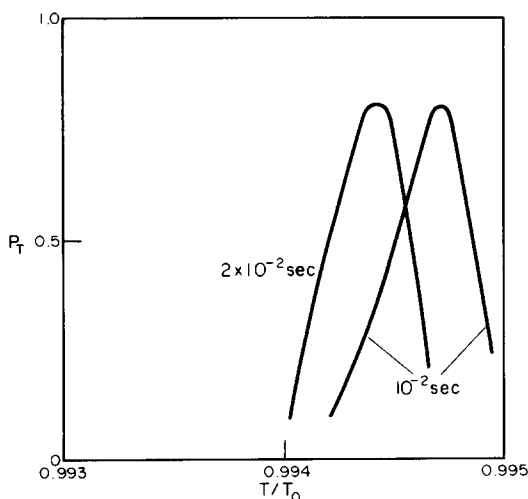Figure 5. Evolution of distribution of temperatures.

Figure 6. Evolution of the distribution of velocities.

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