

## RESEARCH ARTICLE

# Mathematical modeling of vaporization process for a polydisperse ensemble of liquid drops

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In this paper, we study the vaporization process of a polydisperse ensemble of liquid drops on the basis of a nonlinear set of balance and kinetics equations for the particle-radius distribution function and temperature in the gaseous phase. We found an exact parametric solution to this problem using a modified time variable and the Laplace integral transform method. The distribution function of vaporizing drops as well as its moments, the temperature dynamics in gas, and the unvaporized mass of drops are found. The initial particle-radius distribution shifts to smaller particle radii with increasing the vaporization time. As this takes place, the temperature difference between the drops and gas decreases with time. It is shown that the heat of vaporization and initial total number of particles in the system substantially influence the dynamics of a polydisperse ensemble of liquid drops.

## KEYWORDS:

phase transitions, vaporization, integral equations, applied mathematical modeling

## 1 | INTRODUCTION

The processes of interaction of heated gas with evaporating droplets are used in many technological systems (for example, in spray drying or evaporative cooling systems<sup>1,2</sup>). Such processes are controlled by the kinetic mechanisms of interfacial heat and mass transfer. The greatest difficulties arise when studying the dynamic behavior of a polydisperse droplet system, which is described by an integro-differential system of kinetic and balance equations.

In this paper, we consider the evaporation process of a polydisperse system of droplets into a vapor-gas mixture and its subsequent cooling on the basis of an analytical theory developed by analogy with the evolution of spherical crystals in a metastable liquid.<sup>3–11</sup> Following these works, we assume that the evaporating droplets have a spherical shape and do not interact with each other. We also assume that the saturated vapor pressure does not depend on the radius of the droplet, and there is no fragmentation and coagulation of droplets. In addition, we consider the gas and droplets as an adiabatic system, which consists of two locally equilibrium subsystems. Moreover, due to the rapid thermal relaxation of the droplets, their temperature can be considered constant and equal to the temperature of the wet thermometer. Note that these assumptions work in many practically important systems.

The present paper is organized as follows. The governing integro-differential system representing the law of heat conservation and the kinetic equation for the particle-radius distribution function, as well as the initial and boundary conditions is given in Section 2. In addition, this section is devoted to the analytical solutions constructed in a dimensionless form. The behavior of analytical solutions and the main outcomes following from the present analysis are presented in Section 3.

## 2 | THE MODEL AND ITS ANALYTICAL SOLUTION

Let us neglect fluctuations in the vaporization rates of spherical particles and write out the kinetic equation for the particle-radius distribution function  $f(r, t)$  in the form

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial r}(wf) = 0, \quad r > 0, \quad t > 0, \quad (1)$$

where  $r$  and  $t$  represent the spatial and time variables. For the sake of simplicity, we consider the case when the vaporization rate  $dr/dt = w(t) < 0$  of an individual drop is a function of time only.

We assume that the initial distribution of vaporizing droplets is known and given by the initial distribution function  $f_0(r)$  (for instance, the normal, log-normal, square-root-normal, Rosin-Rammler, and Nukiyama-Tanasawa distributions may be mentioned<sup>12</sup>), i.e.

$$f(r, 0) = f_0(r), \quad r > 0; \quad \int_0^\infty f_0(r)dr = 1. \quad (2)$$

In addition, we assume that there are no drops of an infinitely large size in the evaporating system, i.e.

$$f(r \rightarrow \infty, t) \rightarrow 0, \quad t > 0. \quad (3)$$

Let us designate the temperatures of drops and gas through  $T_q$  and  $T$ , respectively. Taking this into account, we write down the heat balance law as

$$(M_g c_{pg} + M_v c_{pv}) \frac{d\theta}{dt} = 4\pi N_0 \rho_q r_i w(t) \int_0^\infty r^2 f(r, t) dr, \quad t > 0. \quad (4)$$

Here  $\theta = T - T_q$ ,  $M_g$  and  $M_v$  are the masses of gas and vapor,  $c_{pg}$  and  $c_{pv}$  are their isobaric heat capacities,  $N_0$  is the initial number of drops in the system,  $\rho_q$  is the density of liquid phase, and  $r_i$  stands for the vaporization heat. Equation (4) should be supplemented with the initial condition of the form

$$\theta(0) = \theta_0, \quad (5)$$

where  $\theta_0$  represents the known temperature.

The integro-differential model (1)-(5) describes the evolution of a polydisperse ensemble of liquid drops in a gas-vapor mixture and its subsequent cooling. In addition, this system determines the distribution function moments of the  $s$ -order given by the following expression

$$\langle r^s(t) \rangle = \frac{N_0}{N(t)} \int_0^\infty r^s f(r, t) dr, \quad t > 0, \quad (6)$$

where  $N(t)$  stands for the current number of drops in the system. So, for example, the initial mean particle radius  $\bar{r}_0$  takes the form

$$\bar{r}_0 = \int_0^\infty r f_0(r) dr. \quad (7)$$

This radius represents the natural characteristic length scale for a given initial particle-size distribution.

For the sake of simplicity, let us introduce the dimensionless variables and parameters as follows

$$\xi = \frac{r}{\bar{r}_0}, \quad \bar{\xi}_0 = \frac{\bar{r}_0}{\bar{r}_0}, \quad g(\xi, \tau) = d_1 f(r, t), \quad g_0(\xi) = d_1 f_0(r), \quad \tau = -\frac{1}{d_1} \int_0^t w(t_1) dt_1, \quad \Delta(\tau) = \frac{\theta(t)}{\theta_0}, \quad \theta^* = \frac{3\mu r_i}{c_{pg}}, \quad (8)$$

$$y(t) = \frac{M_q}{M_{q0}} = \frac{1}{\bar{r}_0^3} \int_0^\infty r^3 f(r, t) dr = y(\tau) = \frac{1}{\bar{\xi}_0^3} \int_0^\infty \xi^3 g(\xi, \tau) d\xi, \quad \mu = \frac{M_{q0}}{M_g}, \quad \frac{M_v}{M_g} = \frac{M_{q0} - M_q}{M_g} = \mu(1 - y). \quad (9)$$

Here  $\xi$  and  $\tau$  represent the dimensionless spatial and time variables,  $g(\xi, \tau)$  and  $g_0(\xi)$  are the dimensionless time-dependent and initial distribution functions,  $\bar{\xi}_0$  is the dimensionless initial mean particle radius,  $\Delta(\tau)$  is the dimensionless temperature

difference,  $y(t) = y(\tau)$  stands for the ratio of the unvaporized mass  $M_q(t)$  of drops to the initial mass  $M_{q0}$  of drops, and  $d_1$  is a characteristic length scale. To chose this scale we should introduce the initial distribution function. So, introducing the normal distribution function

$$f_0(r) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{r-\mu}{\sigma}\right)^2\right] \quad \text{or} \quad g_0(\xi) = \frac{d_1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\xi-\mu/d_1}{\sigma/d_1}\right)^2\right], \quad (10)$$

where  $\mu$  is the mean or expectation of the distribution, and  $\sigma$  is its standard deviation, we can chose any of the parameters  $\bar{r}_0$ ,  $\mu$  or  $\sigma$  as a characteristic length scale  $d_1$ .

The aforementioned model in dimensionless form (8) and (9) becomes

$$\frac{\partial g}{\partial \tau} - \frac{\partial g}{\partial \xi} = 0, \quad \xi > 0, \quad \tau > 0; \quad g(\xi, 0) = g_0(\xi), \quad \xi > 0; \quad g(\xi \rightarrow \infty, \tau) \rightarrow 0, \quad \tau > 0, \quad (11)$$

$$[1 + a_2(1 - y(\tau))] \frac{d\Delta}{d\tau} = -N_0 a_1 \Lambda(\tau), \quad \tau > 0; \quad \Delta(0) = 1, \quad (12)$$

where

$$M_{q0} = \frac{4\pi\bar{r}_0^3\rho_q}{3}, \quad a_1 = \frac{\theta^*}{\theta_0}, \quad a_2 = \frac{\mu c_{pv}}{c_{pg}}, \quad \Lambda(\tau) = \frac{1}{\bar{\xi}_0^3} \int_0^\infty \xi^2 g(\xi, \tau) d\xi.$$

The dimensionless mean particle radius  $\bar{\xi}_0$  and vaporization rate  $d\xi/d\tau$  read as

$$\bar{\xi}_0 = \int_0^\infty \xi g_0(\xi) d\xi, \quad (13)$$

$$w(t) = \frac{dr}{dt} = -w \frac{d\xi}{d\tau}. \quad (14)$$

Thus, expression (14) shows that the vaporization law takes the form of  $\xi = \xi_0 - \tau$ , where  $\xi_0$  is a constant. Let us chose  $\xi_0$  equal to the mean particle radius  $\bar{\xi}_0$ . In this case, we arrive at

$$\xi = \bar{\xi}_0 - \tau. \quad (15)$$

Choosing the vaporization rate as<sup>13</sup>

$$w(t) = -\left(\frac{r}{\bar{r}_0}\right)^{-n} \frac{\alpha_0 \theta(t)}{\rho_q r_i} \quad (16)$$

and combining this law with expression (15), we obtain in dimensionless form

$$w(\tau) = -\left(1 - \frac{\tau}{\bar{\xi}_0}\right)^{-n} \frac{\alpha_0 \theta_0 \Delta(\tau)}{\rho_q r_i}. \quad (17)$$

Here  $\alpha_0$  and  $n$  represent the heat transfer and power coefficients.

Now from expression (8) for  $\tau$ , we obtain

$$\frac{d\tau}{dt} = -\frac{w}{d_1} = \left(1 - \frac{\tau}{\bar{\xi}_0}\right)^{-n} \frac{\Delta(\tau)}{b}, \quad (18)$$

where  $b = d_1 \rho_q r_i / (\alpha_0 \theta_0)$ .

Thus, the model equations, initial and boundary conditions (10)-(13), and (18) written out in dimensionless form describe the vaporization process of a polydisperse ensemble of drops. These equations are used below to determine the analytical solutions.

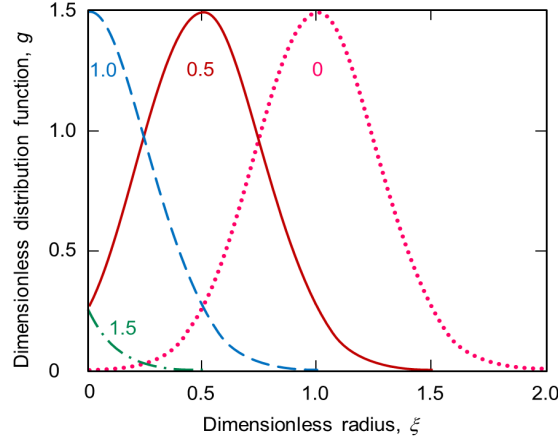
At first, let us apply the Laplace transform to the kinetic equation (11) with respect to the modified time  $\tau$ . Designating the Laplace variable through  $p$ , we obtain

$$\frac{dg^*}{d\xi} - pg^* + g_0(\xi) = 0, \quad g^*(\xi \rightarrow \infty) \rightarrow 0. \quad (19)$$

Here the subscript  $*$  denotes the Laplace transform space.

The solution to equation (19) reads as

$$g^*(\xi) = \int_\xi^\infty g_0(\xi_1) \exp[-p(\xi_1 - \xi)] d\xi_1. \quad (20)$$



**FIGURE 1** The dimensionless distribution function  $g(\xi, \tau)$  versus the dimensional radius  $\xi$  of evaporating drops at different times  $\tau$  (numbers at the curves).

Now taking into account the inverse Laplace transform<sup>14</sup> ( $\delta$  is the Dirac delta function)

$$\exp[-p(\xi_1 - \xi)] \rightarrow \delta(\tau - (\xi_1 - \xi)),$$

we get from (20)

$$g(\xi, \tau) = g_0(\xi + \tau), \quad \xi > 0, \quad \tau > 0. \quad (21)$$

Now integrating equations (12) and (18), we arrive at the dynamical laws  $\Delta(\tau)$  and  $t(\tau)$  of the form

$$\Delta(\tau) = 1 - a_1 N_0 \int_0^\tau \frac{\Lambda(\tau_1) d\tau_1}{1 + a_2 (1 - y(\tau_1))}, \quad \tau > 0, \quad (22)$$

$$t(\tau) = b \int_0^\tau \left(1 - \frac{\tau_1}{\bar{\xi}_0}\right)^n \frac{d\tau_1}{\Delta(\tau_1)}, \quad \tau > 0, \quad (23)$$

where  $y(\tau)$  and  $\bar{\xi}_0$  are defined by formulas (9) and (13).

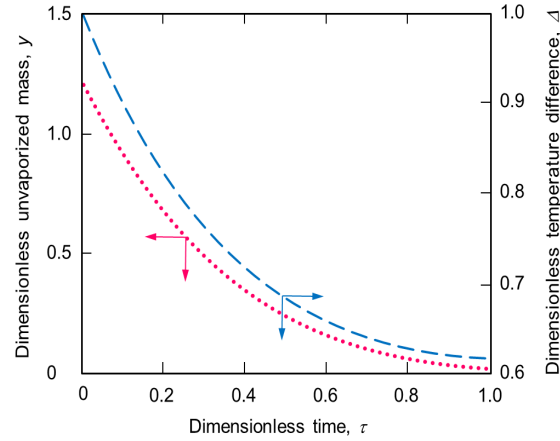
Thus, expressions (21)-(23) entirely determine the analytical solution obtained in a parametric form, where the modified time variable  $\tau > 0$  plays the role of this parameter. Also, let us note that the analytical solutions depend on the initial distribution function  $g_0(\xi)$  that is given by expression (10) in the case of the normal initial distribution.

### 3 | DISCUSSION AND CONCLUSION

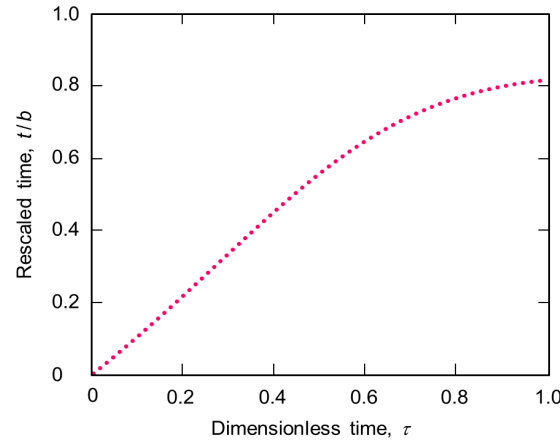
To demonstrate the evolutionary behavior of the particle-size distribution function, we estimate the initial mean particle radius  $\bar{r}_0 = d_1$  as  $10^{-3}$  m. In this case, the mean or expectation  $\mu$  of the initial distribution (10), and its standard deviation  $\sigma$  can be chosen as  $\mu = 10^{-3}$  m and  $\sigma = 0.000267$  m. This choice corresponds to the dimensionless initial mean particle radius  $\bar{\xi}_0 = 1$ .

The distribution function of evaporating drops calculated on the basis of expression (21) is shown in Figure 1. As is easily seen, the initial distribution moves to the left as time increases. Indeed, the initial distribution (dotted line) eventually shifts to the left to the solid curve, transforms into the dashed distribution, and then becomes a dash-dotted line. Physically, this means that large droplets evaporate and reduce their radius in the course of time.

Figures 2 and 3 illustrate the relative unvaporized mass  $y(\tau)$ , relative temperature difference  $\Delta(\tau)$  as well as the rescaled evaporation time  $t/b$  as functions of the modified time variable  $\tau$ . These dependencies are shown accordingly to the analytical solutions (21)-(23). As is easily seen, the unvaporized mass  $y$  of drops and the relative temperature difference  $\Delta = \theta/\theta_0$  between drops and gas decrease as time  $\tau$  increases. As this takes place, the real dimensionless time  $t/b$  grows with increasing the modified time  $\tau$ . It is important to note that when the temperature difference between the gas and the droplets substantially



**FIGURE 2** The ratio  $y(\tau)$  of the unvaporized mass  $M_q(t)$  of drops to the initial mass  $M_{q0}$  of drops (scale of values on the left) and the dimensionless temperature difference  $\Delta(\tau)$  (scale of values on the right) as functions of the modified time variable  $\tau$ . The system parameters are  $N_0 = 10^3$ ,  $a_1 = 10^{-3}$ , and  $a_2 = 10^{-1}$ .



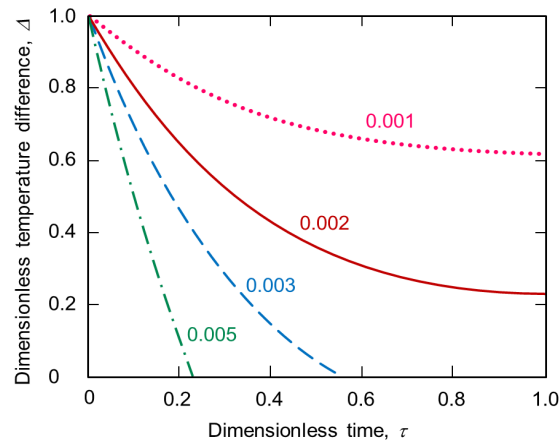
**FIGURE 3** The time  $t$  of evaporation versus the modified time variable  $\tau$ . The system parameters correspond to Figure 2 and  $n = 1$ .

decreases, there is almost no unevaporated mass remaining in the system,  $y \approx 0$ , and the time dependence  $t(\tau)/b$  becomes noticeably different from the linear one.

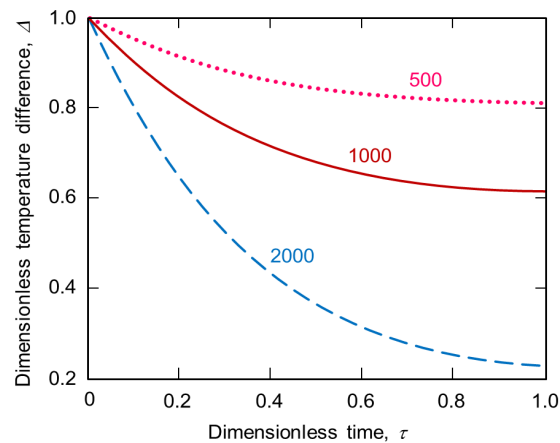
Figures 4 and 5 show that the larger the parameter  $a_1$  (e.g., the larger the heat  $r_l$  of vaporization or the initial mass  $M_{q0}$  of the drops) and the total number  $N_0$  of particles at the initial time, the faster the temperature equalizes between the droplets and the gas. On the other hand, when the parameters  $a_1$  and  $N_0$  decrease, the relative temperature difference  $\Delta$  grows and stabilizes to a certain value as time  $\tau$  increases.

Thus, the exact analytical solutions (21)-(23) constructed in a parametric form enable us to describe the vaporization dynamics of a polydisperse ensemble of drops when neglecting the fluctuations in the evaporation rates of individual particles. Generally speaking, such fluctuations always exist and may play a decisive role in the evolution of particulate assemblages during the initial stages of a phase transformation process.<sup>15</sup> Therefore, it is significant to note that the present analysis should be extended with allowance for the fluctuations in the evaporation rates of individual particles by analogy with the crystallization theory.<sup>16–20</sup>

The next important generalization of the developed theory is to take into account the non-stationary evaporation rates of individual droplets. To solve this problem, it is necessary to derive non-stationary corrections to the evaporation rates of spherical droplets. Such a problem can be solved using the differential series method, like the problem on the growth of spherical crystals in a metastable fluid.<sup>21–23</sup>



**FIGURE 4** The dimensionless temperature difference  $\Delta(\tau)$  as a function of the modified time variable  $\tau$  at different values of the parameter  $a_1$  (numbers at the curves). The system parameters correspond to Figure 2 .



**FIGURE 5** The dimensionless temperature difference  $\Delta(\tau)$  as a function of the modified time variable  $\tau$  at different values of the initial total number  $N_0$  of particles (numbers at the curves). The system parameters correspond to Figure 2 .

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## Author contributions

The authors contributed equally to the present research article.

## Conflict of interest

The authors declare no potential conflict of interests.

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