Application of the homogenous nucleation theory to the study of explosive boiling of superheated liquid drops

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Abstract. In the work, a model of explosive boiling of a single droplet was proposed, which is based on the classical nucleation theory. A criterion is proposed for estimation the droplet's lifetime. Calculations were made for droplets of liquid oxygen in saturated vapor. Analysis is made for influence of the initial temperature and droplet size on its lifetime.

1. Introduction
In the present time the interest to explosive boiling processes is increases. It is related to different technical application and to some fundamental problems. The correct description and understanding of such processes can be helpful for development of engines that used cryogenic liquids or superheated liquid as fuel. The intense phase transitions can take place in superheated liquid which in turn greatly affects the distribution of fuel in the combustion zone.

Spraying cryogenic fuels is a complex physical phenomenon. On the one hand, vapor bubbles form in the liquid, which can lead to fragmentation of the liquid. On the other hand, the droplets intensively evaporate, as a result their temperature decreases rapidly and a solid phase can form. Local zones can also form in which the vapor pressure is higher than the saturation pressure, which causes homogeneous and heterogeneous condensation. All these processes have a significant effect on the process of fuel outflow from the nozzle. It was shown in [1] that the atomization mode depends on the superheating ratio, which is defined as the ratio of saturation pressure at ambient temperature to ambient pressure.

In this work, the destruction of a superheated drop as a result of the formation and growth of vapor bubbles inside it is considered. This process is often called explosive boiling.

2. Formulation of the problem and mathematical description
The phase transition processes are considered on surface and in volume of a droplet with a radius \( R_0 \) and temperature \( T_0 \) placed in an unbounded region with pressure \( p_a \) and temperature \( T_a \). The considered region is filled with saturated vapor of the same substance as the drop. The temperature of the droplet is higher than the saturation temperature at ambient pressure and the liquid is superheated (figure 1).

In superheated liquid bubble nucleation is triggered by local thermodynamic state fluctuations. The nucleation rate per unit volume can be computed based on the classical theory [2]:

\[
I = NB \exp \left( -\frac{W_{cr}}{kT} \right)
\]  

(1)
where \( N \) is number of liquid molecules per unit volume, \( B \) is kinetic coefficient, \( W_{cr} \) is critical nucleation work, \( k \) is Boltzmann constant and \( T \) is temperature of liquid. However, \( B \) and \( N \) are weakly dependent on superheating, therefore, a simplified formula is used for calculations [3]:

\[
\ln I = 88 \frac{W_{cr}}{kT}.
\]  

(2)

![Figure 1. Schematic diagram of the problem.](Image)

The critical nucleation work, which is included in (1) and (2), is calculated as follows:

\[
W_{cr} = \frac{4}{3} \pi r_{cr}^2 \sigma.
\]  

(3)

Here \( \sigma \) is surface tension, and \( r_{cr} \) is the critical size for bubble to grow continuously in superheated liquid.

\[
r_{cr} = \frac{2\sigma}{(p_s - p_{liq})(1 - \rho_v/\rho_{liq})}.
\]  

(4)

Here \( p_s \) is saturation pressure at the temperature of liquid, \( p_{liq} \) is pressure in liquid, \( \rho_v \) is vapor density and \( \rho_{liq} \) is liquid density. Equation (4) is often reformulated by applying the Clapeyron – Clausius equation and the assumption that the vapor density is much lower than the liquid density:

\[
r_{cr} = \frac{2\sigma T_s}{L \rho_v (T - T_s)}
\]  

(5)

Here \( T_s \) is saturation temperature, \( L \) is evaporation heat.

In the general case, the bubble growth rate is determined by the resistance of the repelled liquid (dynamic effects) and the evaporation rate at the interface (thermal effects). However, to solve practical problems, the limiting growth patterns are used. In this work, a dynamic inertial pattern of bubble growth is used, which suggests that the supply the heat to the interface is unlimited. The vapor temperature inside the bubble is equal to the temperature of the liquid, and the pressure inside the bubble is equal to the saturation pressure at the liquid temperature. The bubble growth rate is determined from the solution of the well-known Rayleigh equation:

\[
f = \sqrt{\frac{2 \rho_v (T - p_{liq})}{3 \rho_{liq}}}
\]  

(6)

There can be a large number of bubbles with different sizes in superheated drop at the same time therefore, to describe such a system, a bubble size distribution function \( f \) is introduced. This approach is used to describe the condensation of supersaturated vapor. The product \( f dr \) determines the number of bubbles per unit volume with sizes from \( r \) to \( r + dr \). The kinetic equation for the distribution function is written as follows [4]:
\[ \frac{\partial f}{\partial t} + \frac{\partial}{\partial r} \left( r f \right) = I \delta \left( r - r_{cr} \right). \]  

(7)

Here \( \delta \) is Dirac delta-function, which shows that only bubbles with critical size can form. Using the distribution function, integral characteristics are calculated, such as the number of bubbles per volume unit \( N_b \), the volume of vapor per volume unit \( C_b \), and the average radius of the bubbles \( \bar{r} \):

\[ N_b = \int_{r_{cr}}^{\infty} f dr \]
\[ C_b = \frac{4}{3} \pi \int_{r_{cr}}^{\infty} r^3 f dr. \]  
\[ \bar{r} = \frac{1}{N_b} \int_{r_{cr}}^{\infty} rf dr \]  

(8)

The droplet size changes due to evaporation from the surface and vaporization in its volume. The equation describing changes in droplet size has the following form:

\[ \frac{dR_d}{dt} = \left[ 1 - \frac{\rho_v}{\rho_{liq}} \right] \frac{R_d}{3} \frac{dC_b}{dt} - \frac{j}{\rho_{liq}}. \]  

(9)

Assuming the vapor density is much lower than the liquid density equation (9) is simplified:

\[ \frac{dR_d}{dr} = \frac{R_d}{3} \frac{dC_b}{dr} - \frac{j}{\rho_{liq}}. \]  

(10)

Here \( R_d \) is radius of drop, \( j \) is mass flux from surface of drop. The mass flux is calculated using the formula for intensive evaporation [5]:

\[ j = 0.6 \left( \frac{\rho_v}{\rho_{v,s}} \right)^{0.5} \left( \rho_{v,s} - \rho_v \right) \sqrt{2RT}. \]  

(11)

where \( \rho_{v,s} \) is density of saturated vapor, \( R \) is specific gas constant.

Since the temperatures of the liquid and the vapor inside the bubbles are equal, the following energy equation is used for a two-phase medium:

\[ \rho_d c_{p,d} \frac{dT}{dt} = \left[ \frac{3}{R} \left( jL + q \right) + L \rho_v \frac{dC_b}{dt} \right]. \]  

(12)

Here \( c_{p,d} \) is specific heat capacity of two-phase medium, \( q \) is interphase heat flux. According to the equation (12), the temperature of the liquid changes due to evaporation from the surface, heat transfer between liquid and vapor, and bulk vaporization. Interfacial heat flux is determined by heat conduction:

\[ q = \frac{\lambda}{R_d} \left( T - T_{a} \right). \]  

(13)

To evaluate the droplet's lifetime, a criterion \( \xi \) for its destruction was introduced, which is defined as the ratio of the average distance between of centers of bubbles to the average its diameter. The average distance between centers of bubbles is calculated using the following formula:

\[ l = \sqrt{\frac{1}{N_b}}. \]  

(14)
It is assumed that the drop is destroyed if the average distance between the centers of the bubbles is equal to their average diameter (figure 2).

![Diagram of droplet destruction criteria](image)

**Figure 2.** Schematic diagram of the criterion droplet destruction

### 3. Results and discussion

The calculations were carried out for a drop of liquid oxygen with a radius of 10 mm and 1 mm surrounded by saturated vapor. The ambient pressure was 0.1 bar, the ambient temperature was 72.8 K. The initial droplet temperature was varied in the range from 128 K to 131.2 K.

The time dependences of the dimensionless temperature and the dimensionless drop radius for various values of the initial superheating $\Delta T (\Delta T = T_0 - T_s)$ are presented in figure 3. Figure 3(a) and figure 3(b) show that the curves for different superheating are qualitatively similar. The droplet size is slightly increased (7-13%) and this occurs at the end stage of the droplet's life (Figure 3 (b)). The maximum change in droplet size occurs at the highest superheating (curve 1 in Figure 3 (a)). This fact is explained by higher intensity of bubbles nucleation and growth processes. The changing of droplet size is due to evaporation of the liquid from the surface (decreasing) and vaporization inside the droplet (increasing). Under the considered conditions, the decisive factor is the nucleation and growth of vapor bubbles in the drop volume. At a higher initial temperature, the drop grows to larger sizes. Figure 3 (b) shows that the droplet temperature decreases by less than 1%. This is due to the fact that the destruction time of the drop is much shorter than the time during which the thermodynamic equilibrium between the drop and the environment occurs.

![Dimensionless radius vs. time](image)

**Figure 3.** The time dependences of the dimensionless droplet radius (a) and the dimensionless temperature (b) for various values of the initial superheating: 1 $\Delta T = 55.2$ K, 2 $\Delta T = 56$ K, 3 $\Delta T = 56.8$ K, 4 $\Delta T = 57.6$ K, 5 $\Delta T = 58.4$ K

The nucleation rate strongly depends on the superheating of liquid; therefore, with an increase in the initial temperature of the droplet, the number of bubbles at the moment of the droplet destruction increases, as can be seen in figure 4 (a). The droplet's lifetime decreases with increasing superheating, so the bubbles do not have time to grow significantly.
Figure 4. The number of bubbles per unit volume (a) and the average radius of the bubbles (b) at the moment of the droplet destruction as a function of the initial droplet superheating.

The droplet lifetime decreases monotonically with increasing droplet temperature. However, it does not practically change for drops the different droplet sizes (figure 5). There is a noticeable difference only at a low initial temperature. This is explained by that the pressure in the liquid increases with decreasing droplet size, so the growth rate of vapor bubbles in a large droplet is higher and the lifetime is shorter.

Figure 5. The droplet lifetime as a function of the initial droplet superheating at the different $R_{d0}$

4. Conclusions
The calculations performed for two drops of liquid oxygen showed that the change in the size and temperature of the drop is mainly determined by homogeneous nucleation and the growth of vapor bubbles inside the drop. The size of the droplet, which it reaches at the moment of destruction, increases with increasing initial droplet temperature. The variation of temperature of the drop throughout the process is very slight. The droplet's lifetime strongly depends on the liquid superheating, but weakly depends on the initial droplet size. With increasing initial droplet size, its life time decreases slightly.

References
[1] Yildiz D, Rambaud P, van Beeck J, van BEECK J, and Buchlin J M 2006 Proc. 10th Int. Conf. on Liquid Atomization and Spray Systems (Kyoto) ICLASS06-122
[2] Kashchiev D 2000 Nucleation. Basic Theory with Applications (Oxford: Butterworth-Heinemann)
[3] Skripov V P 1974 Metastable Liquids (New York: Halsted Press)
[4] Hulburt H M, Katz S M 1964 Chem. Eng. Sci. 19 555
[5] Labuntsov D A, Kryukov A P 1979 Int. J. Heat Mass Transfer. 22 989–1002