Simulation of evaporation of mixtures and solutions in the spheroidal state

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Abstract. The paper presents the theoretical dependences of evaporation in the spheroidal state of pure liquids, liquids containing insoluble and partially soluble impurities. The conditions are formulated, upon the occurrence of which a change in the crisis regime of film evaporation to an intensive regime of partially bubble boiling may occur upon contact with a heating surface.

1. Introduction
For quantitative estimates of the physical laws of evaporation of films of pure liquids, desorption of solutions, as well as a complex picture of boiling multicomponent liquid mixtures under conditions of development and change of boiling crises, when the evaporating liquid is separated from the heating surface, theoretical models can be used that reflect individual aspects of the physical picture of the heat and mass transfer processes occurring. As applied to pure liquids, the physical laws governing the occurrence of such processes were studied in papers [1, 2]. However, these classic results cannot be used to describe the picture of the crisis evaporation of liquids containing soluble and insoluble impurities.

2. Problem Statement
It can be assumed that the processes of non-stationary evaporation of solutions, as well as mixtures with insoluble additives should be different from the evaporation of pure liquids. An increase in the concentration of impurities with time in the evaporating spheroid can lead to a change in the physical picture of the crisis evaporation.

Figure 1 shows the scheme of the problem of unsteady evaporation of a flat liquid spheroid with an initial diameter $D_0$ corresponding to the volume $V_0$. The thickness of the spheroid in the process of evaporation is assumed to be constant and equal to $\delta$. In the process of evaporation over time $t$, the current diameter $D$ and volume $V$ of a flat spheroid decrease ($D < D_0$, $V < V_0$). Theoretically, the ultimate point is the time when all the liquid evaporates from a spheroid.

![Figure 1. Scheme of the problem of nonstationary evaporation of a flat spheroid.](image_url)
The current volume $V$, mass $M$ and density $\rho$ of the spheroid will be defined as:

\[ V = V_{\text{IMP}} + V' \quad (1) \]

\[ M = V_{\text{IMP}} \cdot \rho_{\text{IMP}} + V' \cdot \rho' = V\rho_{\text{IMP}} + (1-\chi)\rho' = V[(1-\theta)\rho_{\text{IMP}} + \theta\rho'] \quad (2) \]

\[ \rho = \frac{V_{\text{IMP}} \cdot \rho_{\text{IMP}} + V' \cdot \rho'}{V_{\text{IMP}} + V'} = \chi\rho_{\text{IMP}} + (1-\chi)\rho' = \rho_{\text{IMP}}(1-\theta) + \theta\rho', \quad (3) \]

here: $V_{\text{IMP}}$ and $\rho_{\text{IMP}}$ are the volume and density of impurities (non-evaporating components), respectively; $V'$ and $\rho'$ are the current volume and density of the evaporating liquid, respectively; $\theta = V' / V$ and $\chi = V_{\text{IMP}} / V$ are the current volume fractions of the liquid and impurities in the spheroid, respectively.

When $\chi = 0$, according to (3) we have $\rho = \rho'$, that is, the evaporation of the spheroid is completed as $V \to 0$; for $\chi \to 1$, upon completion of evaporation of the spheroid, a precipitate of volume $V \approx V_{\text{IMP}}$ is formed.

The variable in the problem is $V'$, all other parameters associated with it will also change. In the process of evaporation, there is an increase in the volume fraction $\chi$ or mass fraction of soluble (e.g. salt in water) and insoluble (coal particles in water, plant and biological inclusions, nanoparticles, etc.) impurities in the current volume of the spheroid and a decrease in the parameter $\chi$, determining the relative content of the evaporating component in the spheroid. This leads to a change in the density $\rho$, hydrodynamic pattern of fluid flow in a spheroid, a change in the dynamic balance of the forces keeping the spheroid in suspension above the heating surface. Given the complex interrelated nature of non-stationary processes, we introduce simplifications to the problem, allowing us to obtain approximate analytical solutions.

The solution of the problem will be carried out under the following basic assumptions: the $\delta$, $V_{\text{IMP}}$, $\delta'$ and $\rho_{\text{IMP}}$ values are assumed to be unchanged during the evaporation process; heat transfer and evaporation on the external surfaces of the spheroid are considered negligible compared with the process on the bottom surface facing the heating surface; the temperature of the lower surface of the spheroid is assumed to be equal to the equilibrium thermodynamic temperature of evaporation of a liquid $T''$ at an evaporation pressure.

If we neglect the heat of superheating of steam in the layer $\delta''$, the heat flux equation can be represented as the equality of the sum of the convective and radiative heat fluxes from the heating surface to the bottom surface of the spheroid and the sum of the heat flux spent on the evaporation of the liquid at the bottom of the spheroid, and the heat flux for its heating in the process of moving to the interface:

\[ (\alpha_C + \alpha_R) (T_{\text{SUR}} - T^*) \cdot \pi \cdot D^2 / 4 = r \cdot \frac{d(V\rho)}{dt} + C_{AV} \cdot (T^* - T_{AV}) \cdot d(V\rho) / dt, \quad (4) \]

here: $\alpha_C$ and $\alpha_R$ are the convective and radiation heat transfer coefficients; $T_{AV}$ and $C_{AV}$ are the average temperature and heat capacity of the spheroid in the process of evaporation, which are assumed to be unchanged in the first approximation in the process of evaporation; $t$ - time.

Assuming that the flow of steam in a thin layer between the spheroid and the heating surface is laminar, we can take:

\[ \alpha_C = \lambda^* / \delta^*. \quad (5) \]

It can be shown that:

\[ d(\rho V) = (\pi / 2) \cdot \delta' \cdot D \cdot dD. \quad (6) \]

Taking into account (5) and (6), we bring (4) to the form:

\[ \frac{\lambda^*}{\delta^*} + \alpha_R = 2 \left[ 1 + \frac{C_{AV}(T^* - T_{AV})}{r} \right] \cdot \frac{r \cdot \rho' \cdot \delta}{T_{\text{SUR}} - T^*} \cdot \frac{dD}{D \cdot dt}, \quad (7) \]
The reason why the spheroid is kept suspended above the heating surface is the same: pressure drop, developed due to the action of viscous friction forces during steam outflow along the periphery of the spheroid.

Steam flows around the periphery of the spheroid with a linear velocity \( w'' \) under the influence of excess pressure:

\[
\Delta p = g \cdot \delta \cdot \left( \left[ \rho_{\text{imp}}(1 - \theta) + \theta \rho' \right] - \rho^* \right) = g \delta \left( \left[ \rho_{\text{imp}} \chi + (1 - \chi) \delta' \right] - \rho^* \right). \tag{8}
\]

In this expression, only the second part in square brackets is responsible for the process of active evaporation, as a result of which a dynamic vapor layer \( \delta'' \) thick between the spheroid and the heating surface is formed. The rate of steam flow around the periphery of the spheroid through the magnitude of the total heat flux \( q \) can be defined as:

\[
w'' = q \cdot D / (4 \cdot r \cdot \rho'' \cdot \delta''). \tag{9}
\]

From the condition of the dynamic balance of forces acting on a spheroid:

\[
\frac{\rho''(w'')^2}{2} = \Delta p \tag{10}
\]

can easily determine the rate of steam outflow:

\[
w'' = \sqrt{2g \delta \left( \left[ \rho_{\text{imp}} \chi + (1 - \chi) \rho' \right] - \rho^* \right) / \rho''}. \tag{11}
\]

Taking into account the last expression, the mass of steam flowing along the periphery of the spheroid can be determined by the expression:

\[
dG'' = \xi \cdot \pi \cdot D \cdot \delta'' \cdot \sqrt{2g \delta \left( \left[ \rho_{\text{imp}} \chi + (1 - \chi) \rho' \right] - \rho^* \right) / \rho''} \cdot dt, \tag{12}
\]

where \( \xi \) - the efflux coefficient, taking into account the shape of the peripheral part of the spheroid and the nature of the spatial expiration of steam.

From the material balance of the spheroid follows another expression:

\[
dG'' = (\pi / 2) \cdot \rho' \cdot \delta \cdot D \cdot dD. \tag{13}
\]

From equality (12) and (13) we obtain the expression for the thickness of the vapor layer:

\[
\delta'' = \frac{1}{2 \cdot \xi} \sqrt{\frac{(\rho')^2 \cdot \delta}{2 \cdot g \cdot \rho'' \left( \left[ \rho_{\text{imp}} \chi + (1 - \chi) \rho' \right] - \rho^* \right)}} \frac{dD}{dt}. \tag{14}
\]

Substituting the value of \( dD/dt \) from equation (14) into equation (7), we obtain the expression for the thickness of the vapor layer:

\[
\delta'' = \frac{1}{\sqrt{32 \xi^2}} \sqrt{\frac{\lambda^*(T_{\text{SUR}} - T'')D}{\left[ r + C_{AV} (T'' - T_{AV}) \right]}} \cdot \sqrt{g \delta \rho'' \left( \left[ \rho_{\text{imp}} \chi + (1 - \chi) \rho' \right] - \rho^* \right)}. \tag{15}
\]

Subject to assumption (5), expression (15) takes the form:

\[
\alpha_c = \frac{1}{\sqrt{32 \xi^2}} \sqrt{\frac{\lambda^*[r + C(T'' - T_{AV})]}{(T_{\text{SUR}} - T'')D}} \cdot \sqrt{g \delta \rho'' \left( \left[ \rho_{\text{imp}} \chi + (1 - \chi) \rho' \right] - \rho^* \right)}. \tag{16}
\]

The steam between the spheroid and the heating surface is overheated, as it sets the temperature field in the range from \( T_{\text{SUR}} \) to \( T'' \). Heat consumption for superheating of the generated steam to the average temperature of the vapor layer can be approximately taken into account by entering the approximate expression in the above formulas instead of \( r' \):
Substituting the average thickness of the vapor layer $\delta''$ from (15) into the heat balance equation (17), provided that the radiative heat transfer ($a_C >> a_0$) is neglected, we obtain the equation:

$$
\delta''^4 D^{1/2} D = \frac{\sqrt{\frac{32 \xi}{2 \rho'}}}{4,1\rho''^2} \left[ \frac{\lambda'' (T_{SUR} - T')}{T' - T_{AV}} \right] \left( g \rho'' \left[ \rho_{IMP} + 2(1 - \chi) \rho' - \rho'' \right] \right)^{1/4} dt,
$$

whose integration allows us to obtain an expression for determining the change in the volume of a flat spheroid in the process of evaporation:

$$
V_0^{1/4} - V^{1/4} = \frac{\sqrt{\frac{32 \xi}{2 \rho'}}}{4,1\rho''^2} \left[ \frac{\lambda'' (T_{SUR} - T')}{T' - T_{AV}} \right] \left( g \rho'' \left[ \rho_{IMP} + 2(1 - \chi) \rho' - \rho'' \right] \right)^{1/4} t.
$$

For a spheroid that does not contain impurities ($\chi = 0$), under the condition $\rho' >> \rho''$, expression (19) gives the expression:

$$
V_0^{1/4} - V^{1/4} = \frac{\sqrt{\frac{32 \xi}{2 \rho'}}}{4,1\rho''^2} \left[ \frac{\lambda'' (T_{SUR} - T')}{T' - T_{AV}} \right] \left( g \rho'' \left[ \rho_{IMP} + (1 - \chi) \rho' - \rho'' \right] \right)^{1/4} t,
$$

which coincides with the solution for spheroids of pure liquids [3]. In contrast to (20), the restriction on the use of the solution (19) is the condition $V > V_{IMP}$.

3. Results

It is important to note that setting the conditions at the interface allows one to make assessments of the influence of transfer processes inside the spheroid on the stability of the vapor film separating the spheroid from the heating surface. The importance of such estimates is due to the change in the physical picture of evaporation during the destruction of the vapor film and transient processes of boiling in the process of direct contact of the spheroid with the heating surface.

The stability of the evaporation regime with liquid pushing away from the heating surface by a vapor layer is determined by the value of the parameter $\delta''$. Its increase can be uniquely determined in favor of increasing the sustainability of such a crisis evaporation regime. Therefore, we will dwell in more detail on the main parameters affecting the magnitude of the thickness of the vapor layer.

A preliminary analysis allows us to distinguish the following features of the stationary evaporation process of a spheroid:

1. In the conditions of the earth, a dynamic equilibrium between the spheroid and the horizontal heating surface in the process of evaporation is ensured by the work of viscous friction forces balancing the weight of the spheroid when the steam moves in a thin layer with thickness $\delta''$. However, as $g \to 0$, the influence of the reactive forces $p_N$, arising at the phase transition boundary, becomes strong, which creates conditions for stable separation of the liquid from the heating surface with relatively slow evaporation.

2. The thickness of the vapor layer tends to increase with increasing temperature of the heating surface, which follows from analysis (15) at $\theta = 1,0$ and the heat balance equation (7), which also takes into account radiant heating. According to the estimates made, the share of radiant heat transfer at temperatures $T_{SUR} = 300{\text{÷}}400$ K is about 10% of the total heat flux perceived by the spheroid from the heating surface.

3. An increase in the thickness of the vapor layer should occur with a decrease in the value of $r$, that is, boiling low-boiling working fluids used in vapor compression heat pumps, as well as cryogenic liquids, can occur under conditions of crisis boiling at relatively low temperatures of heating of the heat exchange surfaces.
4. A decrease in the phase transition temperature also contributes to an increase in the thickness of the vapor layer due to an increase in the density of the resulting heat flux.

5. Reducing the weight with changes in $\delta$, $\rho$, $\rho'$, $\rho''$ and $\theta$ values should also contribute to the stabilization of the mode of crisis evaporation.

6. The effect of the parameter $\lambda''$ on the change in $\delta''$ due to the above assumptions is conditional, since it is objectively necessary to consider the value of the total heat flux $q$ through a moving flat vapor layer in which steam is blown from the evaporation surface on the bottom of the spheroid.

The theoretical dependences (15) and (16) indicate the dependence of the heat transfer coefficient $\alpha$ on the degree of porosity $\theta$. That is, if there are inclusions in the spheroid with a density different from that of the spheroid fluid $\rho \neq \rho'$, this circumstance can change the heat exchange conditions during evaporation and affect the thickness of the vapor layer.

Figures 2–4 in dimensionless coordinates show the calculated dependences characterizing the rate of evaporation of liquid spheroids of water and ethyl alcohol with insoluble impurities. The calculations were performed according to (19) for equal periods of time $\Delta t = 10$ s and taking into account the change in the current values of the concentration of insoluble impurities, which were determined at each calculation step $i$, as $\chi_i = V_{\text{IMP}} / V_i$, where $V_i$ - the current estimated value of the spheroid volume. Thus, in the course of the calculations, the conditions $V_i < V_{i-1}$, $\chi_i > \chi_{i-1}$, $V_i > V_{i-1}$ and $\chi_i > \chi_0$ were satisfied for all $t > 0$.

Insoluble impurities can change the characteristics of evaporation of a liquid in the spheroidal state. With increasing current values of their concentration in the spheroid increases and in accordance with (16) increases the intensity of heat transfer. The higher the difference in the densities $\rho_{\text{IMP}}$ and $\rho'$, the more significant are the deviations from the evaporation of spheroids of pure liquids. The influence of the heating surface temperature $T_{\text{SUR}}$ is also significantly.

**Figure 2.** The relative rate of change in the volume of water spheroids $D_0 = 0.03$ m, $\delta = 5 \cdot 10^{-3}$ m, containing insoluble impurities of various densities with an initial concentration of $\chi_0 = 0.3$ at temperatures: a) $T_{\text{SUR}} = 310^\circ\text{C}$; b) $T_{\text{SUR}} = 350^\circ\text{C}$. 
Figure 3. Change of heat transfer coefficient $\alpha$ in the process of evaporation of a model water spheroid at $\chi_0 = 0.3$, with different impurity densities $\rho_{IMP}$ for temperatures: a) $T_{SUR} = 310^\circ C$; b) $T_{SUR} = 350^\circ C$.

Figure 4. The change in the thickness of the vapor dynamic layer $\delta$ in the process of evaporation of a model water spheroid at $\chi_0 = 0.3$, with different impurity densities $\rho_{IMP}$ for the temperature of the heating surface: a) $T_{SUR} = 310^\circ C$; b) $T_{SUR} = 350^\circ C$.

Conclusion
The analysis of the calculated dependences presented in Figures 2–4 also makes it possible to reveal possible changes in the pattern of the evaporation process depending on the impurity density $\rho_{IMP}$. With an increase in the density of impurities due to a decrease in the thickness of the dynamic layer of steam, the current values of the heat transfer coefficient will increase and the probability of a crisis of spheroid evaporation will decrease.

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