Modeling of the droplet surface dried on a solid substrate

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Abstract. The paper presents an approach to modeling the surface of a liquid droplet lying on a solid substrate. Receiving the real shape of the droplet surface plays an important role in modeling the process of drying droplets of liquid dispersed systems on solid diffusion-impermeable substrates. This relates to the strong influence of the characteristics of the droplet surface on the values of the coefficients of heat and mass transfer and the value of the surface area of evaporation. A description of the experimental setup for determining the characteristic parameters of the droplet surface is presented. The formulation and solution to the problem of mathematical modeling of the shape of the droplet’s surface, depending on the wetting angle of the liquid-substrate system, surface tension and droplet parameters, are given. The incorrectness of the assumption about the shape of a droplet as an element of a sphere segment is shown. Some results of visualization of the surface of a droplet for various wettability conditions are presented.

1. Introduction

The process of drying the droplets of liquid dispersed products in real conditions is very difficult to describe. As a rule, many droplets evaporate simultaneously; the evaporation process is non-stationary and takes place in a medium with a non-uniform temperature field [1]. The shape of the droplet changes and a complex circulation of the liquid phase occur inside the droplet during the interaction of the surface of the droplet and the flow of the drying agent. The process of heat exchange between the drying droplet and the drying agent is carried out, as a rule, both by convection and thermal radiation [2].

Accordingly, the theoretical description of the droplet drying process is very complicated so for modeling this process it is necessary to implement a number of simplifying assumptions. As the practice has shown, the most effective way to simulate such processes is to build idealized models of the object and process, and addition to these models certain corrections that take into account the influence of various factors. At the same time, the influence of some factors complicating the model can be excluded [3].

When modeling the process of drying droplets of liquid dispersed systems on solid diffusion-impermeable substrates, the correct modeling of the surface of a droplet plays an important role [4]. The shape of the surface of the droplet lying on the solid substrate depends on the value of the wetting angle, the surface tension coefficient, the angle of inclination of the substrate, the nature of fixing the contact line of the perimeter of the droplet with substrate, the presence or absence of airflow, the velocity and direction of flow of the drying agent [5].

The solution of the droplet shape problem is considered in many papers. For example, in [6] presents the results of the use of infrared thermography methods for measuring the temperature of
droplets. In [7] the dynamics of the geometric parameters of droplets of a water-ethanol solution suspended on polypropylene filaments was investigated using high-speed microphotography.

The modeling of a droplet surface is of great interest not only in the description of drying processes, but also for such processes as extraction, precipitation, coagulation, flotation, dipping and coating processes [8].

2. Experimental part
For the experimental study of the shape of the droplet surface located on the substrate, we applied a special installation (figure 1). This installation consists of a digital measuring microscope (1), a device for positioning the substrate in a predetermined position (2), a black casing (3), and a lighting system (4) that minimizes glares on the surface of the photographed droplet.

![Figure 1. Installation for obtaining characteristics of the surface of droplet lying on the solid substrate.](image)

The liquid droplet of a given volume was dosed onto a substrate located at a pre-set angle, and macro shots of droplets were taken from various angles. The photos taken in transmitted and reflected light from the side (perpendicular to the plane of the substrate) and from the top (parallel to the plane of the substrate) were then taken for analysis.

The photographs were analyzed in a graphical editor in order to obtain experimental data on the value of the wetting angle, the size of the droplet (in particular, the maximum height of the drop), and the wetting perimeter. A profile view of droplet was also received.

Fluoroplastic and aluminum substrates were used as the experimental substrates. Water and liquid from distillers grains were used as the studied liquids. Figure 2 shows a photograph of a droplet of liquid distillers grains on a fluoroplastic substrate whereas Figure 3 shows a photograph of this liquid on an aluminum substrate. The dashed rectangle is the projection of the substrate.

As a result of processing of the experimental data for water and fluoroplastic substrate, the wetting angle was about 113° whereas for water and aluminum it was 55°. The results of processing of experimental data for industrial liquid dispersed products showed that the wettability of the substrate by the liquid strongly depends on the purity of the liquid and the surface cleanliness, on the presence of surface-active substances, impurities, etc. Therefore, depending on the batch (and, consequently, on the operation mode of the distillation column), the measured wetting angles of distillery grain and fluoroplastic vary from 75 to 103°, and for distillery grain and aluminum it vary from 45 to 90°.
3. Mathematical description

For mathematical modeling of the kinetics of droplet drying, it is important to calculate the shape of the surface of the droplet depending on the wettability conditions and the nature of the contact line attachment. In some models the droplet shape is simply taken as a ball segment.

We show that such a simplification of the model’s surface is incorrect, as it does not take into account the influence of mass forces on the curvature of the free surface. The evaluation of the influence of surface and mass forces on the shape of the surface of a droplet is carried out by the value of the Bond number $Bo$:

$$Bo = \frac{\rho gh r_0 (2 \sigma \sin \theta)^{-1}}{\rho g h r_0 (2 \sigma \sin \theta)^{-1}}$$

(1)

With a significant influence of mass forces at the value of $Bo \geq 1$, the curvature of the spherical surface is highly important. With the limiting influence of surface forces the value of the number $Bo < 1$ and the curvature of the spherical surface can be neglected. We estimate the value of the $Bo$ number for droplets of the liquid distillers grains of a given size deposited on the aluminum substrate with a different value of the contact angle of wetting: $\rho = 1012 \text{ kg/m}^3$, $\sigma = 0.055 \text{ N/m}$, $g = 9.8 \text{ m/s}^2$, $r_0 = 0.006 \text{ m}$, $\theta \approx 45^\circ$ to $90^\circ$ and $\delta_m \approx 0.002 \div 0.0035 \text{ m}$ (according to the results of observations), $\delta_m (45) \approx 2.0 \text{ mm}$, $\delta_m (90) \approx 3.5 \text{ mm}$.

Using the equation (1) we obtained the following results:

$$Bo(45^\circ) = 1012 \cdot 9.8 \cdot 0.002 \cdot 0.006 \cdot (2 \cdot 0.055 \cdot \sin(45))^{-1} = 1.27$$

$$Bo(90^\circ) = 1012 \cdot 9.8 \cdot 0.0035 \cdot 0.006 \cdot (2 \cdot 0.055 \cdot \sin(90))^{-1} = 2.12$$

So the assumption about the shape of the droplet’s surface as a segment of a sphere in the modeling will lead to a significant error. An estimate of the deviation of the real surface area of a droplet from the area of a sphere segment is given below.

We present the derivation of equations describing the shape of a droplet lying on a horizontal surface with a width $2b$ (figure 4a – wetting angle less than $90^\circ$; figure 4b – wetting angle more than $90^\circ$).
Problem formulation:

\[ \Delta P_c = \rho g \delta(x) ; \]  
\[ \Delta P_k = \sigma (R_1^{-1} + R_2^{-1}) ; \]  
\[ \Delta P_0 = \Delta P_c + \Delta P_k ; \]  
\[ \rho g \delta(x) + \sigma \cdot (R(x))^{-1} = \rho g C_1 . \]

Boundary conditions:

\[ \delta'(0) = tg(\theta) ; \]  
\[ \delta'(\delta_m) = 0 . \]

When transforming equations (1-6) we obtain:

\[ \delta_m = C_1 - ((a_1 C_1^2 + 1 - \cos \theta) \cdot a_1^{-1})^{1/2} ; \]  
\[ \delta_1 = C_1 - ((a_1 C_1^2 - \cos \theta) \cdot a_1^{-1})^{1/2} . \]

The value \( C_1 \) is necessary to find by iterations from the following equation:

\[ b = - \int_0^{\delta_i} (B_i \cdot (1 - B_i)^{-1})^{1/2} d\delta + \int_0^{\delta_m} (B_i \cdot (1 - B_i)^{-1})^{1/2} d\delta , \]

where

\[ a_i = \rho g \cdot (2\sigma)^{-1} ; \]  
\[ B_i = [a_i (C_1 - \delta)^2 + \cos(\theta) - a_i C_1^2] . \]

If \( \theta \leq 90^\circ \) (for wetting, figure 4a), then when changing the ordinate - the thickness of the layer from 0 to \( \delta_i \) its abscissa monotonously varies from 0 to \( x \). Accordingly, the solution will be:

\[ x = + \int_0^{\delta(x)} (B_i \cdot (1 - B_i)^{-1})^{1/2} d\delta . \]

If the liquid does not wet the surface of the substrate, and \( \theta > 90^\circ \) (figure 4b), then while increasing \( \delta \) the abscissa changes from 0 to \( x_1 \) in the negative direction:

**Figure 4.** Scheme of liquid droplet profile on the plate: \( a \) – wetting angle less than 90°; \( b \) – wetting angle more than 90°.
\[
-x = \int_{0}^{\delta(x)} (B_1 \cdot (1 - B_1)^{-1})^{1/2} d\delta ,
\]  
\quad \text{(14)}

where:

\[
x_1 = -\int_{0}^{\delta_1} (B_1 \cdot (1 - B_1)^{-1})^{1/2} d\delta ;
\]  
\quad \text{(15)}

\[
\delta_1 = (2\sigma \cdot (\rho g)^{-1})^{1/2} ((1 - \cos \theta)^{1/2} - 1).
\]  
\quad \text{(16)}

In the range \(x > x_1\) the profile is calculated from the following equation:

\[
x = x_1 + \int_{\delta_1}^{\delta(x)} (B_1 \cdot (1 - B_1)^{-1})^{1/2} d\delta .
\]  
\quad \text{(17)}

When modeling the surface of a droplet, it is necessary to calculate the volume of the droplet, the perimeter wetted by the droplet, the area of the outer surface of the droplet. For \(\theta \leq 90^\circ\) with droplet profile \(\delta(x)\) we receive:

Profile area \(S_0\):

\[
S_0 = b\delta_m - \int_{0}^{\delta} x(\delta) d\delta ;
\]  
\quad \text{(18)}

Droplet-wetted perimeter:

\[
P_{\text{drop}} = \pi d_{\text{drop}} = 2\pi b .
\]  
\quad \text{(19)}

Droplet’s volume:

\[
V_{\text{drop}} = \pi \int_{0}^{\delta_2} (x(d_m) - x(\delta))^2 d\delta ;
\]  
\quad \text{(20)}

Surface area of the droplet:

\[
S_{\text{drop}} = 2\pi b L = 4\pi \int_{0}^{\delta} (1 + (x(\delta))^2)^{1/2} d\delta ;
\]  
\quad \text{(21)}

where \(L = 2\int_{0}^{\delta} (1 + (x(\delta))^2)^{1/2} d\delta .
\)

For \(\theta > 90^\circ\) with droplet’s profile \(\delta(x)\):

Profile area \(S_0\)

\[
S_1 = (b + x(d_x))\delta_m - \int_{0}^{\delta} x(\delta) d\delta , S_0 = 2S_1 ;
\]  
\quad \text{(22)}

Droplet-wetted perimeter,

\[
P_{\text{drop}} = \pi d_{\text{drop}} = 2\pi b .
\]  
\quad \text{(23)}

Droplet’s volume

\[
V_{\text{drop}} = \pi \int_{0}^{\delta_2} (x(d_m) - x(\delta))^2 d\delta ;
\]  
\quad \text{(24)}

Surface area of the droplet
\[ S_{\text{drop}} = 2 \pi b L = 4 \pi b \int_{\delta_a}^{\delta_b} (1 + (x(\delta))^2)^{1/2} d\delta ; \]  

where \( L = 2 \int_{0}^{\delta_b} (1 + (x(\delta))^2)^{1/2} d\delta . \)

4. Results

We calculated the surface area of the droplet, the volume of the droplet, and the size of the droplet for various wetting cases to obtain a numerical estimate of the deviation of the real surface area of the droplet from the area of the segment of equivalent sphere and the real volume of the droplet from the volume of the segment of equivalent ball.

A number of values were taken (45, 70, 90 and 103°) as a source of data for the contact angle of wetting. The radius of the drop of 4 mm was taken for calculations. The calculation was made from the equations (8), (18-25). Table 1 shows the obtained values of the real surface area of the droplet, the area of the segment of equivalent sphere, the real volume of the droplet, the volume of the segment of the equivalent ball, the maximum thickness of the real droplet as well as the ratio of the areas and volumes of the real droplet and equivalent segments.

| Droplet’s volume \( V_{\text{drop}}, m^3 \) | Wetting angle | Maximum thickness of a droplet \( \delta_m, \text{mm} \) | Surface area of a droplet \( S_{\text{drop}}, m^2 \) | Volume of equivalent ball segment \( V_{b}, m^3 \) | \( V_{\text{drop}}/V_{b} \) | Surface area of the equivalent ball segment \( S_{b}, m^2 \) | \( S_{\text{drop}}/S_{b} \) |
|-------------------------------------------|---------------|---------------------------------|-----------------|-----------------|----------------|-----------------|----------------|
| 3.68\cdot10^{-8}                         | 45°           | 1.285                           | 6.477\cdot10^{-3}| 3.36\cdot10^{-8} | 1.183          | 5.574\cdot10^{-3}| 1.162          |
| 6.321\cdot10^{-8}                        | 70°           | 2.017                           | 1.022\cdot10^{-4}| 5.582\cdot10^{-8} | 1.225          | 6.38\cdot10^{-5} | 1.6            |
| 9.032\cdot10^{-8}                        | 90°           | 2.596                           | 1.323\cdot10^{-4}| 7.63\cdot10^{-8}  | 1.277          | 7.289\cdot10^{-5}| 1.815          |
| 1.169\cdot10^{-7}                        | 103°          | 3.164                           | 1.6\cdot10^{-4} | 9.742\cdot10^{-8} | 1.2            | 8.254\cdot10^{-5}| 1.942          |

As follows from the data in this table, the discrepancy between the values of area and volume ranges from 16 to 27% and depends on the value of the contact angle of wetting. Thus, one cannot assume the form of a droplet as a sphere segment to simulate the surface of a droplet lying on the solid substrate.

Figure 5a presents the results of 3D modeling of the surface of wetting substrates. Figure 5b presents the results of 3D modeling of the surface of non-wetting substrates. The calculation of the surface shape was made from the equations (2)-(17). Droplet’s diameter is 4 mm. Contact angle of wetting is 55° and 113°.
Figure 5. 3D model of liquid droplet lying on solid substrate: a – contact angle of wetting – 55°, b – contact angle of wetting – 113°.

Conclusion

The experimental studies have shown that wettability is an extremely unstable process, which strongly depends on the concentration and nature of impurities in a liquid, the roughness of the substrate surface, the nature of contamination of the substrate surface, etc. As our studies have shown, the value of the contact angle of wetting has a limiting effect on the magnitude of the surface area of the simulated droplet and its shape.

In this case, as a rule, the reference data on wetting angles for most liquids are given through the certain ranges of values, which leads to the need for an experimental determination of the value of wetting angles under specific conditions in order to be able to correctly model the droplet surface.

For modeling the process of drying a droplet, the value of the evaporation surface area and the values of heat and mass transfer coefficients have a particular importance. For a droplet, as a rule, the evaporation surface is equal to the droplet surface and the values of heat and mass transfer coefficients strongly depend on the shape of the droplet surface.

We have shown that to simulate the surface of a droplet lying on the substrate, it is impossible to accept the form of a drop as a segment of a sphere, since such assumption leads to serious errors in calculating the surface area (up to 27% in the case of the contact angle over 90°). Therefore, the correct calculation of the parameters of the surface of a droplet has a generally decisive influence on the accuracy of modeling the process of drying a droplet.

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