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The features of construction the empirical description of the drop contour in automation calculations of the surface properties of the melts

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This paper considers the automation of the process of calculation the density and the surface tension of the melts according to the method of a recumbent drop. To solve the assigned task, it has been derived the empirical formulas of the analytical description of numeral solution Laplace's differential equation for the contour of a drop. It has made possible to automate fully the calculation of thermodynamic characteristics.

***Keywords*: Digital image; algorithm; Laplace's differential equation; density; least square method; surface tension; method of a recumbent drop; Delphi.**

I. Introduction

There are different methods of the experimental definition the surface tension of liquids: method of capillary rise, ring or slab detachment method, method of a recumbent drop, method of a hanging drop, drop weight method, method of the maximum pressure in gas bubble. Method of a recumbent drop gives the most exact result and nowadays it is widely used in the high-temperature searches [1]. It is typical to change the object of research during the experiment because of the interaction with structural materials of the measurement cell and furnace atmosphere for labor intensive and expensive physical and chemical measurements [2]. Therefore, it is very important to reduce the duration of the experiment, to measure all the more features and to automate experimenter labor. Such task becomes possible because of the digital equipment appearance, which can register measuring information and processes to their handling.

II. Formulation of the problem

In this method the metal drop melts on the horizontal refractory substrate or forcibly formed under the sharp edge of the crucible. Drop are photographed at a temperature of shaping and then it is measured to know its maximum diameter (*2r*) and inches under it (*h*). It is known [3] that the contour of a drop is defined by the Laplace's equation of a capillary and it has to be written like the differential second-order equation:

$$\frac{y''}{\left[1+(y')^2\right]^{\frac{3}{2}}}+\frac{y'}{x\left[1+(y')^2\right]^{\frac{1}{2}}}=\frac{(y+y_0)(\rho_1-\rho_2)\cdot g}{\sigma} \qquad (1)$$

where

σ – surface tension, N/m^2;

ρ_2 –density of the medium, where the drop is, kg/m^3;

ρ_1 –density of the medium, which is form the drop, kg/m^3;

g − acceleration of gravity, m/s^2;

y – coordinate of the point on the surface along the vertical axis;

y_0 – coordinate of the point on the top along the vertical axis.

The analytic solution this differential equation doesn't have. An approximate solution can be obtained with a predetermined degree of accuracy. All known techniques described in the literature [3] are based on using of the coupling of the system parameters with certain characteristic dimensions of the experimental drop profile. According to the sheets with theoretical drop shapes, which are calculated in advance, a connection is made between the characteristic dimensions and parameters of the drop, or by the formulas approximating the tabulated values, find the parameters of the system. Calculating the capillary characteristics by using tables is inconvenient and time-consuming.

An analysis of the theoretical aspects of the recumbent drop method has shown that the previously developed formulas and tables are either difficult to apply or not applicable at all for PC calculations, which requires transformations of the Laplace's equation to a form convenient for computer mathematical processing.

III. Description

To find the particular solutions of the differential equation (1) that satisfies the initial conditions $y(0)=0$; $y'(0)=0$ for different values of the capillary constant, let's use the geometric meaning of the first and second derivatives.
As a result, was obtained the expression:

$$\frac{y''}{\left[1+(y')^2\right]^{3/2}}=\frac{1}{R} \qquad (2)$$

which determines the plane curvature of the curve and the first derivative is equal to the tangent of the angle of inclination of the tangent to the axis *0x*. Substituting these values into equation (1), was introduced the substitution:

$$A=\frac{\sigma}{(\rho_1-\rho_2)\cdot g} \qquad (3)$$

So it was observed:

$$\frac{1}{R}+\frac{tg\varphi}{x\cdot\frac{1}{cos\varphi}}=\frac{y+y_o}{A} \qquad (4)$$

$$\frac{tg\varphi}{x\cdot\frac{1}{\cos\varphi}}=\frac{\sin\varphi\cdot\cos\varphi}{x\cdot\cos\varphi} \qquad (5)$$

$$R=\frac{A}{(y-y_0)-A\cdot\frac{\sin\varphi}{x}} \qquad (6)$$

Equation (6) defines the radius of curvature at any point of the meridian section of the drop, but contains an undefined ratio (sin φ)/x. When approaching the top of the drop of $x\to 0$, $y\to 0$, $\varphi\to 0$, the vertex both main droplet radius R_1 and R_2 drops of curvature equal to each other and equal to R_0. From the Laplace's equation (1) for this case was observed

$$R_0=2\cdot A/y_0$$

Having $R_1\to R_2\to R_0= 2\cdot A/y_0$, this was substituted into equation (2) and found the limit of the right side of the resulting expression.

$$\frac{2\cdot A}{y_0}=\lim_{x\to 0}\frac{A}{(y+y_0)-A\cdot\sin\varphi/x}=\frac{A}{y_0-A\cdot\lim\limits_{x\to 0}\frac{\sin\varphi}{x}} \qquad (7)$$

$$\lim_{x\to 0}\frac{\sin\varphi}{x}=\frac{y_o}{2\cdot A} \qquad (8)$$

Were chosen on the meridional section line three sufficiently close to each other points M_{i-1}, M_i and M_{i+1} and drawn through them the normal lines (Fig. 1). The normal line passing through the point M_{1-1} intersects the normal line passing through the point M_i at the point O_{i-1}, and the normal lines passing through the points M_1M_{i+1} intersect at the point O_i. It was denoted the angles formed by the normal lines $M_{1-1}O_{i-1}$, M_iO_i and $M_{i+1}O_i$, respectively, φ_{i-1}, φ, φ_{i+1}.To numerically integrate the differential equation (1) and calculate the droplet shape, it was assumed that for a sufficiently small change in the current angle φ in the range from φ_{i-1} to φ_i, the radius of curvature R_{i-1} (the segment $M_{i-1}O_{i-1}$ or the segment M_i0_{i-1}) of the initial angle φ_{i-1} of the original abscissa x_{i-1} and the initial ordinate V_{I-1} does not change. In the next interval of variation of the angle φ from φ_i to φ_{i+1}, the radius of curvature R_i (of the segment M_iO_i or $M_{i+1}O_i$) or the other is calculated for a new value of the angle φi, the new abscissa xi and the new ordinate yi.

From the rectangular triangle $O_i\,M_{i+1}\,P_{i+1}$ and $O_iM_i\,P_i$ was found:

$$\Delta y_i=|P_i-P_{i+1}|=R_i\cdot\cos\varphi_i-R_i\cdot\cos\varphi_{i+1}=R_i\left[\cos\varphi_i-\cos\varphi_{i+1}\right]$$

$$\Delta x_i=|M_{i+1}P_{i+1}|-|M_iP_i|=R_i\cdot\sin\varphi_{i+1}-R_i\cdot\sin\varphi_i=R_i\left[\sin\varphi_{i+1}-\sin\varphi_i\right]$$

$$y_{i+1}=y_i+\Delta y_i$$

$$x_{i+1}=x_i+\Delta x_i$$

The graphs of the dependences of the coordinates x = x (φ), y = y (φ) of the meridional section of the drop from the current angle φ, and also the volume of the part of the drop between its vertex and the plane y = y_0 = const have functions

$$x=a_x\cdot\varphi^{b_x}\cdot\exp(c_x\cdot\varphi) \qquad (9)$$

$$y=a_y\cdot\varphi^{b_y}\cdot\exp(c_y\cdot\varphi) \qquad (10)$$

$$V=a_v\cdot\varphi^{b_v}\cdot\exp(c_v\cdot\varphi) \qquad (11)$$

at the corresponding values of the parameters a_x,b_x, $c_x a_y$, b_y, c_y, a_v, b_v,c_v.

Therefore, for the empirical description of the numerical solution of the differential equation of the drop form (1), these dependences [4]. The coefficients of the obtained equations are found by the method of rectifying the obtained graphs and introducing new variables. Was found the ratio of the next to the previous value of any of the coordinates

$$\frac{x_{i+1}}{x_i}=\frac{a_x\varphi_{i+1}^{b_x}\exp(c_x\varphi_{i+1})}{a_x\varphi_i^{b_x}\exp(c_x\varphi_i)}=\left[\frac{\varphi_{i+1}}{\varphi_i}\right]^{b_x}e^{c_x[\varphi_{i+1}-\varphi_i]} \qquad (12)$$

Take the natural logarithms from the left and right sides of this relation:

$$\ln(x_{i+1}/x_i)=b_x\ln(\varphi_{i+1}/\varphi_i)+c_x\left[\varphi_{i+1}-\varphi_i\right]=b_x\ln(\varphi_{i+1}/\varphi_i)+c_x\Delta\varphi$$

Denote $\ln(x_{i+1}/x_i)$ by $\tilde{x}$, $\ln(\varphi_{i+1}/\varphi_i)$ trough $\tilde{\varphi}$, then was obtained a linear relationship between the variables $\tilde{x}$ and $\tilde{\varphi}$

$$\tilde{x}=b_x\cdot\tilde{\varphi}+c_x\cdot\Delta\varphi \qquad (13).$$

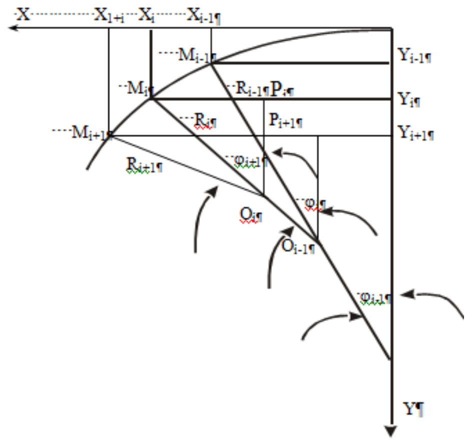

Figure 1. The scheme for constructing the drop elements for numerical integration.

While investigation unknown dependencies it is possible random errors associated with the measurement process. To reduce the effect of random measurement errors, was applied the least squares method, which allows to determine the parameters of the chosen dependence, in which the deviation from the experimental data (in this case, the calculated data) is minimal. There are calculation results (x_1, φ_1), (x_2, φ_2),…,(x_n, φ_n) and the form of the function $\tilde{x} = b_x \cdot \tilde{\varphi} + c_x \cdot \Delta\varphi$. It is necessary to choose b_x *and* c_x so that the sum of the squares of the differences between the empirical and calculated values (deviations) is minimal:

$$\Phi(b_x, c_x) = \sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} [x_i - \tilde{x}]^2 = \min \qquad (14)$$

When the expression (7) is substituted into condition (8) it was obtained:

$$\Phi(b_x, c_x) = \sum_{i=1}^{n} [b_x \cdot \tilde{\varphi} + c_x \cdot \Delta\varphi - x_i]^2 = \min$$

To find the values b_x *and* c_x that convert the left-hand side of the resulting expression to a minimum, it is necessary to equate the derivatives with respect to zero. A function can have an extremum (min) if all its partial derivatives are zero or nonexistent.

$$\frac{\partial\Phi(b_x, c_x)}{\partial b_x} = 0 \qquad \frac{\partial\Phi(b_x, c_x)}{\partial c_x} = 0$$

$$\begin{cases} 2\sum_{i=1}^{n}[b_x \cdot \tilde{\varphi} + c_x \cdot \Delta\varphi - x_i] \cdot \tilde{\varphi} = b_x \cdot \sum_{i=1}^{n} \tilde{\varphi}^2 + c_x \cdot \sum_{i=1}^{n} \tilde{\varphi} \cdot \Delta\varphi - \sum_{i=1}^{n} x_i \cdot \tilde{\varphi} = 0 \\ 2\sum_{i=1}^{n}[b_x \cdot \tilde{\varphi} + c_x \cdot \Delta\varphi - x_i] \cdot \Delta\varphi = b_x \cdot \sum_{i=1}^{n} \tilde{\varphi} \cdot \Delta\varphi + c_x \cdot \sum_{i=1}^{n} \Delta\varphi^2 - \sum_{i=1}^{n} x_i \cdot \Delta\tilde{\varphi} = 0 \end{cases}$$

$$\begin{cases} \underline{\underline{b_x}} \cdot \sum_{i=1}^{n} \tilde{\varphi}^2 + \underline{c_x} \cdot \Delta\varphi \cdot \sum_{i=1}^{n} \tilde{\varphi} = \sum_{i=1}^{n} x_i \cdot \tilde{\varphi} \\ \underline{\underline{b_x}} \cdot \Delta\varphi \cdot \sum_{i=1}^{n} \tilde{\varphi} + \underline{c_x} \cdot \Delta\varphi^2 \sum_{i=1}^{n} 1 = \Delta\tilde{\varphi} \cdot \sum_{i=1}^{n} x_i \end{cases}$$

This is the final form of the normal least-squares method [5]. It was solved the system and found empirical values according to Cramer's formulas. $c_x = \frac{\Delta c_x}{\Delta}$ and

$$b_x = \frac{\Delta b_x}{\Delta}$$

$$b_x = \frac{\Delta b_x}{\Delta} = \frac{\begin{vmatrix} \sum_{i=1}^{n} x_i \cdot \tilde{\varphi} & \Delta\varphi \sum_{i=1}^{n} \varphi \\ \Delta\varphi \cdot \sum_{i=1}^{n} x & \Delta\varphi^2 \cdot n \end{vmatrix}}{\begin{vmatrix} \sum_{i=1}^{n} \varphi^2 & \Delta\varphi \sum_{i=1}^{n} \varphi \\ \Delta\varphi \cdot \sum_{i=1}^{n} \varphi & \Delta\varphi^2 \cdot n \end{vmatrix}} = \frac{\Delta\varphi^2}{\Delta\varphi^2} \frac{\begin{vmatrix} \sum_{i=1}^{n} x_i \cdot \tilde{\varphi} & \sum_{i=1}^{n} \varphi \\ \sum_{i=1}^{n} x_i & n \end{vmatrix}}{\begin{vmatrix} \sum_{i=1}^{n} \varphi^2 & \sum_{i=1}^{n} \varphi \\ \sum_{i=1}^{n} \varphi & n \end{vmatrix}} = \frac{\begin{vmatrix} \sum_{i=1}^{n} x_i \cdot \tilde{\varphi} & \sum_{i=1}^{n} \varphi \\ \sum_{i=1}^{n} x_i & n \end{vmatrix}}{\begin{vmatrix} \sum_{i=1}^{n} \varphi^2 & \sum_{i=1}^{n} \varphi \\ \sum_{i=1}^{n} \varphi & n \end{vmatrix}}$$

$$c_x = \frac{\Delta c_x}{\Delta} = \frac{\begin{vmatrix} \sum \varphi^2 & \sum_{i=1}^{n} x_i \cdot \tilde{\varphi} \\ \Delta\varphi \cdot \sum_{i=1}^{n} \varphi & \Delta\varphi \cdot \sum_{i=1}^{n} x_i \end{vmatrix}}{\begin{vmatrix} \sum \varphi^2 & \Delta\varphi \sum_{i=1}^{n} \varphi \\ \Delta\varphi \cdot \sum_{i=1}^{n} \varphi & \Delta\varphi^2 \cdot n \end{vmatrix}} = \frac{1}{\Delta\varphi} \frac{\begin{vmatrix} \sum \varphi^2 & \sum_{i=1}^{n} x_i \cdot \tilde{\varphi} \\ \sum_{i=1}^{n} \varphi & \sum_{i=1}^{n} x_i \end{vmatrix}}{\begin{vmatrix} \sum \varphi^2 & \sum_{i=1}^{n} \varphi \\ \sum_{i=1}^{n} \varphi & n \end{vmatrix}}$$

After determination the coefficients c_x, b_x was found $a_x = \frac{1}{n} \sum_{i=1}^{n} \left[\frac{x_i}{\varphi_i^{b_x} \exp(c_x \varphi_i)} \right]$ that is, determined all the coefficients of the empirical dependence (3).

Similarly, we find the coefficients $a_y, b_y, c_y, a_v, b_v, c_v$ of dependences (4) and (5), which allows us to determine the volume.

The analytical description of the numerical solution of the differential equation (1) by the empirical formulas (9-11) can be considered quite accurate [6-7]. Thus, on the basis of the empirical dependences obtained, prototypes of the drop contours are obtained. This makes it possible to proceed to the realization of the next stage of identification of drop contours during the experiment and determination of the surface properties of the melts.

IV. CONCLUSIONS

An analytical description of the numerical solution of the Laplace differential equation by empirical formulas was made by using the geometric meaning of the 1-st and 2-nd derivatives. As a result of its application, a new technique for calculating the density and surface tension of melts in the sessile drop method has been developed, which made it possible to perform full automation of calculations on a PC.

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