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ASSESSMENT OF THE RELATIVE ERROR IN SESSILE DROP METHOD AUTOMATION TASK

Assessment of the relative error in the sessile drop method automation. Further development of the sessile drop method is directly related to the development of new techniques and specially developed algorithms enabling automatic computer calculation of surface properties. The sessile drop method mathematical apparatus improvement, drop circuit equation transformation to a form suitable for working, the drop surface calculation method automation, analysis of relative errors in the calculation of surface tension are relevant and are important in experimental determinations. The surface tension measurement relative error, as well as the error caused by the drop ellipsoidness in the plan were determined in the task of the sessile drop automation. It should be noted that if the drop maximum diameter (l) is big or if the ratio of l to the drop height above the equatorial diameter(h) is big, the relative error in the measurement of surface tension by sessile drop method does not depend much on the equatorial diameter of the drop and ellipsoidness of the drop. In this case, the accuracy of determination of the surface tension varies from 1,0 to 0,5%. At lower values the drop ellipsoidness begins to affect the relative error of surface tension (from 1,2 to 0,8%), but in this case the drop ellipsoidness is less. Therefore, in subsequent experiments, we used larger drops. On the basis of the assessment of the relative error in determining the liquid surface tension by sessile drop method caused by drop ellipsoidness in the plan, the tables showing the limits of the drop parameters (h and l) measurement necessary accuracy to get the overall relative error have been made up. Previously, the surface tension used to be calculated with the relative error in the range of 2-3%.

Keywords: *automation, surface properties, physical-chemical experiment, the relative error, absolute error, ellipsoid.*

Левицька Т.О. Оцінка відносної похибки в задачі автоматизації методу лежачої краплі. *У задачі автоматизації методу лежачої краплі дана оцінка відносної похибки визначення поверхневого натягу, викликаної еліпсоїдністю краплі в плані. Складені таблиці із зазначенням меж необхідної точності вимірювання параметрів краплі (h і l) для досягнення спільної відносної похибки. Це дозволило при повній автоматизації розрахунків отримувати значення поверхневого натягу розплавів з високим ступенем точністю, відносна похибка (раніше 2-3%).*

Ключові слова: *автоматизація, поверхневі властивості, метод лежачої краплі, фізико-хімічний експеримент, відносна похибка, абсолютна похибка, еліпсоїдну.*

Левицкая Т.А. Оценка относительной погрешности в задаче автоматизации метода лежащей капли. *В задаче автоматизации метода лежащей капли дана оценка относительной погрешности определения поверхностного натяжения, вызванной эллипсоидностью капли в плане. Составлены таблицы с указанием пределов необходимой точности измерения параметров капли (h и l) для достижения общей относительной погрешности ±0,5%. Это позволило при полной автоматизации расчетов получать значение поверхностного натяжения расплавов с высокой степенью точностью, относительная погрешность ±0,5% (раньше 2-3%).*

Ключевые слова: *автоматизация, поверхностные свойства, метод лежащей кап-*

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[*] *PhD, SHEE «Priazovskyi State Technical University», Mariupol, tlevitiisys@gmail.com*

ли, физико-химический эксперимент, относительная погрешность, абсолютная погрешность, эллипсоидность.

Description of the problem. For the experimental determination of the surface tension of liquids, there are different methods, including sessile drop method gives the most accurate results and is now widely used in high-temperature studies. In the sessile drop method, a drop of molten metal on a horizontal refractory substrate or forced form of a sharp edge of the crucible. Formed drop photographed and these photos increase. Also drop can be projected onto the screen for maximum sharpness in the image contour drops. On the projection photographs or drops build maximum diameter (*l*) and the height above it (*h*). Measurements of the picture and especially spending a tangent, a researcher in making this procedure the elements of subjectivity, the measurement error depends on the quality of the picture. For example, the maximum diameter of the tracing on the eye can give an initial error of 1.5%. It is clear that further development of the method of sessile drop is directly related to the development of new techniques and specially developed algorithms enabling automatic computer calculation of surface properties [1-2]. We have automated technique for solving the basic equation of the surface of the droplets on the basis of advanced mathematical apparatus with the implementation of a system of visual programming Delphi, which significantly expedite the processing of data and implement fully automated calculation of surface tension melts. Nowadays, there is a need to assess the relative error in the determination of the surface tension of the liquid sessile drop method, caused by a drop in terms of ellipsoidal.

Analysis of the last researches and publications. In recent years, more and more attention in the experimental study of the surface tension is given to methods based on the analysis of the digitized image of the zone of two- and three-phase contact. Such an image is obtained using a digital video camera (camera) and the optical system, as shown in [3]. Drop is a figure of rotation around the vertical axis, so its shape can be defined by its meridian section of the curve in the coordinates x, y. Shape of the drop depends on the surface tension forces, which tries to give a drop of a spherical shape, as well as the force of gravity, as a result of which the drop is "flattened". It is known [4] that the contour of the drop is determined by the equation of capillarity Laplace, which can be written in the form of a differential equation of 2nd order. Analytical solution given differential equation has. All known techniques described in the literature [5-6] are based on the communication parameters of the system with some of the characteristic dimensions of the experimental profile of the drop. Tables with theoretical forms droplets that calculated in advance, the link between the characteristic dimensions and parameters of the drop, or formulas approximating table values are system parameters. However, the calculation of capillary characteristics using tables is inconvenient and time-consuming. To date, there is no good time proven, modern, high-precision, experimental methods for measuring surface and interfacial tension, so the development of current and future trends. Improvement of mathematical apparatus by sessile drop method, the transformation equation circuit drops to a form suitable for machining, automation methodology for calculating the droplet surface, analysis of relative errors in the calculation of surface tension are relevant and have a great knowledge of the practice of experimental determinations.

The objective of the article – a task automation by sessile drop method, the estimate of the relative error in the determination of the surface tension caused by the ellipsoidal drop in the plan. Compiled a table showing the limits of the necessary measurement accuracy drops (h and l) to achieve the overall relative error.This greatly improving the accuracy of the method.

Basic material. The calculation of the surface tension on the sessile drop method involves the solution of the basic equation of the droplet surface:

$$\sigma \cdot \left(\frac{1}{R_1} + \frac{1}{R_2} \right) = (\rho_1 - \rho_2) \cdot g \cdot x + \frac{2 \cdot \sigma}{R_0}, \tag{1}$$

where σ – the surface tension at the Radel phases, N/m^2;

R_1 *and* R_2 – the principal radii of curvature of the surface element at a given point, m;

R_0 – radius of curvature at the apex of the drop, m;

ρ_2 – density of the medium in which there is a drop, kg/m^3;

ρ_1 – medium density drop generator, kg/m^3;

g – acceleration due to gravity in m/s^2;

x – coordinate of a point on the surface of the droplet on the vertical axis.

To assess the relative error in the determination of the surface tension of the liquid sessile drop method is proposed to estimate ellipsoidal droplets using eccentricity ε [5]

$$\varepsilon = \sqrt{1-\left(\frac{b}{a}\right)^2}, \tag{2}$$

where a – length of major axis of the ellipse, m;

b – the length of the smaller axis of the ellipse, m.

Scheme for constructing elements of geometry drops for derivation of the equation of the ellipse, assessing the relative error caused by the ellipsoidal drop in terms presented in figure 1.

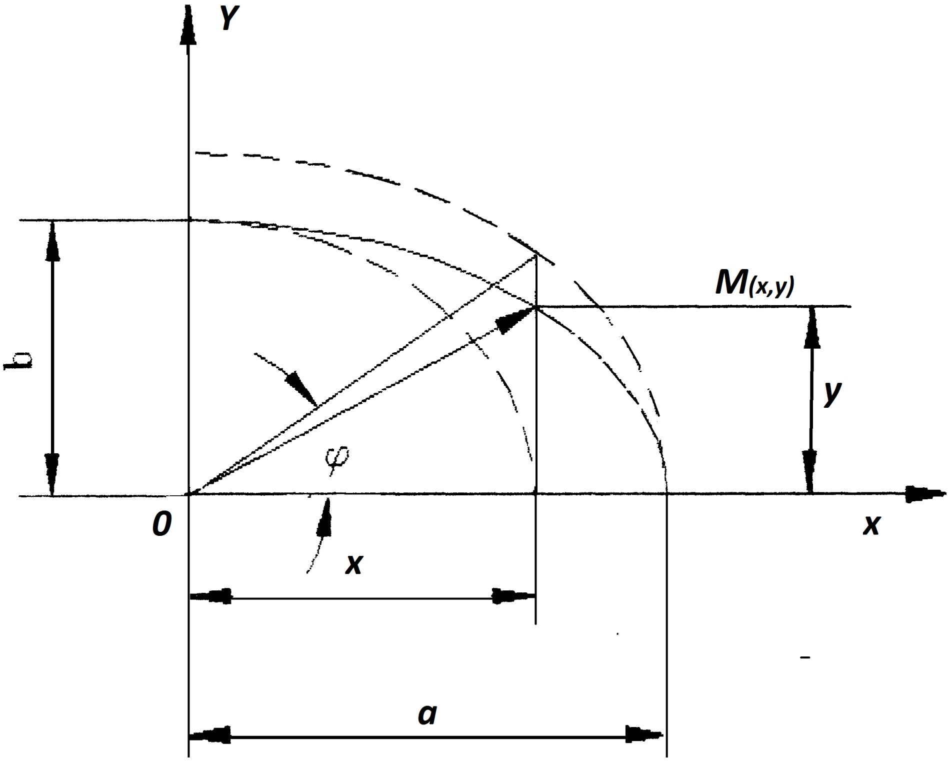

Fig. 1 – Diagram of the elements of geometry drops

In this case, all the dimensions of the ellipse is convenient to write through the length of the semi-major axis and eccentricity. Minor axis b is equal to:

$$b = a \cdot \sqrt{1-\varepsilon^2}\ . \tag{3}$$

We define the average radius of the ellipse. The equation of the ellipse in parametric form:

$$\begin{cases} x = a \cdot \cos\varphi \\ y = b \cdot \sin\varphi \end{cases}. \tag{4}$$

The distance of the current point M (x, y), which lies on the ellipse from the beginning of the coordinate axes is determined (figure 1):

$$r_\tau = \sqrt{x^2+y^2} = \sqrt{a^2 \cdot cos^2\varphi + b^2 \cdot \sin^2\varphi} = a\sqrt{1-\varepsilon^2 \cdot \sin^2\varphi}\ . \tag{5}$$

The average radius of the ellipse is equal to:

$$r_{cp} = \frac{\sum_{i=1}^{n} r_{\tau i}}{\sum_{i=1}^{n} i} = \frac{\sum_{i=1}^{n} r_{\tau i}}{n} \tag{6}$$

or more precisely:

$$r_{cp}=\frac{\int_0^{\pi/2} r_\tau d\varphi}{\int_0^{\pi/2} d\varphi}=\frac{\alpha\cdot\int_0^{\pi/2}\sqrt{1-\varepsilon^2\cdot\sin^2\varphi d\varphi}}{\pi/2}=\frac{2}{\pi}\cdot\left[\varepsilon\cdot\frac{\pi}{2}\right]\cdot a. \qquad (7)$$

Here $\int_0^{\pi/2}\sqrt{1-\varepsilon^2\cdot\sin^2\varphi}\ d\varphi=E\left(\varepsilon,\frac{\pi}{2}\right)$ - 2 elliptic integral of the first kind.

Denoting $2/\pi\cdot E\left(\varepsilon,\frac{\pi}{2}\right)$ through $\mathit{\Phi}(\varepsilon)$, we have the formula to determine the averageradius of the ellipse in the following form:

$$r_{cp}=a\cdot\Phi(\varepsilon). \qquad (8)$$

Maximum absolute error caused by the replacement of the average equatorial radius drops his greatest (a) or lowest (b) size will be respectively equal to:

$$\Delta l(a)=2\cdot\left(a-r_{cp}\right)=2\cdot a\left[1-\mathit{\Phi}(\varepsilon)\right], \qquad (9)$$

$$\Delta l(b)=2\cdot\left(a\cdot\sqrt{1-\varepsilon^2}-a\cdot\Phi(\varepsilon)\right)=2\cdot a\cdot\left[-\frac{b}{a}+\Phi(\varepsilon)\right]. \qquad (10)$$

Graph showing the relationship $\frac{\Delta r}{r_{\text{cp}}}$ and $\Phi(\varepsilon)$ from $\frac{b}{a}$ represented in the figure 2.

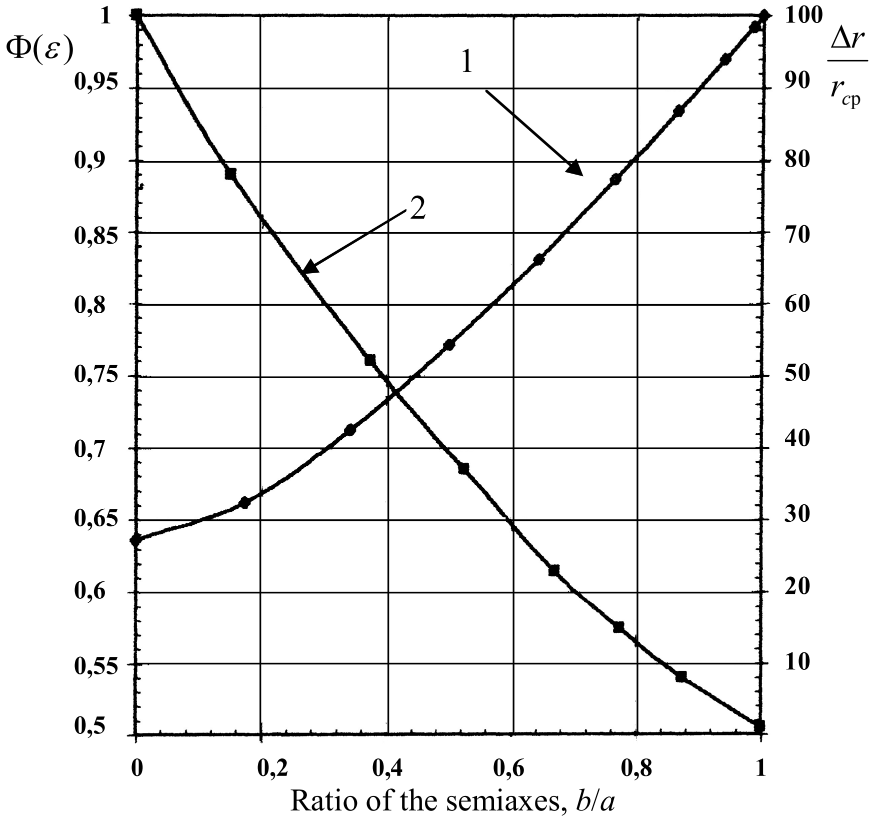

Fig. 2 – Relative error $\Delta r/r_{cp}$ caused by the replacement of the medium-range drop its extreme value, r0: 1 – $\mathit{\Phi}(\varepsilon)=2\pi\int_0^{\pi/2}\sqrt{1-\varepsilon^2\cdot\sin^2\varphi}\ d\varphi$; 2 – $\frac{\Delta r}{r_{\text{cp}}}$

The function value $\Phi(\varepsilon)$ is given in the table.

Table

Value of the function $\Phi_{(\varepsilon)}$ depending on the eccentricity of the ellipse ε or relationship semiaxes *b/a*

ε	*b/a*	$\Phi(\varepsilon)$	$2\cdot(1-\Phi(\varepsilon))$	$2\cdot(\Phi(\varepsilon)-\mathrm{b/a})$
0,0000	1,0000	1,0000	0,0000	0,0000
0,1736	0,9848	0,9924	0,0152	0,0152
0,3420	0,9397	0,9701	0,0598	0,0608
0,5000	0,8660	0,9343	0,1314	0,1366
0,6428	0,7660	0,8869	0,2262	0,2418
0,7660	0,6428	0,8311	0,3378	0,3766
0,8660	0,5000	0,7710	0,4580	0,5420
0,9397	0,3420	0,7120	0,5760	0,7400
0,9848	0,1736	0,6621	0,6758	0,9770
1,0000	0,0000	0,6366	0,7268	1,2732

The relative error of determination of the surface tension in accordance with formula (1), $\frac{\Delta d}{\sigma}=F(l,h)$ and $\sigma=(\rho_1-\rho_2)\cdot g$ is given:

$$\delta(\sigma)=\frac{d\sigma}{\sigma}=\frac{F(l,h)}{(\rho_1-\rho_2)\cdot g}\left[\left|\frac{g}{F(l,h)}\right|d\rho+\left|\frac{\rho_1-\rho_2}{F(l,h)}\right|dg+\left|\frac{(\rho_1-\rho_2)\cdot g}{F^2(l,h)}\right|\left|\frac{\partial F}{\partial h}\cdot\Delta h+\frac{\partial F}{\partial l}\cdot\Delta l+d\overline{F}\right|\right]=$$

$$=\frac{\Delta\rho}{\rho_1}+\frac{\Delta g}{g}+\frac{\partial F}{\partial h\cdot F}\cdot\Delta h+\frac{\partial F}{\partial l\cdot F}\cdot\Delta l+\frac{d\overline{F}}{F}. \qquad (11)$$

Given a formula relative error in determining the surface tension by sessile drop method (11), we have an opportunity to assess the relative error introduced by the ellipticity of the droplet shape in plan view.

$$\delta_\sigma=100\cdot\left|\frac{\Delta\rho}{\rho_1-\rho_2}\right|+100\cdot\left|\frac{\Delta g}{g}\right|+(a\cdot\Delta h+b\cdot\Delta l)+\delta_{(F)}. \qquad (12)$$

Let

$$\Delta l=\Delta l_1+\Delta l_2,$$

where Δl – the total measurement error equatorial diameter drops, m;

Δl_1 – error caused by the inaccuracy of measuring tools, m;

Δl_2 – asbsolute error caused by the ellipsoidal drop by replacing the average droplet radius of its largest or smallest size, m.

Substitute in the formula (11) values (12), determines the relative error of measurement of the surface tension, including the error caused by the ellipsoidal drop.

It should be noted that for large size parameter drops l (or more terms l/h) relative error of measurement of the surface tension by sessile drop method depends weakly on the equatorial diameter of the drop and ellipsoidal drop. In this case, the accuracy of determination of the surface tension varies from 1,0 to 0,5%. At lower values of ellipsoidal drop begins to affect the relative error of surface tension (from 1,2 to 0,8%), but in this case she ellipsoidal drops less. Therefore, in subsequent experiments, we used large droplet sizes.

On the basis of the assessment of the relative error in determining the surface tension of a liquid by sessile drop caused by ellipsoidal drop in the plan, drawn up a table showing the limits of the necessary measurement accuracy drops (*h* and *l*) to achieve the overall relative error $\pm 0{,}5\%$. Previously, the surface tension is calculated in this method with the relative error in the range of 2-3%.

Conclusions

In the task automation sessile drop method evaluated the relative error in the determination of the surface tension caused by the ellipsoidal drop in the plan. Compiled a table showing the limits of the necessary measurement accuracy drops (*h* and *l)* to achieve the overall relative error. This allowed the full automation of calculations to obtain the value of the surface tension of the melt with a high degree of accuracy, the relative error $\pm 0{,}5\%$ (previously 2-3%).

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Reviewer: V.P. Grankin
dr. tech. of sciences, prof., «Pryazovskyi State Technical University»
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© Троханяк В.І.[1], Богдан Ю.О.[2]

ЗАСТОСУВАННЯ МЕТОДУ КІНЦЕВИХ ЕЛЕМЕНТІВ ПРИ ПОБУДОВІ СІТКИ В ANSYS MESHING ДЛЯ CFD МОДЕЛЕЙ

Розроблено методику та здійснено аналіз побудови 2D сітки, використовуючи метод кінцевих елементів в ANSYS Meshing для теплообмінників з коридорним розташуванням труб в пучках та з криволінійним їх розташуванням в компактних пучках труб нової конструкції. Розглянуто особливості та розроблений алгоритм побудови сітки для задач гідро- газодинаміки і тепло- масопереносу. Вибрано найбільш оптимальні та якісні сітки для CFD моделей.

Ключові слова: *метод кінцевих елементів, прикордонний шар, загальна товщина, плавний перехід, гібридна сітка, чотирикутна сітка.*

Троханяк В.И., Богдан Ю.А. Применение метода конечных элементов при построении сетки в ANSYS Meshing для CFD моделей. *Разработана методика и*

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[1] *аспірант, Національний університет біоресурсів і природокористування України, м. Київ,* v1kt0r_t@ukr.net

[2] *ст. викладач, Київська державна академія водного транспорту ім. гетьмана Петра Конашевича-Сагайдачного, м. Київ,* bogdan_yura@mail.ru