Determination of the maximum droplet diameter during centrifugal extraction, soil analysis, contamination and waste disposal

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Abstract. The prospects of the research are determined by the high potential for solving current problems related to environmental problems. Extraction allows not only the purification of chemical production waste, but also the analysis of elements distributed in the soil, which is especially important for migrating contaminants, and contaminants obtained from chemical, paint and varnish and agricultural waste. Examples of such waste are metals and their compounds, fertilizers and pesticides, and radioactive waste. These contaminants enter the human body through food chains, producing toxic, carcinogenic, and mutagenic effects. This approach has several directions that allow us to solve the problem comprehensively. In the first direction of our research, we will consider how this mathematical model can be applied in waste treatment technologies. In the second direction, we will pay attention to soil analysis. In the third research direction, we will focus on optimizing extraction and waste disposal technologies. This paper considers a mathematical model that describes the formation of the shape of droplets when moving in a field of centrifugal forces. When liquid droplets move within liquid or gaseous media, the surface of these droplets undergoes deformation, which can lead to their destruction and the formation of smaller droplets.

1 Introduction

When obtaining rare earth elements, analyzing soils, and determining pollutants, centrifugal extractors are increasingly used [1-8]. The use of centrifugal extractors significantly speeds up the analysis of microcomponents [9-15]. There is a possible destructive effect of radioactivity of elements on extractants especially with high viscosity or small differences in phase densities. For the calculation of such devices, the size of the droplets is important. However, it may vary depending on the radius of the droplets. As a drop moves in another uniformly rotating immiscible liquid, the drop's speed continuously increases. This leads to an increase in the pressure of the oncoming flow, especially in the frontal part, which leads to its destruction [8, 9]. Due to the action of the flow flowing around the drop, a change in its shape is observed, which resembles an asymmetrical concave lens. In turn, the asymmetry of the shape is explained by the action of Coriolis forces.

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It should be noted that when the front and rear sides of the drop are connected, it takes on a toroidal shape. This form, however, is unstable due to surface tension forces, and it quickly breaks up into a collection of smaller droplets. It was experimentally established that the destruction of the drop occurs a little earlier than predicted by calculations [7,9]. This is explained by the fact that when constructing the model, the vibration of the interfacial surface during the movement of the drop was not taken into account.

And when carrying out liquid extraction, the heavy phase spray torch moves from the center to the periphery. As the radius increases due to droplet fragmentation, the droplet size distribution changes. This leads to a change in the phase interface and mass transfer coefficient.

Considering the mechanisms of formation and destruction of a drop, it should be noted that when a drop moves inside another liquid or gaseous medium, they usually undergo destruction, thereby forming more particles [10, 11, 16-20]. This process is widely found in phenomena such as atomization, liquid-liquid extraction, absorption, separation and others. Existing models are usually classified into three main groups depending on the methodology used to describe the crushing process: energetic, oscillatory and aerodynamic [20-29].

Energy model: Based on the conservation of the total energy of the system as a condition for stability. When analyzing this model, it was found that an increase in flow velocity leads to an increase in surface energy. There is a point at which this energy begins to increase indefinitely with a small increase in speed, and this is considered the moment of destruction. The values of the limiting Weber number for this model are in the range We = 2.8-5.41.

Oscillatory model: Based on the assumption that the destruction of a drop occurs when the frequency of its own oscillations corresponds to the frequency of external influences. According to this model, droplet fragmentation will occur at a Weber number We = 4.4.

Aerodynamic approach: Based on the analysis of quasi-stationary deformation of a drop under the influence of an aerodynamic “parachute” in its aft part. According to this model, the moment of destruction will occur when a certain degree of deformation of the parachute is reached. For this model, the limiting Weber number is We = 3.75.

Studies of the mechanism of droplet destruction were carried out in a number of works [24-29], which proposed various mathematical models to describe this process. All these models consider the destruction of droplets in the absence of external mass forces and have their own characteristics depending on the method of describing the fragmentation.

2 Mathematical modeling of the process

All of these destruction methods do not take into account the features of the centrifugal field, such as the inertial force varying along the radius and the Coriolis force, which can cause certain variations in the process of fragmentation of droplets.

When visually observing the destruction of a drop in a centrifugal field, it was found that the drop was deformed with deflection on the front and rear sides without the formation of a “parachute”. The following assumptions were made during the modelling.

Initially, it is assumed that the shape of the drop is like an oblate ellipsoid of revolution. This assumption is based on experimental data describing the movement of droplets under conditions of centrifugal and gravitational fields. Before the destruction process, the shape of the drop remains constant.

The fluids both inside and outside the drop are considered incompressible.

The movement of liquid inside the drop is considered negligible and is not considered in this context.

This model does not consider the vibrations of the droplet surface. From an analysis of the available literature, it follows that this assumption may be justified if the deformation

time of the drop is significantly greater than the period of its own oscillations. In this case, we can talk about quasi-static deformation, and this condition is satisfied in this context.

It is important to note that a laminar boundary layer is formed on the frontal surface of the drop, while a turbulent region appears on the aft part. This fact is also considered in the model.

Additionally, it is assumed that the drop moves in a medium with a quasi-stationary nature of motion. This assumption is based on the results of studies of the movement of droplets under the action of centrifugal forces.

This model also considers that the interface between the drop and the environment behaves like an elastic thin film.

The study of the process of destruction of droplets considers the assumption of non-mixing of incompressible liquids moving inside each other. It was experimentally confirmed that the shape of a liquid drop moving under conditions of uniform rotation at the initial stage approaches the shape of an ellipsoid of revolution, where the minor axis coincides with the direction of movement of the drop. It is assumed that the drop slowly deforms, and at each moment of time its shape remains stable.

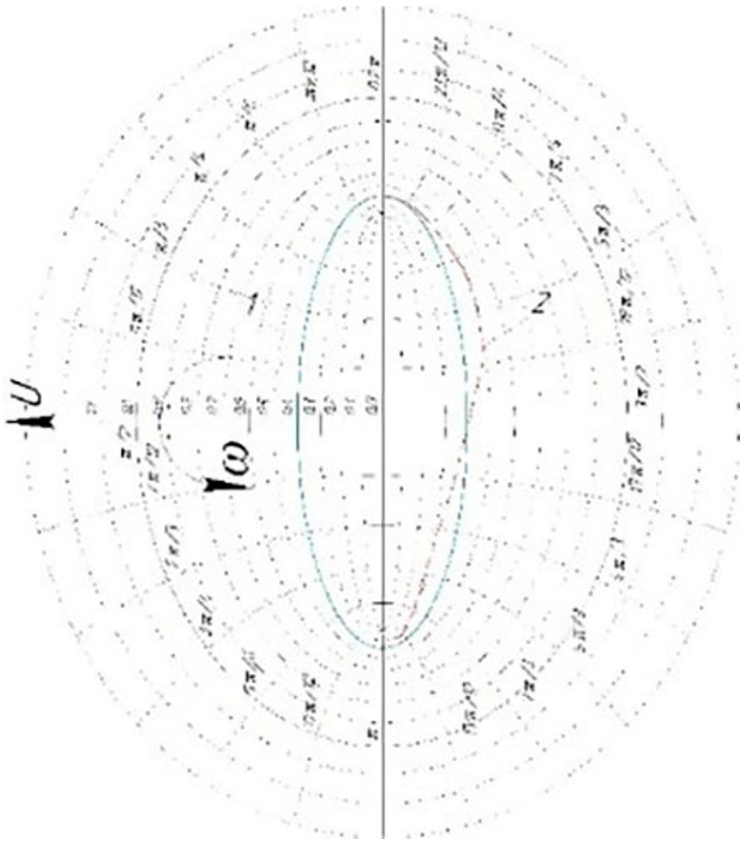

Fig. 1. Flow patterns when a drop moves in an elliptical coordinate system.

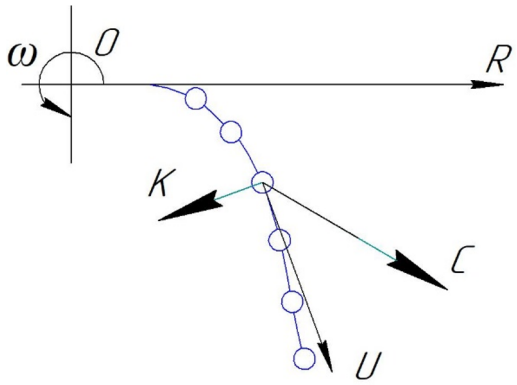

Fig. 2. Schemes of forces acting on a drop and the trajectory of its movement in the polar coordinate system: 1- the shape included in the calculation of the flow potential of the medium around the drop; 2 - real drop shape.

In Figure 2: *U* is drop velocity, *K* is Coriolis force, *C* is centrifugal force.

To ensure stability of the shape of the drop at each moment of time, it is necessary that the pressure inside the drop remains constant at all its points. It is important that the sum of the algebraic pressures acting on the drop from the outside and the internal pressures existing inside the drop is equal to the pressure at the center of the drop. In the absence of external influences (this is a special case), when the drop takes the shape of a sphere, the pressure at its center can be calculated using the following equation: $P_o = \frac{4\sigma}{d}$. We assume that when external conditions change, the pressure component remains constant. Then the condition for stability of the droplet shape can be written as follows:

$$\mathrm{P}_\infty = \mathrm{P}_H \pm \mathrm{P}_K^1 = \mathrm{P}_\mathrm{o} \mp \mathrm{P}_{cc} \pm \mathrm{P}_K^2 - \mathrm{P}_\sigma - \mathrm{P}_c. \quad (1)$$

where: $\mathrm{P_н}$ is pressure from the oncoming flow, $\mathrm{P_к}$ is pressure from the Coriolis forces, $\mathrm{P_{cc}}$ is pressure from the centrifugal force caused by the difference in the densities of liquids inside and outside the drop (index 1 – pressure from the external environment, 2 – pressure from the internal environment), $\mathrm{P_\sigma}$ is pressure from interfacial tension forces, $\mathrm{P_c}$ is pressure averaged over the surface inside the drop. The choice of the sign (+) or (-) for $\mathrm{P_k}$ depends on which side along the drop's path is considered; for $\mathrm{P_{cc}}$ - the sign (+) for the frontal part, and (-) for the rear part of the drop.

To estimate the pressure on the droplet surface, an analysis of the velocity field in the environment is required. It is necessary to take into account that the drops are deprived of internal circulation, which is typical for drops of technical liquids that contain surfactants (surfactants) [30-32]. Boundary layer theory is used for this task. It is assumed that a laminar boundary layer is formed at the front of the drop (see Figure 1), and outside this layer the motion of the medium is considered ideal. Given that the shape of the drop is an ellipsoid of revolution, we can determine the flow potential in elliptical coordinates (λ, η, φ) [30]:

$$\phi_\mathrm{п} = Uc\lambda\eta\frac{\lambda^{-1}-arcctg\lambda}{m}, \quad m = arcsin\frac{1}{\sqrt{\lambda_o^2+1}} - \frac{\lambda_o}{\lambda_o^2+1}. \quad (2)$$

The drop velocity U is determined by the equation [30, 31]:

$$U = 1.74\frac{(\rho_k-\rho_c)^{0.29}\sigma^{0.32}\omega^{0.36}R^{0.18}}{\rho_c^{0.62}\,d^{0.14}} \quad (3)$$

By moving to the coordinates of the oblate ellipsoid of revolution (λ, η), we can determine the velocity components and the asymmetry of the shape relative to the axis passing through the center of the drop parallel to the velocity vector.

$$V_\eta = \frac{\sqrt{1-\eta^2}(1-\lambda arcctg\lambda)}{m\sqrt{\lambda^2+\eta^2}} \quad (4)$$

and

$$V_\lambda = \frac{U\eta(\lambda-(\lambda^2+1)arcctg\lambda)}{m\sqrt{\lambda^2+1}\sqrt{\lambda^2+\eta^2}} \quad (5)$$

where $m = arctg\lambda_0 - \frac{\lambda_0}{\lambda_0^2+1}$.

Then for pressures we obtain the following relations:

$$P_H = 0.5\rho_c(V_\lambda^2 - V_\eta^2) \quad (6)$$

$$P_0 - P_\infty - P_\sigma = 4\sigma d^{-1} - \sigma(r_1^{-1} + r_2^{-1}) \quad (7)$$

$$P_{cc} = 2(\rho_k - \rho_c)\omega^2 R_c\lambda_0\eta \quad (8)$$

$$P_k^2 = -2\rho_k U\omega c\sqrt{\lambda^2+1}\sqrt{1-\eta^2}cos\theta \quad (9)$$

$$P_k^1 = -2\rho_k\omega U m^{-1}c\sqrt{\lambda^2+1}\sqrt{1-\eta^2}cos\theta arcctg\lambda_0 \quad (10)$$

$$P_c = S_n^{-1}\int_0^{2\pi} d\varphi \int_{-1}^{1} P_H\sqrt{\lambda_0^2+1}\sqrt{\lambda_0^2-\eta^2}d\eta \quad (11)$$

Substituting the resulting equations for pressures into (1), we obtain, after transformation, the dependence of the radii of curvature on dimensionless parameters and coordinates which can be written in general form:

$$\sigma(r_1^{-1} + r_2^{-1}) = f(\rho_c, \rho_k, \omega, R, d_k, N, \lambda_0, \eta) \quad (12)$$

Let us assume that the relationship between the main radii of curvature during drop deformation is similar to that which exists for an ellipsoid of revolution:

$$r_1^{-1} + r_2^{-1} = r_1^{-1}\left(1 + \frac{\lambda_0^2+\eta^2}{\lambda_0^2+1}\right). \quad (13)$$

Then substituting (13) to (12) and reducing to dimensionless form, we get [30]:

$$cr_1^{-1} = f(We, Bo, S, T, \lambda_o, \eta) \quad (14)$$

Consequently, the spatial problem of creating a surface was simplified to a plane problem (8) regarding the construction of the meridional section of a drop. For the radius of curvature of this plane curve, the following equation applies [28]:

$r_1^{-1} = \frac{|\vec{r}'\, x\vec{r}''|}{|\vec{r}'|^3}$, where $\bar{r}(\eta, \lambda)$ is radius vector. In elliptic coordinates (λ, η), and also taking ηas a curve parameter:

$$cr_1^{-1} = [(\lambda^2+\eta^2)(\lambda^2+1)(1-\eta^2)\lambda'' + \eta(1-\eta^2)^2(\lambda')^3 - \lambda(2\lambda^2+\eta^2+1)(1-\eta^2)(\lambda')^2 + \eta(1-\eta\eta^2-\lambda^2)\lambda' - \lambda(\lambda^2+1)^2/\left[(\lambda^2+\eta^2)^{3/2}[(1-\eta^2)(\lambda')^2 + (\lambda^2+1)]^{3/2}\right]. \quad (15)$$

Putting and transforming c/r_1 from (14) into (15), we obtain a second-order differential equation that describes the shape of the meridional curve of the drop. An analytical solution to this equation is not available, so we will resort to an algorithm for sequentially constructing this curve. It is important to note that the shape we create will vary depending on the values of the numbers We (Weber number), Bo (Bond number), S and T. To determine these parameters, we will set the condition under which the drop will be destroyed - this is the condition of the curve touching, representing the front part of the drop, with a curve representing the rear part of the drop.

First we set the values of We (Weber number), Bo (Bond number), S, T and λ_0 (initial coordinate λ). Then we construct a curve according to equation (15) using the Runge-Kutta method, starting from the point $\lambda = \lambda_1$, simultaneously moving in the direction 1-2-3 and 1-4-3 (see Figure 2). At the initial point it is also assumed that λ' = 0, which can be obtained from the physical picture of the deformation and means that in a small vicinity of the frontal point the pressure is symmetrical relative to it.

After the step-by-step construction of curves 1-2-3 and 1-4-3, it is necessary to carefully check the fulfillment of the following conditions, as described in studies [31, 32]:

It is necessary to make sure that the curve is closed at point 3.

And one should ensure drop volume is maintained.

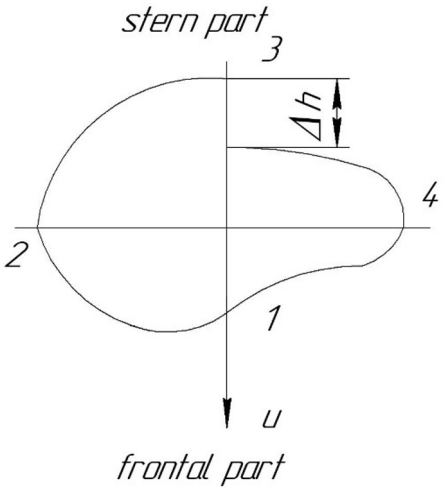

Fig. 3. Drop formation curves.

It is needed to check the coincidence of the shape coefficients λ_ω, which were initially specified, with the values obtained on the constructed curve.

After completing the construction of the drop shape, it is necessary to check the condition for its stability, which is that curves 2-1-4 and 2-3-4 touch each other. If such a touch does not occur, we adjust the value of the We parameter, since this value plays a key role in the gravitational field.

A special case was also considered when S = 0, which means there is no pressure from the Coriolis force and corresponds to the gravitational field. In this case, the Bond number has a certain form: $\mathrm{Bo} = \frac{(\rho_K - \rho_c) g d^2}{\sigma}$. The calculation results demonstrate that a change in the Bo criterion in the range from 0 to 20 leads to a change in the Weber number (We) during the crushing process in the range from 10.5 to 13.5. Comparing these data with studies of droplet fragmentation in a gravitational field in devices such as Venturi scrubbers [30-32], it can be noted that under those conditions the Weber number (We) varies over a wider range, namely from 9 to 24. However, it should be noted that that this analysis does not take into account the value of the number Bo, which can also have an impact on the crushing process and can be entered into the calculations: $Bo = \frac{(\rho_K - \rho_c) a d^2}{\sigma}$, where a is the acceleration of the liquid particle in the flow, it is necessary note a fairly good agreement between the obtained data.

The results of calculations for the process of droplet fragmentation in a centrifugal field, taking into account the non-zero value of the parameter S (which means the influence of the Coriolis force), were processed using the function $\mathrm{We} = ABo^{\alpha} S^{\beta} T^{\gamma}$ of the least squares method. This made it possible to obtain a dependence expressed as follows:

$$\mathrm{We} = \mathrm{Bo}^{0,21} \mathrm{S}^{-0,46} \mathrm{T}^{-0,4.} \quad (16)$$

Transforming (15) into a function for the maximum droplet diameter, we obtain

$$d_{kp} = 3{,}9 \frac{(\rho_K - \rho_c)^{0,14} R^{0,14} \sigma^{0,83}}{\rho_K^{0,27} \rho_{sr}^{0,71} U^{1,67}}. \quad (17)$$

To confirm the accuracy of the obtained expression (17), we conducted experiments to study the process of droplet fragmentation in a centrifugal field. When comparing the experimental data with the theoretical data (see Figure 3), it became obvious that the actual destruction of the droplets occurs slightly earlier than predicted by our theory [29].

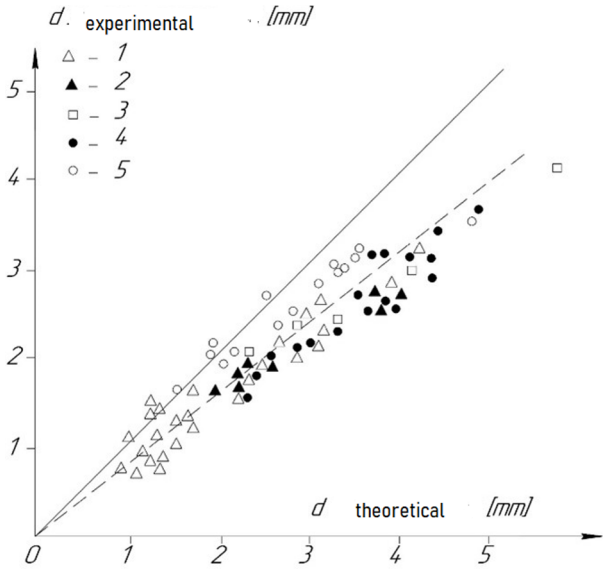

Fig. 4. Results of comparison of droplet diameter, theoretical with experimental: 1 - Water-diisopropyl alcohol; 2 - tricresyl phosphate – water; 3- water - kerosene; 3 - water-toluene; 4- CCL_4 – water.

The reason for this difference is that the original theoretical model did not take into account the vibrations of the droplet surface. In reality, during the initial deformation, the vibrations of the drops have an amplitude that is insignificant compared to the thickness of the drop. However, when a sufficiently thin layer is formed between the front and rear surfaces of the drop, the amplitude of vibrations becomes comparable to the thickness of this layer, which can lead to earlier destruction. If we take this fact into account and make an amendment to the theoretical dependence (dashed line in Figure 4), then the final equation will have the following form:

$$d_{kp} = 3{,}25\frac{(\rho_K-\rho_c)^{0,14}R^{0,14}\sigma^{0,83}}{\rho_K^{0,27}\rho_{sr}^{0,71}U^{1,67}}. \quad (18)$$

The dependence (18) is recommended for calculating the maximum stable diameter of droplets in a centrifugal field. This value should be considered when calculating mass transfer processes in areas where a dispersed phase is present [32-38].

3 Conclusion

Analyzing the data obtained, several important conclusions can be drawn.

Extraction is presented as an effective and reliable tool necessary when using natural resources and reducing negative impacts on the environment.

The extraction process addresses the problems of migration of pollutants and nutrients in the soil.

The process of rupture of a drop of heavy liquid as it moves in a centrifugal field depends on several key parameters: the Bond number (Bo), which reflects the interaction of surface tension and gravitational forces; density relationships between the drop and the environment; and the number S, which evaluates the influence of the Coriolis force on the rupture process.

The mechanism of drop destruction is the deflection of the frontal and rear parts of the drops until they touch their surfaces.

Fluctuations of the droplet surface contribute to the limiting droplet size not exceeding 17%.

Nomenclature

$Bo = \frac{(\rho_K - \rho_c)\omega^2 R d^2}{\sigma}$ - Bond number;
c – scale factor of elliptic coordinates, m;
d_o – hole diameter, m;
$d_к$ – average drop diameter, m;
h – height of the nozzle passage opening, m;
P – pressure, H/m^2;
R, r – considered rotor radius, m;
$S = \frac{\rho_c \omega U d^2}{\sigma}$ - a number characterizing the ratio of Coriolis forces to surface tension forces;
$T = \frac{\rho_K}{\rho_c}$ - density ratio of droplet and medium liquids;
$We = \frac{\Delta\rho\omega^2 R^3}{\sigma}$ – Weber number;
U – drop speed, m/s;
Θ – the angle between the direction of the Coriolis force and the axis λ;
V – speed of the continuous phase, m/s;
λ, η, φ – elliptical coordinates;
ρ_c, ρ_D – density of continuous and dispersed phases, kg/m^3;
ρ_K – drop density, kg/m^3;
ρ_{sr} – mixture density, kg/m^3;
ω_o – angular velocity of the rotor, s^{-1};
ω_L – angular velocity of liquid, s^{-1};
σ - surface tension, N/m.
Δ - difference.

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