Determination of droplet size and flow breakup mechanisms in centrifugal contact devices

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Abstract. This article investigates the mechanisms of droplet breakup and the determination of droplet size in centrifugal contact devices, focusing on phase separation and mass transfer processes. The study highlights the critical role of turbulent pulsations and the rotational speed of the rotor in influencing droplet deformation and breakup. Based on the Kolmogorov-Obukhov theory of turbulence, the paper presents theoretical and experimental approaches to predict droplet behavior and optimize the geometry of contact devices. Key findings demonstrate that increased rotor speed and nozzle design significantly impact droplet size reduction, improving interaction efficiency between phases. The results are applicable to the optimization of centrifugal apparatuses used in chemical processes and phase separations.

1 Introduction

Understanding the processes and studying the mechanisms of droplet crushing in turbulent flows of centrifugal apparatuses is key to intensifying mass transfer processes and increasing the efficiency of process equipment, especially in phase separation and chemical reactions. The main factors influencing the droplet crushing process are rotor rotation speed, nozzle sizes and physical and chemical properties of liquids. Under centrifugal field conditions, liquid droplets are exposed to the action of turbulent pulsations, which can lead to their deformation, destruction into small fractions and, as a consequence, to acceleration and improvement of interaction between different phases contacting in the apparatus [1]. In turn, increasing the contact surface between the phases through droplet crushing in the apparatuses operating in the centrifugal field significantly improves the efficiency of the processes carried out in the equipment.

Modern requirements for production processes determine the need for a high degree of dispersion of phases to achieve optimal characteristics of the final product. For instance, in pharmaceutical production, the homogeneity of emulsions directly depends on the size and distribution of droplets, which affects the stability and bioavailability of dosage forms. Similarly, in petroleum refining, effective phase separation makes it possible to improve product quality while reducing the cost of feedstock purification and processing.

Thus, studying the mechanisms of droplet crushing in centrifugal apparatuses, the influence of different nozzle designs on the crushing efficiency and analyzing modern

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research in this area is of certain scientific interest. Modern research aimed at improving the droplet crushing efficiency are both experimental and numerical methods. For instance, numerical simulation of crushing processes using computational fluid dynamics makes it possible to predict droplet behavior under different conditions and optimize the geometry of contact devices [2], while experimental research on physical models of apparatuses makes it possible to visualize crushing processes and validate mathematical models. The integration of machine learning and artificial intelligence methods into the process of experimental data analysis and modeling opens new possibilities for describing and predicting the nature of complex interactions in multicomponent systems, which can significantly improve the accuracy and reliability of droplet crushing models. The goal of this research is to advance our understanding of droplet crushing processes for modeling, performance improvement, and optimization of centrifugal machines.

2 Materials and methods

The theoretical basis for droplet fragmentation in turbulent flows was laid in the research of Kolmogorov and Obukhov [3]. In the mentioned theory, it is assumed that a liquid ring of dispersed phase exiting the disperser slot is split into numerous jets that act as drop formation centers. Under the influence of hydrodynamic pressure and counterflow of the continuous phase, as well as as as a result of collisions of the flow with the elements of nozzles or separation discs, the jets are subject to destruction due to discontinuous changes in velocity caused by turbulization of the flow, and other external factors, which leads to the formation of a stream of droplets. The inhomogeneity of the flow during the droplet motion causes additional stresses on its surface, resulting in its deformation, destruction and fragmentation.

Based on the above theory of isotropic turbulence, it is possible to describe the process of droplet fragmentation in turbulent flows that do not mix with the main liquid, for instance, in two-phase flows in contact devices of centrifugal apparatuses, where the speed of turbulent pulsations plays an important role. It is stated in [3] that the main parameter determining the droplet breaking in turbulent flow is the Weber number (We), which describes the ratio of inertial forces and surface tension. The conditions of droplet destruction are determined by the physical and chemical properties of the liquid and depend on the non-uniformity of dynamic heads on the surface of dispersed particles [4]. The latter corresponds to conditions when turbulent pulsations have a small scale, and the difference in phase velocities leads to a violation of surface tension. In the reverse situation, when the flow is featured by large-scale turbulent currents and the values of phase densities are close, the droplet will be stable and will be carried by the flow rather than destroyed by it. Hence, we can conclude that the drop destruction occurs mainly under the influence of such turbulent pulsations, the velocity of which is proportional to the size of the drop itself dk, and in this case the following expression can be considered valid:

$$\mathrm{V_k} \sim (\bar{\varepsilon} \cdot \mathrm{d_k}/\rho_c)^{1/3}, \tag{1}$$

here $\bar{\varepsilon}$ is the value of turbulent energy dissipation per unit mass of fluid flowing out of the bore, ρ — medium density.

For droplets in the transition regime between laminar and turbulent flow, as well as in the state of the droplet before its breakup, the average value of the droplet diameter can be determined from the assumption that the viscosity and inertia forces (Re) and the surface tension and inertia forces (We) are in balance. In this case, calculations are simplified because the values of Re and We are taken close to unity, which makes it possible to analyze the main mechanisms of droplet fracture and the effect of flow on its shape and behavior. Thus, the average values of droplet diameter can be determined from the following condition:

$$1/\Re \cdot \bar{d_k} + \mathrm{We} \cdot \bar{d_k} \approx 1, \tag{2}$$

which reflects that when a fluid particle breaks, the kinetic energy it has is balanced by the work done by the forces of viscosity and surface tension:

$$V_d^2 \cdot \rho \approx \mu \cdot V_d \cdot d_k^2 + \sigma \cdot d_k^2, \tag{3}$$

here σ — surface tension, μ — viscosity. Then, provided that there are no viscous forces, the droplet size can be expressed as follows:

$$d_k = \frac{\sigma^{3/5}}{\bar{\varepsilon}^{2/5} \cdot \rho_c^{1/5}}. \tag{4}$$

To take into account the influence of viscous forces, expression (4) for determining the average drop diameter should be written in the following form:

$$d_k = \frac{\sigma^{3/5}}{\bar{\varepsilon}^{2/5} \cdot \rho_c^{1/5}} + \frac{\mu}{\bar{\varepsilon}^{1/5} \cdot \rho_c^{2/5}}, \tag{5}$$

However, this theoretical dependence gives a possibility to get an idea only about the order of droplet size, stable under conditions of turbulent flow in the centrifugal field. In reality, the characteristic droplet sizes are influenced by numerous factors that are not taken into account by this theory. These include forces arising in the centrifugal field at slip of liquid relative to the rotor, counter flows of phases, collisions of drops with contact elements and walls of the rotor, resulting in unpredictable changes in the trajectory of movement of both dispersed and continuous phases. To take into account the above factors in the mathematical description of the process it is possible to express a generalized dependence in the form of:

$$\frac{d_k}{h_R} = K\left(\frac{\sigma}{\Delta\rho \cdot V_d^2 \cdot h}\right)^a \left(\frac{\mu_c}{\Delta\rho \cdot V_d \cdot h}\right)^b \left(\frac{Q_d + Q_c}{Q_d}\right)^c, \tag{6}$$

here Q — phase flow rates, h — nozzle bore height, h_R — mixing chamber width, K — proportionality factor; a, b, c — indices of degrees of the equation terms characterizing the contribution of specific components, indices d, c — denote the values related to the dispersed and solid phases, respectively.

As a result of the literature review, it was found that modern research not only confirms, but also complements the existing theory, as well as offers ways to improve the design of apparatuses and contact devices installed in them for effective droplet crushing. For instance, [5] investigates the differences in droplet crushing when using vortex flow and dual flow nozzles, making it possible to optimize the separation process and improve the characteristics of the final product.

Other authors [6, 7], emphasize the importance of numerical simulations in studying droplet crushing parameters such as mechanical stresses and droplet residence time in nozzles. Specific research in this area pays attention not only to the droplet crushing processes themselves, but also to the droplet size distribution, which is especially important in the design of efficient mass transfer devices. For instance, in the work on estimating the disperse composition of droplets, it was found that changing the nozzle design and rotor speed significantly affects the droplet sizes and their phase distribution [8].

The use of computational fluid dynamics (CFD) methods makes it possible to predict droplet sizes and investigate crushing mechanisms, as well as to use the results of numerical experiments for risk analysis and assessment of accident consequences [9-12]. Detailed models of interaction between droplets and turbulent flows were described in [13, 14], where statistical data on droplet breakup in turbulent flows were analyzed and the dynamics of droplet deformation under such conditions were studied. In specific works it is shown that modern research based on computational fluid dynamics methods achieves high accuracy in modeling the processes of coalescence and droplet crushing sufficient to justify design decisions in the design and optimization of apparatuses with dispersants and nozzles operating under centrifugal field conditions. The applicability of CFD for modeling phase interaction in turbulent flows is confirmed in [15], where parameters of droplet dispersibility and their stability at high rotational velocities are analyzed.

Recent experiments [16, 17] evaluated the effect of nozzle geometry and scaling on oil droplet fragmentation during emulsion atomization, and pay attention to the effect of droplet and carrier fluid viscosity. It was observed in [18] that at high viscosity ratio, the droplet can deform strongly before breaking, which is also confirmed in one of the papers [19], which proposes a dual droplet breaking mechanism model covering the whole turbulence spectrum. Current research actively employs adaptive meshes and high-resolution numerical modeling schemes to make it possible to capture the details of droplet formation and crushing dynamics with a high degree of accuracy.

The results of such research provide new possibilities for optimization of separation processes in various industries; however, for more accurate modeling of droplet crushing processes it is important to take into account nonlinear interactions between phases and the influence of dynamic changes in flow geometry; therefore, it seems promising to experimentally determine the influence of various factors on the characteristic droplet size.

3 Results and discussion

Nozzle design is a key factor in determining droplet crushing efficiency. Research shows that nozzles with additional flow turbulization tend to provide better droplet crushing than other types due to more efficient energy distribution and uniformity of droplet formation. Experimental research was conducted using centrifugal apparatuses equipped with X-shaped nozzles [20].

The main objective of the experiment was to determine the dependence of droplet size on the rotor speed at a given size of the outlet bore (d0=2 mm). To estimate the droplet size in the apparatus with a transparent body and rotor, stroboscopic illumination was used. The following systems of substances were chosen for research: kerosene - water, isoamyl alcohol - water and hydrogen tetrachloride - water. The choice is conditioned by different ratios of values of surface tension, density and viscosity of the substances. Kerosene and isoamyl alcohol have lower density but much higher viscosity compared to water, while carbon tetrachloride, on the contrary, has higher density than water but similar viscosity.

Fig. 1 shows the results of experimental research on the dependence of droplet size on the angular speed of the rotor and on the composition of phases, which shows that with increasing rotor speed the droplet diameter decreases significantly, and the nature of this dependence is determined by the properties of the separated substances.

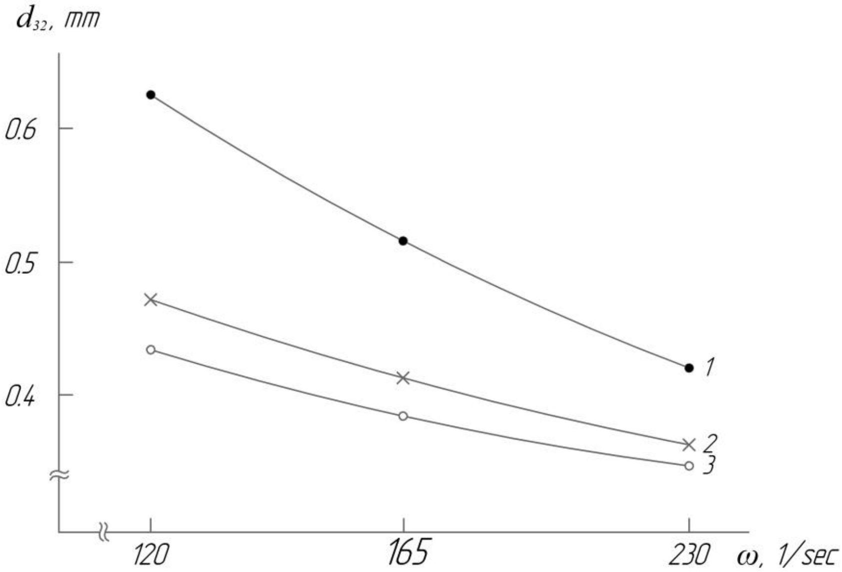

Fig. 1. Weighted average specific surface of droplet diameter as a function of rotor speed for different systems: 1 - kerosene and water, 2 - isoamyl alcohol and water, 3 - water and carbon tetrachloride.

It can be concluded from the obtained results that regardless of rotor speeds the largest droplets are observed in the kerosene-water system. The latter can be explained by a relatively small difference in the density of substances, as a result of which the inertia forces acting on the droplets are less significant compared to other systems. In addition, kerosene has a lower viscosity compared to isoamyl alcohol, so turbulent pulsations and collision with oncoming flow or contact devices contribute less to droplet breakup than in the other cases considered, since the droplets have fewer internal forces that could contribute to their breakup under the influence of external factors.

The graph (Figure 1) shows that increasing the rotor speed leads to a decrease in droplet size for all cases, but the kerosene-water system shows the greatest change in droplet size compared to the other systems. In more viscous media (for instance, isoamyl alcohol and water), due to higher internal tension, the droplets break up more intensively even at low turbulent pulsations and low rotor speeds. This also contributes to the fact that the largest droplets are observed when researching the first system of substances. In the case of the second system, the droplet diameter is significantly smaller, despite the fact that kerosene and water have similar density ratios to the isoamyl alcohol-water system. The viscosity of isoamyl alcohol is much higher than that of kerosene, which means that the second system is more susceptible to shear stresses and the deformation of droplets under the action of external forces is more intense, which contributes to their effective crushing even at low speeds. In this case also plays a role of surface tension, which in isoamyl alcohol with water can be lower than in kerosene, which contributes to easier droplet breaking in conditions of low values of rotor angular speed.

The smallest droplets are observed in the third system (water - carbon tetrachloride), which is explained by the combination of high density and low viscosity of carbon tetrachloride, as well as the nature of the interaction of this substance with water. Significant difference in densities causes large gradients of forces acting on the phases during rotation of the rotor of the apparatus, which leads to a more intense crushing of droplets. The low viscosity of carbon tetrachloride (close to the viscosity of water) makes the droplets less resistant to external influences, resulting in easy deformation and fragmentation under turbulent conditions, unlike high-viscosity liquids such as isoamyl alcohol, which can maintain their integrity under the same conditions. The surface tension at the interface between carbon tetrachloride and water is lower than in other systems, which means the droplets are more prone to loss of shape. The strong differences in density and low viscosity lead to more intense turbulent pulsations, which exerts a greater shear force on the droplets and favors their fragmentation. Thus, the high density of carbon tetrachloride, combined with low viscosity values and low surface tension, results in the finest droplets in the water-carbon tetrachloride system compared to other systems.

It is important to note that the rotor speed has a direct effect on the droplet crushing intensity. The higher the angular velocity of the rotor, the greater the inertial forces that contribute to the stretching and breaking of the droplets. In particular, at high values of viscosity of the dispersed phase there is a significant deformation of droplets before their destruction. This feature should be taken into account when designing the contact zone of centrifugal apparatuses working with highly viscous liquids, for instance, in the petrochemical industry.

To estimate the size of dispersed particles, we used the inverse of the specific surface of phase contact, namely, the specific surface weighted average diameter as an averaged characteristic of a polydisperse system:

$$d_{32} = \frac{\sum n_i \cdot d_i^3}{\sum n_i \cdot d_i^2} \tag{7}$$

As a result of experimental data processing, the refined dependence (6) for determining the droplet diameter was obtained:

$$d_{32} = 0{,}79 \cdot d_0^{0.78} \cdot R^{0.22} \left(\frac{\sigma}{\Delta\rho \cdot \omega^2 \cdot R \cdot d_0^2}\right)^{0.26} \left(\frac{\mu_d}{\mu_c}\right)^{-0.44} \tag{8}$$

Results analysis shows that capillary forces (interfacial surface tension) and the level of centrifugal field influence significantly on the droplet diameter, and the stability of the formed droplets depends on the combination of rotational speed and geometric parameters of the nozzle. It was found that the use of nozzles with increased contact area makes it possible to significantly reduce the droplet size, especially at high rotor speeds. In particular, modeling has shown that reducing the nozzle diameter leads to an increase in the outlet pressure, which also affects the character of droplet crushing.

However, this increases the probability of cavitation in the flow, which can negatively affect the efficiency of the apparatus. Under certain conditions, a transition from laminar to turbulent flow regime is observed, which leads to a sharp decrease in droplet size and an increase in dispersion. This confirms that optimization of nozzle design and selection of correct rotation parameters can significantly improve the processes of droplet crushing in centrifugal devices. It is also necessary to take into account the ratio of viscosity and density values of solid and dispersed phases, but the influence of phase flow rates does not have a significant impact. Consequently, there is a need for careful design of not only the geometry of the rotor and the working space of centrifugal devices, but also the flow area of contact devices (dispersants) to achieve optimal conditions of droplet crushing, which is especially important when scaling processes at industrial plants.

A comparative analysis with previous research [5-17] confirms that the proposed models and experimental data are consistent with existing theories and extend them, to some extent taking into account additional factors affecting the droplet crushing process. In particular, numerical models based on CFD methods have shown a high degree of consistency with experimental results, which makes it possible to use them for further optimization of centrifugal apparatus designs, but only under the condition of extensive physical experiments that allow us to verify the adequacy of the models used for research under specific conditions.

4 Conclusion

Jets of liquid flowing from dispersants in the centrifugal field, under the influence of hydrodynamic pressure and counterflow of the continuous phase, as well as as as a result of collisions of the flow with contact devices, are subject to destruction. This process is caused by discontinuous changes in velocity caused by turbulization of the flow and other external factors, which subsequently leads to the formation of a stream of droplets. Analysis of experimental data showed that droplet crushing is a function of turbulent pulsations, which are formed as a result of rotor rotation. It was found that the droplet size decreases as the rotor speed increases, and the nature of this change is determined by the physical and chemical properties of the separated substances.

The research results are consistent with the theoretical assumptions that the increase in turbulence in the flow increases the probability of droplet crushing. At high rotational velocities, the inertia forces have an additional effect on the droplets, which contributes to their more intensive destruction. In addition, the data showed that Coriolis and centrifugal acceleration forces also have a significant effect on the droplet crushing process, which means that increasing rotor speed and modeling the configuration of the nozzle devices can significantly improve phase interaction and increase the performance of the apparatuses, since droplet sizes in centrifugal apparatuses determine the efficiency of mass transfer processes.

The data obtained emphasize the importance of considering the physical and chemical properties of liquids in the design of centrifugal apparatuses. Particular attention should be paid to turbulence parameters and nozzle configuration, as they play a crucial role in determining the efficiency of droplet crushing processes. In particular, modern numerical simulation methods such as computational fluid dynamics (CFD) make it possible not only to predict droplet size under different conditions, but also to optimize the design of apparatuses to achieve higher performance. This opens new perspectives for contact device design and process efficiency improvement.

Thus, the mathematical description of droplet crushing processes in a centrifugal field is of scientific interest both for the optimization of existing apparatuses and for the design of new contact devices. However, for more effective control of dispersing processes and phase interaction in solving the objectives of centrifugal apparatus optimization, further development of the above research is necessary.

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