

CFD analysis of water-in-oil droplet formation within a co-flow channel

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ABSTRACT

Two-phase systems are important tools for droplet formation that have received much attention in recent decades due to their vast applications. In the present work, the process of water-in-oil droplet formation, in a coaxial geometry using the fluid volume method, and impact of effective parameters such as dispersed phase velocity and density and also interfacial tension are investigated. The results are used to produce spherical γ -alumina particles by the oil drop method. In this study, using a laboratory setup, the factors affecting the droplet formation process are investigated. Results are validated against laboratory data. The measurement error is about 5% for droplet size and about 4% for sphericity. Studies show that although the mentioned parameters have a great effect on droplet size and separation time, the dependency of droplets diameter on interfacial tension and dispersed phase density is higher. Increasing the interfacial tension causes increasing droplets size and separation time. Also increasing the density of the dispersed phase reduces the diameter of the droplets and increases separation time. Increasing the velocity also had a small effect, but lead to an increase in size and reduces droplets separation time.

KEYWORDS

Droplet formation, Two-phase flow, Co-flow channel, VOF method, Computational fluid dynamics

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1. Introduction

Multiphase flow is the simultaneous flow of several thermodynamic phases next to each other, where these phases interact with each other. In the process of droplet formation in the liquid phase, two-phase flow is the simplest and the most important one. These processes play an important role in the fields of chemical, Lab-on-Chip, drug delivery, encapsulation, and nanomaterials synthesis [1].

In the process of droplet formation, the continuous forming of small droplets with the same distance from each other is very important. Experimental works face limitations such as the very small geometry, the difficulty of manufacturing the equipment, the high cost, and time-consuming experimentations that the CFD can overcome.

A survey of the recent studies indicates that the process of formation and control of droplets is very complex due to the presence of various parameters such as interfacial tension, viscosity, surfactant, density, geometry, and so on. The effect of these parameters on different geometries has been investigated by experiments and simulations [2-5].

In the present study, the simulation of droplet formation due to the mixing of two immiscible fluids is studied. The Eulerian-Eulerian method for both phases in a coaxial geometry is used. To capture the interface volume of fluid (VOF) method has been used. The results of this study can be used to produce γ -alumina spherical particles by oil drop method. Droplet simulation using computational fluid dynamics can be effective in designing a suitable system for the production of uniform spherical particles as well as controlling their sphericity. The effect of the dispersed phase velocity, density, and surface tension are investigated.

2-Numerical method

2-1- VOF model theory

The method of the volume of fluid was employed to solve the governing equations. This method uses a finite volume constant lattice to calculate the position of the interface between two immiscible fluids. In this method, a volume fraction function is used to distinguish between two phases. A value of zero indicates the presence of the first fluid and a value of one indicates the presence of a second fluid. On the computational range, the volume fraction values between these two values indicate the existence of an interface.

2-2- Governing equations

Two fluids are considered incompressible, Newtonian, The process is performed without any external force.

Governing equations include two main equations: continuity equation and Navier-Stokes,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \bar{U}) = 0 \quad (1)$$

$$\rho \left(\frac{\partial \bar{U}}{\partial t} + \bar{U} \cdot \Delta \bar{U} \right) = -\nabla P + \mu \Delta^2 \bar{U} + \rho g + F_\sigma \quad (2)$$

2-3- Fluid properties and boundary conditions

Deionized water is considered as a dispersed phase and oil is considered as a continuous phase. In this research, a pressure-based solver has been used. The inlets of water and oil phases were set as velocity inlet, the outlet boundary condition was set as atmospheric pressure and no-slip condition was used for walls.

3- Simulation results

3-1- The effect of dispersed phase velocity

The result indicates that droplet size increases with increasing dispersed phase velocity. Fig 1 shows the simulation results after 16 sec. According to Weber's number in equation 3,

$$We = \frac{\rho U^2 D_d}{\sigma} \quad (3)$$

by increasing the dispersed phase velocity, the inertial force dominates, and the balance between interfacial tension and inertial forces is determined by the transition from the dripping regime to the jetting regime. When the velocity reaches 0.013 m/s, the droplet formation regime changes to the jetting regime. Feng et al.[6] and Carsten et al.[7] found similar results in their studies.

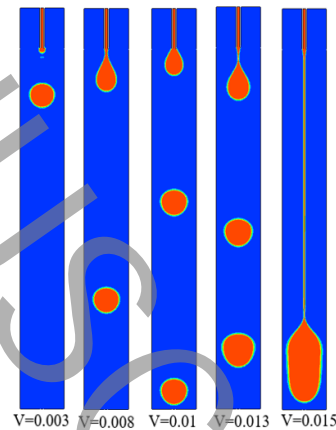


Fig 1- Effect of dispersed phase velocity on droplet size at $t = 16$ s

3-2- Effect of interfacial tension

By increasing the surface tension force, the value of Weber number and Bond numbers decreases according to equations 3 and 4,

$$Bo = \frac{\rho g D_d^2}{\sigma} \quad (4)$$

as a result, the surface tension force overcomes the force of inertia and gravity, and becomes the dominant force in the process of droplet formation. If the surface tension force increases, the force between the molecules increases and causes the separation of the droplet to be delayed, increasing the size of the formed droplet.

Reducing the interfacial tension causes the droplet to break and separation requires less force. Therefore, the separation time of the droplet and droplet size is reduced. Fig 2 shows the simulation results. These results are in line with those reported by Jinsong et al [8].

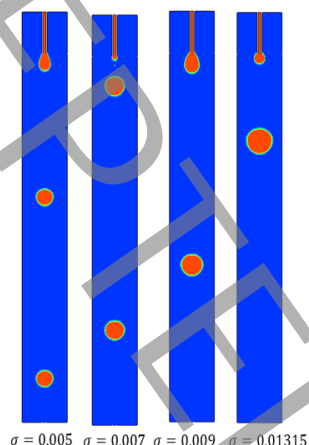


Fig 2- Effect of interfacial tension on droplet size

3-3- Effect of dispersed phase density

The simulation result shows that the droplet size decreases with increasing dispersed phase density. Fig 3 depicts the simulation results. When density increases, the effect of the gravitational force is greater than the buoyancy force and the droplet separates faster from the capillary tube and is unable to grow. These findings were confirmed by Zhe et al [9].

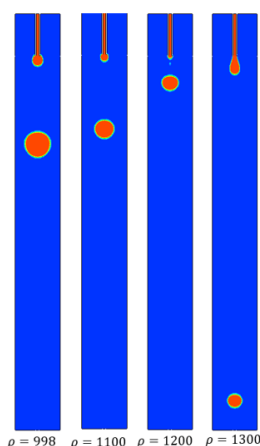


Fig 3- Effect of dispersed phase density on droplet size at $t = 11$ s

4- Conclusions

In the present research work, the process of droplet formation in a coaxial geometry was investigated using

the volume of fluid method. Deionized water was used as the dispersed phase and oil was considered as the continuous phase. The results revealed that increasing the dispersed phase velocity increases the droplet size. Further increase in velocity, changes the flow regime from dripping to jetting. Increasing the interfacial tension increases the droplet size. The droplet size also decreases with increasing dispersed phase density. The results of this study can be used in designing a suitable system for the production of uniform γ -alumina spherical particles.

5- References

- [1] S. G. Sontti and A. Atta, Numerical Insights on Controlled Droplet Formation in a Microfluidic Flow-Focusing Device, *Industrial & Engineering Chemistry Research*. 59(9)(2020) 3702–3716.
- [2] M. Rahimi, S. Yazdanparast, and P. Rezai, Parametric study of droplet size in an axisymmetric flow-focusing capillary device, *Chinese Journal of Chemical Engineering*, 28(4)(2020) 1016–1022.
- [3] C. Deng, H. Wang, W. Huang, and S. Cheng, Numerical and experimental study of oil-in-water (O/W) droplet formation in a co-flowing capillary device, *Colloids and Surfaces A: Physicochemical and Engineering Aspects.*, 533(2017) 1–8.
- [4] T. Chekifi, Computational study of droplet breakup in a trapped channel configuration using volume of fluid method, *Flow Measurement and Instrumentation*, 59(2017) 118–125.
- [5] W. Lan, S. Jing, X. Guo, and S. Li, Study on 'interface – shrinkage – driven' breakup of droplets in co-flowing microfluidic devices, *Chemical Engineering Science.*, 158 (2017) 58–63.
- [6] F. Bai, X. He, X. Yang, R. Zhou, Three dimensional phase-field investigation of droplet formation in microfluidic flow focusing devices with experimental validation, *International Journal of Multiphase Flow*, 93 (2017) 130–141.
- [7] C. Cramer, P. Fischer, and E. J. Windhab, Drop formation in a co-owing ambient fluid, *Chemical Engineering Science*, 59 (2004) 3045–3058.
- [8] J. Hua, B. Zhang, and J. Lou, Numerical simulation of microdroplet formation in coflowing immiscible liquids, *AIChE Journal*, 53(10)(2007) 2534–2548.
- [9] Z. Q. Huang and H. Wang, VOF Simulation Studies on Single Droplet Fluid Dynamic Behavior in Liquid–Liquid Flow Process, *Journal of Chemical Engineering of Japan*, 51(1)(2018) 33–48.