Modelling the dispersed phase holdup in a pulsed disc and doughnut liquid-liquid extraction columns (PDDC) using the Volume of Fluid (VOF) method

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Highlights

- A PDDC is simulated for application in nuclear fuel cycle.
- The VOF method is fast and suitable for holdup predictions at higher phase velocities.
- At higher phase velocities, k-epsilon turbulence model gives superior agreement.
- At lower phase velocities, k-omega-SST model is better for VOF method.
- VOF is computationally less expensive and more simple than Eulerian multiphase turbulence models

1. Introduction

In the contemporary landscape of chemical reactors, pulsed disc and doughnut liquid-liquid extraction columns (PDDCs) have emerged as a promising alternative to conventional stirred tank reactors for applications in the nuclear fuel cycle, owing to their higher safety and mass transfer.[1] Till now, turbulent flow simulations for PDDCs have been performed mostly with Eulerian models,[2] where both phases are modeled as an interpenetrating continuum. In these models, two continuity and momentum equations are solved concomitantly including the interphase momentum exchange for each phase that makes the calculations expensive and time consuming. As an alternative, the Volume of Fluid (VOF) method treats both liquid phases as an effective fluid, and only one continuity and one momentum equation, along with the turbulence models, are solved, which makes this method less computationally expensive and conceptually more simple than Eulerian models. While the VOF model has previously been utilized in bubble columns to forecast bubble plume characteristics,[3] its application to pulsed columns remains largely unexplored.

Herein we employed the turbulent VOF method to simulate the dispersed phase holdup (or volume fraction of the dispersed phase) in PDDC liquid-liquid extraction columns. The dispersed phase holdup is one of the most important parameters in extraction columns that govern the mass transfer coefficient. The quality of the simulations was contrasted to dispersed phase holdup measurements conducted in a homemade PDDC liquid-liquid extraction column to transfer aqueous nitric acid to a tributyl phosphate (TBP) phase as a model of more complex plutonium and uranium extraction from waste nuclear fuel.

2. Experimental methodologies

A series of nitric acid extraction experiments were carried out in a PDDC liquid-liquid extraction column (i.d. = 7.5 cm i.d., active section height = 2 m,) consisting of 70 pairs of discs (6.35 cm diameter) and doughnuts (3.5 cm diameter) (**Figure 1a**). The continuous phase was a 3 M aqueous solution of nitric acid and the dispersed phase solvent was 30% tri-butyl phosphate. As the organic phase was dispersed, stainless steel was used to fabricate the disc and doughnut internals. Sinusoidal pulses with pulsation intensities in the range 9.36-18.72 mm/s were applied in the column (**Figure 1b**). The total superficial velocities of the different phases (V_c-cont. phase; V_d-disp. phase) were varied from 1.25-3.75 mm/s. The dispersed phase holdups were measured after reaching steady state using the volume displacement method.

3. Computational details (VOF method)

In the VOF method, both fluid phases are considered as one effective fluid and only one continuity and one momentum equation are solved. In the momentum equation, the surface tension force is taken explicitly into account to capture the liquid-liquid interface. For this purpose, a continuous surface tension model was solved for resolving the interfacial surface curvature. The density and viscosity of the effective fluid were calculated by adding the continuous and dispersed phase densities and viscosities weighted by their respective phase fractions. To reconstruct the interface, the advection equation of the phase fraction was solved, and the relative velocity between the phases was implemented to retain the two fluid natures of the system. This relative velocity was calculated by introducing an artificial compression factor that acted only at the proximity of the liquid-liquid interface. The advection equation was solved using the flux corrected technique allowing a precise interfacial modeling.

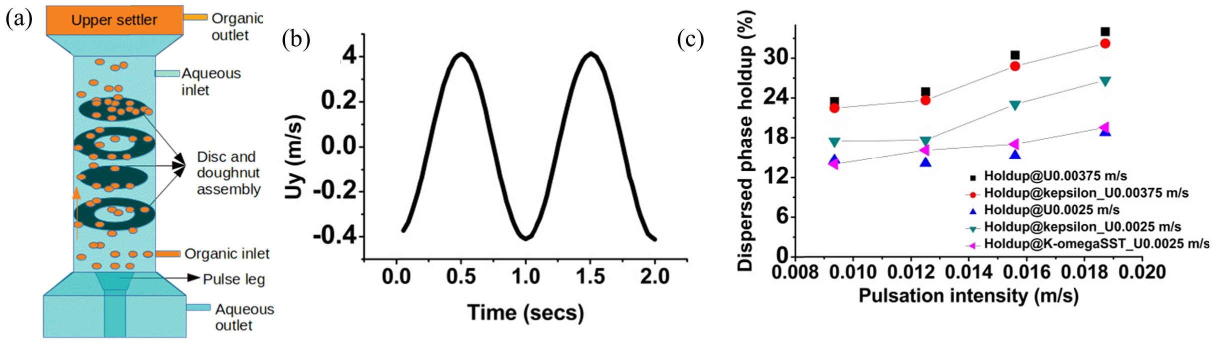

Figure 1. (a) Scheme of a PDDC, (b) velocity pulses, and (c) evolution of the dispersed phase holdup against the total superficial phase velocities (dots) and comparison with simulations using the VOF method (lines).

4. Results and discussion

The results in the PDDC liquid-liquid extraction column show that, regardless of both phase velocities, the dispersed phase holdup increases at higher pulsation intensities (**Figure 1c**). This trend can be attributed to the fact that, by increasing the pulsation intensity, drop breakage dominates coalescence and as a result the settling velocity of the drops decreases resulting in a higher holdup. The simulations of dispersed phase holdup using the Volume-of-Fluid (VOF) method coupled with k-epsilon and k-omega-SST turbulence models for a PDDC shows validity of the k-epsilon model at higher velocities (3.75 mm/s) but is inadequate at lower velocities, specifically at 2.5 mm/s. These results can be explained by the over-prediction of the turbulent energy dissipation rate at lower phase velocities.[4] In this view, the k-Omega-SST model with low Reynolds number wall treatment was chosen, yielding predictions of the dispersed phase holdup with reasonable agreement with the experimental values even at lower velocities, such as 2.5 mm/s. At higher phase velocities (3.75 mm/s), the k-epsilon turbulence model predicts the turbulent properties, such as the turbulent kinetic energy and dissipation rate with reasonable accuracy. Therefore, low Reynold's number wall treatment was not necessary and good agreement between the experimental and simulated dispersed phase holdups could be achieved with standard wall treatment.

5. Conclusions

Predictive analysis of dispersed phase holdup utilizing multiphase Volume-of-Fluid (VOF) simulation coupled with k-epsilon and k-omega-SST turbulence models was efficient to model the dispersed phase holdup in PDDC liquid-liquid extraction columns. Notably, the VOF method demonstrates efficacy particularly at higher phase velocities, whereas the conventional k-epsilon model exhibits limitations at lower velocities. In such case, utilization of the k-omega-SST model yields superior predictions compared to the k-epsilon turbulence model. All and all, the VOF method can be used to simulate pulsed extraction columns as an alternative to the computationally expensive Eulerian multiphase turbulent models. The VOF method represents a robust and viable approach for scaling up a PDDC liquid-liquid extraction columns at increased throughputs for plutonium and uranium extraction from waste nuclear fuel.

References

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