

Experimental and numerical study of bubble formation in supersaturated liquids

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Highlights

- A meso-scale model for phase transition is proposed
- The model will be expanded with experimental results
- The rate of bubble formation increases with the supersaturation

1. Introduction

The fundamental understanding of bubble forming in natural and industrial settings still represents a challenge as a consequence of the complex interactions between the different transport phenomena present in bubbly flows. From the industrial perspective, phase transition appears in several applications such as fermenters or in electrolytic processes, for instance the electrolysis of brine or in solar-to-fuel applications for hydrogen production [1], where the presence of bubbles can greatly influence the performance of the aforementioned applications. For this reason, improved fundamental insight is required to bring important advances to the state-of-the-art design and optimization of such processes.

The use of Computational Fluid Dynamics (CFD) to study complex multiphase systems has gained popularity in the past years due to the many possibilities offered by the increasing computational power. With a multiscale approach, different levels of detail (length scales) can be found in literature to study bubbly flows. At the meso-scale, Euler-Lagrange (E-L) models offer the advantage of including large scale bubble dynamics while still being less computationally expensive than Direct Numerical Simulations (DNS) [2]. However, despite the great potential provided by CFD, experimental studies for validation are still essential to further develop and extend the models and assess their validity.

The main objective of this project is to investigate the hydrodynamics and mass transfer in large scale bubble columns with heterogeneous bubble formation due to supersaturation, using a mesoscale model combined with experimental validation. In particular, the aim will be at studying rates of bubbles formation, the resulting bubble size distributions and boundary layer effects at different supersaturation ratios.

2. Methods

The Discrete Bubble Model (DBM) is an Euler-Lagrange type model where the liquid phase is described as a continuum and the gas bubbles as discrete Lagrangian elements. Their motion is tracked with Newton's laws of motion where bubble interactions (such as collisions, coalescences and breakups) are accounted for in a deterministic fashion [3]. In addition, mass transfer between the two phases with a species transport equation is included. This is essential to describe the desaturation of a liquid solution, as well as heterogeneous bubble formation on a selected substrate, which is implemented in the model via the nucleation of bubbles on specific sites on the surface with predefined surface density, cavity sizes and other properties (to be determined from experiments). On those sites, nucleated bubbles can grow due to mass transfer and ultimately detach and rise offering space to a newly forming bubble.

Empirical information on nucleation rates for a given substrate is scarce. As a consequence, a dedicated setup was built consisting of two vessels: an upstream vessel to dissolve a gas in a liquid (e.g. carbon dioxide in water) under pressure (8 bar), which is connected to a second vessel where a saturated solution can be transferred to. In this measurement tank, the pressure is released under fine-grained control, altering the equilibrium of the solution thus obtaining a supersaturated liquid. Bubbles forming on a surface are recorded with a high speed camera and analyzed with a Digital Image Analysis (DIA) algorithm [3] to obtain relevant

information such as bubble nucleation density, bubble size distributions and growth rates as a function of operating conditions and substrate materials and characteristics.

3. Results and discussion

With the experimental setup, the formation of bubbles on different materials (e.g. plastic, metals etc.) and different liquids or gases will be investigated. Of special importance will be the characterization of the surface in terms of nucleation sites densities and sizes and the associated nucleation rates and related bubble sizes distributions. The detailed nucleation data is subsequently used as empirical data for the nucleation model in the DBM.

With the model a surface consisting of randomly positioned nucleation sites with a random size was simulated. As shown in Figure 1, the CO₂ concentration in water determines the total number of bubbles in the column. The total number of bubbles present in the column is higher at higher supersaturation ratios, since the bubbles grow and detach faster on the nucleation sites, while additionally the detachment from the surface starts significantly earlier because of the high mass transfer gradient. A significant decrease in the number of bubbles after longer times on stream for the case with the highest supersaturation, which can be attributed to the depletion of the dissolved component in the liquid. Experimental validation and extension to other cases is currently ongoing.

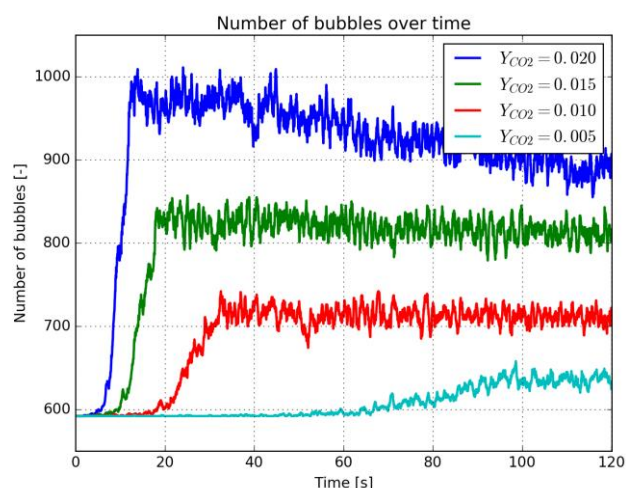


Figure 1. Number of bubbles over time in a box containing a water-CO₂ mixture with bubble nucleation at the bottom surface due to supersaturation. The lines represent different starting mass fractions of CO₂ dissolved in water, while the saturation mass fraction is $Y \approx 0.0017$.

4. Conclusions

A meso-scale model for phase transition in a supersaturated liquid is developed and initial results are presented. A surface was simulated with randomly distributed nucleation sites. Exploratory simulations show that the extent of supersaturation has a pronounced effect on the rates of bubble generation and on the bubble size distribution, where more and larger bubbles are present at higher supersaturation ratios. The model will be extended with empirical information on the basis of experimental data obtained from a dedicated experimental setup.

References

- [1] J. Jia et al., Nat. Commun. 7, 13237 (2016).
- [2] M. van Sint Annaland, N.G. Deen, J.A.M. Kuipers, Heat and Mass Transfer, Springer, Berlin, 2003.
- [3] Y.M. Lau, W. Bai, N.G. Deen, J.A.M. Kuipers, Chem. Eng. Sci. 108 (2014) 9-22.

Keywords

Multiphase modeling; CFD; Phase transition; Bubbly flows