ASTFE
American Society
of Thermal and Fluids Engineers

8th Thermal and Fluids Engineering Conference (TFEC)
March, 26-29, 2023
Partially Online Virtual and at University of Maryland, MD Conference

TFEC-2023-46636

HYBRID VOLUME OF FLUID (VOF) AND LAGRANGIAN APPROACH FOR SIMULATING INTERACTIONS BETWEEN DISPERSED BUBBLES AND LARGE INTERFACES IN TWO-PHASE FLOW

Xiang Zhang, Alexander S. Rattner*

The Pennsylvania State University, University Park, PA 16802, USA

ABSTRACT

In many two-phase flow and heat transfer processes, gas and liquid structures of widely varying physical scales interact. For example, in flow-boiling, mm-scale dispersed bubbles may depart from nucleation sites on walls, interact with bulk liquid flow, and ultimately coalesce with cm-scale gas slugs. It can be prohibitively computationally expensive to directly resolve this range of scales with interface capturing simulation methods, such as the Volume of Fluid (VOF) approach. For such flows, we propose that the dynamics of small bubbles can be modeled with Lagrangian approaches, which treat them as point particles tracked on a coarse mesh that resolves large scale transport. In this study, a hybrid VOF-Lagrangian solver is developed to characterize the coupling between micro-scale bubble transport and macro-scale hydrodynamics in such multiscale two-phase flows. The Lagrangian model tracks the trajectory of individual injected discrete small bubbles, accounting for effects such as buoyancy, pressure, virtual mass, drag, and turbulent dispersion. Once bubbles exceed a threshold packing density or overlap with VOF structures, they are converted to the grid-scale vapor phase. An empirical bubble-lifetime model is implemented to account for the finite coalescence times of bubbles at free surfaces. Contributions of this effort include programmable closure for bubble lifetime at the free surface (before popping/coalescence), a pinning force method for bubbles at the free surface, and Lagrangian-to-VOF transition of bubbles based on packing density. The accuracy of this approach is being assessed using experimental high-speed video data for bubble trajectories at free surface of a bubble column.

KEY WORDS: Two-phase flow, Multiscale interaction, Simulation, Hybrid VOF and Lagrangian approach

1. INTRODUCTION

There are several classes of simulation methods for multiphase flows, which are well suited to different flow regimes and physical scales [1-3]. In direct interface tracking/capturing methods, the governing equations are based on the local instantaneous conservation equations. As these methods are often considered “direct numerical simulations,” they can often be applied without additional closure models for sub-grid-scale transport. Such methods are well suited to studying local transport processes such as small vortices behind bubbles and bubble-bubble interactions. However, due to high computational costs, such approaches are typically only applied to “small problems,” such as flows with a single bubble or to a few interacting bubbles [4-7]. Volume of fluid (VOF) algorithms are the most commonly methods for direct interface capturing simulations, and are available in many commercial CFD packages. In typical VOF methods, single velocity and pressure fields are solved, which apply in both phases. An additional scalar “marker” or volume fraction field ($\alpha \in [0,1]$) is advected by the flow, which indicates the local fluid phase. This α field can be used to evaluate local material properties and surface tension forces due to interface curvature.

In Lagrangian simulation approaches, flow fields are solved for a “background” continuous fluid phase and sub-grid-scale dispersed phase particles (*e.g.*, droplets, bubbles) are modelled as superimposed point-particles with individual state equations for trajectory and other properties. Varying degrees of interaction can be considered for forces and transport between the phases or different Lagrangian particles. Prior studies have

*Corresponding Author: Alex.Rattner@psu.edu

employed Lagrangian approaches to model small dispersed bubbles in continuous liquid environments, often for bubble-column applications. However, such simulations have generally simplified processes at the main free-surface gas-liquid interface. This interface has often been treated as an artificial boundary condition or a buffer zone without dynamics [8-10].

The present study proposes a hybrid VOF-Lagrangian simulation approach with improved fidelity of processes at such large-scale interfaces in adiabatic bubbly flows. The macro-scale continuous liquid and gas phases are modelled with a VOF approach, which can predict waves at the free surface. Subgrid scale bubbles are modelled with a Lagrangian approach. Additional closure models are added to account for multiscale interaction, including bubble pinning at the macroscale free surface, finite popping/coalescence times of bubbles at the free surface, and coalescence of dispersed Lagrangian bubbles into the continuous VOF gas phase. Experimental visualization studies of a small oil-air bubble column are being used to assess this simulation approach. The proposed methods could be extended to study flow boiling processes in which nucleating vapor bubbles merge and interact with larger two-phase structures.

2. SIMULATION APPROACH

The hybrid solver is an extension of the OpenFOAM VOF and Lagrangian solver *interDPMFoam*, with extensions for Lagrangian-to-continuous gas transition (*e.g.*, bubble popping / coalescence) and bubble pinning forces at the VOF free surface. The continuous liquid and gas phases are modelled with the following conservation equations for continuity, momentum, and advection of the macro-scale interface (liquid volume fraction field α_L). These equations are weighted by the instantaneous volume fraction of the continuous phases in each cell/face: α_c.

$$\frac{\partial \alpha_C}{\partial t} + \nabla \cdot (\alpha_C \, \vec{u}_C) = 0 \tag{1}$$

$$\frac{\partial(\rho_C \, \alpha_C \, \vec{u}_C)}{\partial t} + (\vec{u}_C \cdot \nabla)(\rho_C \, \alpha_C \, \vec{u}_C) + (\rho_C \, \alpha_C \, \vec{u}_C) \cdot \nabla \vec{u}_C = -\nabla(\alpha_C P) + \nabla \cdot \bar{\bar{\tau}} + \alpha_C \rho_C \vec{g} + \vec{f}_\sigma + \vec{f}_{L \to E} \tag{2}$$

$$\frac{\partial(\alpha_C \, \alpha_L)}{\partial t} + \nabla \cdot (\vec{u}_C \, \alpha_C \, \alpha_L) = 0 \tag{3}$$

Here, $\vec{f}_\sigma$ is the macro-scale volumetric surface tension force at curved interfaces, applied as a volumetric source on the interface containing cells. $\vec{f}_{L \to E}$ is the net volumetric force between the continuous and dispersed phases in each cell. Transfer of volume from the dispersed bubbles to continuous gas due to bubble popping or coalescence is applied explicitly at the end of each simulation time step. Therefore, the governing differential equations are not modified with corresponding source terms.

Trajectories of discrete dispersed gas bubbles are modelled with Newton's equation of motion accounting for forces from buoyancy and gravity (F_b), drag (F_D), pressure gradients (F_P), virtual mass (F_D), and lift due to continuous-phase velocity gradients (F_L). An additional force is applied to bubbles near the VOF liquid-gas interface to represent *pinning* (F_{IP}). This cancels out the components of other forces normal to the VOF interface, effectively constraining bubbles at the free surface while allowing them to slide, as is often observed.

$$m_B \frac{du_B}{dt} = F_b + F_P + F_D + F_L + F_{VM} + F_{IP} \tag{4}$$

Dispersed bubble coalescence with the continuous VOF gas phase is evaluated explicitly at the end of each time step. The residence time of Lagrangian bubbles at the macro-scale VOF interface is tracked, and reset to zero if bubbles move away from the interface. If a bubble's residence time at the free surface exceeds a correlation value, it is transferred to the continuous gas phase (*i.e.*, popped). If the Lagrangian phase volume fraction in a cell $(1 - \alpha_C)$ exceeds a threshold packing density, the bubbles are assumed to have coalesced and are similarly converted to the continuous gas phase. converted to the grid-scale vapor phase.

3. EXPERIMENTAL ASSESSMENT OF SIMULATION METHOD

A bubble column experimental facility was developed to investigate adiabatic bubbly flow hydrodynamics in a square glass tube with 40×40 mm inner dimensions. The schematic and typical visualization in front view of the experimental facility are illustrated in Fig. 1. The base of column is capped with a flange-like connector, which is used for mounting and sealed with silicone sealant. A 25 mm diameter, 1.6 mm thick porous stainless-steel disc is sandwiched between the flange and gas injector as a sparger. The gas injection volumetric flow rate is controlled and monitored by a syringe pump. Due to its low viscosity and surface tension, PSF-5cSt Pure Silicone Fluid (supplied by Clearco Products Co., Inc.) was selected as the working fluid.

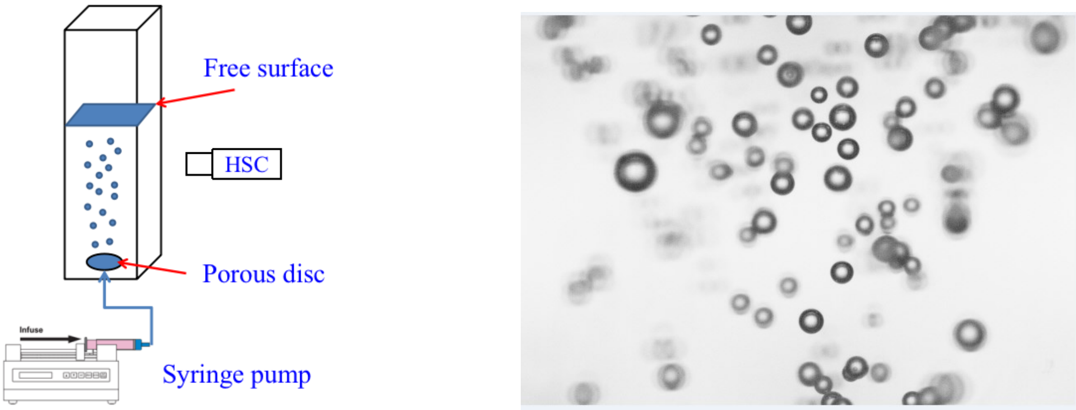
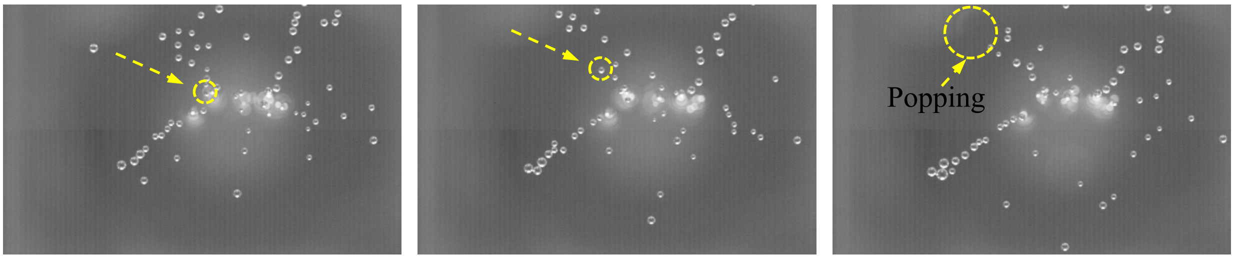


Fig. 1 Schematic and typical visualization of experimental facility.

Visualizations were collected with a high-speed camera. An image processing technique was developed to extract bubble diameters using the ImageJ software [11]. Fig. 2 shows a representative path of a 450 µm diameter bubble on the free surface, which propagates outward (up the curved meniscus) until it pops after approximately 440 ms. For the observed range of bubble sizes, the bubble lifetime at the free surface can be correlated with a linearly with bubble diameter. As shown in Fig. 3, larger bubbles last longer at the interface before popping. Three consecutive images each before and after popping are used to estimate the uncertainty in the bubble size and lifetime, which is less than 9%.



(a) 0 ms (b) 180 ms (c) 440 ms

Fig. 2 Visualizations of bubble propagation and popping at the free surface.

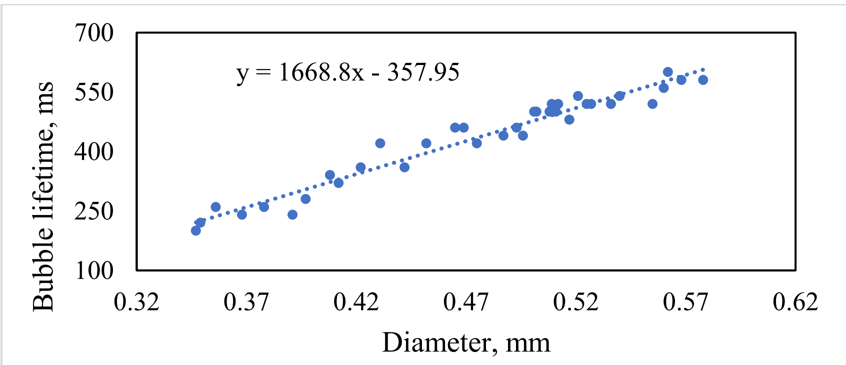


Fig. 3 Relationship between bubble lifetime and diameter.

4. CORRESPONDING SIMULATION STUDY

A corresponding 3D simulation domain was studied with uniform cell size 2×2×2 mm. A static contact angle of 5 degrees was imposed on the side walls for the highly wetting oil-glass pair. This forms a slightly curved free surface, causing Lagrangian bubbles pinned on the free surface to propagate outward due to buoyancy. Dispersed bubbles were injected into the domain at 2 ml min^{-1} with a size distribution based on experimental observations (0.34 to 0.59 mm). Fig. 4 shows representative results using the hybrid solver. The white dots represent the dispersed bubbles in liquid and free surface. Consistent with the experimental results, bubbles persist on the interface for a period of time and propagate outside from the injection domain before popping. Quantitative comparison between simulation and experimental bubble trajectories and free-surface waves is underway.

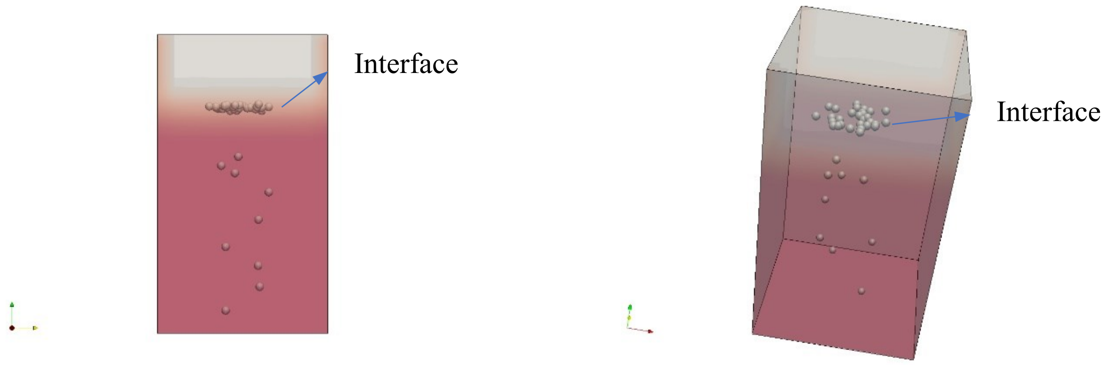


Fig. 4 Simulative results using the hybrid solver.

5. CONCLUSIONS

In the present study, a hybrid VOF-Lagrangian solver is developed to characterize the coupling between micro-scale transport and macro-scale hydrodynamics at the gas-liquid interface in a bubble column. The approach captures macro-scale interface effects (*e.g.*, waves) as well as phenomena such as bubble pinning, finite bubble lifetimes at the free surface before popping, and bubble coalescence at high packing density. Experiments are being analyzed to assess the computational approach. Extensions are being developed to account for similar multiscale interactions in flow boiling.

ACKNOWLEDGEMENTS

The authors wish to acknowledge generous support from the U.S. National Science Foundation (CBET-1652578).

REFERENCES

[1] R. Sungkorn, J. J. Derksen, and J. G. Khinast, “Euler–Lagrange Modeling of a Gas–Liquid Stirred Reactor with Consideration of Bubble Breakage and Coalescence,” AIChE J., vol. 58, no. 5, pp. 1356–1370, 2012, doi: 10.1002/aic.

[2] N. G. Deen, M. van Sint Annaland, and J. A. M. Kuipers, “Multi-scale modeling of dispersed gas-liquid two-phase flow,” Chem. Eng. Sci., vol. 59, no. 8–9, pp. 1853–1861, 2004, doi: 10.1016/j.ces.2004.01.038.

[3] D. Zhang, N. G. Deen, and J. A. M. Kuipers, “Numerical simulation of the dynamic flow behavior in a bubble column: A study of closures for turbulence and interface forces,” Chem. Eng. Sci., vol. 61, no. 23, pp. 7593–7608, 2006, doi: 10.1016/j.ces.2006.08.053.

[4] J. C. Cano-Lozano, R. Bolaños-Jiménez, C. Gutiérrez-Montes, and C. Martínez-Bazán, “The use of Volume of Fluid technique to analyze multiphase flows: Specific case of bubble rising in still liquids,” Appl. Math. Model., vol. 39, no. 12, pp. 3290–3305, 2015, doi: 10.1016/j.apm.2014.11.034.

[5] F.Tocci, “Assessment of a hybrid VOF two-fluid CFD solver for simulation of gas-liquid flows in vertical pipelines in OpenFOAM,” POLIMI Dr. Thesis, no. January 2016, p. 100, 2016, doi: 10.13140/RG.2.2.20229.29929.

[6] L. C. Malan, A. G. Malan, S. Zaleski, and P. G. Rousseau, “A geometric VOF method for interface resolved phase change and conservative thermal energy advection,” J. Comput. Phys., vol. 426, p. 109920, 2021, doi: 10.1016/j.jcp.2020.109920.

[7] A. S. Rattner and S. Garimella, “Taylor flow in intermediate diameter channels: Simulation and hydrodynamic models,” Int. J. Heat Mass Transf., vol. 103, pp. 1108–1124, 2016, doi: 10.1016/j.ijheatmasstransfer.2016.07.012.
[8] Y. M. Lau, W. Bai, N. G. Deen, and J. A. M. Kuipers, “Numerical study of bubble break-up in bubbly flows using a deterministic Euler-Lagrange framework,” Chem. Eng. Sci., vol. 108, pp. 9–22, 2014, doi: 10.1016/j.ces.2013.12.034.
[9] R. Sungkorn, J. J. Derksen, and J. G. Khinast, “Euler–Lagrange Modeling of a Gas–Liquid Stirred Reactor with Consideration of Bubble Breakage and Coalescence,” AIChE J., vol. 58, no. 5, pp. 1356–1370, 2012, doi: 10.1002/aic.
[10] N. G. Deen, M. van Sint Annaland, and J. A. M. Kuipers, “Multi-scale modeling of dispersed gas-liquid two-phase flow,” Chem. Eng. Sci., vol. 59, no. 8–9, pp. 1853–1861, 2004, doi: 10.1016/j.ces.2004.01.038.
[11] A. A. Jasim, A. J. Sultan, and M. H. Al-Dahhan, “Impact of heat exchanging internals configurations on the gas holdup and bubble properties in a bubble column,” Int. J. Multiph. Flow, vol. 112, pp. 63–82, 2009, doi: 10.1016/j.ijmultiphaseflow.2018.11.008.
[12] C. W. Hirt and B. D. Nichols, “Volume of fluid (VOF) method for the dynamics of free boundaries,” J. Comput. Phys., vol. 39, pp. 201-225, 1981, doi.org/10.1016/0021-9991(81)90145-5.