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Bubble Breakup Sensitivity on Local Surface Tension Modification in LES of Turbulent Slug Flow

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ABSTRACT

Understanding the complex behaviour of two-phase flow during accidental conditions in nuclear power plants requires evaluating flow properties under varying conditions. This study aims to investigate the interface breakup in the tail of a Taylor bubble in slug flow. Such breakup occurs on spatial and temporal scales that are typically much shorter than those of fluid dynamics. Our model for interface breakup is based on grid-scale surface tension models that modify the physical surface tension in accordance with the local curvature of large interfaces. The primary focus is the development and implementation of grid- and subgrid-scale models of artificial surface tension, which are able to manipulate the Taylor bubble breakup dynamics.

Two-dimensional simulations are conducted with the modified interFoam Volume of Fluid (VOF) solver in OpenFOAM. The study provides valuable insights for the development and testing of grid- and subgrid-scale models to manipulate bubble coalescence and breakup behaviour. Findings reveal that Taylor bubbles in water-air mixture are significantly influenced by the modelling of the surface tension, with increased total surface tension near the sharp interfaces leading to decreased bubble breakup and vice-versa. The shape of Taylor bubbles is also notably affected by the surface tension, particularly at the bubble nose and tail region.

1 INTRODUCTION

Nuclear power, an essential contributor to the world's low-carbon energy mix, remains an area of continuous innovation and research, with safety considerations being of paramount importance. Understanding the behavior of two-phase flow during accidental conditions is crucial for the safe and continuous operation of nuclear power plants. Such scenarios often involve complex fluid dynamics, including the formation, interaction, and disintegration of gas bubbles in a liquid flow, thereby necessitating an in-depth analysis of these phenomena. In this context, Taylor bubbles, large gas bubbles moving in a liquid counter-current flow, present a critical aspect that requires detailed investigation due to their impact on heat transfer and overall reactor safety.

The flow and dynamics of Taylor bubbles are influenced by a variety of factors. Notably, the bubble's interaction with turbulent flow leads to a chaotic flapping motion at the bubble's skirt, instigating a gradual breakup of the bubble. Our study takes a closer look at the conditions under which this breakup occurs, with particular emphasis on the role of surface tension. This research builds on previous work that proposed using counter-current turbulent flow to maintain the bubble in an equilibrium position for extended periods, thereby allowing for in-depth observation of its decay [1]. First experiments of the Taylor bubble in the counter-current turbulent flow were performed by Martin [2]. He demonstrated that the bubble velocity in the counter-current slug flow cannot be adequately represented by the existing theories for co-current background flow or stagnant liquid at that time. Recent experiments of the Taylor bubble in the counter-current regime were performed with high-speed camera in visible light and a disintegration rate of the bubble has been measured as well as the speed of the waves on the Taylor bubble interface which also eventually leads to bubble breakup [1], [3].

In our study, we focus particularly on the physics of bubble breakup and coalescence, as well as on developing corresponding numerical models compatible with the Large Eddy Simulation method (LES). Both topics are still in early stages of the development [4]. Shape and behaviour of a Taylor bubble depends on properties of the gas-liquid mixture. Araujo [5] has performed a comprehensive study on how flow properties impact the shape and behavior of Taylor bubbles in laminar conditions, using two-dimensional simulations. Other numerical simulations of slug flow have consistently observed increased bubble breakup in turbulent regime [6] and therefore different coalescence [7] or breakup models need to be applied.

In this paper we propose a new grid-scale surface tension model which models local surface tension coefficient as a function of interface curvature. We have developed the model within OpenFOAM framework and tested it with two-dimensional simulations of Taylor bubble in counter-current flow.

1.1 Implications in nuclear industry

Understanding the behaviour of gas bubbles within a nuclear power plant is crucial to its efficient and safe operation. Our study is trying to show that locally enhanced grid-scale surface tension at higher curvatures could lead to slower bubble breakup. This finding has notable implications for the nuclear industry, as bubble formation and breakup can influence reactor operation, thermal efficiency, and safety protocols.

The formation, growth, and breakup of bubbles occur in the boiling coolant in a nuclear reactor. In these systems, heat from the nuclear reaction is used to boil water, and the steam produced is used to drive a turbine and generate electricity. The behaviour of the bubbles in the coolant can significantly impact the efficiency of this process.

From a safety perspective, enhanced bubble breakup, resulting in smaller bubbles, is generally desirable. Smaller bubbles provide a larger total surface area for a given volume of gas, which improves heat transfer from the nuclear fuel to the coolant. This helps keeping the fuel rods cooler and enhances the reactor's overall thermal efficiency.

On the other hand, larger bubbles or vapor films could lead to an undesirable condition known as "film boiling," where a layer of steam forms on the fuel rods, significantly reducing the heat transfer efficiency and potentially leading to overheating of the fuel rods. This condition is known as "Departure from Nucleate Boiling" (DNB), and it must be avoided to ensure the safe operation of the reactor.

While our study develops a numerical grid-scale surface tension model aimed at reducing bubble breakup in CFD simulations, in a nuclear reactor, one might consider strategies to do the opposite—i.e., to increase bubble breakup. Potential strategies for that could include the addition of specific surfactants to the coolant, careful control of temperature and pressure, controlling bubble size at the point of formation, or even the application of external vibrations or mechanical disturbances. However, each of these strategies comes with its own set of challenges. The feasibility of such methods needs to be carefully evaluated, considering potential impacts on other aspects of reactor operation, the stability of the proposed changes under reactor conditions, and the overarching imperative of maintaining safety at all times.

2 THEORETICAL AND NUMERICAL BACKGROUND

A two-phase mixture of gas and liquid is modelled using the one-fluid formulation of the Navier-Stokes equations with the Volume-Of-Fluid (VOF) approach for interface capturing. In this method a void fraction α is introduced and the advection equation for this quantity is the following:

$$\partial_t \alpha + \boldsymbol{u} \cdot \nabla \alpha = 0$$

with partial time derivative ∂_t, velocity vector u and gradient operator ∇. The fluid mixture is described by the incompressible Navier-Stokes equations, i.e. the mass conservation equation,

$$\nabla \cdot \boldsymbol{u} = 0$$

and momentum conservation equation

$$\partial_t(\rho \boldsymbol{u}) + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \rho \boldsymbol{g} + \nabla\left(\mu_{eff}(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T)\right) + \sigma(\boldsymbol{\kappa})\boldsymbol{\kappa}\boldsymbol{\delta}(\boldsymbol{n})\boldsymbol{n}$$

with mass density ρ, pressure p, gravitational acceleration $\boldsymbol{g}$, effective mixture viscosity μ_{eff}, surface tension coefficient $\sigma(\boldsymbol{\kappa})$, interface curvature $\boldsymbol{\kappa}$, interface normal unit vector $\boldsymbol{n}$ and interface Dirac delta function $\boldsymbol{\delta}(\boldsymbol{n})$.

Viscosity at the interface was calculated with linear averaging, namely:

$$\mu = \alpha_l \mu_l + \alpha_g \mu_g,$$

where α_l is the fraction of the liquid phase and α_g is fraction of the gas phase in the given computational cell, respectively. Similarly, μ_l and μ_g are the corresponding liquid and gas viscosities.

The described equations were solved in open-source computer program OpenFOAM v10 [8]. We have used a modified interFoam solver, which enables the usage of the Diagonally Implicit Runge-Kutta (DIRK) time integration schemes integrated with PLIC geometric reconstruction. Used numerical schemes are second-order accurate in space and time. This solver was based on a solver developed in OpenFOAM v4 by Frederix et al. [6]. Turbulence at the sub-grid scales was modelled by the WALE model. A recycling boundary condition was used at the inlet in order to achieve a fully developed turbulent flow. The flowrate was also adjusted at every timestep so that the net force on the bubble is always zero and the bubble stays at approximately constant position throughout the simulation.

In the present study, the fluid properties were selected to reproduce the water-air mixture at 20 degrees Celsius. We have studied the case where the pipe diameter was 26 mm and pipe length 52 cm. The corresponding dimensionless numbers are presented in Table 2, where the Reynolds number is computed for the single-phase flow of liquid upstream of the bubble.

Table 1: Morton, Froude, Eotvos and liquid Reynolds numbers

Mo	Fr	Eo	Re
2.60E-11	0.113	90.90	5600

2.1 Numerical mesh

Two-dimensional simulations have been performed in order to reduce the computational costs. Firstly, we have constructed five different meshes to perform the mesh convergence study. We have used equidistant cells in both *x* and *y* direction. N_x is the number of cells in streamwise direction and N_y is number of cells in wall normal direction. In the spanwise direction we have used only one cell with appropriate boundary condition, therefore making it a two-dimensional simulation.

Table 2: Different meshes used for mesh convergence study.

Mesh	N_x	N_y	N
1	52	26	1352
2	104	52	5408
3	208	104	21632
4	416	104	43264
5	416	208	86528

2.2 Modelling of surface tension coefficient

Surface tension is the property of the cohesive forces in the liquid surface that allows it to resist an external force. It is conventionally defined for interface between two immiscible fluids, such as water and air. Here, the surface tension coefficient is a constant value at a given temperature and pressure.

However, when considering curved surfaces, such as in small droplets or bubbles, surface tension can have a more complicated behaviour that is not captured by scales simulated with continuum approximation. This is also true for other mechanisms that control bubble breakup and coalescence. The bubble breakup observed in the VOF simulations is therefore usually larger than in experimental measurements.

In this paper we therefore propose a numerical model for the surface tension coefficient, denoted as σ, as a function of the normalized curvature, denoted as κ, which ranges from 0 to N, but reaches maximum value at $\kappa = 1$. In all models, σ_0 is the baseline surface tension coefficient, and C is a parameter that controls the magnitude of the curvature effect.

The sigmoid model is given by:

$$\sigma(\kappa) \; = \; \sigma_0[1 + \frac{C}{(1 + exp(-k(\kappa - 0.5)))}],$$

where k controls the steepness of the transition. This model has an "S"-shaped curve, with a rapid transition around κ = 0.5 as shown in Figure 1. We have done the study where we have changed the C value as: [0, 1, 5, 10] and k value as [1, 10, 100].

Curvature is mathematically defined as:

$$\kappa = \frac{1}{R},$$

where R is radius of the circle fitted to the interface.

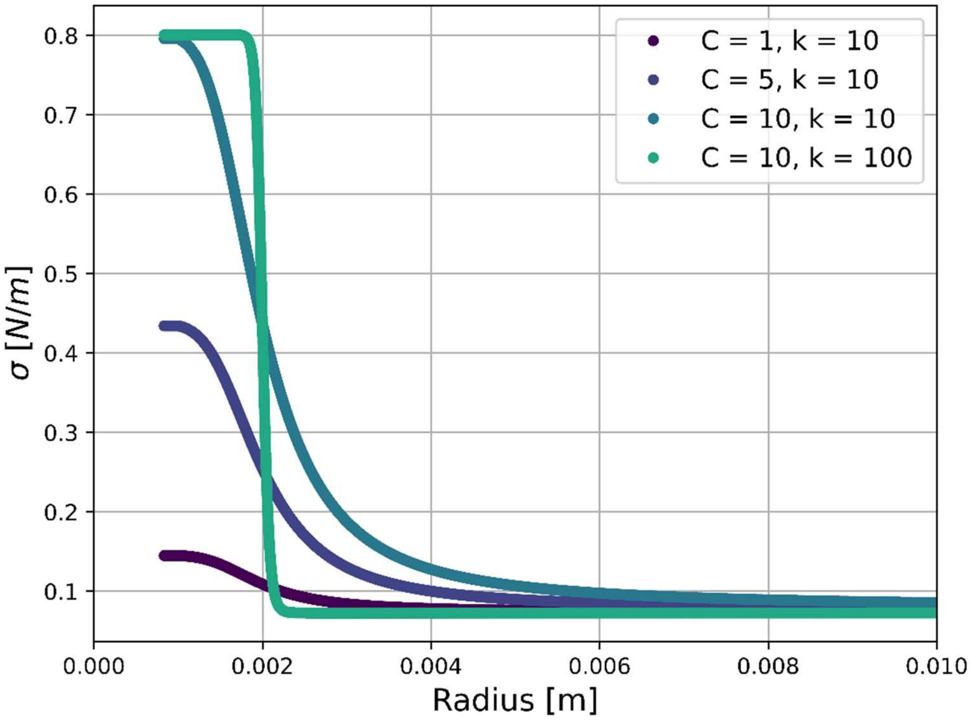

Figure 1: Model for surface tension coefficient as a function of curvature.

The proposed model specifically impacts surface tension at larger curvatures while maintaining a constant surface tension at lower curvatures. This approach is designed to align with the empirically determined surface tension of a water-air mixture as measured on a flat surface. While the exact enhancement proposed cannot be directly validated, employing this model will facilitate the assessment of two significant factors:

1. The influence of increased surface tension on the bubble breakup process.
2. Bridging the gap between experimental and numerical results, thereby enhancing the comparability of these findings.

3 RESULTS

3.1 Mesh convergence study

Initially, we undertook a mesh convergence study, analysing fundamental parameters such as bubble shape and breakup rate in relation to mesh refinement. Figure 1 depicts the Taylor bubble's shape alongside trailing bubbles for various mesh sizes, as detailed in Table 2. Notably, a finer mesh more accurately captures the bubble interface, resulting in reduced bubble breakup. Properly capturing this bubble interface is of paramount importance. Nevertheless, the grid refinements, which would properly capture all processes of the interface breakup and generation of small bubbles are several orders of magnitude smaller than the meshes used in the present study.

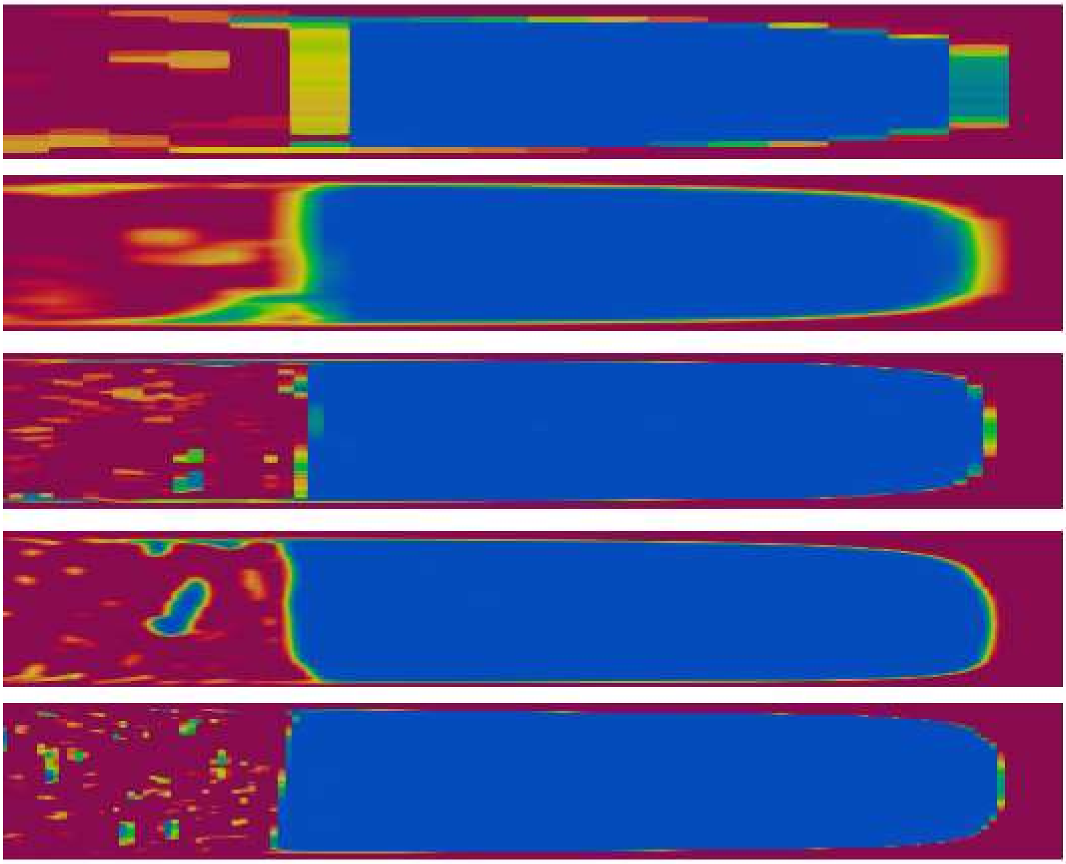

Figure 2: Bubble shape for meshes 1-5 from top to bottom after t=1s

Table 2 presents the time-averaged void fraction (α) values at the outlet for different mesh sizes. As anticipated, the finest mesh records the lowest value, while the coarsest mesh indicates the highest. The difference is substantial, with a disparity spanning nearly two orders of magnitude. While there isn't a pronounced trend among medium meshes, it's evident that even with a finer mesh, bubble breakup is reduced but never completely eliminated.

Table 3: Bubble breakup rate as a function of mesh. We show average α at the outlet.

Mesh	**1**	**2**	**3**	**4**	**5**
Bubble breakup rate	0.01365	0.00899	0.00387	0.00874	0.00075

3.2 Parametric study

Parametric study has been conducted for three values of C and three values of k, therefore in total we have conducted 9 different simulations shown in Table 4. The benchmark simulation with C = 0 is shown in Table 3.

Figure 3 illustrates the bubble shape for various values of parameter C at t=10s. It is evident that with higher C values, the bubble shape undergoes significant alterations, deviating from the observed experimental shapes [5]. However, this also results in a marked reduction in bubble breakup.

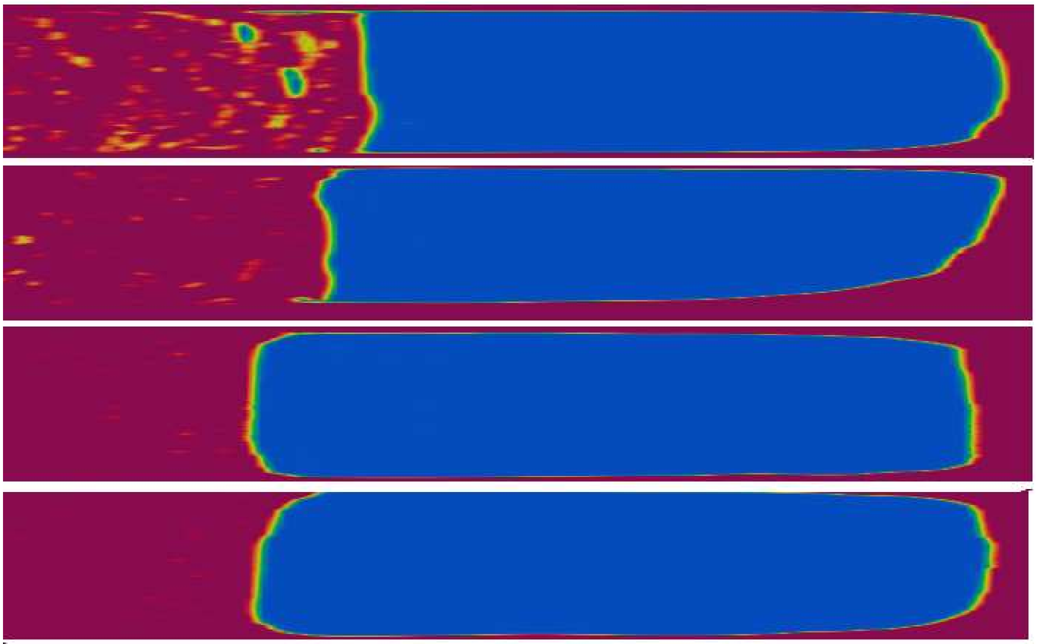

Figure 3: Bubble shape after t=10s for C=0, 1, 5, 10 from top to bottom and k=10.

The reduced bubble breakup rate can be also seen in Table 4. For small values of C, we do not observe significant difference with the base case with C=0, but for larger values of C we observe significantly lower bubble breakup (about one order of magnitude), which confirms the plausibility of the proposed model. The influence of the value k is insignificant for bubble breakup. The experimental value of 3.4e-05 [1] is still smaller than in numerical simulations but considerably closer with the newly proposed model. Further evaluation of the proposed model will be made with three-dimensional simulations.

Table 4: Bubble breakup rate as a function of parameters C and k. We show time-averaged α (t=20s) at the outlet.

k \ C	1	5	10
1	2.77e-03	5.058e-05	9.013e-05
10	1.49e-03	8.577e-05	4.299e-04
100	3.99e-03	4.856e-04	4.073e-04

4 CONCLUSIONS

In this context, we performed two-dimensional simulations using the modified interFoam VOF solver with additional grid-scale surface tension model in open-source software OpenFOAM. This approach proved instrumental in generating valuable insights for the development and testing of grid- and subgrid-scale models aimed at manipulating bubble coalescence and breakup behavior.

Our findings highlight that surface tension considerably affects Taylor bubbles in water-air mixtures. Specifically, local artificial enhancement of surface tension near the sections of the interface with large curvature leads to a reduction in bubble breakup. Notably, the shape of Taylor bubbles, particularly at the bubble nose and tail region, is significantly influenced by surface tension modifications. Additional closures for surface tension in the scope of LES are therefore crucial for better comparison of experimental results with numerical. This study contributes to understanding and the development of models capable of capturing and manipulating coalescence and breakup behaviour in the LES of turbulent slug flow.

In future research, we aim to apply this model to three-dimensional simulations of Taylor bubbles in counter-current flows. Additionally, we plan to refine the model to minimize its dependency on mesh size.

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