



# EFFECT OF INTERFACIAL FORCE ON FLOW BEHAVIOR AND LIQUID FILM THICKNESS IN THREE-PHASE TAYLOR FLOW

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## 1. ABSTRACT

This study investigates the effect of interfacial force on the flow behaviour and liquid film thickness in three-phase Taylor flow using the MPPICInterFOAM solver. Within this solver, the interface force model was modified to prevent particle penetration through the gas-liquid interface. Simulations demonstrated that increasing the interfacial force coefficient significantly increases film thickness by up to 25%, within the study range, and alters particle distribution within liquid slugs. These findings contribute to optimizing three-phase flow parameters for advanced heat transfer applications such as nanofluids and chemical microreactors.

## 2. INTRODUCTION

Two-dimensional (2D) nanomaterials, such as graphene and hexagonal boron nitride, are of particular interest in heat transfer applications involving electronics and microchannel heat sinks, due to their exceptional thermal properties (e.g., thermal conductivity) [1]. Various techniques, including chemical, electrochemical, and mechanical methods, are employed to produce, synthesize, and extract these nanomaterials. As a microreactor technology, three-phase Taylor flows have also emerged as a significant area of interest for optimizing the continuous flow synthesis and extraction of micro- and nanomaterials. Segmented flows, characterized by a train of gas bubbles segmented by liquid slugs, offers considerable advantages such as a large interfacial surface-to-volume ratio, efficient mixing, and effective thermal control [2].

The current study explores the use of three-phase Taylor flow microreactors for extracting nanomaterials to enhance heat transfer. Understanding the flow characteristics, particularly the dynamics of particles within liquid slugs and the liquid film layers around bubbles, is essential for developing an efficient approach for selective particle manipulation. A key parameter in this context is the interaction between dispersed particles and the interface between bubbles and the surrounding slurry. This parameter is typically assumed in numerical studies without any explicit validation. Using a modified OpenFOAM solver, MPPICInterFOAM, simulations were conducted to investigate the influence of interfacial force on the behaviour of particles in the liquid regions, especially near the interface between the liquid and gas and within the liquid film regions.

## 3. METHODOLOGY

The OpenFOAM solver MPPICInterFOAM was utilized to simulate three-phase Taylor flow within a capillary tube of one millimetre diameter and twenty-five millimetres length. This solver integrates the Volume of Fluid (VOF) method for capturing the gas-liquid interface with the MPPIC Lagrangian approach for particle tracking. A modification to the interface force model was implemented to adjust particle hydrophobicity and prevent particles from moving through the gas-liquid boundary. This force is defined [3]:

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$$F_{int} = -C_{int} m_p \nabla \alpha \quad (1)$$

where  $C_{int}$  represents the physical nature of the particle surface and shape,  $m_p$  is the particle mass, and  $\alpha$  is the volume fraction of the liquid phase. The modification also eliminated residual values of parameters that incorrectly generate the force far from the interface, making the results and revised open-source solver applicable for accurately modelling other generic multiphase flow problems. In addition to the interface force, the solver accounts for drag, lift, gravity, pressure gradient, and viscous forces. The governing equations include the continuity equation for mass conservation and the momentum equation considering four-way coupling [4].

Simulations were conducted on a High-Performance Computing (HPC) system, analysing the effect of the interface force on flow behaviour, specifically film thickness. The investigation explored a range of interface force coefficients ( $C_{int}$ ) from ten to five thousand.

#### 4. RESULTS

The interfacial force was found to be one of the most dominant factors affecting particle dynamics and distribution in this study. Figure 1 illustrates that an increase in the interfacial force coefficient results in a continuous rise in film thickness, up to 25%, within the studied range. This increase in film thickness is attributed to the higher ratio of particles present within the film layer compared to the total number of particles in the entire domain, as shown in Figure 1. Further examination of the flow fields in Figure 2 indicates that increasing  $C_{int}$  leads to a higher concentration of particles in the outer circumferential regions of the liquid slug. This, in turn, reduces the concentration of particles in the central area of the liquid slug.

This phenomenon occurs because an elevated interfacial force coefficient exerts a stronger repulsive force on particles as they approach the liquid-gas interface. Consequently, these particles are directed towards the liquid phase, where they are influenced by the global flow behaviour within the liquid slug. The circulations within the liquid slug, characteristic of segmented liquid-gas flows, intensify with the rise of the interfacial force coefficient. This increased vorticity enhances the likelihood of more particles being propelled into the region between the bubble nose and the wall. Furthermore, the emergence of a small-scale vortex in the bubble nose region for  $C_{int} < 100$  restricts particle flow at the entrance to the thin film. In contrast, an increase in the interfacial force coefficient was found to have a negligible effect on the overall bubble morphology.

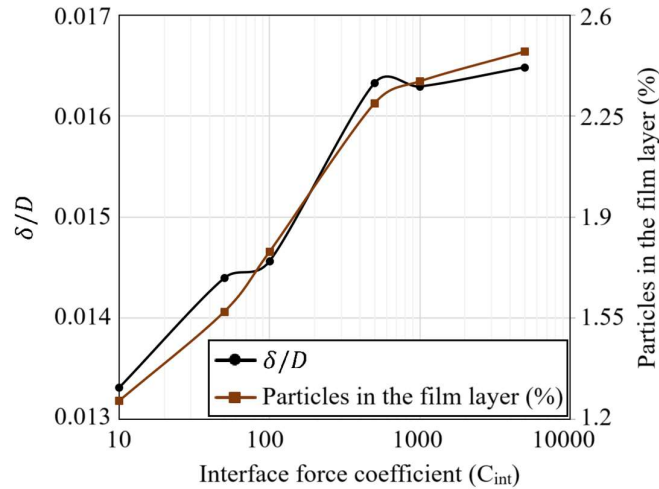


Figure 1: The effect of the interfacial force coefficient  $C_{int}$  on the film thickness (primary y-axis) and the percentage of the particles in the film layer to the total particles in the flow field (secondary y-axis).  $Re = 100$ ,  $\phi = 3 \times 10^{-4}$ ,  $d_p = 400 \text{ nm}$ .

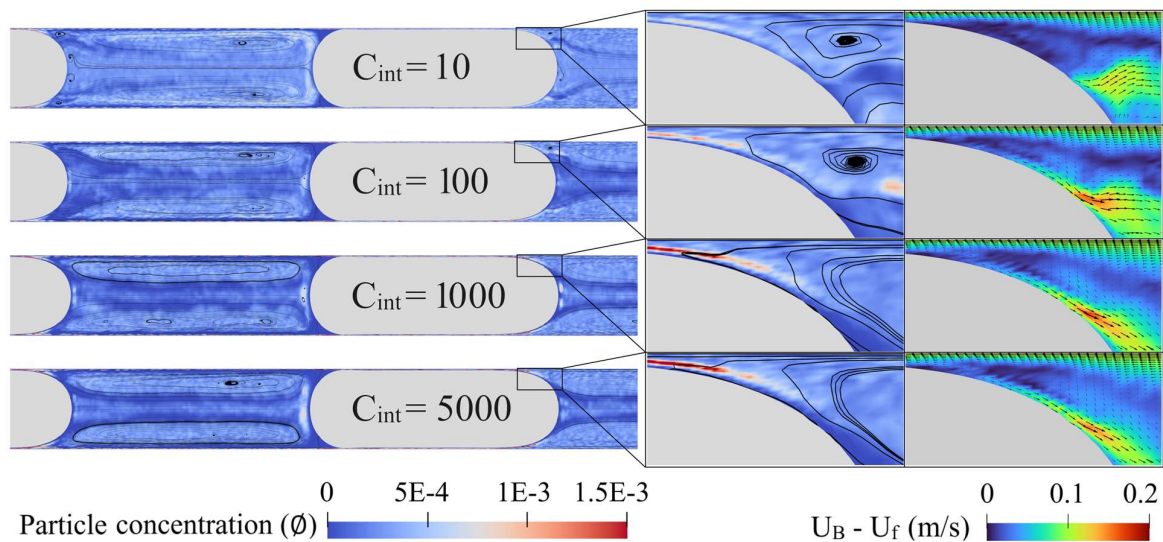


Figure 2: Flow field and particle distribution for different values of interfacial force coefficient  $C_{int}$ .  $Re = 100$ ,  $\phi = 3 \times 10^{-4}$ ,  $d_p = 400 \text{ nm}$ .

## 5. CONCLUSIONS

The study demonstrated that interfacial force is a dominant factor affecting particle dynamics and liquid film thickness in three-phase Taylor flow. By modifying the MPPICInterFOAM solver to prevent particle penetration through the gas-liquid interface, the simulations showed a continuous increase in film thickness, up to 25%, with higher interfacial force coefficients. This increase is due to the higher particle concentration within the film layer, influenced by stronger repulsive forces at the liquid-gas interface. The research highlights the importance of understanding interfacial forces for optimizing simulations of micro- and nano-particles, such as graphene, for heat transfer applications. Future work should focus on further refining the interface force model and exploring its impact on other flow parameters to enhance the efficiency of microreactors in material synthesis and extraction post-processes.

## ACKNOWLEDGMENT

This research was supported by the Higher Committee for Education Development in Iraq (HCED) Scholarship program, a Royal Academy of Engineering/Leverhulme Trust Research Fellowship [LTRF2122-18-108], and an EPSRC research grant [EP/Z002540/1].

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