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ABSTRACT

A direct numerical simulation (DNS) study is performed to investigate the flow field and interfacial species transfer around freely rising Taylor bubbles in a cylindrical pipe. The Eötvös number Eo is varied from 4.9 to 8.7, the bubble Reynolds number Re from 36 to 303, and the Schmidt number Sc from 1 to 256, covering both the laminar–turbulent transition and fully turbulent regimes. The predicted bubble shape, liquid-film thickness, terminal Froude number, and terminal Sherwood number are compared with experimental data and established correlations, showing good agreement and thereby validating the simulations. On the basis of the validated DNS results, detailed characteristics of the flow and concentration fields are analyzed. At $Eo = 4.9$, the wake is non-axisymmetric, consistent with the transition regime. At higher Eo , corresponding to the fully turbulent regime, a large open recirculation zone develops downstream of the bubble. A peak in the concentration fluctuation c' is observed within the liquid film. Its magnitude increases with increasing Schmidt number and follows a scaling law $c' \sim Sc^{1/4}$. In the wake, a pronounced peak in c' occurs near the wall jet and decays gradually downstream. The wake statistics further suggest scaling behaviors of $\bar{c} \sim Sc^{1/4}$ and $c' \sim Sc^{1/4}$, although additional cases are required for confirmation. Overall, this study demonstrates that DNS is a powerful tool for revealing detailed mechanisms of turbulent flow and interfacial species transfer associated with Taylor bubbles. A key remaining challenge is robust control of parasitic currents, which may become significant owing to interactions between the sharp gas–liquid interface and turbulent fluctuations.

KEYWORDS

Taylor bubble, Direct numerical simulation, Multiphase flow, Volume-of-fluid, Turbulence, Interfacial species transfer

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I. INTRODUCTION

Taylor bubbles are long, bullet-shaped gas bubbles that rise or are transported through a liquid in a tube or channel.^{1,2} They are typically several pipe diameters in length and occupy nearly the entire cross-sectional area of the conduit.³ As a result, a thin annular liquid film forms between the bubble and the wall, and the flow consists of alternating Taylor bubbles and liquid slugs. Taylor bubbles and the associated slug flow occur in many engineering applications, including oil and gas pipelines, chemical reactors, boiling systems, and microchannel mixers. Consequently, Taylor bubbles have been extensively studied over the past decades.

Experiments remain an essential approach for investigating bubbly flows, and a large body of experimental work on Taylor

bubbles is available in the literature. Polonsky *et al.*⁴ measured the motion of a single elongated bubble in a vertical pipe under stagnant, upward-flowing, and downward-flowing conditions to clarify the relationship between Taylor-bubble dynamics and the surrounding velocity field. Fabre and Figueroa-Espinoza⁵ experimentally investigated the transition from symmetric to asymmetric Taylor-bubble shapes in both laminar and turbulent flows.

Some experimental studies have focused on mass transfer. Filla⁶ measured the liquid-phase resistance associated with the absorption of a CO₂ slug in water. Hosoda *et al.*⁷ investigated mass transfer from single CO₂ bubbles in vertical pipes using stereoscopic image processing and developed a corresponding correlation, considering pipe diameters of 12.5, 18.2, and 25.0 mm. Kastens *et al.*⁸ measured the flow field and mass transfer from single CO₂ Taylor bubbles in

vertical minichannels with diameters of 6.0, 7.0, and 8.0 mm. Kexel *et al.*⁹ studied how the fluid dynamics around Taylor bubbles influences the selectivity of fast gas–liquid reactions in methanol. Mei *et al.*¹⁰ proposed a Sherwood-number scaling law based on a normalized time and incorporating the dimensionless liquid-slug length, as well as the Péclet and Dean numbers.

Other experimental work has emphasized hydrodynamics and interface dynamics. van Hout *et al.*¹¹ investigated a single Taylor bubble rising in a vertical pipe filled with stagnant water, for a pipe diameter of 25.0 mm and a Reynolds number of 4350. Nogueira *et al.*¹² examined film thickness, mean velocity profiles, and shear-stress distributions for Taylor-bubble flows across the laminar-to-turbulent transition. Liberzon *et al.*¹³ observed upward-propagating capillary waves on the surface of short Taylor bubbles. Kren *et al.*¹⁴ analyzed interface dynamics in vertical counter-current flow and quantified the propagation speeds of interfacial waves using cross-correlations of time-dependent interface fluctuations.

Experiments provide the most direct information about Taylor bubbles. However, owing to technical challenges, it is difficult to measure all details of the flow and species concentration fields surrounding the bubbles. With the rapid development of high-performance computing, computational fluid dynamics (CFD) has become an increasingly important tool for understanding bubbly flows.

A major challenge in numerical simulations of gas–liquid flows is accurately tracking or capturing the thin gas–liquid interface. Several numerical methods have been developed to compute the phase boundary, account for the local surface tension force, and resolve its temporal evolution. These include the front-tracking (FT) method,¹⁵ the volume-of-fluid (VOF) method,¹⁶ and the level-set (LS) method.¹⁷ Another difficulty is modeling turbulence, which often occurs in the bubble wake. The interaction between turbulence and interface instability renders the flow and species transport around Taylor bubbles extremely complex.

Numerical studies of Taylor bubbles have been widely reported in the literature. Some studies have performed two-dimensional simulations, neglecting the effects of three-dimensional turbulent structures.^{18–22} Other studies have focused on low-Reynolds-number flows, in which the motion is laminar.^{23,24} In these cases, turbulence was not considered.

Reynolds-averaged Navier–Stokes (RANS) simulations with turbulence models are frequently used to study turbulent flows. Taha and Cui²⁵ simulated Taylor bubbles in vertical tubes using the VOF method and the renormalization group (RNG) k – ϵ model. Using the same VOF and RNG k – ϵ model, Shin *et al.*²⁶ investigated Taylor bubbles in vertical and bent pipes. Alekseev and Lukyanov²⁷ employed the VOF method with the k – ω SST turbulence model to validate their numerical results, including the liquid film shear stress, the Taylor bubble nose shape, and the film thickness. Ambrose *et al.*²⁸ observed oscillatory behavior of Taylor bubbles, finding that the oscillation frequency inversely depends on the square root of the average bubble length, in agreement with experimental data.

Some studies have employed large eddy simulation (LES) or detached eddy simulation (DES) methods to capture turbulence. Frederix *et al.*²⁹ performed a LES–VOF study of turbulent co-current Taylor bubble flow, considering Eötvös numbers Eu ranging from 25 to 187. Shaban and Tavoularis³⁰ simulated turbulent flows induced by Taylor bubbles rising in a stagnant liquid column and analyzed

the pressure and temperature fields resulting from the interaction of the bubbles with a heated tube wall. Wang *et al.*³¹ and Wang *et al.*³² applied a stress-blended eddy simulation (SBES) model, in which RANS and LES are blended using a shielding function, in their simulations.

Only a few studies have reported direct numerical simulations (DNS) of Taylor bubbles. Zimmer and Bolotnov³³ simulated the slug-to-churn transition in vertical two-phase flows using a front-tracking (FT) method, with a Reynolds number of 2600. They analyzed the flow structures in the bubble wake and the evolution of the bubble interface during the transition from the slug flow regime to churn-turbulent regime. Frederix *et al.*³⁴ simulated a Taylor bubble with $Re = 5300$ using the VOF method, and examined the turbulent kinetic energy (TKE) budgets ahead of the bubble, in its wake, and across the interface. Nop *et al.*³⁵ performed FT-based DNS of a Taylor bubble at $Re = 1423$ and compared their results with experiments. Overall, DNS of turbulent flows around Taylor bubbles has only emerged in recent years, while the previous studies mainly focused on pure multiphase hydrodynamics without interfacial species transfer. DNS studies of interfacial species transfer around Taylor bubbles are still lacking in the literature. This problem is significantly more challenging because it involves high Péclet-number transport coupled with turbulent interfacial dynamics.

DNS is a powerful tool for understanding the physics of turbulent flows and the associated interfacial species transfer around Taylor bubbles, since it provides highly detailed information. However, one of the major difficulties in DNS of turbulent Taylor bubbly flows is the extremely high computational cost. In addition, performing a DNS study requires careful control of unphysical parasitic (or spurious) currents, which often arise in interface tracking or capturing methods owing to inaccuracies or inconsistencies in surface tension calculations. These parasitic currents become even more significant when interface instabilities interact with turbulent vortices. In this study, we simulate the fluid flow and interfacial species transfer of single freely rising Taylor bubbles in a vertical pipe using DNS. The Reynolds numbers range from 36 to 303, and the Eötvös numbers from 4.9 to 8.7, covering laminar–turbulent transition to fully turbulent regimes. The objectives of this study are to investigate the physics of Taylor bubbles and the associated interfacial species transfer, and to establish reliable flow and species transfer data that can supplement experiments for validating turbulence models.

The remainder of this paper is structured as follows. Section II presents the governing equations and the numerical methods. Section III introduces the test cases. The main results on fluid flow and species transfer are discussed in Sec. IV. Finally, Sec. V summarizes the conclusions.

II. MATHEMATICAL EQUATIONS AND NUMERICAL METHODS

A. Governing equations

Figure 1 schematically illustrates the freely rising Taylor bubble in a pipe that is simulated in this study. The Taylor bubble can be divided into a nose, a film, and a tail,³⁶ while a wake forms downstream of the bubble. In a stagnant liquid, the Taylor bubble rises owing to the buoyancy force resulting from the density difference between the gas and the liquid. The rise velocity stabilizes when the

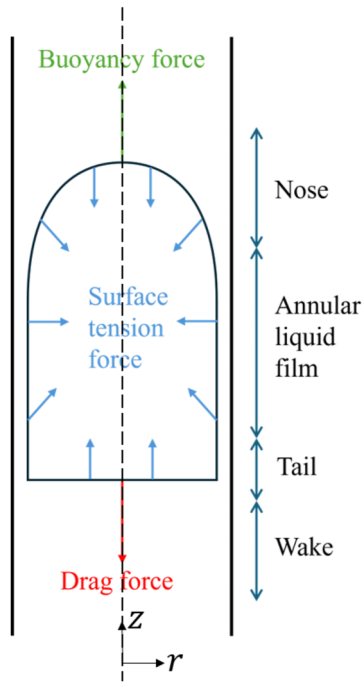


FIG. 1. Schematic of a freely rising Taylor bubble with the forces acting on it.

buoyancy force balances the drag force exerted by the surrounding liquid.

The governing equations that describe the conservation of mass, momentum, bubble color function, and species concentration are

$$\frac{\partial u_i}{\partial x_i} = 0, \quad (1)$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_j u_i)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ji}}{\partial x_j} + \rho g_i + f_{\sigma i} - \rho a_{Fi} + s_i, \quad (2)$$

$$\frac{\partial \alpha}{\partial t} + \frac{\partial(u_i \alpha)}{\partial x_i} + \frac{\partial[\alpha(1-\alpha)U_{ri}]}{\partial x_i} = 0, \quad (3)$$

$$\frac{\partial c}{\partial t} + \frac{\partial(u_i c)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\mathcal{D} \frac{\partial c}{\partial x_i} \right) + s_c. \quad (4)$$

The viscous stress component τ_{ji} in the momentum equation (2) is calculated as

$$\tau_{ji} = \bar{\mu} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad (5)$$

where $\bar{\mu}$ is the phase-averaged dynamic viscosity, which is calculated as

$$\bar{\mu} = \frac{\alpha(1-\alpha)}{(1-\alpha)\mu_g + \alpha\mu_\ell}, \quad (6)$$

where μ_ℓ and μ_g are the dynamic viscosities of the liquid and the gas phases, respectively. A surface tension force $f_{\sigma i}$ is given at the bubble interface, expressed as

$$f_{\sigma i} = \sigma \kappa \frac{\partial \alpha}{\partial x_i}, \quad (7)$$

where σ is the surface tension coefficient. The curvature κ is calculated as

$$\kappa = -\nabla \cdot \left(\frac{\nabla \alpha}{|\nabla \alpha|} \right). \quad (8)$$

The computational domain is translated with the bubble to keep it stationary in the computational frame. The frame velocity is controlled using a proportional–integral–derivative (PID) controller, such that

$$\Delta u_{Fi} = \frac{1}{\Delta t} \left(K_P e_i + K_I \int_0^t e_i dt + K_D \frac{e_i - e_{i,old}}{\Delta t} \right), \quad (9)$$

where Δu_{Fi} is the change of the frame velocity after time step Δt . This results in a frame acceleration rate $a_{Fi} = \Delta u_{Fi} / \Delta t$. K_P , K_I , and K_D are the proportional, integral, and derivative parameters of the PID controller, respectively. Their values are set to 0.1, 0.3, and 0.1 in this study. e_i is the distance vector between the current bubble center and its target location. $e_{i,old}$ is the value of e_i in the previous time step. s_i is another artificial force, which is used to control the parasitic currents.

U_{ri} in the color function equation (3) is an artificial compression velocity that is used to sharpen the captured interface. $\mathcal{D}$ is the species diffusion coefficient, which is calculated as

$$\mathcal{D} = \frac{\alpha(1-\alpha)}{(1-\alpha)\mathcal{D}_g + \alpha\mathcal{D}_\ell}, \quad (10)$$

where $\mathcal{D}_g$ and $\mathcal{D}_\ell$ are the species diffusion coefficients of a scalar c in the gas and liquid phases, respectively. Since the species concentration c is a passive scalar, whose transport does not affect the other equations, it is possible to solve several species transport equations (4) for different species diffusion coefficients with the same flow field. A source term s_c is given in the species transport equations to ensure that the species concentration in the gas phase is uniformly 1.

B. Dimensionless numbers and correlations

On the basis of the governing equations, we can define dimensionless numbers that characterize Taylor bubble flow and species transfer. The Eötvös number Eu is defined as

$$Eu \equiv \frac{(\rho_\ell - \rho_g)gD^2}{\sigma}, \quad (11)$$

which represents the ratio of buoyancy force to surface tension force. The Morton number Mo is defined as

$$Mo \equiv \frac{\mu_\ell^4 g (\rho_\ell - \rho_g)}{\rho_g^2 \sigma^3}, \quad (12)$$

which characterizes the combined effects of viscous and gravitational forces relative to surface tension. The capillary number Ca is defined as

$$Ca \equiv \frac{\mu_\ell u_b}{\sigma}, \quad (13)$$

which represents the ratio of the viscous force to the surface tension force. The buoyancy Reynolds number N_f is defined as

$$N_f \equiv \frac{\sqrt{gD^3(\rho_\ell - \rho_g)\rho_\ell}}{\mu_\ell}, \quad (14)$$

which quantifies the ratio of the buoyancy force to the viscous force. Nogueira *et al.*³⁷ suggested using N_f to classify the wake downstream of a Taylor bubble as a laminar wake ($100 < N_f < 500$), a transition wake ($500 < N_f < 1500$), and a turbulent wake ($N_f > 1500$). The Froude number Fr is defined as

$$Fr \equiv \frac{u_b}{\sqrt{(\rho_\ell - \rho_g)gD/\rho_\ell}}, \quad (15)$$

where u_b is the bubble rise velocity. Fr characterizes the ratio of the inertial force to the gravitational force. Sometimes, the bubble Reynolds number Re is used instead of the Froude number Fr , and is defined as

$$Re = \frac{u_b D}{\nu_\ell}, \quad (16)$$

where the pipe diameter D is used as the characteristic length scale.

Brown³⁸ theoretically derived an expression for the bubble film thickness δ as a function of the bubble rise velocity u_b , the superficial liquid velocity u_c , and the pipe radius $R = D/2$, given by

$$\delta = \left\{ \frac{3\nu}{2g(R-\delta)} [(R-\delta)^2 u_b - R^2 u_c] \right\}^{1/3}. \quad (17)$$

Additionally, multiple correlations are available to estimate the terminal Froude number Fr_∞ , which is the mean Froude number as the bubble rise velocity becomes statistically stationary. For instance, Wallis³⁹ suggested the correlation

$$Fr_\infty = 0.345(1 - e^{-0.01N_f/0.345})(1 - e^{(3.37 - Eo)/m}),$$

$$m = \begin{cases} 25 & \text{if } N_f < 18, \\ 69 N_f^{-0.35} & \text{if } 18 < N_f < 250, \\ 10 & \text{if } N_f > 250. \end{cases} \quad (18)$$

Tung and Parlange⁴⁰ suggested the correlation

$$Fr_\infty = \sqrt{0.136 - 0.944 \frac{\sigma}{\rho_\ell g D^2}}. \quad (19)$$

Viana *et al.*⁴¹ suggested the correlation

$$Fr_\infty = \frac{0.34}{(1 + 3805/Eo^{0.306})^{0.58}} \quad (20)$$

for large buoyancy Reynolds numbers ($N_f > 200$).

The species transfer in the Taylor bubble flow is characterized by the Schmidt number Sc , which is defined as

$$Sc \equiv \frac{\nu_\ell}{\mathcal{D}_\ell}, \quad (21)$$

where ν_ℓ is the kinematic viscosity of the liquid phase, and the Sherwood number

$$Sh \equiv \frac{k_\ell D}{\mathcal{D}_\ell}, \quad (22)$$

where k_ℓ is the averaged species transfer coefficient at the gas-liquid interface. Sometimes the Schmidt number and the Reynolds number are combined, yielding the Péclet number, defined as

$$Pe \equiv ScRe = \frac{u_b D}{\mathcal{D}_\ell}. \quad (23)$$

Van Baten and Krishna⁴² suggested that the Sherwood number follows the scaling law

$$Sh \sim Pe^{0.5}. \quad (24)$$

Hosoda *et al.*⁷ developed an empirical correlation

$$Sh_{d_{eq}} = (0.489\lambda^2 - 0.691\lambda + 2.064)Pe_{d_{eq}}^{0.5}, \quad (25)$$

where $Sh_{d_{eq}}$ and $Pe_{d_{eq}}$ are the corresponding dimensionless numbers computed with the equivalent spherical diameter d_{eq} as the characteristic length scale, instead of the pipe diameter D . This model is valid in the range $0.61 \leq \lambda \leq 2.0$ and was constructed on the basis of experiments carried out for $12.5 \text{ mm} \leq D \leq 25 \text{ mm}$.

C. Numerical methods

The solver is developed based on the multiphase flow solver InterFOAM from OpenFOAM 22.12. The governing equations (1)–(4) are solved with the finite volume method (FVM) in this solver. The solution is advanced in time with the second-order implicit backward method. The convection terms of the momentum and species equations (2) and (4) are discretized with a second-order central difference scheme.

In the standard InterFOAM solver, an interface compression term is implemented in the color function equation (3) to sharpen the interface. In the FVM, Eq. (3) is discretized in a control volume as

$$\frac{\partial \alpha}{\partial t} + \sum_f (\alpha u_i)_f S_{i,f} + \sum_f (\alpha(1-\alpha)u_{ri})_f S_{i,f} = 0, \quad (26)$$

where $S_{i,f}$ denotes the surface vector component of face f of the corresponding control volume. The flux of the first convective term $(\alpha u_i)_f$ is discretized using a second-order van Leer scheme.⁴³ The second flux $(\alpha(1-\alpha)u_{ri})_f$ is initially discretized using an interface compression scheme, in which $u_{ri,f}$ is calculated as

$$u_{ri,f} = n_{i,f} \min [C_\alpha |\mathbf{u}_f|, \max (|\mathbf{u}_f|)]. \quad (27)$$

The max operator in the equation gives the maximum value of the velocity magnitude over all faces of the local control volume. The constant C_α is set to 1 in this study. $n_{i,f}$ is a component of the interface-normal direction vector $\mathbf{n}_f$, which is calculated as

$$\mathbf{n}_f = \frac{(\nabla \alpha)_f}{|(\nabla \alpha)_f + \delta|}, \quad (28)$$

where δ is a small value. Then, a multidimensional universal limiter with explicit solution (MULES) algorithm is used in the solver to correct the compression velocity $u_{ti,f}$ to ensure the local conservation of each phase and that α is bounded between 0 and 1. We have used the standard InterFOAM solver based on this method to simulate a single rising bubble with interfacial species transfer⁴⁴ and multiple bubbles.⁴⁵

The standard interFoam solver has been successfully applied to many two-phase flow problems. However, when the flow around a Taylor bubble becomes turbulent, DNS using the standard interFoam formulation can still exhibit significant parasitic currents. This is due to the interaction between interfacial instabilities and transient turbulent vortices, which amplifies spurious velocities.

To mitigate parasitic currents, we employ staggered meshes in the present study instead of body-fitted meshes. Although this approach introduces geometric inaccuracies in representing the pipe wall surface, it enables the generation of meshes with exceptionally high quality, characterized by a unit aspect ratio and near-zero skewness. This substantially reduces parasitic currents, which are known to be highly sensitive to mesh quality.

Additionally, it is found that the parasitic currents make the slip boundary condition at the gas–liquid interface no longer valid, which is nonphysical. We compute the tangential velocity at the interface with

$$u_{t,i} = u_i - (u_j n_j) n_i. \quad (29)$$

The dissipation rate due to its gradient in the interface-normal direction is calculated as

$$\varepsilon_t = \mu n_j n_k \frac{\partial u_{t,i}}{\partial x_j} \frac{\partial u_{t,i}}{\partial x_k}. \quad (30)$$

The value of ε_t is zero if the slip boundary condition is perfectly satisfied at the interface. However, the VOF results show that it is nonzero, owing to parasitic currents. We use ε_t to quantify the strength of the parasitic currents. Using the relative velocity $u_i - u_{i0}$, where u_{i0} is the bubble velocity in the moving frame, as the characteristic velocity, we are able to construct an artificial force

$$s_i = -A_s \rho \alpha (1 - \alpha) (u_i - u_{i0}) \left(\frac{\varepsilon_t}{\mu} \right)^{1/2}, \quad (31)$$

which is added to the momentum equation (2) to subtract the kinetic energy at the interface, and thus control the parasitic currents and stabilize the interface. The constant A_s is set to 1. As can be seen, s_i becomes zero (i.e., vanishes) if no parasitic currents occur.

III. DESCRIPTION OF TEST CASES

In this study, we try to represent the experiments on freely rising Taylor bubbles by Kastens and others.^{8,9,46,47} The main parameters in these experiments are shown in Table I.

We adopt the same fluid properties as in the experiment, which considers CO₂ bubbles rising in water. The Schmidt number for CO₂ in water is ~600. However, resolving species transport at such a high Schmidt number is not feasible in DNS with our available computational resources. Therefore, we perform simulations at reduced Schmidt numbers ($Sc = 1, 4, 16, 64$, and 256) to investigate the effect of the Schmidt number on interfacial species transfer.

TABLE I. Main parameters for the test cases.

	Case A	Case B	Case C
D (mm)	6	7	8
λ	1.43	1.43	1.43
Eu	4.9	6.7	8.7
N_f	1456	1834	2241
Ca	9×10^{-5}	3.1×10^{-4}	5.3×10^{-4}
Mo	2.6×10^{-11}	2.6×10^{-11}	2.6×10^{-11}
Sc	1–256	1–256	1–256
Flow regime	Transition	Turbulence	Turbulence

The computational domain is a vertical pipe of height $H = 8D$. Using the PID controller [Eq. (9)], the domain is translated to follow the rising bubble at the same instantaneous velocity. As a result, the bubble center remains fixed in the computational frame throughout the simulation. A uniform velocity field $(0, 0, -u_b)$ is prescribed at the upper and side-wall boundaries, where u_b is the transient bubble rise velocity. A fixed relative pressure $p = 0$ is imposed at the lower boundary. A no-slip boundary condition with $\alpha = 0$ is given at the wall surface. The concentration c is set to zero at the top boundary

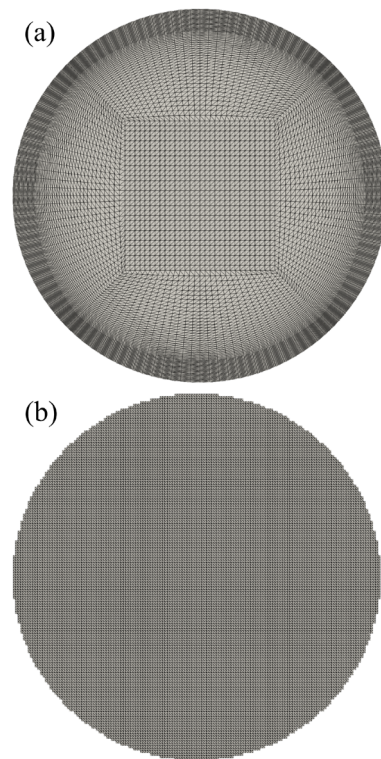


FIG. 2. Computational meshes in a cross-section considered in the study. (a) Mesh I is a body-fitted mesh with 1.4×10^7 cells, a maximum aspect ratio of 8.3, and a maximum skewness of 0.88. (b) Mesh II is a staggered mesh with 2.1×10^7 cells, a uniform aspect ratio of 1.0, and a uniform skewness of 0.0. Mesh II is finally selected for the DNS.

(inlet), while a zero-gradient condition is applied at the remaining boundaries.

Two types of meshes are considered in this study. The first mesh (mesh I) is a body-fitted mesh, with cells clustered near the wall. A cross-sectional view of this mesh is shown in Fig. 2(a). The mesh quality, characterized by a maximum aspect ratio of 8.3 and a maximum skewness of 0.88, is excellent for single-phase simulations. Mesh II is a staggered mesh. Although it introduces some geometric inaccuracy near the wall, it provides nearly perfect mesh quality, with a uniform aspect ratio of 1.0 and zero skewness. Based on the effect of these two meshes on parasitic currents (see Sec. IV A), mesh II is selected for the DNS study. Approximately 2.1×10^7 cells are used in all DNS cases. In addition, case C is also computed using two coarser resolutions, namely, 1.2×10^7 cells (mesh II2) and 6.3×10^6 cells (mesh II3), to assess the sensitivity of the DNS results to mesh resolution. In addition, we have calculated a test case in a longer pipe ($H = 10D$) using the resolution of mesh II3 to evaluate the effect of the computational domain.

Adaptive time stepping is employed in the DNS. On the basis of our previous DNS studies of bubbly flows, both the maximum Courant number (based on the fluid velocity) and the maximum interface Courant number (based on the interfacial velocity) are limited to 0.15. Using mesh II under these Courant–Friedrichs–Lewy (CFL) constraints, the mean time steps are 2.3×10^{-6} s for case A, 3×10^{-6} s for case B, and 2.2×10^{-6} s for case C.

IV. RESULTS AND DISCUSSION

A. Preparation for the computation

To investigate the influence of the numerical method on parasitic currents, case C is computed using the two meshes shown in Fig. 2, with and without extracting kinetic energy associated with parasitic currents at the bubble interface. Figure 3 presents snapshots of the instantaneous velocity magnitude obtained using the different approaches.

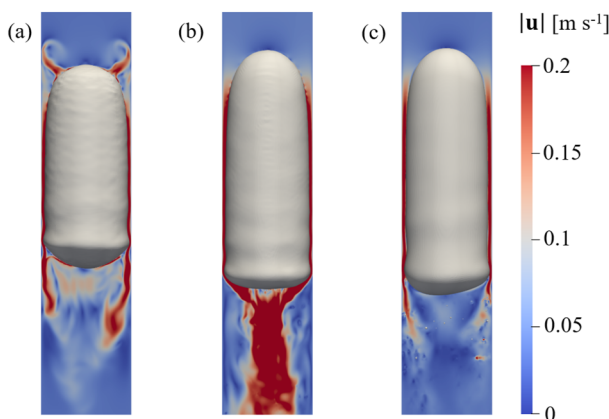


FIG. 3. Numerical results for the instantaneous velocity magnitude $|u|$ of case C: (a) using a body-fitted mesh; (b) and (c) using a staggered mesh respectively without and with extraction of kinetic energy due to parasitic currents at the interface. The method in (c) is used in the DNS study.

When the body-fitted mesh is used [Fig. 3(a)], significant non-physical recirculation is observed near the bubble nose, despite the excellent mesh quality for single-phase simulations. These spurious flows near the bubble nose largely disappear when the staggered mesh is employed [Fig. 3(b)]; however, oscillations remain visible along the interface. More importantly, liquid attaches to the bubble tail owing to an unrealistic bubble shape, leading to an over-predicted bubble Reynolds number. It should be noted that the errors induced by the parasitic currents cannot be effectively suppressed solely by increasing the mesh resolution.

When the staggered mesh is combined with kinetic-energy extraction at the interface, parasitic currents are effectively suppressed and a much smoother and more realistic interface is obtained [Fig. 3(c)]. A recirculation zone forms downstream of the bubble, consistent with the experimental observations by Kexel *et al.*⁹ On the basis of these results, this method is adopted for the DNS study.

Figure 4 shows the time evolution of the bubble Reynolds number $Re(t)$ and the Sherwood number $Sh(t)$ at $Sc = 1$. Both quantities oscillate about constant mean values after $t = 0.4$ s, indicating that

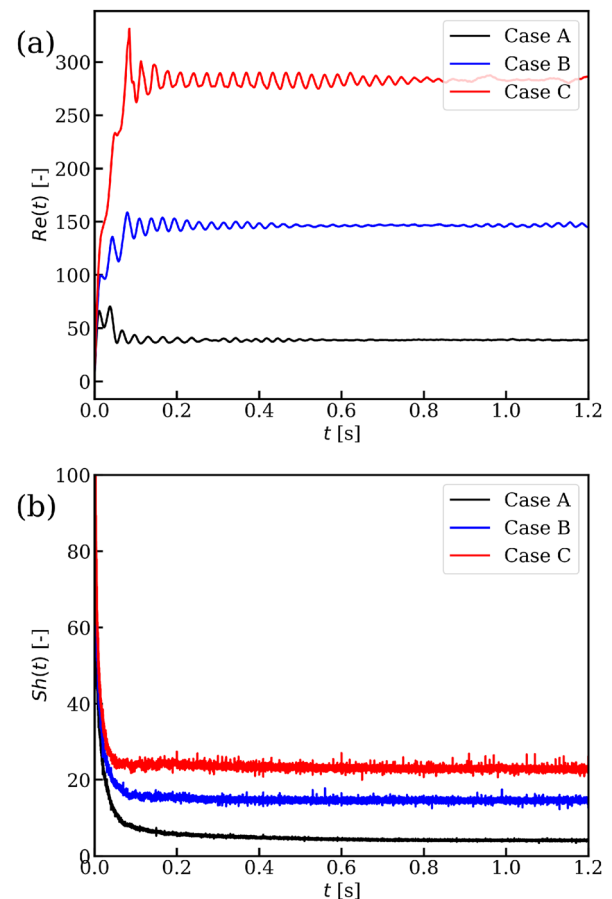


FIG. 4. Time evolution of (a) transient Reynolds number $Re(t)$ and (b) Sherwood number $Sh(t)$ at $Sc = 1$.

the flow and concentration fields have reached a statistically stationary state. We therefore continued the simulations for at least an additional 1 s to collect the statistics.

Figure 5 shows the mean axial velocity u_z and mean radial velocity u_r obtained using different mesh resolutions. It can be observed that insufficient mesh resolution may lead to an over-prediction of the deviation in u_z . The difference between the results obtained with meshes II and II2 provides an estimate of the numerical uncertainty in the present DNS. Nevertheless, this uncertainty does not affect the analysis in this study. Additional mesh-independence and validation studies were also conducted, including assessments of the effects of mesh resolution on the predicted bubble Reynolds number and Sherwood number. These results are presented and discussed in the following sections.

Figure 6 shows the mean vertical velocity u_z along the pipe axis. In the present DNS study ($H/D = 8$), the upper boundary is located $2D$ above the bubble head, while the lower boundary is located $3.25D$ below the bubble tail. Because the liquid ahead of the rising bubble is quiescent, both the velocity and pressure fields remain nearly uniform within $\sim 0.75D$ upstream of the bubble head, indicating that the

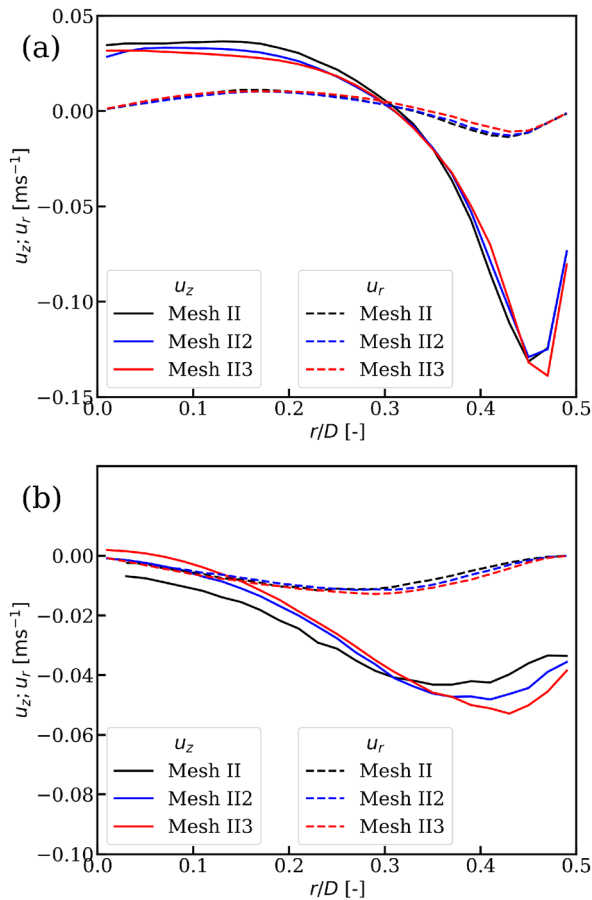


FIG. 5. Mean axial velocity u_z and radial velocity u_r in cross-sections (a) $0.1D$ and (b) $0.5D$ from the bubble tail. The results obtained using mesh II (2.1×10^7 cells), mesh II2 (1.2×10^7 cells), and mesh II3 (6.3×10^6 cells) are compared.

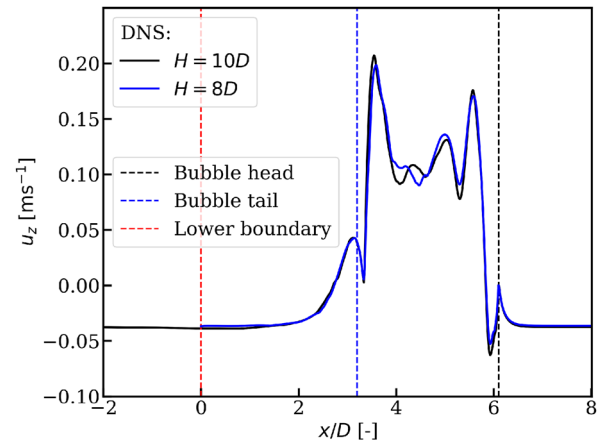


FIG. 6. Effect of pipe height H on mean axial velocity u_z at the pipe axis. The locations of the bubble head, bubble tail, and the lower boundary in the DNS are indicated.

upper boundary has a negligible influence on the bubble dynamics. As shown in Fig. 6, the mean vertical velocity u_z becomes nearly constant for $x/D \leq 1$, while the lower boundary of the DNS domain is located at $x/D = 0$. This result suggests that the influence of the outlet boundary is confined to a narrow region close to the boundary. By contrast, the statistical quantities reported in this study are sampled at $x/D = 2.75$ and 3.75 , which are well outside the affected region. Therefore, the influence of the lower boundary on the reported DNS statistics is negligible. It can also be observed in Fig. 6 that u_z changes very slightly as H/D increases from 8 to 10.

B. Shapes of Taylor bubbles

The gas-phase color function α is time-averaged to obtain the mean field $\bar{\alpha}$. The bubble interface, defined by $\bar{\alpha} = 0.5$, is shown in Fig. 7. The DNS results are compared with the experimental measurements of Kastens *et al.*⁸ for $D = 6$ mm (case A) and $D = 8$ mm

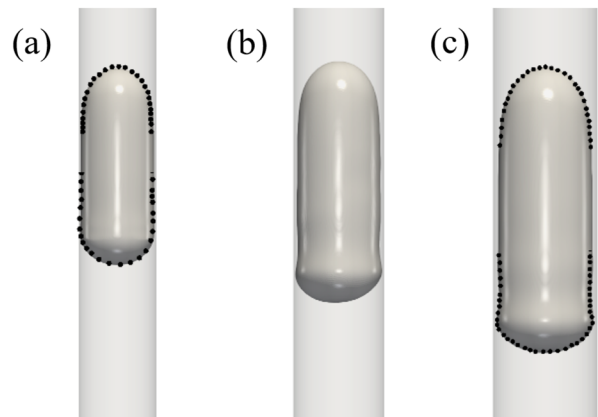


FIG. 7. Bubble shapes indicated by $\bar{\alpha} = 0.5$ for (a) case A, (b) case B, and (c) case C in Table I. The DNS results (in gray) are compared with experimental data digitized from Kastens *et al.*⁸ (solid circular symbols).

(case C), which are indicated by solid circular symbols in Fig. 7. Overall, the DNS predictions agree well with the experimental data. As the pipe diameter increases, the bubble tail becomes flatter, which promotes the formation of a recirculation zone in the wake.

The bubble film thickness is not uniformly distributed. Near the bubble tail, the interface first contracts and then expands. This behavior produces a local maximum film thickness $l_{\max}$, and a local minimum film thickness $l_{\min}$. The values of $l_{\max}$, $l_{\min}$, and the film thickness at the bubble mid-length, l_m , are compared with the correlation equation (17) proposed by Brown, see Fig. 8.³⁸ Overall, the correlation lies between $l_{\min}$ and $l_{\max}$. At larger Eo , where the bubble Reynolds number is higher, the correlation prediction approaches $l_{\min}$ more closely.

C. Flow fields and statistics

Figure 9 compares the DNS results for the bubble terminal Froude number with the experiments by Kastens *et al.*⁸ and the correlations proposed by Wallis,³⁹ Tung and Parlange,⁴⁰ and Viana *et al.*⁴¹ Overall, the DNS results are in good agreement with the experiments, although slightly lower Fr_{∞} values are observed at large Eo . Results from lower-resolution DNS are also shown for comparison, indicating that Fr_{∞} is over-predicted when the mesh resolution is insufficient.

At higher Eo values (6.7 and 8.7), the DNS results fall between the correlations of Wallis³⁹ and Viana *et al.*⁴¹ However, at a lower Eo of 4.9, both DNS and experiments show smaller Fr_{∞} values. This discrepancy arises because the buoyancy Reynolds number for this case is $N_f = 1456$, near the upper end of the transition regime ($500 < N_f < 1500$),³⁷ and much higher than the critical value of 200 reported by Viana *et al.*⁴¹ Despite this, the flow at $Eo = 4.9$ is nearly laminar, resulting in a thinner liquid film and lower bubble rise velocity than predicted by the correlations.

Figure 10 shows snapshots of the instantaneous velocity vectors of the liquid phase in the wake of the bubble. The bubble is shown in three dimensions to illustrate its three-dimensional shape. The velocity vectors, however, are plotted on a cross-sectional plane

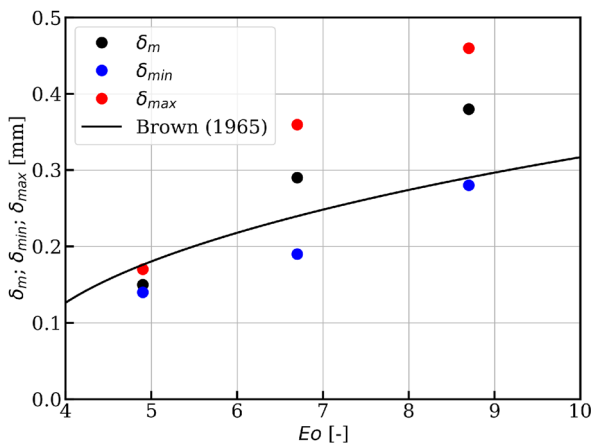


FIG. 8. DNS results for film thickness $l_{\max}$, $l_{\min}$, and δ_m , compared with Eq. (17) proposed by Brown.³⁸

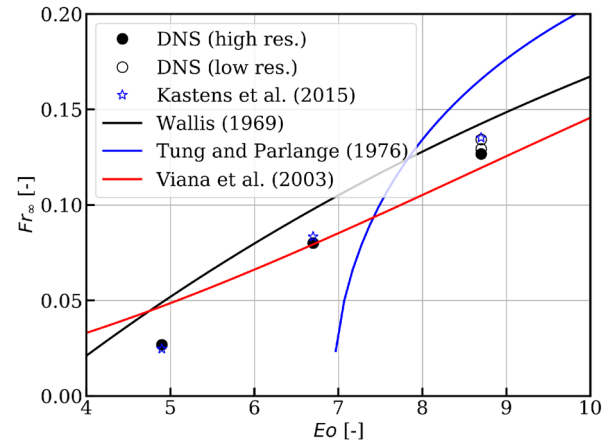


FIG. 9. Comparison of the DNS results for bubble terminal Froude number with the experiment by Kastens *et al.*⁸ and the correlations proposed by Wallis,³⁹ Tung and Parlange⁴⁰ and Viana *et al.*⁴¹

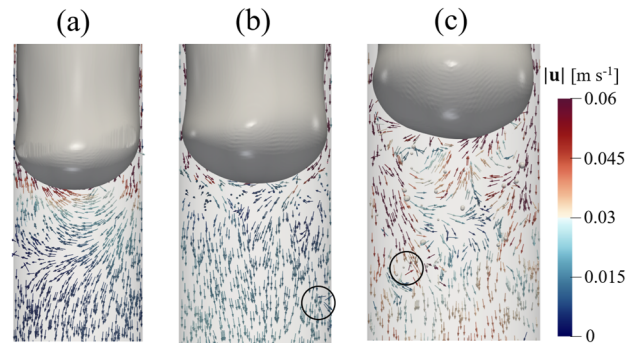


FIG. 10. Snapshots of instantaneous velocity vectors in the wake colored with the velocity magnitude for (a) case A, (b) case B, and (c) case C. The vortices outside the primary recirculation region are indicated by circles.

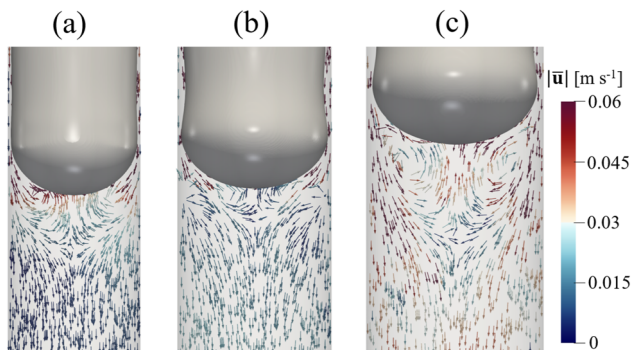


FIG. 11. Snapshots of mean velocity vectors in the wake colored with the velocity magnitude for (a) case A, (b) case B, and (c) case C.

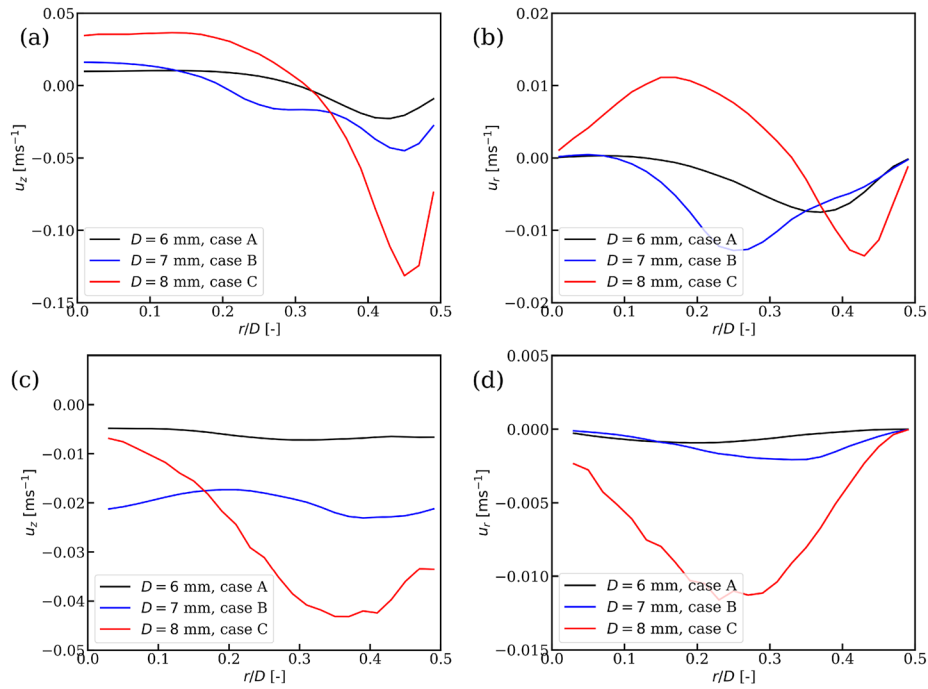


FIG. 12. Mean axial velocity u_z [(a) and (c)] and radial velocity u_r [(b) and (d)] in cross-sections 0.1D [(a) and (b)] and 0.5D [(c) and (d)] from the bubble tail.

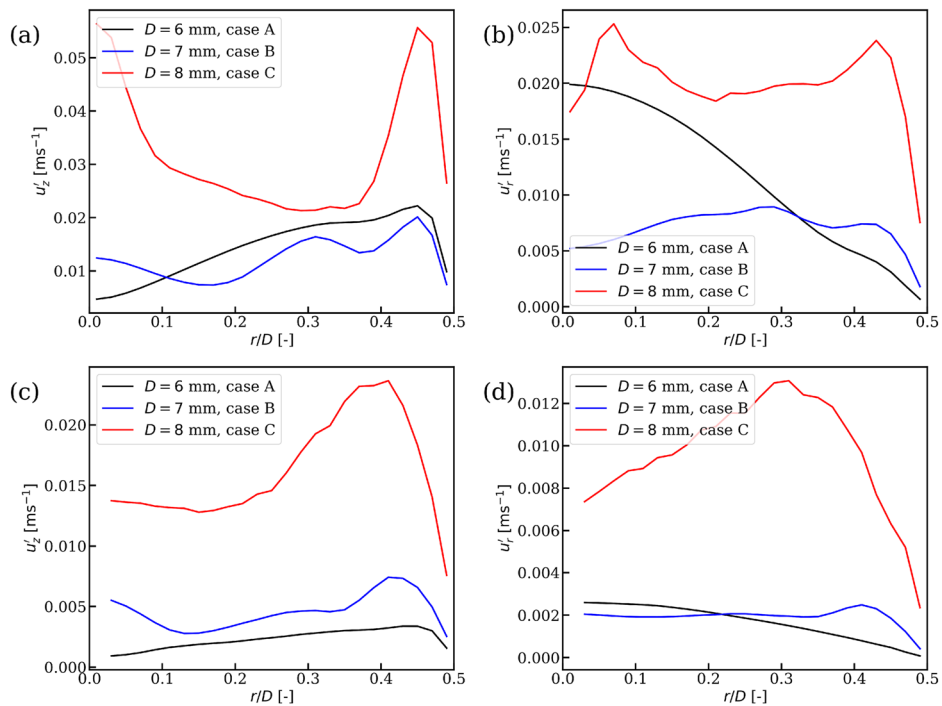


FIG. 13. rms axial velocity u'_z [(a) and (c)] and radial velocity u'_r [(b) and (d)] in cross-sections 0.1D [(a) and (b)] and 0.5D [(c) and (d)] from the bubble tail.

to show the wake recirculation structures more clearly. Case A ($D = 6$ mm) is still within the transition regime, as suggested by Nogueira *et al.*³⁷ The non-axisymmetric wake is clearly visible in Fig. 10, indicating that the liquid flows from the right side to the left at this instant. The time-averaged velocity vectors [Fig. 11(a)] reveal two vortices near the bubble tail and the pipe wall.

Cases B and C are in the fully turbulent regime. Randomly located recirculation regions can be observed far from the bubble tail in these cases [Figs. 10(b) and 10(c)], consistent with the observation that open wakes with recirculatory flow exist in the fully turbulent regime.³⁷ The vortices indicated by the mean velocity vectors gradually shift toward the pipe axis as Eo increases [Fig. 11(b)] and also become larger.

We perform time-averaging of the velocity field to obtain the mean axial and radial velocities (u_z and u_r) and their rms values (u'_z and u'_r). Figure 12 shows the distributions of u_z and u_r in cross-sections located $0.1D$ and $0.5D$ downstream of the bubble tail. A wall jet develops along the pipe wall at the Taylor bubble tail, where the liquid leaving the thin film accelerates along the boundary. This is clearly visible as a high downward velocity in Fig. 12(a). The wall jet velocity increases with increasing Eo . At $Eo = 8.7$ (case C), a distinct backflow is observed, indicated by positive u_z and u_r . In the cross-section $0.5D$ downstream of the bubble tail, u_z and u_r remain nonuniformly distributed, but are negative, suggesting that this cross-section is near the outer edge of the recirculation zone.

Small recirculation zones are also observed near the bubble tail at $Eo = 4.9$ (case A) and $Eo = 6.7$ (case B), indicated by positive u_z [Fig. 12(a)]. However, u_r remains negative in these cases, suggesting that the liquid flows radially inward around the bubble tail. Further downstream, both u_z and u_r become nearly uniform across the cross-section.

The rms velocities u'_z and u'_r exhibit peak values along the wall jets (Fig. 13), which increase with Eo and gradually decay with distance from the bubble tail. Another peak appears near the pipe center at the bubble tail, arising from the instability of the gas–liquid interface; this peak disappears further downstream. In case A ($D = 6$ mm), a pronounced peak of u'_r is observed near the bubble tail and pipe axis [Fig. 13(b)] owing to the non-axisymmetric wake [Fig. 10(a)]. The rms velocities in cases A and B decrease to very small values at the cross-section located $0.5D$ downstream of the bubble tail.

D. Concentration fields and statistics

The species transport equation is solved for five Schmidt numbers ($Sc = 1, 4, 16, 64$, and 256) using the simulated flow field. Snapshots of the instantaneous concentration fields c for case C are shown in Fig. 14. Typical turbulent structures, manifested as chaotic and random concentration patterns, are clearly visible. As the Schmidt number increases, the concentration fluctuations exhibit smaller length scales.

Figure 15 shows the DNS results for the terminal Sherwood number Sh_∞ , compared with the experiments by Kastens *et al.*⁸ and the correlation [Eq. (25)] proposed by Hosoda *et al.*⁷ Owing to computational limitations, the maximum Schmidt numbers used in the DNS are smaller than that of CO_2 in water, which is of the order of 600. As shown in the figure, the DNS results are in good agreement with both the experiments and the correlation. The calculated

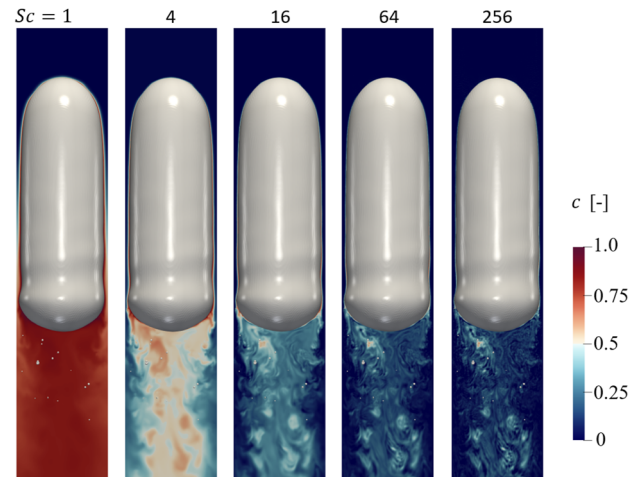


FIG. 14. Snapshots of instantaneous concentration fields for case C ($D = 8$ mm) at different Schmidt numbers.

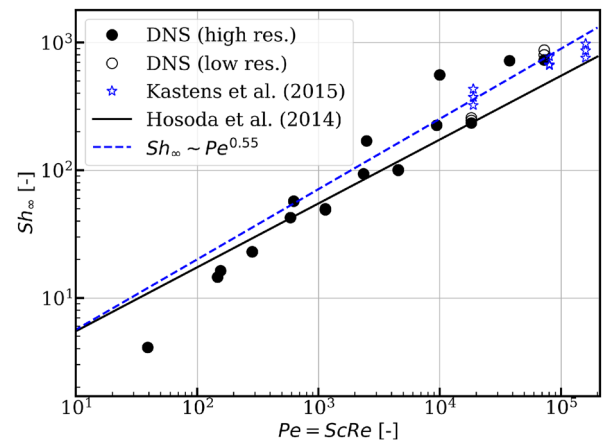


FIG. 15. Comparison of DNS results for bubble terminal Sherwood number Sh_∞ with the experiment by Kastens *et al.*⁸ and the correlation proposed by Hosoda *et al.*⁷

Sherwood numbers can be well fitted by the scaling law $Sh_\infty \sim Pe^{0.55}$ as $Pe \geq 600$, which is close to the scaling law $Sh_\infty \sim Pe^{0.5}$ for freely rising single bubbles.⁴⁴ When the mesh resolution is insufficient, DNS tends to over-predict Sh_∞ at high Péclet numbers. Furthermore, Sh_∞ might also be overestimated when parasitic currents are non-negligible. In the present study, we are still not able to fully control the parasitic current.

While Fig. 15 presents the terminal Sherwood numbers for all cases, we focus only on the statistics of fully turbulent species transfer (case C). Figure 16 shows the radial distribution of the mean concentration $\bar{c}$ at the bubble mid-length. The dashed lines for $\bar{\alpha} = 0.01$ and 0.99 are also shown in the figure to indicate the location of the resolved gas–liquid interface. The diffusion of the species originates from the inner side of this interface. The gradient of $\bar{c}$ increases with increasing Schmidt number, while it remains

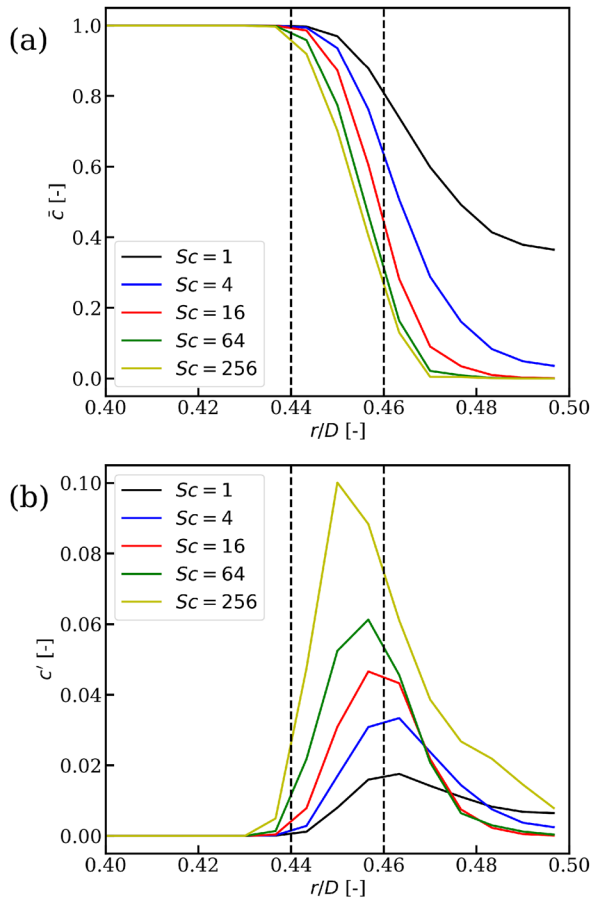


FIG. 16. (a) Mean concentration $\bar{c}$ and (b) its rms value c' in the cross-section at the bubble mid-length for different Schmidt numbers (case C, $D = 8$ mm). The resolved gas-liquid interface is indicated by the region between the two dashed lines.

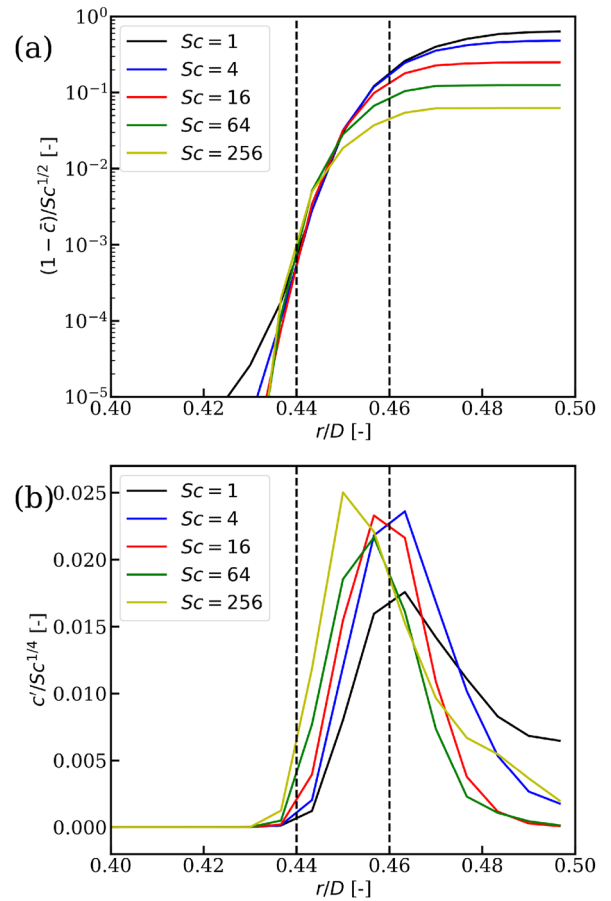


FIG. 17. (a) Normalized mean concentration $(1 - \bar{c})/Sc^{1/2}$ and (b) its rms value $c'/Sc^{1/4}$ in the cross-section at the bubble mid-length for different Schmidt numbers (case C, $D = 8$ mm). The resolved gas-liquid interface is indicated by the region between the two dashed lines.

close to zero near the wall. The profiles of $(1 - \bar{c})/Sc^{1/2}$ as a function of r/D for all Schmidt numbers nearly collapse near the interface [Fig. 16(a)], indicating that the local Sherwood number Sh_{loc} , defined as

$$Sh_{loc} = \frac{\mathcal{D} D}{\mathcal{D}_\ell} \left. \frac{d\bar{c}}{dr} \right|_{\bar{a}=0.5}, \quad (32)$$

follows the scaling law $Sh_{loc} \sim Sc^{0.5}$. This is consistent with the scaling of the global terminal Sherwood number, $Sh_\infty \sim Pe^{0.5}$. Additionally, fluctuations of c in the film are observed [Fig. 16(b)]. The peak of these fluctuations shifts toward the gas-liquid interface as Sc increases. The rms concentration c' follows the scaling $c' \sim Sc^{1/4}$, and so the scaled profiles $c'/Sc^{1/4}$ are generally identical [Fig. 17(b)].

Figure 18 shows the radial distributions of the mean concentration $\bar{c}$ and its rms value c' in the wake, comparing different Schmidt numbers. As expected, the mean concentration in

the wake decreases with increasing Sc , reflecting reduced molecular diffusion and weaker mixing. A local minimum of $\bar{c}$ occurs near the wall ($r/D = 0.5$), coinciding with the wall-jet region. The associated concentration gradient becomes progressively steeper as Sc increases.

Consistently, c' exhibits a pronounced peak near the wall jet, which decays with increasing downstream distance from the bubble tail. Toward the pipe center, both $\bar{c}$ and c' become more uniformly distributed, since the wake vortices [Figs. 10(c) and 11(c)] enhance radial mixing.

Figure 19 further shows that the profiles of $\bar{c}$ and c' collapse reasonably well when scaled by $Sc^{1/4}$, particularly at higher Schmidt numbers. These DNS results suggest scaling laws $\bar{c} \sim Sc^{1/4}$ and $c' \sim Sc^{1/4}$ in the wake. However, the Schmidt numbers considered in this DNS study are significantly lower than those encountered in real Taylor bubble systems, such as CO_2 dissolution in water. The obtained scaling laws should be further validated using additional cases.

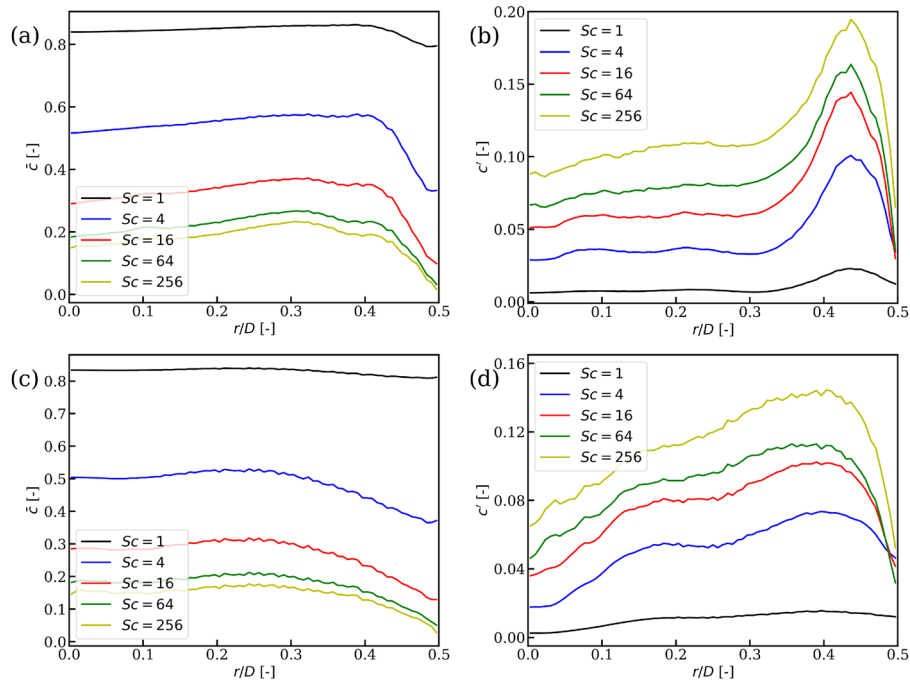


FIG. 18. Distributions of mean concentration $\bar{c}$ [(a) and (c)] and its rms value c' [(b) and (d)] for different Schmidt numbers in the cross-sections $0.01D$ [(a) and (b)] and $0.5D$ [(c) and (d)] downstream of the bubble (case C, $D = 8$ mm).

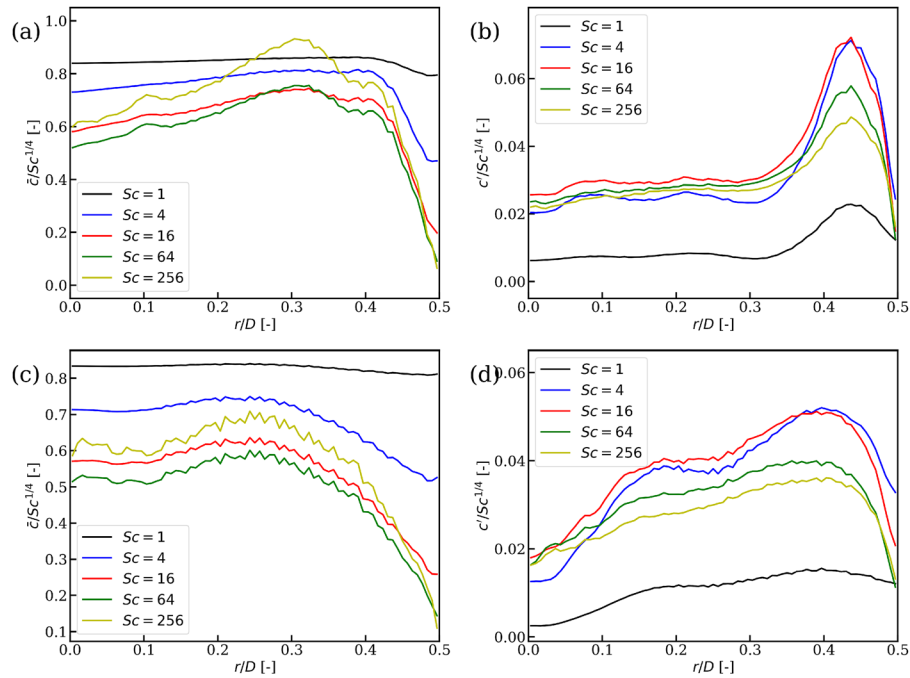


FIG. 19. Distributions of normalized mean concentration $\bar{c}/Sc^{1/4}$ [(a) and (c)] and its rms value $c'/Sc^{1/4}$ [(b) and (d)] for different Schmidt numbers in the cross-sections $0.01D$ [(a) and (b)] and $0.5D$ [(c) and (d)] downstream of the bubble (case C, $D = 8$ mm).

V. CONCLUSIONS

We performed a DNS study of the fluid flow and interfacial species transfer around single freely rising Taylor bubbles in a vertical pipe. The Eötvös number was varied from 4.9 to 8.7, the Reynolds number from 36 to 303, and the Schmidt number from 1 to 256. The properties of water and CO₂ were used, except that the Schmidt number was reduced compared with that of CO₂ in water owing to computational constraints. Turbulent motions were resolved directly without using any turbulence models. The gas–liquid interface was captured using a VOF method. To minimize parasitic currents, a staggered mesh with uniform aspect ratio 1.0 and skewness 0.0 was employed. In addition, we proposed a new method for controlling parasitic currents by extracting the kinetic energy associated with the parasitic currents near the interface. This method effectively suppresses parasitic currents and improves the robustness of the simulations.

We compared the bubble shape, film thickness (δ_m , $\delta_{\min}$, and $\delta_{\max}$), terminal Froude number Fr_∞ , and terminal Sherwood number Sh_∞ with experiments and established correlations to validate our DNS results. The simulations provide detailed information about the flow and concentration fields around the Taylor bubbles. The DNS results show a non-axisymmetric wake at $Eo = 4.9$, consistent with the transition regime described by Nogueira *et al.*³⁷ As the Eötvös number Eo increases, the bubble tail becomes flatter. The interface contracts near the tail and then expands, resulting in a minimum film thickness $\delta_{\min}$ that is much lower than the mean thickness δ_m . A wall jet forms as the liquid leaves the thin film, indicated by a high downward velocity u_z and peaks in the rms velocities u'_z and u'_r . This wall jet generates a large recirculation region downstream of the bubble at high Eo . In these cases, the recirculation region is open, and some randomly located vortices can be observed far from the bubble, although they are not present in the time-averaged field.

The instantaneous concentration field in case C reveals typical chaotic and irregular turbulent structures, which extend to smaller length scales as the Schmidt number increases. Diffusion occurs from the inner side of the resolved gas–liquid interface, while the mean concentration $\bar{c}$ approaches a constant value near the wall. The distance required to reach this constant value decreases with increasing Schmidt number. The DNS results show a peak in the concentration fluctuation c' within the film, which grows with increasing Schmidt number. To the best of our knowledge, this phenomenon has not been reported previously. Additionally, c' follows the scaling law $c' \sim Sc^{1/4}$ in the film. In the wake, the mean concentration is lowest near the wall and becomes nearly uniform toward the pipe axis. A peak in c' is also observed in the wake, located near the wall jet, and it gradually decays downstream. This fluctuation also increases with increasing Schmidt number. The mean concentration $\bar{c}$ and the concentration fluctuation c' generally follow the scaling laws $\bar{c} \sim Sc^{1/4}$ and $c' \sim Sc^{1/4}$ in the wake. These scaling behaviors have not been reported previously either.

The study demonstrates that DNS is a powerful tool for revealing detailed features of turbulent flow and species transfer around Taylor bubbles. However, controlling parasitic currents is critical, since they become significant when the sharp gas–liquid interface interacts with turbulent motions. While this study presents effective

strategies to mitigate parasitic currents, further efforts are required to fully suppress them. In addition, the highest Schmidt number considered in this DNS study is $Sc = 256$, which remains significantly lower than the value for CO₂ in water. As a result, the scaling relationships derived here should be interpreted with caution when extended to higher Schmidt and Péclet number regimes. For example, the present data suggest a scaling $Sh \sim Pe^{0.55}$, which provides the best fit to the DNS results. However, this deviates slightly from the classical scaling $Sh \sim Pe^{0.5}$, indicating remaining uncertainty in the extrapolation to realistic operating conditions. Therefore, further high-Schmidt-number simulations or experimental validation are required to confirm the applicability of these scaling laws in practical CO₂–water systems.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Yan Jin: Conceptualization (equal); Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (lead); Project administration (equal); Resources (equal); Software (equal); Supervision (lead); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Kamal Ouro-Koura:** Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Writing – original draft (equal); Writing – review & editing (equal). **Arne Speerforck:** Conceptualization (equal); Project administration (equal); Software (equal); Supervision (equal); Writing – review & editing (equal). **Michael Schlüter:** Conceptualization (equal); Funding acquisition (lead); Project administration (equal); Resources (equal); Software (equal); Supervision (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

NOMENCLATURE

a_{Fi}	artificial acceleration rate to keep bubble location (m/s ²)
c	species concentration
Ca	capillary number
D	pipe diameter (m)

$\mathcal{D}$	mean diffusion coefficient (m^2/s)
$\mathcal{D}_g$	diffusion coefficient in gas phase (m^2/s)
$\mathcal{D}_\ell$	diffusion coefficient in liquid phase (m^2/s)
Eo	Eötvös number
$f_{\sigma i}$	surface tension force [$\text{kg}/(\text{m} \cdot \text{s}^2)$]
Fr	Froude number
Fr_∞	terminal Froude number
Mo	Morton number
N_f	buoyancy Reynolds number
$n_{i,f}$	interface-normal direction vector
Pe	Péclet number
Re	bubble Reynolds number
s_c	source term in species equation (s^{-1})
s_i	artificial force to extract kinetic energy due to parasitic currents [$\text{kg}/(\text{m} \cdot \text{s}^2)$]
Sc	Schmidt number
Sh	Sherwood number
Sh_∞	terminal Sherwood number
U_{ri}	compression velocity component (m/s)
u_i	velocity component (m/s)
$u_{t,i}$	tangential velocity component at interface (m/s)

Greek

α	bubble color function
δ_m	mean film thickness (m)
$\delta_{\max}$	maximum film thickness (m)
$\delta_{\min}$	minimum film thickness (m)
ε_t	dissipation rate due to parasitic currents [$\text{kg}/(\text{m} \cdot \text{s}^3)$]
κ	curvature of gas–liquid interface (m^{-1})
λ	ratio of equivalent bubble diameter to pipe diameter
$\bar{\mu}$	mean dynamic viscosity [$\text{kg}/(\text{m} \cdot \text{s})$]
$\bar{\mu}_g$	dynamic viscosity of gas [$\text{kg}/(\text{m} \cdot \text{s})$]
$\bar{\mu}_\ell$	dynamic viscosity of liquid [$\text{kg}/(\text{m} \cdot \text{s})$]
$\bar{\rho}$	mean density (kg/m^3)
σ	surface tension coefficient (kg/s^2)

Abbreviations

DNS	direct numerical simulation
FT	front-tracking
LES	large eddy simulation
LS	level-set
RANS	Reynolds-averaged Navier–Stokes
VOF	volume-of-fluid

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