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Validation of Interface Capturing and Tracking techniques with different surface tension treatments against a Taylor bubble benchmark problem ☆

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ABSTRACT

The validation and verification of models and numerical methods for interfacial two-phase flow simulation is still a challenge and standards have not yet been established. Mostly comparing with analytical solutions, many validation studies so far have considered simple or simplified two-phase flow scenarios. While this is mandatory for method development, complementary, validation against more complex test-cases is essential, in order to prove the method's final scope of capabilities. However, one reason for the absence of such two-phase flow benchmark studies is the lack of freely accessible, detailed and high-quality experimental data.

The Priority Program SPP 1506 *Transport Processes at Fluidic Interfaces* by the German Research Foundation DFG proposes a benchmark problem for validation of interfacial two-phase flow solvers by means of specifically designed experiments for Taylor Bubble Flow. The benchmark experiments aim at providing detailed and local data as a basis for validation. This contribution demonstrates its use by assessing and approving the reliability and accuracy of the solvers used by several research groups within the priority program. Special emphasis is set upon different approaches to surface tension calculation both for interface capturing and interface tracking methods. Data and material of the presented benchmark can be freely downloaded from the website of SPP 1506 (http://www.dfg-spp1506.de/taylor-bubble).

1. Introduction

Taylor bubbles are elongated bubbles which almost completely fill the cross-sectional area of (commonly) straight channels – without wetting its confining walls but being surrounded by a thin liquid film. The flow of multiple subsequent Taylor bubbles in a channel is known as *Taylor flow* (also: bubble train flow), where a *liquid slug* separates two subsequent Taylor bubbles.

Taylor flow in narrow channels is used in many micro-fluidic applications, inter alia, micro-process engineering, catalysis (coated monolith reactors), material synthesis, analysis of biological or chemical probes. Recent reviews of Taylor flow are given in [1,2].

Main advantages of Taylor flow in milli- or micro-channels are its

- high values of specific exchange area (interfacial area density per unit volume), and consequently its high heat and mass transfer rates,
- low axial dispersion due to separation of the liquid by bubbles into distinct slugs,
- high mixing rates within the liquid slugs due to recirculation and
- short diffusion lengths for mass transfer from the gaseous phase through the thin liquid film to the channel wall (e.g., a catalytic wash-coat).

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1.1. Hydrodynamics of Taylor bubbles

The hydrodynamics of Taylor bubbles in small (milli/micro-) channels is predominately determined by viscous (friction) and surface tension forces, with the inertial forces becoming important only at higher flow velocities. The relevant dimensionless groups are the Capillary number $\mathrm{Ca} = \eta_L U_B/\sigma$ (ratio of viscous to surface tension force) and the Reynolds number $\mathrm{Re} = \rho_L d_h U_B/\eta_L$, where U_B denotes the magnitude of the bubble velocity, d_h the hydraulic diameter of the channel, σ the surface tension, and ρ_L and η_L the liquid density and dynamic viscosity, respectively.

As for the current state of scientific knowledge, it is stated in [1] that, while hydrodynamics of formed Taylor bubbles in fully developed flow and pure liquid systems is generally understood for cylindrical channels, further research is especially required for non-cylindrical channels. Since the interfacial area density is a central measure with respect to process intensification and performance of milli/micro-apparatus, the interfacial surface of a Taylor bubble at specific operation conditions is of pivotal interest. Moreover, diffusion lengths in Taylor bubble flow are directly related to process intensification and performance as well. Hence, due to their direct accessibility, relevant target quantities of experimental and theoretical studies are mostly related to the bubble's interface geometry:

Liquid film thickness. For cylindrical channels of diameter d the liquid film thickness δ is constant along the circumference of the bubble surface for a wide range of Ca and can be described by $\delta_F/d_B = 0.66\mathrm{Ca}^{2/3}/(1+3.33\mathrm{Ca}^2/3)$ – cf. [3,4]. The effect of inertial forces on the liquid film thickness is not significant up to $\mathrm{Re} \approx 50$ for $\mathrm{Ca} < 0.01$ [4, Fig. 5].
For quadratic channel cross-sections, it is known that the liquid film thickness is not constant, but varies along the circumference of the bubble's surface. For Ca in the range $0.04\ldots0.1$ transition takes place and the Taylor bubble can no longer be considered axis-symmetric [5,6], while for even lower values of Ca the bubble clearly penetrates into the corners of the channel.
Bubble shape. The front and rear end of the bubble obey the shape of hemispheres for low values of Ca. The higher the values of Ca, the lower the interfacial curvature on the channel axis at the bubble rear and the higher the curvature at its front. For high values of Ca the bubble's rear shows a dent, where the curvature of the trailing menisci becomes negative. Within the liquid slug a bypass flow can be observed for $\mathrm{Ca} > 0.7$, while for $\mathrm{Ca} < 0.7$ there is a recirculation flow [7].
For quadratic channel cross-sections the shape deformation of the Taylor bubble's front and rear is known to behave qualitatively similar to the circular case. Latest three-dimensional numerical studies [8] of Taylor bubble flow of viscous squalane and nitrogen in a quadratic channel show steepening of the front shape and flattening at the bubble's rear – in good agreement with experimental results. However, this study has been restricted to moderate/high values of Ca.

1.2. Validation benchmark with Taylor bubbles

Taylor bubbles as a validation benchmark provide the essential advantage of being predominantly governed by the Capillary number as control parameter: for given fluids the Capillary number can be varied by one to two orders of magnitude by changing the bubble velocity. Alternatively, an even larger variation can be achieved by changing the liquid's viscosity. A pivotal measure for validation of the hydrodynamics, employing different numerical methods and codes is the three-dimensional shape of the Taylor bubble for distinct values of Ca.

Ultimately, with the Taylor bubble validation benchmark, we aim at providing a comprehensive assessment and objective measure of accuracy and reliability of interfacial two- phase flow solvers. For this purpose, we propose this validation benchmark based on specifically designed high-resolution experiments to assess the interfacial shape of a Taylor bubble.[1] It is believed that such a detailed benchmark for two-phase flow is of similar use as single-phase benchmarks such as the 'NACA airfoil' [9,10] or the 'Ahmed car body' [11–13] for external flow configurations, and the rearward facing step [14] or the turbulent channel flow of [15] as for internal flow configurations, which have become established over the last two decades.

In this study, we perform Direct Numerical Simulations (DNS) of a single rising Taylor bubble in a square milli-channel, in order to examine the influence of various numerical methods for surface tension calculation for both interface capturing and interface tracking methods. Hence, our main focus is on the quantitative comparison of the shape of a rising Taylor bubble by means of geometrical target quantities (such as distances, curvatures and film thickness) at locations, where deficiencies in surface tension calculation procedures become visible. We compare different interfacial two-phase solvers and their underlying numerical methods – namely the Volume-of-Fluid (VoF) and Level-Set (LS) interface capturing methods as implemented in the codes FS3D, TURBIT-VOF and DROPS, and the Arbitrary Lagrangian Eulerian (ALE) interface tracking method of OpenFOAM – with detailed and local data obtained by high-resolution X-ray tomography.

In doing so, we present a code-to-experiment comparison for a realistic three-dimensional Taylor bubble flow problem. However, we shall also emphasize the relevance of basic (mostly simple or simplified) test cases for verification and validation (V&V) during method development. Targeted method development would be infeasible without such test cases, which enable to focus on single aspects of two-phase flow in a more isolated manner than it is possible with benchmarks exhibiting a complex interplay of multiple two-phase flow aspects. Simplifications or simplified scenarios often allow for an explicit analytical (or, exact) reference solution, with which numerical results can be compared. Both for interface capturing and for interface tracking methodologies such V&V test cases can be set out in two categories, namely purely numerical verification cases to test numerical algorithms or discretization methods regarding distinct terms within the governing equations, and physical validation cases to assess a selected model with respect to its capability to correctly capture a distinct interfacial condition, transport process or phenomenon. Advection tests, for instance, prescribe simple constant (translation and rotation advection tests) and complex, possibly time-varying (shear and deformation advection tests) velocity fields in order to evaluate numerical errors related to the advection term or algorithm, and to assess the corresponding interface-stability and shape-preserving properties of the method. Established cases with simple constant velocity fields are interface translation (cf. [16,17]) and rotation tests, e.g. the well-known Zalesak disk [18]. Moreover, tests in which complex velocity fields are prescribed have been established, such as interface shear and deformation tests as proposed in [19–21], to mention a few. Validation tests for surface tension implementations cover both static resp. steady and dynamic resp. unsteady cases, and help to assess the interfacial balance of surface tension, viscous and inertia effects. Well-known representatives are the static drop in equilibrium ('equilibrium rod') by Brackbill et al. [22–24], the so-called Bretherton problem for an elongated bubble in a tube [25] and the creeping flow around a single spherical

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[1] Detailed velocity field data shall be provided in a forthcoming publication in order to complement the present Taylor bubble benchmark.