Accuracy of two-phase flow simulations: The Taylor Flow benchmark

Sebastian Aland[1], **Christoph Lehrenfeld**[2,*], **Holger Marschall**[3], **Christoph Meyer**[4], and **Stephan Weller**[5]

[1] Institut für Wissenschaftliches Rechnen, TU Dresden, 01099 Dresden, Germany
[2] Institut für Geometrie und Praktische Mathematik, RWTH Aachen, Templergrabern 55, 52056 Aachen, Germany
[3] Center of Smart Interfaces, TU Darmstadt, Petersenstr. 17, 64287 Darmstadt, Germany
[4] Institut für Mehrphasenströmungen, TU Hamburg-Harburg, Eißendorfer Straße 38, 21073 Hamburg, Germany
[5] Angewandte Mathematik III, Dept. Mathematik, Universität Erlangen-Nürnberg, Cauerstr. 11, 91058 Erlangen, Germany

We detail on the relevance and characteristics of a Taylor Flow benchmark recently proposed within the framework of the Priority Program 'Transport Processes at Fluidic Interfaces' by the German Research Foundation (DFG-SPP1506).

1 Benchmarks for Two-Phase Flows

Numerical simulations of two-phase flows have reached a certain level of importance for process intensification and optimization in industry involving microfluidic applications. Improved schemes and algorithms for numerical simulations of systems with two immiscible fluids continuously arise and are subject to ongoing research efforts. However, the most common approach to verification and validation (V&V) of such methods is to qualitatively compare obtained interface shapes with those of reference solutions. For validation, such reference solutions commonly are compared to the bubble-shape diagrams of Clift et al. [1], Banga and Weber [2] or the interfacial shape from dam break experiments [3]. For verification, often Zalesak's moving disc [4] and the well-known Raleigh-Taylor instability are used. Such simple or simplified test problems can be very helpful for code development but they clearly are not sufficient for a comprehensive assessment in V&V context.

In the absence of exact, resp. analytical, reference solutions, numerical benchmarking (i.e. code-to-code comparison) is needed to assess the accuracy of the numerical models more rigorously. An important step in this direction was the benchmark proposed by Hysing et al [5] in 2009. It considers a single rising bubble in a liquid column in 2D and quantitatively compares benchmark quantities as rise velocity, bubble position and circularity over time. The original paper considers Level-Set and ALE methods, later Aland and Voigt [6] applied it to diffuse interface models. Although this benchmark has been intensely used since its publication, in the authors' view it lacks some aspects.

The benchmark idea in [5] is based on a code-to-code comparison, which certainly has to be considered critical given the fact that different approaches to numerical simulations of two-phase flows might yield apparently similar and physically plausible results while failing to reproduce experimental results quantitatively. Agreement among distinct methods are delusive and might be caused by (even different) errors and shortcomings of the underlying schemes or algorithms. Moreover, a single benchmark based on code-to-code comparison might involve the risk of another even more surreptitious problem: within one numerical approach two errors might compensate each other while reproducing the results of this single benchmark in what one would call 'good agreement'.

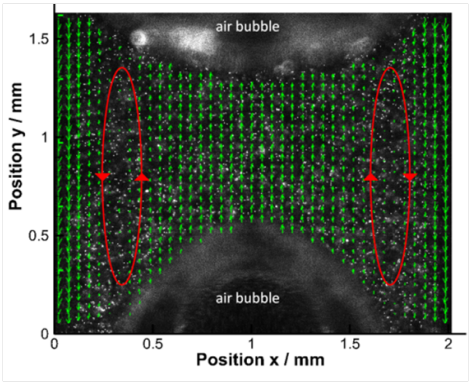
Another aspect to be addressed here in order to stress the need for further two-phase flow benchmarks is the somewhat limited scope in [5]: It is only interesting for 2D codes (effectively excluding pure 3D codes) and for a rather small range of surface tension coefficients. However, surface tension is of major importance for all codes aiming at two-phase flow simulations, since in many applications surface tension effects are predominant or at least play a central role. A simple bubble rise scenario as used in [5] can not assess the case of large surface tensions, since this just leads to spherical bubbles, making the surface evolution almost trivial.

It is the goal of this paper to promote an additional (complementary) benchmark which is highly sensitive to a large range of surface tensions and suitable for validation both in 2D and 3D based on high-resolution experiments. Such a benchmark has been recently detailed in a joint collaboration of different numerical and experimental groups within the framework of a Priority Program by the German Research Foundation (DFG-SPP1506). The benchmark considers a Taylor-Flow problem, which is of practical relevance. Section 2 gives an overview into the topic of Taylor-Flow. The mathematical model and the benchmark setup are described in Sec. 3. A collection of first results is presented in Sec. 4. Finally, Sec. 5 concludes this paper and gives an outlook on ongoing work.

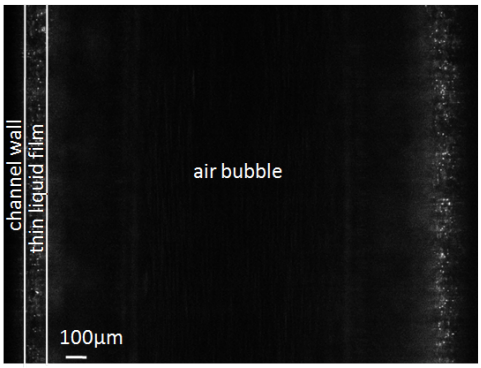
2 Taylor Flow

Taylor flow is encountered in many practical applications, such as multiphase monolith microreactors [7], heat-exchanger reactors [8] or fuel cells [9]. The Taylor flow regime in gas-liquid two-phase flow is characterized by a sequence of elongated

* Corresponding author: email lehrenfeld@igpm.rwth-aachen.de, phone +00 49 241 80 93954, fax +00 49 241 80 92394



(a) Recirculation flow pattern in a liquid slug of an upward gas liquid Taylor flow measured by micro-PIV.



(b) Raw μPIV image of the thin liquid film and the Taylor bubble. The film thickness is magnitudes smaller than the diameter.

Fig. 1: Raw μPIV images for the measurement of the flow fields around Taylor bubbles.

gas bubbles (Taylor bubbles), which move within a capillary channel. Although Taylor bubbles typically have diameters of approximately the channel width, there exists a liquid film between the Taylor bubbles and the channel wall. The surrounding fluid region at the front and rear of the Taylor bubbles separates the subsequent Taylor bubbles from each other (liquid slugs).

Figure 1a presents a typical sketch of the front and the rear of two Taylor bubbles in a minichannel as well as the recirculation within the liquid slug of an upward gas-liquid Taylor flow. Notably, Taylor flow in mini- or microchannels exhibits many advantages, e.g. low axial dispersion (due to separation by slugs), high heat and mass transfer rates (due to high interfacial area density per unit volume), high mixing rates within the liquid slugs (due to recirculation) and short diffusion lengths for mass transfer due to a characteristically thin liquid film between interface and channel wall (see Fig.1b). The film thickness certainly is a key parameter being important in many applications, such as catalyst coating in monolith reactors [10] and mass transfer from the channel wall to the liquid [7, 11], for instance. Restricting ourselves further to cases where surface tension effects become predominant, another advantage is that many aspects of the hydrodynamics of Taylor flow such as the liquid film thickness and the bubble shape depend mainly on one single parameter, i.e. the capillary number $\mathrm{Ca} := \eta_L \mathbf{u}_B / \tau$, where $\mathbf{u}_B$ denotes the bubble velocity, η_L the dynamic viscosity of the liquid and τ the surface tension coefficient.

The central characteristics of Taylor flow regime is its regularity in geometrical quantities that is all bubbles have approximately the same dimensions (i.e. length, width and mean curvatures). Moreover, the slug lengths (i.e. the distance between two successive bubbles) is nearly constant. Besides their dimensions and the slug length one of the main advantages for experimental investigations of Taylor flow regime is its high comparability (which however demands for exact reproducibility of experimental conditions). As for the numerical simulations, Taylor bubble flow is utmost demanding and there are numerous (sometimes method dependent) challenges. The thin liquid film between bubble surface and channel wall requires highly accurate schemes and efficient local mesh adaptivity. Moreover, considering the case of low Ca numbers, an accurate numerical model to surface tension becomes pivotal in order to capture correctly the bubble's shape (and consequently its drag).

Based on these characteristics Taylor flow forms an excellent and demanding gas-liquid two-phase flow system to study systematically. Therefore, Taylor flow is well suited for the validation of mathematical models and numerical methods for two-phase flow simulations. The investigations on Taylor bubbles are carried out both experimentally and numerically within the Priority Program by the German Research Foundation (DFG-SPP1506) 'Transport Processes at Fluidic Interfaces'. Despite the fact that square shaped channels are generally used in applications (e.g. monolith reactors) most investigations have been published for circular cross sections. Because hydrodynamics of Taylor flow in square channels are different from those of circular tubes (i.e. expansion of the bubble in the corners of the channel) the hydrodynamic characteristics in capillaries with *both circular and square* cross sections are subject to the presented benchmark of SPP 1506 as described in the remainder. So far, comparison studies were devoted to the Taylor bubble's interfacial shape only (cf. section 4). Validation studies regarding the flow field are to follow. Most experimental investigations deal with the flow field within the liquid slug, while little is known about the velocity profile in the liquid film surrounding the gas bubble (i.e. the liquid film between the bubble and the channel wall), especially in mini- or microchannels. An experimental challenge lies in the requirement that bubbles are symmetrical to the capillary centerline which is difficult to achieve in a vertical alignment of the capillary. Nevertheless, recently experimental investigations of the velocity fields both in the liquid slug and in the liquid film have been performed successfully. The corresponding validation study will be subject to a future publication.

3 Two-Phase Flow Model and Taylor Flow Setup

We consider a two-phase flow situation with two different immiscible incompressible fluids (here fluid/gas) which may move in time and have different material properties ρ_i (density) and μ_i (viscosity), $i = 1, 2$. The domain Ω is partitioned into the subdomains $\Omega_1(t)$ and $\Omega_2(t)$, $\overline{\Omega} = \overline{\Omega}_1(t) \cup \overline{\Omega}_2(t)$, $\Omega_1(t) \cap \Omega_2(t) = \emptyset$, each of them containing one of the phases. These phases are separated from each other by the interface $\Gamma(t) = \overline{\Omega}_1(t) \cap \overline{\Omega}_2(t)$. We assume isothermal conditions and assume that both

phases are pure substances. The normal velocity of the interface is denoted by $V_\Gamma = V_\Gamma(x,t) \in \mathbb{R}$. As we do not consider phase transition, from the immiscibility assumption it follows that $V_\Gamma = \mathbf{u} \cdot \mathbf{n}_\Gamma$ holds at the interface, where $\mathbf{u}$ denotes the fluid velocity and $\mathbf{n}_\Gamma$ the unit normal on Γ. We consider the following (standard) sharp interface model (in strong formulation and assuming interfacial no-slip) for the *fluid dynamics* of such a two-phase *incompressible* flow:

$$\begin{cases} \rho_i(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla\mathbf{u})) &= \operatorname{div}\sigma_i + \rho_i \mathbf{g} \\ \operatorname{div}\mathbf{u} &= 0 \end{cases} \quad \text{in } \Omega_i(t),\ i=1,2, \qquad (1)$$

$$[\sigma \mathbf{n}_\Gamma] = -\tau\kappa\mathbf{n}_\Gamma - \nabla_\Gamma \tau \quad \text{on } \Gamma(t), \qquad (2)$$

$$[\mathbf{u}] = 0 \quad \text{on } \Gamma(t), \qquad (3)$$

$$V_\Gamma = \mathbf{u}\cdot\mathbf{n}_\Gamma \quad \text{on } \Gamma(t). \qquad (4)$$

Here κ denotes the mean curvature and σ_i are the stress tensors within the bulk of the two phases, for which standard closure for Newtonian fluids is applied. The equations are further coupled through the two (vector-valued) interface conditions (2) and (3) which describe the mass and momentum jump conditions.

Diffuse interface models are also used to numerically simulate the two-phase flow situation. The corresponding equations are specified in [12] and can be seen as an approximation to the above sharp interface formulation (under the assumption of small mobility and interface thickness).

As indicated above in Sec. 2 Taylor flow exists in a large range of configurations. Within the scope of this collaboration we considered upward rising Taylor flow/bubbles which are *pressure driven*, i.e. gravity effects do not play an important role. The capillary number Ca is chosen in the order of 0.1 which leads to significant effects of surface tension forces. We further restrict ourselves to very *laminar* flow (Reynolds number $Re := \rho_L d_H \mathbf{u}_B/\eta_L < 20$, where ρ_L is the density of the liquid and d_H the hydraulic diameter of the channel). This allows us to consider *quasi-stationary* situations, which are easier to assess for a comparison between simulations and experiments. A low Reynolds number also results in a small film thickness between the bubble and the channel wall. To achieve such a configuration small capillaries (diameter $\approx$ 2mm) and a substance system of air (for the bubble) and a water-glycerol mixture (for the surrounding fluid) are used. As in realistic applications the ratio between densities and viscosities in liquid and gas phase are in the order of 1000.

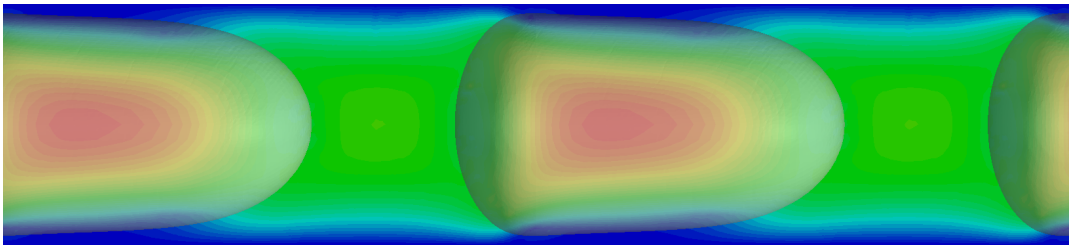


Fig. 2 Example of a quasi-stationarily rising Taylor flow. Flow is going from left to right. Coloring indicates absolute velocity.

4 Results

Two different collaboration projects were carried out in the context of Taylor Flow. Both projects compared experimental data to numerical simulations, albeit in different settings.

The first project focused on 2D numerics, and was therefore limited to experimental data obtained from a round capillary (since the surface tension in all experimental setups is relatively high, rotational symmetry of the bubble can then be safely assumed) [12]. Participating numerical codes were based both on a classical sharp-interface approach and also on a diffuse-interface model. For the sharp-interface model, two numerical codes using Arbitrary Lagrangian Eulerian (ALE) coordinates and a moving mesh were used and for the diffuse-interface approach two different but similar mathematical models were compared. Data from all codes was compared to each other in a purely numerical benchmark with varying capillary numbers and also to experimental data obtained from X-ray measurements. By using a high-energy synchrotron radiation source, very precise measurements of the bubble shape were obtained.

The different mathematical models and numerical codes lead to results that were in very good agreement to each other. The difference of the simulated bubble shapes to the experimental data was somewhat higher. While the exact reason for this slight disagreement is unclear as of yet, measurement errors in the experiment could explain part of this problem.

The second project focused on square channels and 3D numerical codes. The numerical codes are all based on a sharp-interface model but use different numerical approaches. Two codes use an Interface Capturing approach using Finite Volumes with the VOF method on structured grids, one uses a Level-Set function for Interface Capturing in an adaptive Finite Element framework and the fourth code uses an Interface Tracking Finite Volume method on unstructured moving (and matching) grids. In [13] these codes were used to validate against each other and against an experimental bubble shape, which has been obtained from X-ray measurements in the same manner as in the rotational symmetric case. The Bubble shapes are compared at lateral and diagonal cuts through the flow domain. Comparison shows a good agreement for all codes and the measurements.

5 Outlook

Benchmarking is a valuable tool to assess the accuracy of two-phase flow codes. We present a novel quantitative benchmark problem which considers a Taylor flow setup and goes beyond any other existing benchmark proposal. Advantages include

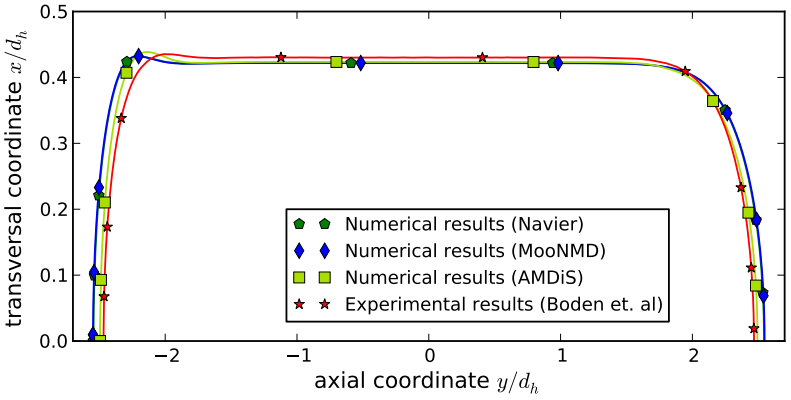


Fig. 3: Overview over a simulated Taylor bubble in different numerical codes and experiment, from [12].

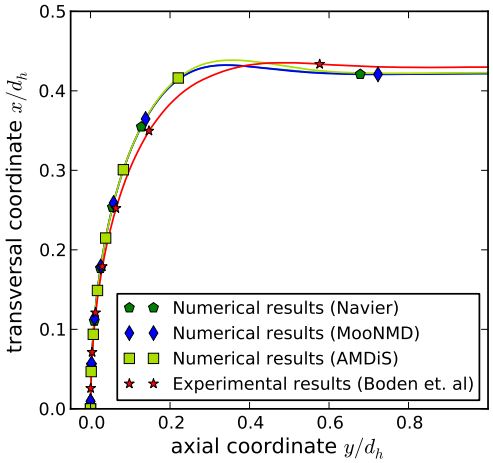


Fig. 4: Close-up view of the rear of the bubble, from [12].

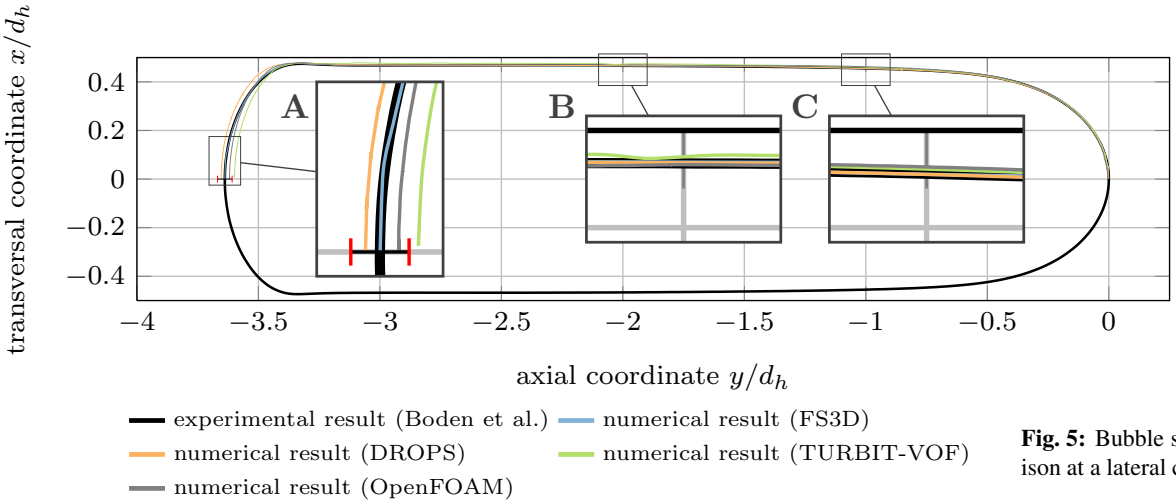


Fig. 5: Bubble shape comparison at a lateral cut, from [13].

the experimental accessibility and comparability, the sensitivity to a large range of surface tensions and the practical relevance of the proposed setup.

The first two studies have been performed [12, 13] and showed that it was possible yet demanding to obtain agreement between the codes and the experimental data. It is planned to put detailed data of the different codes and experiments online as supplementary material to the corresponding papers as well on the SPP homepage (*www.dfg-spp1506.de/taylor-bubble*). Other research groups are encouraged to join by contacting the authors. The next step will be to extend the hydrodynamic benchmark to species transfer. This may include transport between the bulk phases (e.g. a dissolving gas bubble) and/or on the fluid interface (e.g. a single insoluble surfactant). In both cases the comparison between mathematical models, numerical codes and experiments is expected to be of great relevance to rigorously assess the capabilities of numerical simulations.

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