**Influence of Capillary number on the droplet shape, film thickness, and pressure drop in a liquid-liquid Taylor flow inside a microcapillary**

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**Abstract**

Numerical analysis of a two-dimensional, axisymmetric, incompressible, laminar liquid-liquid Taylor flow in a vertically upward circular microchannel is carried out in the present study. The focus is laid on fluid flow characteristics in the slug flow regime. Although many researchers have performed numerical and experimental studies of two-phase flows in narrow channels, their efforts seem to have been fairly successful in explaining the underlying mechanisms of fluid flow phenomena, especially for slug flow regime. Here, an attempt has been made to explore the hydrodynamics of such flows. In the present study, dodecane and Pd5 have been used as the carrier phases and water as the dispersed phase. The internal diameter of the circular microchannel is 1.5 mm with its wall being insulated. The flow and volume fraction equations are solved by the finite volume approach (FVM). The volume of Fluid (VOF) method has been adopted for capturing the two-phase interface. The effect of Capillary number on film thickness and interfacial pressure drop is explained. The film thickness is found to increase with Capillary number and is in a close match with the correlations available in the literature. The pressure drop per unit length obtained from simulations is compared with the standard correlations available in the literature. The pressure drop across the unit cell is found to be in accordance with the phenomenological model. It is observed that the pressure drop at the two-phase interface has a higher contribution to the total pressure drop over other of pressure drops in the channel, with ~50-55% in dodecane-water and ~55-62% in Pd5-water systems. In addition, the distribution of the velocity, axial, and wall pressure fields inside the microcapillary are also discussed.

1. **Introduction**

Two-phase slug flow, whether it be gas-liquid or liquid-liquid, is used for high heat removal with low coolant flow rate. The potentiality of these flows with respect to the liquid-only flows has been studied and reported by many researchers ([1-14]. Taylor flow (Slug flow) regime is the most useful flow regime since it covers a large portion in the flow regime map [15,16]. Taylor flow is characterized by a sequence of liquid droplets (or bubbles) filling the entire flow channel with liquid slugs between two consecutive droplets. In Taylor flows, the presence of a thin liquid film between the wall and droplets, and Taylor vortices inside the liquid slugs play a vital role in heat and mass transfer processes. In gas-liquid flows, the role of the gas phase in the heat transfer process is often neglected due to its lower thermal conductivity. Introducing an immiscible liquid droplet in place of gas bubble significantly increases the heat transfer rates. Asthana et al. [17], Ookawara et al. [18], Song et al [19], and Urbant et al. [20] have discussed a wide variety of applications of liquid-liquid slug flows, such as in polymerase chain reaction, Nitration of benzene to toluene, micro separation, and electronics cooling, respectively.

1. **Literature review**

A wide number of numerical and experimental studies have been performed by eminent researchers to explore the hydrodynamics of gas-liquid as well as liquid-liquid Taylor flows. Hirt and Nichols [21] have presented the VOF technique for the numerical treatment of free boundaries associated with the computational mesh of Lagrangian-Eulerian and Eulerian elements. Brackbill et al.[22] proposed a novel method for modeling surface tension effects on the fluid motion. The model has been extensively used by several groups of researchers [23,10,24,2,1,25,34]. The internal recirculation within the slugs was experimentally visualized by Particle Image Velocimetry (PIV) technique by [26], whereas in numerical studies the recirculations are visualized in bubble/droplet frame of reference [13]. Taha and Cui [27] implemented VOF technique to describe the motion of gas bubbles in stagnant as well as flowing liquids and validated their results with the published experimental results of White and Beardmore [28]. Gupta et al.[23] performed simulations on a two-dimensional, horizontal, axisymmetric domain (d = 0.5mm, L = 10d) using VOF multiphase method to explore the hydrodynamics of air-water Taylor flows inside the microchannel. They developed a methodology for simulating slug flows using the VOF method, which has been widely used by many researchers [10,1,13]. The formation of the Taylor bubble and its formation period in channels of a circular cross-section having a different diameter, with air-water and air-octane systems, were reported in [29, 30]. In their numerical work on slug flows in T-Junction microchannels, Santos and Kawaji [31] and Nichita et al. [32] numerically studied the effect of wall wettability on the flow physics of gas-liquid Taylor flows in a T-junction microchannel. Farhangi et al.[33] numerically studied the hydrodynamics of a single bubble rising in a vertical tube using a two-dimensional axisymmetric model. They investigated the effect of different parameters such as surface tension, channel height, initial bubble radius and liquid viscosity on the shape and velocity of the bubble. The effect of gravity on the flow and heat transfer mechanisms of gas-liquid two-phase flows was explained by Leung et al. [6] through their experimental work. Unequal film thicknesses were found at the bottom and top walls of the channel. Based on their experimental findings, a model was proposed to predict the velocity profile in the film region Through their micro-PIV experiments, and numerical studies on gas-liquid Taylor flows in a horizontal circular channel, Gupta et al. [35] explained the significance of the third dimension on the bubble shape and fluid flow. An asymmetry was observed in the bubble shape which was also in close agreement with their experimental results. Gupta et al. [24] conducted experimental and numerical studies on liquid-liquid Taylor flows in a circular channel to explore the flow characteristics. Hexadecane and water were employed as the continuous and dispersed phases, respectively. They have explained the applicability of Bretherton's model [36] in predicting the pressure drop and film thicknesses at low viscosity ratios, and have also proposed expression for predicting the normalized pressure drop in a unit cell. Based on this literature survey it is understood that the flow and thermal characteristics of Taylor flows depend on several parameters. Most of the studies are done using gas-liquid flows, whereas only a few studies have been conducted so far with liquid-liquid flows. Liquid-liquid flows are efficient in dissipating high heat fluxes and also promote the mixing performance due to a higher thermal conductivity of dispersed liquid unlike the gas phase in gas-liquid flows. This study is aimed at a systematic simulation of liquid-liquid Taylor flows in a circular microchannel to acquire a thorough knowledge of the flow characteristics in microchannels. The study numerically investigates the dependence of the two-phase flow on important flow parameters such as homogeneous void fraction, slug and droplet lengths, and Capillary number. The corresponding numerical results of the present are compared with widely accepted correlations.

1. **Simulation methods**
   1. **Governing equations**

The present work deals with two-phase Taylor flow inside a circular microchannel where both phases are liquids. Each of the two fluids is considered to be incompressible, Newtonian, immiscible and without any phase change. Volume-of-fluids (VOF) interface capturing technique [21] has been adopted to track the two-phase interface between the fluids. The governing equations of continuity, momentum, and volume fraction as well as surface tension modeling [22], which are solved by the numerical model for multiphase flow, can be obtained from [23].

* 1. **Computational domain**

A fully-developed liquid-liquid slug flow can be modeled in a periodic unit cell due to its periodic and regular nature [13]. The periodic unit cell consists of two halves of continuous phase liquid at either end of the disperse phase droplet which is situated at the center of the unit cell. The position of dispersed phase droplet remains unchanged in the unit cell when observed from a reference frame moving with a velocity equal to that of the droplet. Hence, the flow can be considered as steady in the moving frame of reference. Figure 1 shows the above-mentioned unit cell having a periodic inlet and outlet at its ends.

* 1. **Methodology**
     1. **Moving domain method**

The dynamic mesh motion method, available in ANSYS Fluent, is incorporated to model the two-phase flow in the present study due to its lower computational cost over stationary domain method.

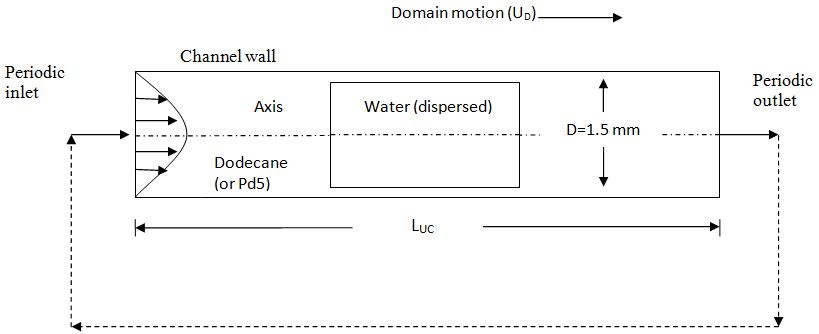
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Fig. 1. Schematic diagram of the computational domain.

The moving domain method is employed to carry out the present simulations since the flow domain moves with the droplet velocity (*U*D), and hence, the shape of the domain also changes over time. Rigid body treatment is used as both the domain as well as the incoming stream move in the same direction. Also, the dynamic layering technique is adapted to update the mesh at each time step. It should be noted that at the beginning of each time-step, the droplet velocity is calculated using Eq. (11) and is supplied to the solver by user-defined C routines.

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| --- | --- |
|  | (11) |

The homogeneous void fraction (β) can be obtained by the following expression:

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| --- | --- |
|  | (12) |

where, αD is volume fraction of the disperse phase droplet, and uTP is the mixture velocity in m/s.

* + 1. **Boundary and initial conditions**

In the present study, a two-dimensional, axisymmetric (x-r), laminar, incompressible liquid-liquid slug flow (or droplet-train flow) inside a circular microchannel is considered. Periodic velocity inlet and pressure outlet boundary conditions are applied at both ends with no-slip at the channel wall. The radial and axial velocity components are transformed to the upstream boundary from the downstream boundary. The continuous phase liquid is allowed to enter the domain at a constant velocity. At the beginning of each simulation, the solution domain has a liquid droplet having a size equal to the required volume fraction. The entire flow channel is initialized with a uniform pressure of zero Pascal and fully-developed parabolic velocity profile having an average mixture velocity equal to the incoming primary (continuous) phase fluid. The periodic velocity boundary condition mentioned above is achieved by wrapping the axial and radial velocity fields at the downstream boundary to the upstream boundary using user-defined C routines in the solver as shown in the equations below:

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| --- | --- |
|  | (13) |
|  | (14) |
|  |  |

* + 1. **Numerical schemes**

The commercial code ANSYS Fluent 15.0 was employed to perform this study. The volume of Fluid (VOF) multiphase method was adopted to capture the interface between the two phases. A first-order implicit scheme using non-iterative solver was adopted for the unsteady formulation of flow equations. The gradients of various flow parameters were evaluated using the Green-Gauss node based method. Geo-Reconstruct algorithm for the discretization of volume fraction was used. A maximum Courant number of 0.25 was adapted for the volume fraction equation. Variable time-stepping strategy with global Courant number of 0.25 was used for momentum, pressure and energy equations. Body force weighted scheme for solving pressure equation, and QUICK scheme for solving the convective terms of momentum equations was employed. The surface tension coefficients at the dodecane-water and Pd5-water interfaces were 0.052 and 0.0397 N/m, respectively.

1. **Results and discussion**

In the present work, dodecane and Pd5 are considered as the continuous phase liquids and water as the dispersed phase liquid. The thermo-physical properties of the working fluids are listed in Table 1. The diameter of the circular channel is 1.5mm. The simulation is performed for different dispersed phase volume fraction 0.15 < αD < 0.75, and mixture velocities 0.0566 < uTP < 0.113 (for dodecane-water system) and 0.0168 < uTP < 0.0335 (for Pd5-water system), whereas the Capillary number in both cases of working fluids is identical and lies in the range 0.0015 <CaC < 0.00302. Table 2 gives details of various parameters considered during this numerical study. A single rectangular droplet is initially placed in the computational domain. Each simulation begins with a continuous liquid (dodecane or Pd5) and dispersed droplet at rest.

Table. 1. Thermophysical properties of working fluids at room temperature and atmospheric pressure.

|  |  |  |  |
| --- | --- | --- | --- |
| Material | Density  [kg/m3] | Viscosity  [kg/m s] | Interfacial Tension  [N/m] |
| Water | 996.1 | 0.00091 | ---- |
| Dodecane | 754.3 | 0.00139 | 0.0520 |
| Pd5 | 911.8 | 0.00358 | 0.0397 |

Table. 2. Flow parameters considered in this numerical study.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Dodecane-water system | | | | | |
| Case | uTP (m/s) | α | LUC(mm) | CaC | ReC |
| 1 | 0.057 | 0.183 | 11.88 | 0.0015 | 46.1 |
| 2 | 0.057 | 0.437 | 8.246 | 0.0015 | 46.1 |
| 3 | 0.057 | 0.527 | 5.67 | 0.0015 | 46.1 |
| 4 | 0.057 | 0.631 | 6.165 | 0.0015 | 46.1 |
| 5 | 0.057 | 0.735 | 6.66 | 0.0015 | 46.1 |
| 6 | 0.068 | 0.735 | 6.66 | 0.0018 | 55.3 |
| 7 | 0.079 | 0.735 | 6.66 | 0.00212 | 64.5 |
| 8 | 0.091 | 0.735 | 6.66 | 0.00242 | 73.7 |
| 9 | 0.102 | 0.735 | 6.66 | 0.00272 | 82.9 |
| 10 | 0.113 | 0.735 | 6.66 | 0.00302 | 92.1 |
| Pd5-water system | | | | | |
| 12 | 0.0168 | 0.449 | 9.87 | 0.0015 | 6.41 |
| 13 | 0.0201 | 0.449 | 9.87 | 0.0018 | 7.69 |
| 14 | 0.0235 | 0.449 | 9.87 | 0.00212 | 8.97 |
| 15 | 0.0268 | 0.449 | 9.87 | 0.00242 | 10.25 |
| 16 | 0.0302 | 0.449 | 9.87 | 0.00272 | 11.53 |
| 17 | 0.0336 | 0.449 | 9.87 | 0.00302 | 12.81 |

* 1. **Computational mesh**

The computational mesh used in the simulations consists of 85,000 square elements. Near-wall mesh treatment is performed by following the guidelines of Gupta et al.[23] to capture the thin liquid film between the wall and droplet. Figure 4 shows the droplet shape for three different mesh sizes, viz. 65000, 85000, and 100,000 elements. It can be seen that the droplet shape obtained from 85000 and 100000 elements size are same and the mesh having 85,000 elements has been adopted throughout the study.

* 1. **Hydrodynamics**

The hydrodynamics of liquid-liquid Taylor flows are explored in the present section. The film thickness, pressure drop, velocity field, recirculation within the flow, and droplet shapes have been studied. Also, the results obtained from the present CFD study have been compared with the standard correlations available in the literature.

* + 1. **Film thickness**

In this section, the CFD results of film thickness neighboring a liquid droplet have been compared with Bretherton's free slip model [36] and Aussillous and Que're's (A&Q) [37] semi-empirical correlation. Bretherton developed the model to evaluate the film thickness with an assumption of δF << R, whereas A&Q proposed their model by relaxing the Bretherton's hypothesis. Variation of film thickness with the Capillary number (for Do-W case) is depicted in Fig. 5. It is observed that film thicknesses near the water droplet, obtained from CFD simulations, are in accordance with Bretherton's free slip model of gas-liquid flow. Although Bretherton's model is applicable for gas-liquid Taylor flows, present simulation results were found to be in a close match with the model because of the lower viscosity ratio in the present case [24]. Throughout the simulations, the homogeneous void fraction was kept constant ( β=0.753) and the average mixture velocity at the inlet was varied in the range 0.057−0.1132 m/s. In addition, a region of non-uniform film thickness was observed for lower values of homogeneous void fraction (β=0.2) which is in accordance with the previous literature [39-41].

* + 1. **Droplet shape**

The droplet profiles at different mixture velocities ( 0.057 < uTP < 0.1132 m/s) obtained from CFD simulations of dodecane-water system are shown in Fig. 6. Shown in figure 6 are the profiles of water droplet when the flow has been developed hydrodynamically and droplet shapes become independent of the dispersed phase volume. It is observed that the film thickness between the water droplet and channel wall increases with the Capillary number. The possible reason for this relationship between the film thickness and the mixture velocity is that the curvature of the leading meniscus (droplet nose) increases when the mixture velocity is increased, whereas, the curvature of the trailing meniscus (droplet tail) of the droplet is constant.

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| Fig. 4. Droplet volume fraction for different mesh sizes. | Fig. 5. Variation of the continuous phase film thickness with the Capillary number (Do-W system). |

For all the Capillary numbers considered in the present study, a ripple (waves or undulations) at the rear end of the droplet is observed. These ripples at the rear end of droplet indicate the zones of sharp pressure jumps near the liquid-liquid interface. Similar observations were reported by Bretherton [36], Gupta et al. [24], Fukagata et al. [11], and Asadolahi et al. [14] in their gas-liquid slug flow studies. Figure 6 also shows the variation of wall pressure along the axial length of the channel at different mixture velocities for a given β. It is clear from Figs. 6(a) and (b) that the pressure difference over the frontal region is higher than the pressure drop over the rear region.

* + 1. **Pressure field**

In this section, an effort has been made to study the pressure field in the two-phase liquid-liquid Taylor flow, where dodecane and Pd5 are continuous phases in different cases respectively, and water is considered as the dispersed phase. The total pressure drop during the two-phase flow occurs due to three major contributing factors: (a) slug (ΔPslug); (b) film (ΔPfilm); and (c) the interfacial (ΔPinterface) pressure drops [38].

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| **E:\Varying carrier phase\origin graph for paper\nose coincident PD vs Ca.jpg** | **E:\Varying carrier phase\origin graph for paper\Tail Coincident PD vs CA.jpg** |
| (a) | (b) |
| Fig. 6. Variation of droplet shape and wall pressure along the axial length of the channel for different Capillary number at β=0.735. In (a) the droplet fronts are coincident and pressure at the droplet front has been shifted to zero, whereas, in (b) the tails of the droplets are coincident, and the minimum pressure near the droplet tail has been shifted to zero. | |

Slug pressure drop can be evaluated from Hagen-Poiseuille's equation (Eq. 1) due to fully developed flow in the primary phase slug. The same equation was also used by Gupta et al. [24] in their liquid-liquid Taylor flow study where hexadecane and water were used as continuous and dispersed phases, respectively.

|  |  |
| --- | --- |
|  | (1) |

Figure 7 shows the variation of the wall and axial pressure along the axial length of the channel. It is observed that, in the region of uniform film thickness, the pressure gradients are identical in both the phases. Fouilland et al. [40] assumed random pressure gradients at the annulus and core, and have given a solution for velocity profile using an analytical, annular, laminar-laminar flow solution for gas-liquid Taylor flows, whereas, Gupta et al. [24] derived an expression for evaluating the film pressure drop considering equal pressure gradients, unlike arbitrary gradients.

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|  | (2) |

Figure 8(a-b) shows the comparison of interfacial pressure drop across the interface between the two fluids obtained from simulations with that obtained from Eq. (3). The interfacial pressure drop could be calculated by differencing the pressure between the droplet nose and tail. In all the cases considered in the present work, interfacial pressure drop has a significant contribution (~50-55% and ~55-62% for dodecane-water and Pd5-water cases, respectively) to the overall drop in pressure in contrast to other pressure drops.

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| --- | --- | --- |
|  | | (3) |
|  | (4) |

Figure 8(c) compares the normalized pressure drop in the microchannel obtained from Eq. (4) and present simulations. In both simulations as well as the analytical model, it is observed that the normalized pressure drop (ΔP/L) increases with mixture velocity. However, the analytical model has a higher rate of increase as compared to CFD results. Also, a significant deviation in the interfacial pressure drop is observed between the numerical results and those obtained from the Bretherton's model for an inviscid bubble. The possible reasons for this could be the high viscosity ratios, which in our case, for both system of working fluids, i.e., dodecane-water and Pd5-water, are 0.254 and 0.655, respectively unlike 0.02(approx.) for the gas-liquid flows considered by Bretherton. Hence, it is highly recommended to look for better models to predict the interface pressure drop and overall pressure drop for a liquid-liquid Taylor flow covering low as well as a high range of viscosity ratios.

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| Fig. 7. Variation of the wall and axial pressure along the axial length of the channel for uTP =0.0566ms-1 and β=0.0735 for the dodecane-water system. (The dashed line represents the axial pressure shifted by Laplace pressure difference, which is equal to 75 Pa (approx.)). | (a) |
| **Q:\CONFERENCES And JOURNALS\Journals\5 Liquid-Liquid Taylor flow_optimal pressure drop\Results\origin graphs\new\3b pd5.jpg** | **Q:\CONFERENCES And JOURNALS\Journals\5 Liquid-Liquid Taylor flow_optimal pressure drop\Results\origin graphs\new\13.jpg** |
| (b) (c)  Fig. 8. Interfacial pressure drop and pressure drop per unit length as a function of Capillary number. (a) Comparison of interfacial pressure drop across the droplet as obtained from CFD simulations and Eq. (3) for the dodecane-water system. (b) Comparison of interfacial pressure drop across the droplet as obtained from CFD simulations and Eq. (3) for Pd5-water system. (c) Comparison of pressure drop per unit length over a unit cell obtained from CFD simulations and Eq. (4). | |
|  | |
| **E:\Varying carrier phase\origin graph for paper\Ux vs R and Ud.jpg** | |
| Fig. 9. Comparison of the normalized velocity profile in the middle of liquid slug for four different mixture velocities with the fully-developed single-phase parabolic velocity profile for the case 10. The horizontal dash-dotted line shows the normalized droplet velocity and the vertical dotted line shows the zone of stagnation at r/R=0.7. | |

* + 1. **Velocity field**

Figure 9 shows the effect of mixture velocity on the velocity field along the radial direction in the middle of a slug. Also, shown in the figure are the normalized velocity profiles of fully-developed, laminar liquid-only flow, and the droplet velocity (UD/uTP) (horizontal dash-dotted line) for a mixture velocity of 0.0566 m/s. The velocity profiles indicate that the velocity at the axis has reached 1.8 times that of the average velocity. For none of the mixture velocities, the flow has become fully-developed. As suggested by Shah and London [43], the length required to achieve hydrodynamically fully-developed single-phase flow (L/d~0.055Re), it would take a length of 2.535d for the lowest Reynolds number (Re = 46.1) considered in our simulations for the dodecane-water system of fluids. The liquid slug lengths in our cases are between 0.65–0.75d, hence a velocity gradient in the radial direction occurs at the beginning of liquid slug, which restricts the flow to show the plug flow behavior. It can be seen in Fig. (9) that at r/R = 0.7, the liquid near the axis is moving with a higher velocity with respect to the water droplet, while the liquid ahead of r/R = 0.7 moves with a lower velocity than that of the droplet. This indicates that there exists a recirculation inside the liquid slugs when observed in droplet frame of reference, where the location of the stagnant liquid is at about r/R = 0.7.

1. **Conclusions**

The paper has presented the numerical study on the hydrodynamics of a two-dimensional, axisymmetric, incompressible, laminar liquid-liquid Taylor flow in a circular channel of diameter 1.5mm. VOF technique was employed to capture the interface of the two-phase flow. Two different fluids, namely dodecane and Pd5 were used as the continuous phases, and water was used as the dispersed phase. The effect of Capillary number on various flow parameters was explored. The thickness of the thin liquid film between the wall and droplet was observed to be increasing with mixture velocity. Also, it showed a good match with Bretherton's model. The presence of a ripple near the trailing meniscus of the droplet was witnessed, which occurs due to sharp pressure jumps. The pressure gradients in both phases were identical in the region of uniform film thickness. The results of interfacial pressure drop have shown a considerable contribution of approximately 50-55% and 55-62% for dodecane-water and Pd5-water systems, respectively, to the overall pressure drop. However, a large deviation in the interfacial pressure drop was observed between the CFD results and those obtained from Bretherton's model for an inviscid bubble, suggesting the formulation of an expression to calculate the pressure drop which could cover a wide range of viscosity. The overall pressure drop per unit length of the unit cell increased with an increase in Capillary number.

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