Computational modelling of slug flow in a capillary microreactor

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Abstract

The benefits of slug flow capillary microreactor exhibit the ability to adjust two individual transport mechanisms, i.e. convection inside the slug and diffusion between two consecutive slugs. The mass transfer rate is enhanced by internal circulation, which arises due to the shear between slug axis and continuous phase or capillary wall. The knowledge of circulation patterns within the slug plays an important role in the design of a capillary microreactor. Apart from this, well defined slug flow generation is a key activity in the development of methodology to study hydrodynamics and mass transfer. In the present paper we discuss computational fluid dynamics (CFD) modelling aspects of internal circulations (single phase) and slug flow generation (two-phase).

Key words: Microreactor, Slug Flow, CFD, Free Surface Modelling, Volume of Fluid (VOF).

1 Introduction

Liquid-liquid slug flow is a flow of two immiscible liquids, characterised by a series of liquid slugs (plugs) of one phase separated by the other. Since

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both phases move alternatively, each slug serves as an individual processing subvolume. These subvolumes are highly regular and guarantee well defined interfacial area for transfer processes (for example, mass transfer). The mass transfer takes place by two mechanisms: convection within the slug and diffusion between two slugs. The convection is due to the internal circulations within each slug because of the shearing action between slug axis and capillary wall while the diffusion is because of concentration gradients between two consecutive slugs. The first phenomenon depends on physical properties of fluids, slug geometry and flow velocity while the later is depending on the interfacial area available for transfer and concentration gradient between two slugs. In order to study all these phenomena, it is imperative that the fluid dynamics of the system has to be understood well. In addition to this, there are other issues such as circulation patterns within the slug, pressure drop, type of mixing element to generate the slug flow and stability of the flow, all of which should be considered while designing such reactors.

There are several CFD studies available on the behaviour of drops or bubbles in tubes ([17], [18]). These studies can be extended to slug flow microreactor by taking care of additional forces (e.g. capillary force). In addition to that, most of the microreactors are made up of materials such as silicon, quartz, polymers and metals that have well defined physical and chemical properties which have to be considered during CFD modelling. Though microreactor technology is a new area for chemical engineers, many studies on single phase and two phase flow are available (for example, [10], [16], [23]). Slug flow has been studied by many researchers and it is referred as bubble train flow or Taylor bubble flow for gas-liquid slug flow while segmented flow, liquid train or slug flow for liquid-liquid slug flow. The CFD simulations to study the hydrodynamics of bubble train flow have been carried out in [14] considering it as a single phase since the gas has very less density and viscosity compared to the liquid with which it is in contact. The simulations with reaction engineering models for liquid-liquid slug flow were carried out in [8] and reported that increased flow velocity enhances the mass transfer by inducing stronger internal circulations within the slugs. Further, a numerical model was developed to predict the internal flow patterns of the fluid segments [11] and the transfer of the dissolved chemical species within and across the segments for liquid-liquid slug flow. The flow was represented by two stagnant and adjacent rectangular units which were linked at both ends to form a continuous loop. The model was validated with different sets of experimental results and showed accurate prediction of flow field and mass transfer.

The interface between the slugs is important in evaluating the performance of the reactor and therefore free surface modelling is necessary. This is one of the challenging research areas for mathematicians with respect to providing an efficient solver. VOF and levelset approaches belong to the two best possible implicit free surface reconstruction methods, while particularly VOF is relatively simple to treat topological changes of the interface and is naturally conservative. This method was extensively used for many applications (for example, [2], [5], [7], [15]). The velocity field and bubble profile in a vertical gas-liquid slug flow inside the capillaries has been obtained in [19] and it was found to be in good agreement with published experimental measurements. In their study, the motion of single Taylor bubble rising in a flowing liquid was simulated using a finite volume discretisation. Recently, the mass transfer coefficients have been investigated from rising Taylor bubbles to liquid in circular capillaries using CFD [22]. The bubble was considered as void which was acting as a free surface with the surrounding liquid phase. The simulations were performed over a unit cell by keeping the bubble stationary and moving the system with the average rise velocity.

The above mentioned literature shows the potential of CFD methodology in the prediction of flow behaviour of immiscible fluids. In this paper, a single phase and a two-phase CFD methodology is described. The first part of the paper deals with the single phase CFD simulations to study the flow behaviour within each individual slug while the second is about an attempt to generate the slug flow using free surface methodology. Effects of operating parameters on internal circulation and slug flow generation are discussed. The numerical challenges in the free surface modelling are also presented.

2 Single Phase Simulations

2.1 Problem Details and Solver

The experiments for slug size measurement were carried out on a device proposed in [8] and are described in short in the following two phase simulations section. Water was used as an aqueous phase while cyclohexane was an organic phase. The slug size was measured at each average flow velocity and the corresonding deviation from mean size at all flow velcities was investigated. The geometries of aqueous and organic phases were retrieved from the experimental snapshots as shown in Figure 1. Each slug was considered separately as a single phase domain and solved individually.

During the experiments it was revealed that the organic slug leaves a wall film (approximately 1% of radius of the slug) due to the superior wetting properties of the capillary material. This film gives lubricating action to the enclosed aqueous slug and therefore it moves with slightly greater velocity than the average flow velocity. This velocity difference of average flow and enclosed slug flow can be investiaged by assuming the steady state velocity profile in the film region as given in [6] for pipeline flow of capsules. The following equation relates the slug flow velcity u_s and average flow velocity u_{avg} as

$$u_s = \frac{2}{1 + (R_s/R)^2} u_{avg} \tag{1}$$

where R_s and R are the radius of enclosed slug and capillary, respectvely. However, the capillary radius and enclosed slug radius are related as

$$R_s = R - h \tag{2}$$

Where h is film thickness which was calculated from Brethertons law [1]

$$h = 1.34RCa^{2/3}. \tag{3}$$

Therefore, two cases were considered during simulations: without film and with film. In the case of aqueous slug, the domain for without and with film was the same (Figure 2a) while the radius was changed with film thickness for aqueous slug with film. For organic slug without film, the domain was considered as a closed geometry (Figure 2b) while in the case of film there was film flow inlet and outlet (Figure 2c). The front and back interface of all slugs was assumed to be the same (symmetric) at each flow velocity though there was convective flow in and out of the organic slug with film. The slug lengths used for simulation were 2.379 and 4.758 mm for aqueous slug while 0.561 and 1.122 mm for organic slug.

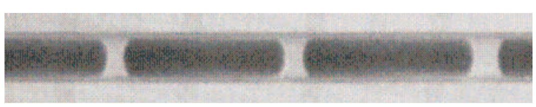

Fig. 1. Liquid-liquid slug flow showing stained aqueous phase and colourless organic phase

The in-house developed open-source Finite Element CFD Tool, FEATFLOW [21], was used for all simulations considering the following assumptions:

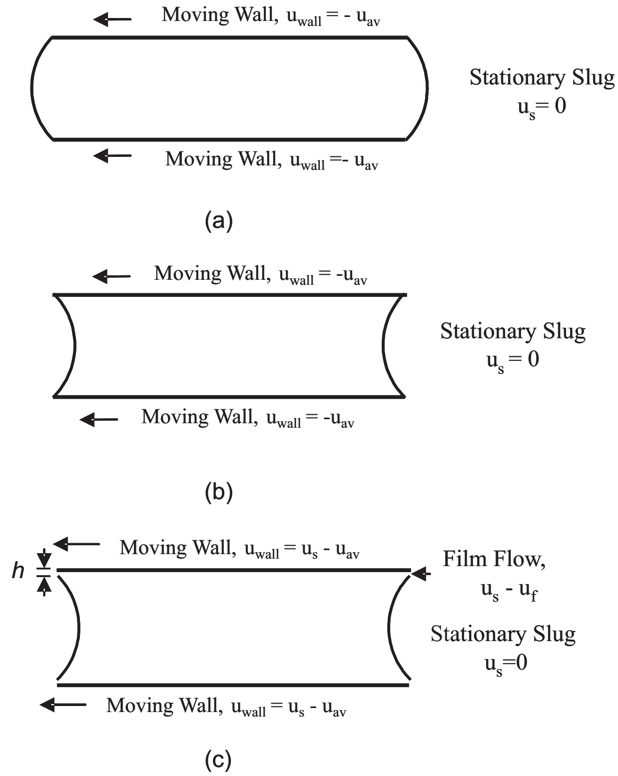

Fig. 2. Computational domains and boundary conditions for single-phase simulations (u_{wall} is wall velocity): (a) Aqueous slug without and with film, (b) Organic slug without film and (c) Organic slug with film

1. front and back interface of each slug were the same
2. the slug size was the same for all flow velocities
3. the problem was considered as two-dimensional and non-stationary
4. the fluid in each slug was considered to be Newtonian, incompressible and isothermal

The following incompressible Navier-Stokes equations were solved for velcoity u and pressure p:

$$u_t - \nu \Delta u + u \cdot \nabla u + \nabla p = 0, \nabla \cdot u = 0 \qquad \Omega \in \mathbb{R}^2 \times [0, T] \tag{4}$$

Here, ν is the kinematic viscosity and T is the time. The FEATFLOW package gives freedom to use two different approaches namely, a coupled approach and a projection approach to treat the discretised nonlinear system. The coupled approach solves for velocity and pressure simultaneously, promises best stability behaviour but requires largest numerical efforts while the projection solver decouples velocity and pressure, reduces the problem to the solution of a sequence of scalar problems [21] and is well suited for nonstationary configurations. So, in this study, the projected solver was used to simulate the flow field.

2.2 Numerical Grid, Boundary Conditions and Solution

In this study, the geometry considered is shown in Figure 2, with front interface being concave and with a back interface being convex for aqueous slug and vice versa for the organic slug. The structured two-dimensional coarse grid was generated with the help of the in-house developed Design and Visualization Software Resource (DeViSoR 2.1). The grid was refined near the walls and corners of the geometry for improving the resolution. The boundary conditions of aqueous phase are the same for slug without and with film. Since there was no inflow and outflow in aqueous slug and organics slug without film, Dirichlet type boundary condition was used. In organic phase domain with film (of thickness h), there was film inlet and outlet, and Neumann type boundary condition was used. The negative x-velocity was given to the capillary wall which moved it in negative direction while the slug was kept stationary. The film and interface velocities were defined relative to the negative wall velocity.

Initially, the simulations were carried out in order to make the solution grid independent using different levels of refinement. Stationary flow fields were achieved with equidistant time stepping of 0.01 and total time of 30s for each slug. Similarly equidistant time stepping of 0.25 was used for visualization of General Mesh Viewer (GMV) outputs. The GMV outputs were taken with the same level of refinement. The Sun-Fire-880 computer system with 900 MHz Sparcv9 processor was used for simulation. The total time required for a single simulation was 416s (12288 cells) and 872s (20480 cells) for aqueous (L = 2.379 mm) and organic (L=1.122 mm) slug respectively.

2.3 Results and Discussion

The velocity vectors and a schematic diagram of the velocity patterns within the aqueous slug without film are shown in Figure 3. As can be seen, the

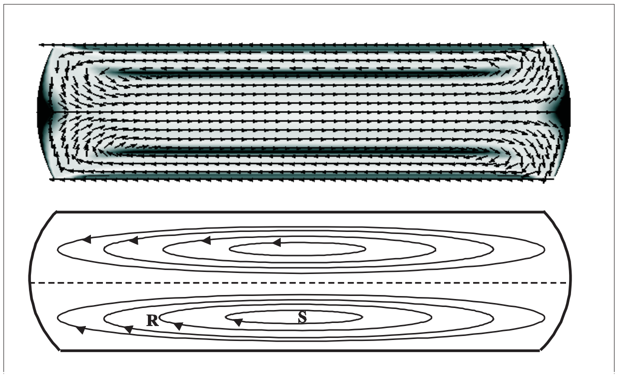

Fig. 3. CFD simulated velocity vectors and schematics of velocity patterns showing recirculation zone (R) and stagnant zone (s)

maximum velocity is at the centre and minimum velocity at the wall, showing a fully developed parabolic (Poiseuille) profile. Two flow patterns were observed within each slug: a recirculation zone at the centre and in the wall proximity and two stagnant zones in between them. When the slug moves through the capillary, due to the shear between slug axis and capillary wall, the liquid in the centre moves to the front end of the slug, where it touches the front interface and returns back along the wall of the capillary while at the back end, liquid moves from the wall to the centre of slug and thus circulation takes place. Thus, the parabolic profile is bidirectional showing a maximum velocity at the centre of the slug, zero velocity at some radial position r^0 (stagnant zone) and negative velocity at the wall surface (see Figure 4). Similar type of study was made in [20] for liquid slug of gas-liquid flow through circular and square cross section capillaries. The average flow velocity has strong effects on the bidirectional profile or recirculation. With increase in the average flow velocity, internal circulation increases, and thereby enhances convective mass transfer.

These recirculation patterns are strongly influenced by the slug geometry. If the length of the slug is less than its diameter (for example, organic slug, L = 0.561 mm), the velocity patterns are totally different than the slugs with lengths greater than their diameters. In many chemical engineering studies, it is required to produce slugs with length less than its diameter. So, many simulations were carried out to study such behaviour. In few simulations, dead zones rather than recirculation were observed. Sometimes it shows that the front part of the slug has dead zones and the back part has circulation at the corners only. Increasing the length of the slug, the velocity profile in the slug approached to parabolic (Poiseuille) profile. In the case of slugs with

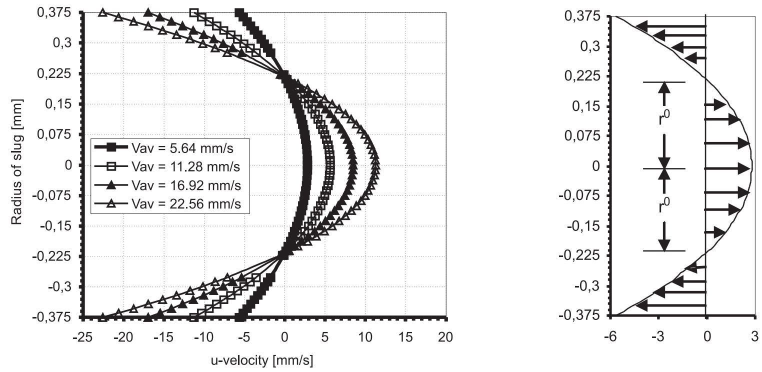

Fig. 4. Parabolic velocity profile inside the slug (aqueous slug, length = 2.379 mm and diameter = 0.75 mm)

film, the aqueous slug has the same profile while in the organic slug it is slightly disturbed near the interface due to film inlet and outlet, however a fully developed profile was observed at the centre. The film thickness shows no strong effect on the velocity profile because it is very small as compared to the diameter of the slug. Thus, from single phase simulations it was observed that for a slug with length greater than its diameter, intensity of internal circulation increases with increase in the average flow velocity and the film has no significant effect on it.

3 Two Phase Simulations

3.1 Problem Details and Solver

The well defined and stable slug flow is suitable for investigations of two phase liquid-liquid reactions because it ensures a uniform interfacial area to fulfil the basic requirement for mass transfer. So, in this section, we will concentrate on the generation of slug flow. The schematic representation of the experimental set-up for slug flow generation is shown in Figure 5. It shows that two liquids are introduced by continuously operating high-precision piston pumps into a 120^0 Y-piece mixing element. The capillary microreactor made up of a polymer, PTFE (Poly-tetra-fluoro-ethylene) and having a diameter of 0.5-1 mm was attached directly downstream of the Y-piece. The length of the capillary micrometer depends on the residence time required and was kept 1 m in the present study. The experiments were carried out over a range of 0-300 ml/hr average flow velocity.

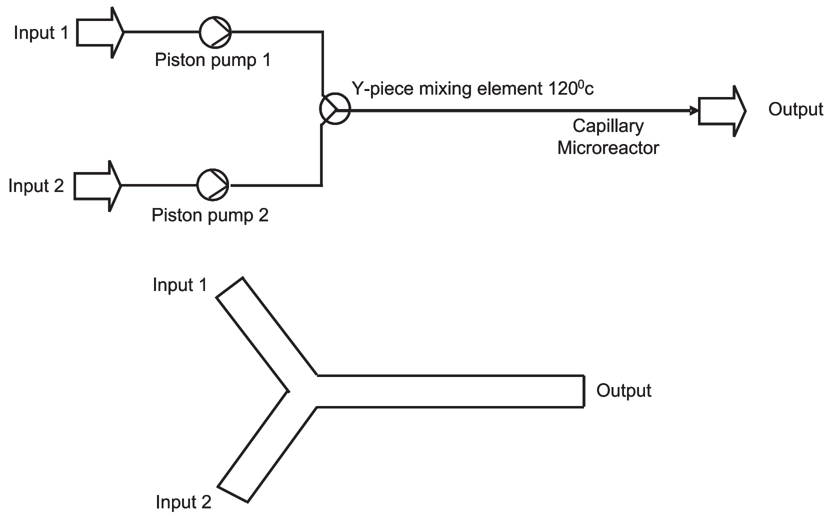

Fig. 5. Schematics of experimental set up and computational domain

To generate the slug by numerical experiments, a corresponding free surface methodology was developed. The description of the free surface is one of the challenging tasks and can be done by two approaches: Eulerian and Lagrangian. In liquid-liquid slug flow, the problem is relatively simple since the flow is quite stable while in the case of immiscible flow with large viscosity and density differences (for example, air-water flow) the interface may undergo severe deformations and break up. The difference between the Eulerian and Lagrangian approach is that the mesh remains fixed with the flow moving through it in the first case while the mesh moves with the same speed of the fluid in the later case. In the Lagrangian approach the mesh distortion leads to limitations and thus only simple non-intersecting interfaces can be represented. So, we have followed the Eulerian approach which formulates the interface tracing by two methods: front tracking and volume tracking. The Volume of Fluid (VOF) methodology was developed [12] which relies on the fact that two or more phases are not interpenetrating and for each additional phase we add the volume fraction of the phase in the computational cell. In each control volume the volume fractions of all phases sum to unity. This methodology has several advantages namely reasonable accuracy, relative simplicity and it can solve highly complex free surface flows. It solves the incompressible Navier-Stokes equations for velocity u

and pressure p:

$$u_t + \nabla \cdot (uu) = -\frac{1}{\rho}[\nabla p - \nabla \cdot (2\mu S)] + \frac{1}{\rho}F_{SF}, \nabla \cdot u = 0 \tag{5}$$

where S is the deformation tensor which is given by,

$$S = \frac{1}{2}(\nabla u + [\nabla u]^T). \tag{6}$$

Where F_{SF} is continuum surface force vector. The above equation is dependent on the volume fractions of all phases through the propeties ρ and μ. These properties were calculated by the following equations:

$$\rho = \sum \alpha_k \rho_k \tag{7}$$

and

$$\mu = \frac{\sum \alpha_k \rho_k \mu_k}{\sum \alpha_k \rho_k} \tag{8}$$

where α_k, ρ_k and μ_k are the volume fraction, density and viscosity of the kth fluid, respectively. In a two-phase system, the following possibilities arises in a perticular cell

$$\alpha_2 = \begin{cases} 0, & \text{(Fluid 1)} \\ 1, & \text{(Fluid 2)} \\ 0 < \alpha_2 < 1, & \text{(Interface between two fluids)} \end{cases} \tag{9}$$

The interface between two fluids was tracked by volume fraction function, α_k. It convects with the flow and conservation of this function can be represented with the help of interface mass balance conditions by pure convection equation:

$$\frac{\partial \alpha_k}{\partial t} + u \cdot \nabla \alpha_k = 0 \tag{10}$$

The volume fraction for the primary phase was not solved and was obtained from the following equation:

$$\sum \alpha_k = 1 \tag{11}$$

In a capillary microreactor, modelling of surface tension and wall adhesion effects are important in addition to mass and momentum. The surface tension is due to the strong intermolecular attractive forces between molecules in a fluid which holds the molecular strongly and minimises the surface area of slug. While the wall adhesion is due to the stronger attractive forces between liquid molecules and the wall and thus the fluid makes some contact angle with the wall. In the present work, the continuum surface force (CSF) model proposed in [3] was used to model surface tension. With this model, the addition of surface tension to the VOF calcualtion results in a source term in momentum equation. The surface curvature was computed from the local gradients in the surface normal at the interface. Thus, the source term in the momentum equation was specified as follows

$$F_{SF} = \sigma \kappa \boldsymbol{n} \left[\frac{\alpha_1 \rho_1 + \alpha_2 \rho_2}{\frac{1}{2}(\rho_1 + \rho_2)} \right] \tag{12}$$

where $\boldsymbol{n}$ is the surface normal and κ is the curvature which are given as

$$\boldsymbol{n} = \nabla \alpha_2 \tag{13}$$

$$\kappa = -(\nabla \cdot \hat{n}) = \frac{1}{|\boldsymbol{n}|} \left[\left(\frac{\boldsymbol{n}}{|\boldsymbol{n}|} \cdot \nabla \right) |\boldsymbol{n}| - (\nabla \cdot \boldsymbol{n}) \right] \tag{14}$$

The surface normal $\boldsymbol{n}$ was evaluated in the cell where α_2 has value greater than 0 and less than 1 i.e. interface containing cell. The geometric construction scheme (Piecewise linear interface calculation, PLIC) was used to calculate the inteface position in the cell. In the case of wall adhesion, rather than imposing the boundary condition at the wall itself, the contact angle that the fluid is assumed to make with the wall is used to adjust the surface normal in the cells near the wall. If θ_w is the contact angle at the wall then the surface normal at the live cell next to the wall is

$$\hat{\boldsymbol{n}} = \hat{\boldsymbol{n}_w} cos\theta_w + \hat{\boldsymbol{t}_w} sin\theta_w \tag{15}$$

Where $\hat{\boldsymbol{n}_w}$ and $\hat{\boldsymbol{t}_w}$ are the unit vectors normal and tangential to the wall, respectively.

At the moment, the above equations were solved with the help of finite volume (FVM) based commercial fluid flow solver Fluent 6.1 (Fluent Inc., USA). However, due to the superior experience for the single phase flow particularly in three dimensional problems, FEATFLOW is our preferred candidate for the future. So we have already started to implement the same system of the equations in our finite element (FEM) based FEATFLOW. At Present, we are missing surface tension and wall adhesion effects in it.

The geometry for the two-phase simulations is shown in Figure 5. The unstructured rectangular grid generated with the help of Gambit 2.2 (Fluent Inc., USA) was used for simulation. The grids were refined in the vicinity of Y-junction in order to improve the resolution.Two equal flow rates were given at the two inlets. In some simulations, those were used as constants while in some simulations they were defined sinusoidal. At the outlet, the Neumann type boundary condition was used. The flow fields were achieved with equidistant time stepping of 3×10^{-5} and with maximum time 20 s. However, the other parameters were kept same like single phase simulations.

3.2 Results and Discussion

The laboratory experiments were carried out for a cyclohexane-water system. The two liquids were introduced at two inlets at constant pressure using precision piston pumps. Initially one phase flows into the microreactor through Y-junction, while the other to cross the junction, thereby both phases struggle to flow and produce alternate slugs. The experiments were carried out for capillary diameter ranging from 0.5 to 1 mm. Well defined slug flow was observed in the capillaries. In the case of gas-liquid pipe flow, the slug flow is generated from stratified flow [13] by natural growth of hydrodynamic instabilities and liquid accumulation is due to instantaneous imbalance between pressure and gravitational forces caused by pipe undulations. In the experiments, the inputs were given at constant pressure, the mixing element (Y-type in the present study) plays an important role in the generation of slug flow. The literature shows that slug flow was generated in the microreactor for different applications using different type of mixing elements. The T and cross type of elements were used to generate the slug flow in [4] and reported that the comparison between these two devices shows no significant difference. Further, Y type mixing element was used for the production of slug flow in the capillary microreactor in [8] and reported that well defined slug flow was generated with the deviation of $\pm 5\%$ from mean slug size at same average flow velocity.

In order to generate slug flow by CFD methodology, the simulations were carried out for the same experimental operating conditions using different immiscible fluid systems. As a first attempt, two sinusoidal inputs were given for two phases in order to understand if the hydrodynamics instabilities are one of the reason to generate the slug flow. Initially, the simulations were carried out without surface tension and wall adhesion. In this case, at low flow velocities, both phases flow as parallel flow with wavy interface. With

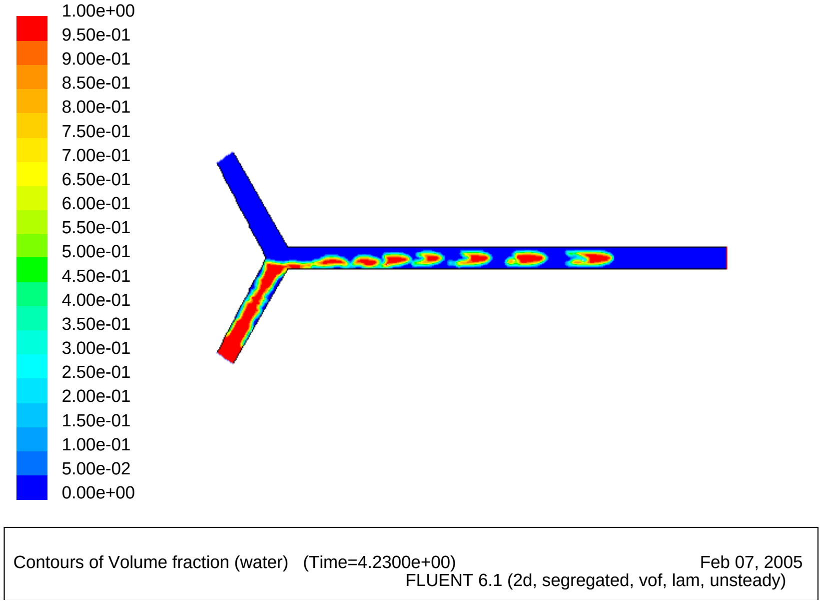

Fig. 6. Flow simulation without wall adhesion in a microreactor of 1 mm diameter for oil-water system. (u_1=10 mm/s and u_2= 10 mm/s)

the further increase in the flow velocities of both phases, the waves grow and finally they show waves as big as a slug. However, it shows deformed interfaces which was connceted to the bottom of other slug. The connecting layer between two slugs was found to be reduced along the lenght of the capillary. Then the surface tension was implemented and identical flow rates were given and it was observed that the secondary phase flows in the form of deformed bubbles and there is no interaction with the wall as shown in Figure 6.

Further, wall adhesion and surface tension was implemented in Fluent solver and simulations were carried out. Refer [9] for further details of surface tension and wall adhesion. The contact angle was given explicitly from the measured experimental values (80 - 90^0). The mesh was refined further to a size smaller than 0.001× slug diameter (capillary diameter). A time step of $1 - 5 \times 10^{-5}$ used for simulations and well defined slug flow was observed. The well defined slug flow at inlet velocity of 10 mm/s for each phase is shown in Figure 7. As can be seen, the liquid travels thorugh Y-junction as a parallel flow to a certain distance and due to wall adhesion the interfece makes an angle with the wall and thus slug formation takes place. The size of the two consecutive slug is same because of equal input flow which was given at the inlet. Thus, it shows that wall adhesion palys an important role

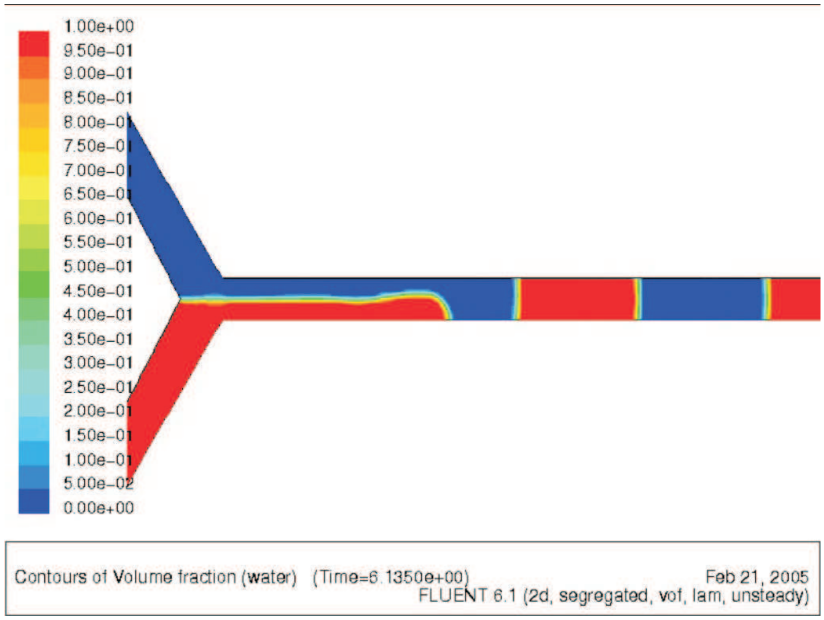

Fig. 7. Slug flow formation at Y-junction in a capillary microreactor of 1 mm diameter for oil-water system. (u_1=10 mm/s, u_2= 10 mm/s, θ_w=90^0)

in slug flow generation. Also it was observed that wall adhesion influences the calcualtion of surface normal.

In the laboratory experiments, the slug flow was observed at all flow velocities. Similar to the this, the well defined slug flow was observed in the simulation with surface tension and wall adhesion for different immiscible fluid systems. The study will be continued by implementing the surface tension and wall adhesion in the FEM solver FEATFLOW and the performace of both solvers will be compared. Further, the detailed characterisation of slug size, mass transfer and chemical reaction will implemented in the FEM solver. Before comparing these numerical results with experimental, there is need to consider three dimensional effect in the slug flow generation. This target can certainly be achieved with more successor works.

4 Conclusion

The velocity patterns and slug flow generation have been studied with the help of CFD modelling. The bidirectional velocity profile i.e. internal circulations within each slug with length greater than its diameter were observed. The increase in the average flow velocity showed increase in the intensity of internal circulations. The present two-phase flow methodology shows an appropriate step towards the generation of well defined slug flow. In the future, the present study can be improved by optimised numerics with the inclusion to predict mass transfer and chemical reaction in more realistic situation.

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