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Study of Flow Patterns of Water-ionic Liquid System in T-junctions using Computational Fluid Dynamics Simulations: Effect of Channel Geometry and Superficial Velocity

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Recovery of mixed plastics using liquid-liquid extraction is an emerging area of research. Green solvents like ionic liquids (IL) and efficient techniques like microchannels for extraction have considerable potential in extraction of plastics to maximize both solvent and plastic recovery with microchannels. New flow patterns have been observed experimentally for flow of greener solvents in microchannels and no reports of Computational Fluid Dynamics (CFD) simulations for such patterns are reported in literature. In the present work, CFD simulations for water-IL system in rectangular microchannels for the experimental conditions reported in literature have been carried out for different operating conditions, geometric parameters and physical properties of liquids in contact with each other in a two phase flow. Qualitative predictions for slug, plug, parallel and throat-annular flos show good agreement with experimental results while rivulet flows could not be predicted. Predictions in drop flow showed considerable deviations from experimental observations. Quantitative predictions for plug lengths were analysed for the experimental conditions reported in the literature. The deviations of 7-8% have been reported as compared to experimental results. This study shows the capability of numerical simulations to predict different flow patterns and depicts the potential for carrying out simulations for dissolution of plastics in microchannels in future

1. Introduction

Liquid liquid extraction (LLE) technique using green solvents for recovery of bioactive products like microalgae using ultrasound (Papadaki et al., 2016), for extraction of valuable compounds using microextractors (Pataro et al., 2019) or extraction of Polyhydroxybutyrate (PHB) from bacteria (Abate et al., 2022) has gained extensive prominence in last decade. However, extraction of plastics using such techniques has yet not received the required attention. The extraction of recoverable plastics faces several challenges like separation of solvents after recovery of plastics. As mentioned by (Zhao et al., 2018) in their review on separation of solvents reported that extraction of recoverable plastics undergoes the process of dissolution. This involves solvent diffusion and chain disengagement. The chain disengagement causes the plastic to be converted to polymer. Mostly organic solvents like xylene, toluene, turpentine etc. have been tried for this purpose. The major success of plastic recovery using LLE lies in the quality and efficiency of solvent recovery. Ionic liquids (IL) consist of green solvents and high extraction efficiency and can be easily recovered. Microchannels posses the qualities of high surface area to volume ratio. Most important factors for having high extraction efficiencies depends on flow patterns followed by mass transfer and provides good promise for both high plastic and solvent recovery. Several experimental and Computational Fluid Dynamics (CFD) studies depicting the importance of flowpatterns on mass transfer can be found in a few reviews (Ganguli and Pandit, 2021;Ganguli et al., 2023). The influence of interfacial forces may be defined by a variety of dimensionless numbers, such as the Capillary number (Ca) = $(\mu U_{bulk})/\sigma$, which is the ratio of the viscous force to the surface tension force, and the Weber number (We)= $(\rho U^2_{bulk} d)/\sigma$, which is the ratio of the inertia force to the surface tension force. The influence of inertial forces is defined by the Reynolds number ($Re=dU\rho/\mu$). Flow patterns help in deciding the solvent properties operating parameters like velocity etc. Knowing the right flow patterns helps in choosing right geometry in case of microchannels.

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The conventional flow patterns in microchannels include plug flow and parallel flow which depend on geometric operating conditions, physical properties of liquids. It was hence thought worthwhile to present the prominent research works (both experimental and CFD) in microchannels with IL as organic phase in the forthcoming sections.

1.1 Experimental studies

(Yagodnitsyna et al., 2016) have described some of the prominent experimental works of different two phase LL flow patterns. Similarly, for systems like water-IL were investigated by (Yagodnitsyna et al., 2017) and (Yagodnitsyna et al., 2020) where flow patterns like plug flow, slug flow, parallel flow, rivulet and throat annular flow were found. Mass transfer during extraction of calcium from aqueous phase using IL as solvent is (Marsousi et al., 2019) where high extraction efficiencies upto 94% in spiral microchannels while it is only 10% in conventional microchannels. The authors attributed the enhancement in mass transfer to flow pattern specifically the mixing in the droplet and the bulk phase between two droplets during their movement in the microchannels.

1.2 Computational Fluid Dynamics (CFD) studies

Several research works in CFD simulations for predicting flow patterns are reported in literature but have been restricted to plug flow and parallel flow regime. Effect of flow patterns on mass transfer have been carried out only by few researchers. Hence, only two important works which depict the capability of CFD to predict extraction efficiency and dependence on flow patterns are elaborated in this section. Different approaches to track the interface to understand flow patterns in CFD include the Volume of Fluid (VOF), Level-Set (LS) and Combined Level-Set and VOF (CLSVOF). Volume of Fluid (VOF) is the most utilized interface tracking to understand liquid-liquid interface dynamics in a microfluidic device. (Gómez-Pastora et al., 2018) carried out both experimental and CFD studies using the VOF approach coupled with convection-diffusion equation and the Navier-Stokes governing equations of mass and continuity to predict extraction efficiency. A good agreement between the simulated and experimental results was observed. (Tsaoulidis and Angeli, 2015) carried out CFD simulations for circular capillaries with diameters in range of 0.5 mm to 2 mm in plug flow regime to study mass transfer during extraction of uranium oxide ions from nitrous solutions using ionic liquids. The CFD simulations were carried out without interface tracking methods assuming wall moving with plug velocity. The authors found reasonably good predictions for mass transfer for different geometrical configurations.

2. Objective of the work

Literature work shows that extraction in microchannels is restricted to only slug and parallel flow while many other flow patterns which exist with IL as solvent have numerically not been explored. Further, the effect of mass transfer when these flow patterns occur have also not been explored but the numerical techniques illustrated in Section 1.2 predict both flow patterns and mass transfer well for conventional flow patterns. As a first step towards recovery of solvent in plastic recovery with IL's the primary objective is to carry out CFD simulations and predict the flow patterns like plug, slug, throat annular, rivulet and parallel flow (as per the terminology followed by (Yagodnitsyna et al., 2017)) both qualitatively and quantitatively and validate the predictions with the experimental results of (Yagodnitsyna et al., 2017) reported for two different geometries.

3. Mathematical modeling

3.1 Geometric details

Figure 1A shows the 3D geometry used for the simulations while Figure 1B represents the corresponding grid used. The grid sensitivity for the geometries considered for simulations have been carried out for the plug flow case as a mandatory aspect of CFD simulation (though not shown here). Three different mesh elements namely 343280 (coarse), 415570 (medium) and 485600 (fine) elements were chosen. It was observed that the highest deviation between the mesh elements of coarse and medium meshes are around 10 % while for the medium and finest mesh are around 2%. Hence, the mesh elements with 415570 elements have been used for all the simulations.

3.2 Method of solution and Boundary condition

Both the faces on the top and bottom of the vertical limb are velocity inlets for the two fluids (IL (top) and water (bottom) respectively) while the far end of central horizontal limb represents the outlet shown in Figure 1. The outlet is represented as pressure outlet. All the other faces are modelled using the no-slip wall boundary condition. The spatial derivatives were discretized using the QUICK scheme while a first-order implicit method was used for the discretization of the temporal derivatives. The Pressure Implicit with Splitting of Operator (PISO) algorithm was used for the pressure-velocity coupling in the momentum equation

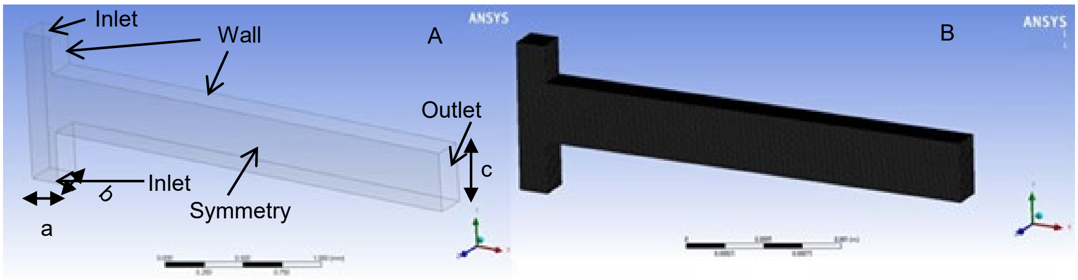

Figure 1. Geometric details for the case of 100 x 400 µm as used by (Yagodnitsyna et al., 2017) in their experimental investigations (A) Geometry (B) Mesh. a and b represent width and breadth of channel (100 µm) while c represents the height of the channel (400 µm in this case)

4. Results and discussion

CFD simulations were carried out for the two geometries and operating conditions considered by (Yagodnitsyna et al., 2017). VOF method has been used for all simulations considered in the study using Ansys Fluent 18.1.

4.1 Flow patterns

The focus of the study in this section is to understand the effect of operating conditions and physical properties of dispersed and continuous phases. The flow patterns in liquid-liquid systems have been defined in different ways by different authors. In the present work we follow the terminology of (Yagodnitsyna et al., 2017). The simulation results are qualitatively compared with the experimental photographs for various flow patterns in literature.

Table 1: Physical properties of liquid

Physical properties	Ionic liquid	Water
Density (kg/m^3)	1420	997
Viscosity mPa s	41	0.894
Interfacial tension, mN/m	12.3	

Table 2: Flow patterns for different bulk velocities and dimensionless numbers for both dispersed and continuous phases

Flow pattern	**U_w (mm/s)**	**U_{IL} (mm/s)**	**Re_d**	**Re_c**	**Ca_d**	**Ca_c**	**We_d**	**We_c**
Plug	0.15	0.3	0.0017	0.03	0.001	1.09E-05	1.66E-06	2.92E-07
Drop	2.9	14.5	0.0804	0.52	0.048	2.11E-04	3.88E-03	1.09E-04
Slug	115.7	0.06	0.0003	20.64	0.0002	8.41E-03	6.65E-08	1.74E-01
Throat annular	28.9	14.5	0.0804	5.16	0.048	2.10E-03	3.88E-03	1.08E-02
Parallel	290	14.5	0.0804	51.75	0.048	2.11E-02	3.88E-03	1.09E+00
Rivulet	580	1.16	0.0064	103.5	0.004	4.22E-02	2.49E-05	4.36E+00

Table 1 summarizes the properties of the fluids used for simulations and calculations pertaining to dimensionless number. Table 2 summarizes the dispersed phase and continuous phase Reynolds, Capillary and Weber numbers used for the study of the different flow regimes. The hydraulic diameters of both cases are the same 160 µm. Presently, all the predictions of (100 x 400 µm) are presented since all other simulations except the slug flow showed similar predictions for both geometries. To optimize the computational time and effort the length of the CFD domain is limited to 4 to 7 times lower than actual domain while retaining the requirements for proper flow. An important finding from the Table 2 is that the Capillary number of the continuous phase controls the flow regimes. As the Ca number increases, the regimes change from one regime to other characterized by plug regime for lowest Ca number and rivulet for highest Ca number. Figure 2 (i) shows the flow patterns predicted by CFD simulations while Figure 2 (ii) shows the experimental results of (Yagodnitsyna et al., 2017). Qualitative predictions of single plug by CFD simulation shows excellent agreement with experimental photographs of published literature as depicted in Figure 2 (a).

Figure 2 (b) however shows that CFD simulations are unable to predict the number and size of the droplets formed as observed by (Yagodnitsyna et al., 2017).

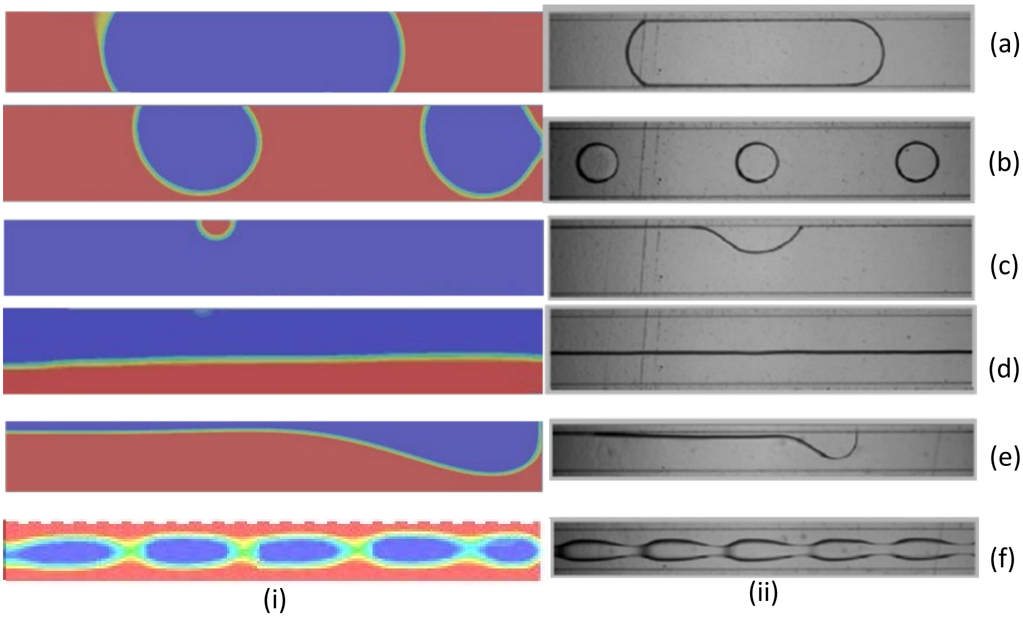

Figure 2. Flow patterns (i) CFD predictions blue color denotes dispersed phase while red is continuous phase volume fractions (ii) Experimental photographs (with permission from (Yagodnitsyna et al., 2017). (a) Plug flow (b) Drop flow (c) Slug flow (d) Parallel flow (e) Slug flow (120 x 240 μm) (f) Throat annular flow. All simulations except (e) are for (100 x 400 μm)

Discrepancies in simulation predictions were observed in drop flow regime (Fig. 2b). Two droplets were observed from the simulation results with shape nearly equal to channel diameter and one of the wall being wetted by dispersed phase while the corresponding experimental photographs show 3 droplets with size much lesser than the channel diameter and no wetting of surfaces. The probable reasons for discrepancy might be due to the fact that (i) contact angle change might be dynamic in nature (ii) the droplet size might not be spherical in simulation and due to symmetry boundary condition assumption the droplet shape is erroneously predicted. For slug flow the CFD predictions for both geometries have been presented in Figure 2c and 2e and show good agreement between experimental observations and simulation predictions. Figure 2c shows an isolated hemispherical droplet at a distance without a tail while experimental photographs show a trailing line of the dispersed phase. Further, the shape and size of the slug between the prediction and experimental photograph has substantial deviation (quantitative measurements of experimental data are not available). However, in Figure 2e the experimental observations and simulation predictions show a good qualitative match. Here, the trailing dispersed phase is visible from the volume fractions of dispersed phase. Figure 2d shows the CFD predictions and experimental observations of parallel flow. As clearly depicted the simulations show good qualitative match with experimental results. Figure 2f shows the simulation results and experimental observations of throat annular flows. The simulations for throat annular flows and successful predictions have been done for the first time as per the published literature data. The number of ovular cells predicted by the CFD simulations agreed well with the experimental data. While the information of cell sizes are not available the present results are a significantly encouraging results since such type of flows are difficult to simulate. Efforts to simulate rivulet flow have been made but encouraging results were not found and hence have not been presented.

4.2 Effect of bulk velocity and flow ratio on plug dynamics

In the previous subsection, the flow patterns arising due to an interplay of inertial, viscous and surface tension forces. (Yagodnitsyna et al., 2017) have mentioned in their published work regarding lack of data on properties of plug flow. CFD simulations were performed for both geometries and plug lengths were found through image processing of the simulated results. Figure 3A shows that there is a linear increase in plug velocity with that in the bulk velocity. It is interesting to note that the simulations underpredict the values of the experimental measurements till bulk velocity of 0.7 m/s after which it over predicts. This may be attributed to the fact that the error bars in the experimental investigations are higher at the lowest and the highest bulk velocities and predictions are well within the range. Another important aspect which needed investigation was the slug length to diameter ratio. This is an important factor due to the internal and external circulations that occur due to the varying slug length to diameter ratio which enhances mixing and in turn mass transfer.

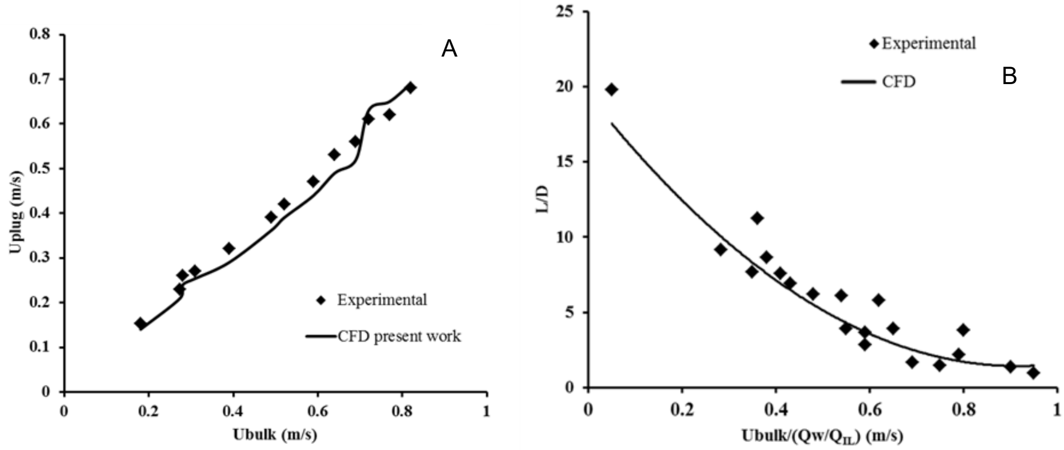

Figure 3. Simulated v/s experimental results to study properties of plug flow for geometry 100 x 400 µm (A) Variation of plug velocity with bulk velocity (B) Comparison of plug velocity and plug length to diameter ratio with dimensionless ratio of bulk velocity and flow ratio

The abscissa has been considered the same as that of (Yagodnitsyna et al., 2017). The predictions match well with the experimental data with most of the points within a deviation of 8 %.

5. Discussion

In Section 4, both qualitative and quantitative predictions by CFD simulations have been presented. It is interesting to note that the capability for simulations to predict the flow patterns would help researchers to carry out mass transfer studies in different regimes. It is worthwhile to mention that both experimental and simulation studies for mass transfer have been carried out in plug flow or parallel regimes where mixing is limited in the form of internal circulations inside the plugs or outside between two consecutive plugs in the case of plug flow regime and at the interface in parallel flow regime. Since the extraction of mixed plastics is a new system experimental studies can be explored in microchannels using IL's. Further, simulation studies can complement experimental investigations well and operated under different flow regimes to study mixing and pressure drop. It is anticipated that throat annular flows would give better mixing characteristics than plug flow regimes with lower pressure drop than micromixers thus providing higher mass transfer without increase in pressure drop. While the above discussion needs significant amount of further studies there is definitely lot of promise for extraction of mixed plastics in different regimes.

6. Conclusions

Qualitative predictions have shown good agreement with experimental results in cases of plug, slug, parallel and throat annular flows. The following conclusions were drawn as follows:

1 Drop flow predictions show considerable discrepancies. Drop sizes in case of drop flow are highly over predicted and attach to one of walls which is not observed in experimental investigations reported in the literature.

2. Throat annular flows have been successfully simulated with excellent agreement with respect to experimental measurements in terms of both number and size of the cells.

3. Predictions of slug flows were found to be dependent on geometry of the microchannel. Of the two geometries considered one of the geometries had good agreement with experimental observations while the other deviated around 10%.

4. Rivulet flows could not be predicted and have not been reported presently.

5. Quantitative results of bulk v/s plug velocity and slug length v/s non-dimensionalized bulk velocities showed good agreement with experimental results.

6. CFD predictions support the conclusions of literature that the plug length can be described as a function of bulk velocity very well and does not depend on aspect ratio of channels.

7. Rigorous simulations studies to simulated drop regime and rivulet regimes needs to be taken up by researchers.

8. Experimental and simulation studies involving extraction of mixed plastics using microchannels needs to be taken up and extensive simulations needs to be carried out for the throat annular regime in terms of its ability to possess enhanced mixing characteristics

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Notations

Ca – Capillary number, (-)
d – channel diameter, μm
D – slug diameter, μm
L – slug length, μm
Q – flow rate, lit/min
Re – Reynolds number,(-)
U – velocity, (m/s)
We – Weber number, (-)

Subscripts

c – continuous phase
d – dispersed phase
bulk – bulk phase
w – water
IL – ionic liquid

Symbols and Abbreviations

ρ – density (kg/m^3)
μ – viscosity (kg/m s)
σ – surface tension (N/m)
CFD – Computational Fluid Dynamics
CLSVOF – Combined LevelSet and VOF
LS – LevelSet method
VOF – Volume of Fluid method

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