

Numerical study of two phase fluid flow in a T-junction microchannel

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Abstract

Numerical Investigation of two phase (gas-liquid & liquid-liquid) fluid flow in a T-junction rectangular microchannel was carried out. The model was developed in both 2D and 3D cases in ANSYS Fluent 18.2 Academic research software using volume of fluid method (VOF). In this work, the effect of various parameters such as: fluid properties, channel properties, slug size, pressure drop on hydrodynamics in the microchannel were studied and discussed. It was observed that the Pressure drop predicted by 3D model is higher than the 2D model that may be because of curvature and hence the internal pressure in 3D model is approximately double of 2D model. In addition, it was also observed that the slug volume decreases more rapidly with increasing flow ratio. The flow velocities were varied in the range of 0.025 m/s to 0.50 m/s. Results obtained from simulations are compared with available literature and experimental data [1] and found encouraging trends and in-line with that of experimental results already published.

Keywords: Hydrodynamics; slug flow; CFD; microchannel

1. Introduction

A micro-structured device deals various advantages in various applications such as: heat exchangers, microreactors, microelectronics, micro-electro-mechanical systems (MEMS) etc. Heat and mass transfer is enhanced due to high surface to volume ratio in microfluidic devices compared to conventional devices [2]. In these devices, small amount of fluid can be processed with enhanced outcome e.g. in biomedical engineering, various medical tests were performed on a single microfluidics chip. Various flow patterns have been reported in microchannel i.e. slug flow, bubbly flow, churn flow, annular flow etc. The arrangement of the different fluid flow pattern is totally depends on the thermo-physical property of fluids and geometry of the object [2, 3]. The flow pattern analyses [4, 5, 6] depicting development of fluid flow with above thermo-physical properties and characteristics of geometry, shows that slug flow leads over the other flow pattern in terms of enhancement of heat and mass transfer in microfluidic devices. Mass transfer between two fluids generally depends on two factors: firstly the internal circulation within each slug and secondly the concentration gradients between adjacent slugs [7, 8]. In fact, these devices builds the interfacial zone and rate of self-blending because of development of small size air bubble/droplets [9] which improves rate of heat and mass transfer [10, 11]. Further, during slug formation, microfluidic frameworks offer tremendous scope in the process of computerization and revamping of substance and unified mechanical frameworks. A number of numerical analysis has been accounted, for on immiscible liquid-liquid and gas-liquid two phase flow system by VOF model, which is one of the most famous and feasible technique to track the interfacial properties by calculating volume fraction. Various researchers [1, 12, 13, 14, 15] had considered this technique for analysis of hydrodynamics of gas-liquid two phase flow, dependency of slug flow on different

parameters. Taha and Cui [16] did detail study on hydrodynamic of slug flow in both 2D and 3D dimension with moving frame and also studied distribution of shear stress, various shapes of bubble and there speed inside the channel with the help of volume of fluid method. Desssimoz et al. [17] performed simulation on 2D geometry with T & Y structured and they found that frictional pressure drop is comparatively high in T-junction than the Y-junction. Thin film and wettability are the main characteristics of slug formation were studied using VOF model in T-junction microchannel 2D geometry [2, 12, 18, 19].

From the above collected works, it was realised that the majority of the researchers focused on hydrodynamics, heat, and mass transfer in microchannel but still have some issues likewise effects of material of construction of the channel and their geometry, variation in pressure drop in 2D and 3D models, and several other fluids have not been reported. Based on above, a detailed study of hydrodynamics of slug flow with varying fluid properties and operating parameters using VOF technique have been reported in this paper. The channel used in this investigation was a T-junction micro-channel, in which the flow velocity of both the phases was kept in the range of 0.025 to 0.50 m/s. Furthermore, the simulation results obtained were compared with available results [1] and found similar trend.

2. Mathematical Model

In this work, a mathematical model was taken to simulate the hydrodynamics of two phase flow by VOF model in fluent software under slug flow regime. The hydrodynamics of such flows can be pronounced by incompressible Navier-Stokes equations. These equations, continuity, momentum and volume fraction equation for multiphase flow are as follows:

Equation of continuity:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\vec{v}) = 0 \quad (1)$$

Equation of motion:

$$\frac{\partial(\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot [\mu(\nabla \vec{v} + \nabla \vec{v}^T)] + \vec{F}_{SF} \quad (2)$$

$$\vec{F}_{SF} = \rho \vec{g} + \vec{F} \quad (3)$$

Volume fraction equation:

$$\frac{\partial \phi}{\partial t} + \vec{v} \cdot \nabla \phi = 0 \quad (4)$$

where ρ denotes the density, μ the dynamic viscosity, \vec{v} the velocity vector, ϕ the volume fraction, p the pressure and \vec{F}_{SF} the surface tension force. The continuum surface force (CSF) model [20] was used in equation (2), surface forces are sum of two forces; surface tension force and gravitational force but in case of microchannels gravitational force are negligible therefore only the surface tension act as a source term in the equation of motion [2]. The surface tension (\vec{F}_{SF}) per unit volume in Eq. 2 can be evaluated as:

$$\vec{F}_{SF} = \sigma k_n \left[\frac{\phi_1 \rho_1 + \phi_2 \rho_2}{\frac{1}{2}(\rho_1 + \rho_2)} \right] \quad (5)$$

$$k_n = -(\nabla \cdot \hat{n}) \quad (6)$$

where σ denotes the surface tension and k_n the interface curvature and these are calculated from the divergence of unit normal surface $\hat{n} \left(= \frac{\vec{n}}{|\vec{n}|} \right)$, where surfce normal, $\vec{n} = \nabla \phi$

The volume fraction (ϕ) in the interface tracking algorithm was calculated by solving Eq. (4) and it becomes zero for continuous phase and one for dispersed phase. The hydrodynamics of the individual phases are defined and all phases obtain a volume fraction in the computational cell in domain as well as at the interface. For multiphase flow, if the known volume fraction of one phase is ϕ_1 , the density (ρ), and viscosity (μ) in all cell can be evaluated using Eqs. (8 and 9):

$$\rho = (1 - \phi_1) \rho_2 + \phi_1 \rho_1 \quad (8)$$

$$\mu = (1 - \phi_1) \mu_2 + \phi_1 \mu_1 \quad (9)$$

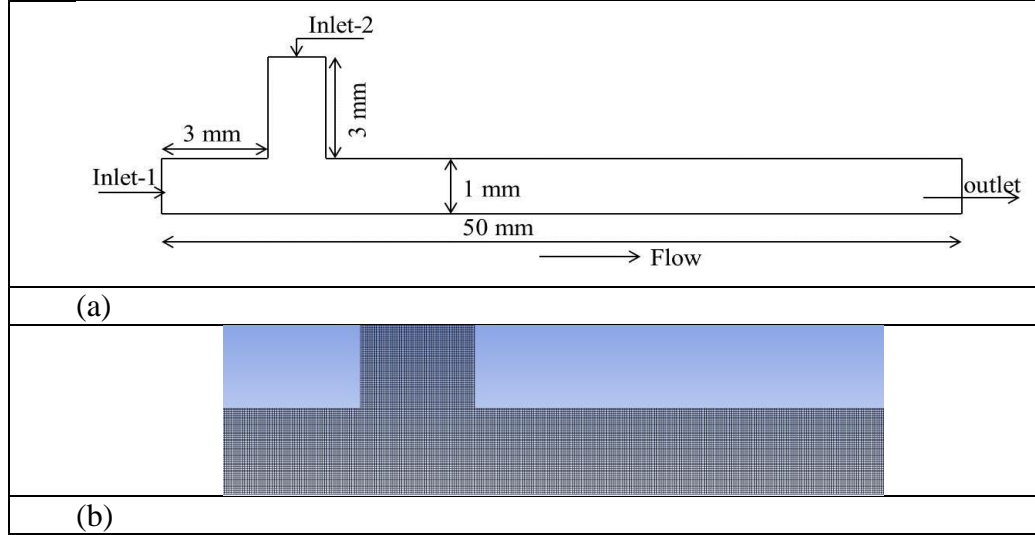


Fig. 1 (a) Geometry, (b) Meshing

Table 1: Physical properties of fluids for two phase flow system

Fluid	Density (ρ) (kg/m ³)	Dynamic viscosity (μ) (kg/m.s)	Interfacial surface tension (σ) (N/m)
Water	998.2	0.001003	0.072
Air	1.225	1.7894×10^{-5}	
Cyclohexane	780	0.000982	0.05
Water	998.2	0.001003	
Furfural	1160	0.00149	0.03
Iso-octane	692	0.0005	

3. Numerical Scheme

The hydrodynamics of two phase flow has been investigated numerically using VOF method in a two dimensional (2D) geometry to save computational time and energies. Fig. 1 represents the channel geometry, boundary conditions and mesh was created by Ansys pre-processor solver. T-junction geometry has two inlets; one fluid was introduced horizontally called continuous phase and other vertically called dispersed phase. At the outlet boundary condition, a constant atmospheric pressure was applied. The simulations were carried out for different fluids in CFD software ‘ANSYS FLUENT 18.2’ with double-precision solver. Mesh size was taken to be $2.0 \mu\text{m}$ to ensure solution independent from mesh and found reproducible simulation results. The present mesh contains 132500 hexahedral cells. The simulation are carried out using unsteady state transient time, pressure based solver and Courant no (Cr) were fixed at 0.25. The time step size 10^{-6} sec was used in this simulation. The stationary wall no slip shear condition and wall adhesion is

turned on and default contact angle was set at 90° . The value of surface tension was set according to systems, which is given in Table 1. Pressure-implicit with staggering option (PISO) scheme was used for pressure-velocity coupling with constant neighbour correction factor value equal to one. For the discretization, gradient of scalars i.e. pressure, velocity and volume fraction were calculated using Green-Gauss cell-based method. Pressure staggering option (PRESTO!) scheme for pressure gradient, second order upwind scheme for velocity gradient and Geo-reconstruct scheme were taken for volume fraction as solution parameters. Non-iterative time advancement first order implicit transient formulation was also taken into account. The convergence condition for continuity and velocities were fixed as 10^{-3} . The simulations were carried out on a workstation.

4. Results and Discussion

A rectangular channel of hydraulic diameter 1 mm and 50 mm length with 3 mm side entry length was used in this investigation. The slug velocities of fluids were taken from 0.0025 to 0.50 m/s. The properties of working fluids used in this study have already been shown in Table 1.

4.1 Effect of flow rate on slug formations:

The slug volume is the important parameters in two phase flow for determination of mass transfer between the slugs in microchannels [2]. As evident from literature, some researchers have developed correlations for estimation of slug size, which are in terms of flow ratio of fluids, diameter of channel, volume fraction and physical properties of fluids. In this study, the effect of gas flow rate on slugs was investigated, which is presented in Fig. 2. The result obtained from simulation are plotted and correlated with [21, 22]. It was observed that the slug length decreases linearly with gas velocity at constant liquid velocity. The results obtained were compared with the available data in literature and it was observed that the trends found in this study are in line with that predicted by [22].

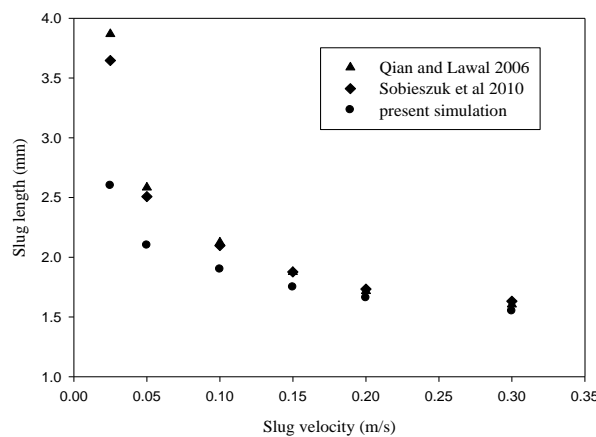


Fig. 2: Effect of gas velocity on slug length at constant liquid velocity, $U_L = 0.025$ m/s

Further, the effect of flow ratio on slug volume for furfural and iso-octane were studied and results obtained were compared with data due to Kashid and Agar [1], presented in Fig. 3(a). It is clearly depicted from the figure that the trend is similar with almost equal decrement of slug volume but the value of slug volume is little more than that of [1]. This variation might be due the change in fluid (cyclohexane-water system). Further, the figure also depict that the slug volume decreases with the increment of slug velocity because of rapid penetration of one phase into others, which leads to high interfacial area and thus resulted enhancement in rate of mass transfer between

slugs at given flow rate. In addition, the effect of flow ratios on slug volume was also studied. Three different flow ratios were taken i.e. 1, 2 and 3, as shown in Fig. 3(b). It was observed that the slug volume decreases more rapidly with increasing flow ratio and thus high mass transfer rates between adjacent slugs were achieved.

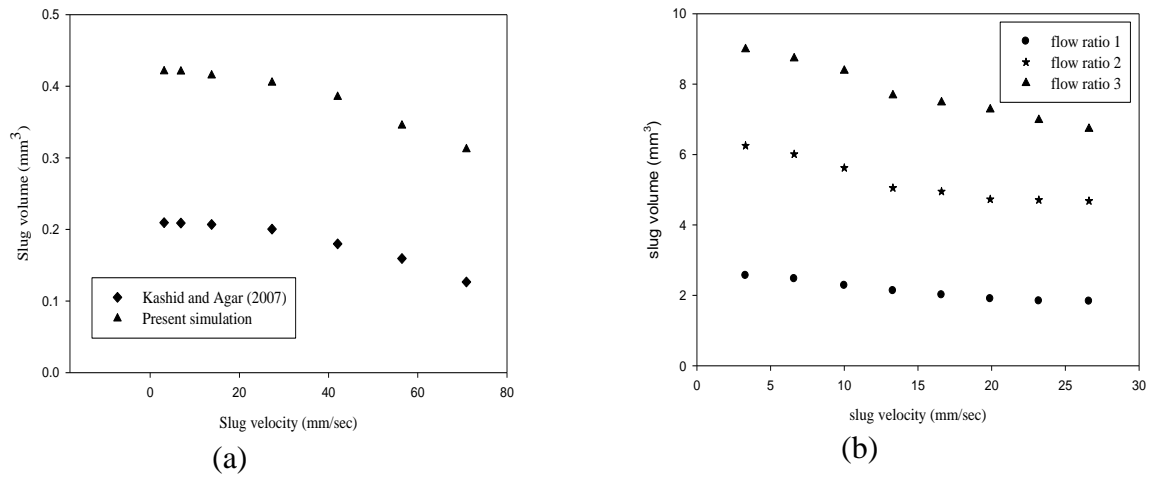


Fig. 3: Effect of flow rate on slug volume (a) identical flow rate (b) different flow ratio

4.2 Comparison of 3D and 2D model:

The total pressure drop in the two phase slug flow has mainly due to two forces: (a) pressure drop due to viscous force and (b) pressure drop due to interfacial tension (Laplace pressure). The total pressure drop in 2D model was less than the 3D model because in 2D only one radius of curvature captured, therefore interfacial tension is just half of 3D model as shown in Fig. 4.

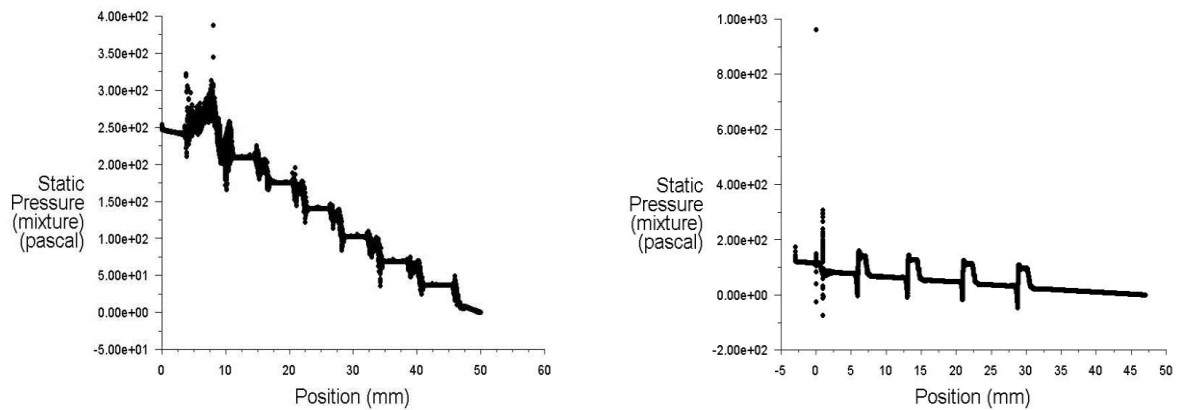


Fig. 4: Static pressure variation in the microchannel for (a) 3D (b) 2D T-junction microchannel ($U_G = U_L = 0.025$ m/s, interfacial tension (σ) = 0.072 N/m and $\theta = 90^\circ$)

4.3 Effect of fluids on slug flow:

A simulation of varying fluids was carried out on hydrodynamics of two phase flow mainly slug flow in a T-junction rectangular microchannel. The increase in fluid viscosity and decrease in surface tension are key parameters to increase Capillary number and hence the formations of slugs by shearing flow regime presented in Fig. 5 (c). At high surface tension the formation of slugs by

squeezing flow regime presented in Fig. 5 (a). The slugs formed followed by shearing flow regime more uniformly at surface tension 0.05 N/m as shown in Fig. 5(b). Further, we observed that the mixing in Shearing flow regime has lower than squeezing regime; therefore the mixing is diminished in which fluids have high viscous and low surface tension.

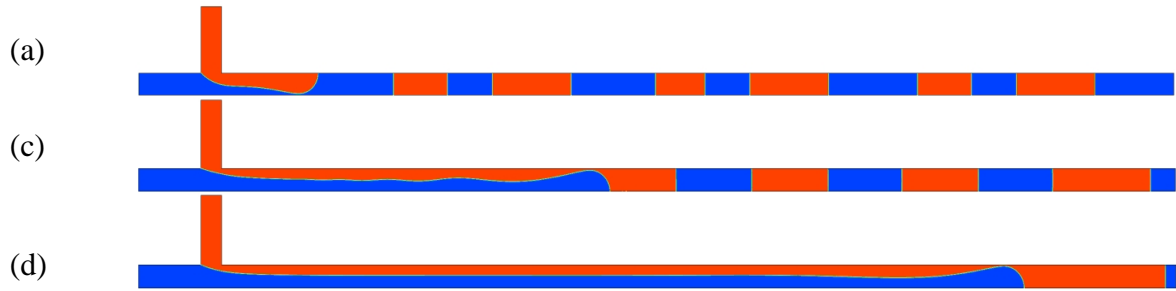


Fig. 5 (a) air-water, (b) cyclohexane-water and (c) furfural-isooctane system at equal flow velocity 0.025 m/s

4.4 Effect of materials on slug flow:

A channel of 1 mm diameter and length 50 mm was constructed with varying materials simulations were performed on hydrodynamics of slug flow in microchannel presented in Fig. 6. The Figure demonstrates that the formation of slugs via squeezing regime and uniformly throughout the channel in the case of high density material i.e. copper.

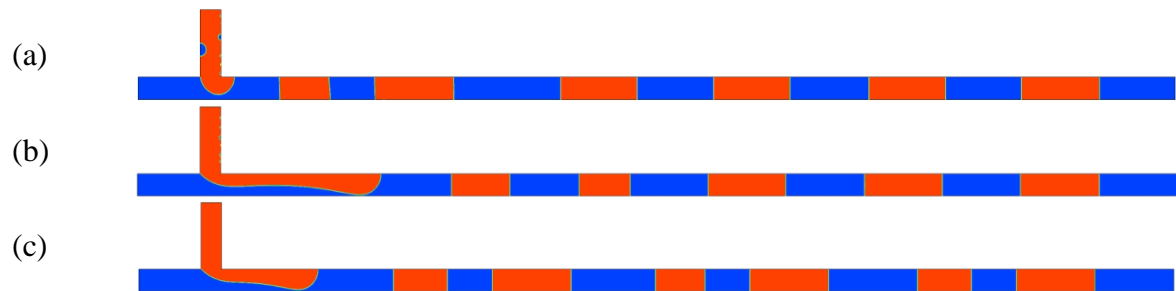


Fig. 6 (a) copper, (b) steel and (c) aluminium at equal flow velocity 0.025 m/s

5. Conclusion

In this work, the hydrodynamics of slug flow using two phase flow (air-water, cyclohexane-water and furfural-iso-octane) in a T-junction microchannel was studied by VOF model. The simulation results are validated with [1] and observed similar trend. Squeezing flow regime was found at high surface tension and thus high mixing between adjacent slugs were observed. Slug volume decreases with increasing slug velocity due to one phase penetrates into others quickly achieves high interfacial area and thus enhanced the rate of mass transfer between slugs in the channel. The pressure drop in 2D model was lower than the 3D model because in 2D case only one radius of curvature captured, therefore interfacial tension is just half of 3D model. Further, it was observed that the hydrodynamics of slug flow depends upon materials of construction, fluid properties, flow ratios, and surface wettability.

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References

- [1] Kashid, M.N. and Agar, D.W., Hydrodynamics of liquid–liquid slug flow capillary microreactor: flow regimes, slug size and pressure drop. *Chemical Engineering Journal*, 131(1-3), (2007)1-13. <https://doi.org/10.1016/j.cej.2006.11.020>
- [2] Khan, W., Chandra, A.K., Kishor, K., Sachan, S. and Alam, M.S., Slug formation mechanism for air–water system in T-junction microchannel: a numerical investigation. *Chemical Papers* 72 (11), (2018), 2921–2932. [Doi: 10.1007/s11696-018-0522-7](https://doi.org/10.1007/s11696-018-0522-7)
- [3] Padoin, N., de Souza, A.Z., Ropelato, K. and Soares, C., Numerical simulation of isothermal gas– liquid flow patterns in microchannels with varying wettability. *Chemical Engineering Research and Design*, 109, (2016.), 698-706. <https://doi.org/10.1016/j.cherd.2016.03.027>
- [4] Triplett, K.A., Ghiaasiaan, S.M., Abdel-Khalik, S.I. and Sadowski, D.L., Gas–liquid two-phase flow in microchannels Part I: two-phase flow patterns. *International Journal of Multiphase Flow*, 25(3), (1999), 377-394. [https://doi.org/10.1016/S0301-9322\(98\)00054-8](https://doi.org/10.1016/S0301-9322(98)00054-8)
- [5] Kawahara, A., Sadatomi, M., Nei, K. and Matsuo, H., Experimental study on bubble velocity, void fraction and pressure drop for gas–liquid two-phase flow in a circular microchannel. *International Journal of Heat and Fluid Flow*, 30(5), (2009), 831-841. <https://doi.org/10.1016/j.ijheatfluidflow.2009.02.017>
- [6] Kawahara, A., Sadatomi, M., Nei, K. and Matsuo, H., Characteristics of two-phase flows in a rectangular microchannel with a T-junction type gas-liquid mixer. *Heat Transfer Engineering*, 32(7-8), (2011), 585-594. <https://doi.org/10.1080/01457632.2010.509752>
- [7] Burns, J.R. and Ramshaw, C., The intensification of rapid reactions in multiphase systems using slug flow in capillaries. *Lab on a Chip*, 1(1), (2001), 10-15. [Doi: 10.1039/B102818A](https://doi.org/10.1039/B102818A)
- [8] Dumann, G., Quittmann, U., Groschel, L., Agar, D.W., Worz, O. and Morgenschweis, K., The capillary-microreactor: a new reactor concept for the intensification of heat and mass transfer in liquid–liquid reactions. *Catalysis Today*, 79, (2003), 433-439. [https://doi.org/10.1016/S0920-5861\(03\)00056-7](https://doi.org/10.1016/S0920-5861(03)00056-7)
- [9] Günther, A. and Jensen, K.F., Multiphase microfluidics: from flow characteristics to chemical and materials synthesis. *Lab on a Chip*, 6(12), (2006), 1487-1503. [Doi: 10.1039/B609851G](https://doi.org/10.1039/B609851G)
- [10] Talimi, V., Muzychka, Y.S. and Kocabiyik, S., Slug flow heat transfer in square microchannels. *International Journal of Heat and Mass Transfer*, 62, (2013), 752-760. <https://doi.org/10.1016/j.ijheatmasstransfer.2013.03.035>
- [11] Bandara, T., Nguyen, N.T. and Rosengarten, G., Slug flow heat transfer without phase change in microchannels: A review. *Chemical Engineering Science*, 126, (2015), 283-295. <https://doi.org/10.1016/j.ces.2014.12.007>
- [12] Kashid, M.N., Renken, A. and Kiwi-Minsker, L., CFD modelling of liquid–liquid multiphase microstructured reactor: Slug flow generation. *Chemical Engineering Research and Design*, 88(3), (2010), 362-368. <https://doi.org/10.1016/j.cherd.2009.11.017>
- [13] Abadie, T., Aubin, J., Legendre, D. and Xuereb, C., Hydrodynamics of gas–liquid Taylor flow in rectangular microchannels. *Microfluidics and nanofluidics*, 12(1-4), (2012), 355-369. [doi: https://doi.org/10.1007/s10404-011-0880-8](https://doi.org/10.1007/s10404-011-0880-8)
- [14] Chandra, A.K., Kishor, K., Mishra, P.K. and Alam, M.S., Numerical investigations of two-phase flows through enhanced microchannels. *Chemical and biochemical engineering quarterly*, 30(2), (2016), 149-159. <https://doi.org/10.15255/CABEQ.2015.2289>
- [15] Kishor, K., Chandra, A.K., Khan, W., Mishra, P.K. and Siraj Alam, M., Numerical study on bubble dynamics and two-phase frictional pressure drop of slug flow regime in adiabatic T-junction square microchannel. *Chemical and biochemical engineering quarterly*, 31(3), (2017),

- 275-291. <https://doi.org/10.15255/CABEQ.2016.877>
- [16] Taha, T. and Cui, Z.F., Hydrodynamics of slug flow inside capillaries. Chemical Engineering Science, 59(6), (2004), 1181-1190. <https://doi.org/10.1016/j.ces.2003.10.025>
- [17] Dessimoz, A.L., Cavin, L., Renken, A. and Kiwi-Minsker, L., Liquid-liquid two-phase flow patterns and mass transfer characteristics in rectangular glass microreactors. Chemical Engineering Science, 63(16), (2008), 4035-4044. <https://doi.org/10.1016/j.ces.2008.05.005>
- [18] Santos, R.M. and Kawaji, M., Numerical modeling and experimental investigation of gas-liquid slug formation in a microchannel T-junction. International Journal of Multiphase Flow, 36(4), (2010), 314-323. <https://doi.org/10.1016/j.ijmultiphaseflow.2009.11.009>
- [19] Santos, R.M. and Kawaji, M., Developments on wetting effects in microfluidic slug flow. Chemical Engineering Communications, 199(12), (2012), 1626-1641. [doi: https://doi.org/10.1080/00986445.2012.660712](https://doi.org/10.1080/00986445.2012.660712)
- [20] Brackbill, J.U., Kothe, D.B. and Zemach, C., A continuum method for modeling surface tension. Journal of computational physics, 100(2), (1992), 335-354. [https://doi.org/10.1016/0021-9991\(92\)90240-Y](https://doi.org/10.1016/0021-9991(92)90240-Y)
- [21] Qian, D. and Lawal, A., Numerical study on gas and liquid slugs for Taylor flow in a T-junction microchannel. Chemical Engineering Science, 61(23), (2006), 7609-7625. <https://doi.org/10.1016/j.ces.2006.08.073>
- [22] Sobieszuk, P., Cygański, P. and Pohorecki, R., Bubble lengths in the gas-liquid Taylor flow in microchannels. Chemical engineering research and design, 88(3), (2010), 263-269. <https://doi.org/10.1016/j.cherd.2009.07.007>