AJChE 2017, Vol. 17, No. 1, 82 – 90

# Numerical Investigation on Multiphase Flows in Various Configurations of Microchannels Using Computational Fluid Dynamics

**Mohd Fadhil Majnis *,[1]**
**Mohamad Rawad Jalwan [1]**
[1] Department of Chemical and Petroleum Engineering, Faculty of Engineering, Technology and Built Environment, UCSI University Kuala Lumpur, Malaysia
*e-mail: fadhil@ucsiuniversity.edu.my

A two-dimensional domain of multiphase flow analyses in this study using the Volume of Fluid (VOF) model was carried out in order to simulate and predict the fluid flows and mixing performance of two miscible liquids in various microchannel configurations. The various microchannels configurations were designed accordingly and the simulation was carried out based on the justified conditions, assumptions and considerations by using the commercial computational fluid dynamics (CFD) software, FLUENT. The grid type and size of the computational domain were verified in terms of stability by performing the grid independence analysis. The result showed that static mixing would be possible to achieve in various configurations of microchannels, however, the simulation results predicted that it appeared to be more efficient in complex and retrofitted microchannels. It showed the potential to promote and enhance chaotic advection, compositions distribution, and diffusivity as compared to basic microchannels that are mostly dependent only on the injection focus. Furthermore, the Reynolds number appeared to be a significant factor to enhance the mixing performance in microchannel beside the configurations.

**Keywords :** CFD; VOF model; microchannel; multiphase flow; mixing performance; Reynolds number

## INTRODUCTION

Microfluidics is a study of designing, formulating and fabricating integrated unit operations with microchannels serving as the fluid path at a microscale hydraulic diameter that less than 1 mm, which deals with the microscale volume of fluids that less than 1 µl (Kee 2011, Watts and Wiles 2007). The science emerged in the early 1980's and since it had developed significantly in terms of continuous fluid flow, droplet formation, and operations such as mixing, reacting and heat exchanging. The operations take place in the internal packing of the microdevices (inside the microchannel which is referred as the configuration). Examples of these devices which arose in the early 1990's include micro-reactors, micromixers, micro-pumps, and micro-heat exchangers (Watts and Wiles 2007). The idea of these devices had initially appeared with the development of micro-technologies for chemical processing in contrast with the conventional chemical processing at macro-scale through chemical process intensification, which, in turn, deals with designing and analyzing methodologies and equipment (integrate reactions and unit operations) to enhance the system's overall performance by reduction in the chemical plant order of magnitude (Stankiewicz and Moulijn 2000, 2004).

The chemical processing micro-devices had been involved in several studies and experiments ranging from microscale volumetric titrations, catalysis (homogeneous and heterogeneous) and catalytic oxidation to micromixing of fluids and much more (Bajus 2012). It demonstrated to be a valuable subject in chemical engineering and it accomplishes the miniaturisation of the macro-scale conventional chemical process devices when designed, analysed, fabricated and implemented adequately. Similarly to developed technologies for the design and analysis of conventional macroscale chemical processing devices, the process of designing and analysing these micro-devices prior to its fabrication is based on mathematical modelling and computer simulations respectively in order to predict its performance according to the application required.

Computational fluid dynamics (CFD) serves as a prediction tool to solve fluid flows problem by means of mathematical modelling and numerical simulation. Fluid flows generally in fluid mechanics are governed by a set of partial differential equations which represent laws for mass, momentum and energy conservation. In this study, the simulation of multiphase flows in the various configuration of the microchannel was carried out using CFD software, FLUENT. The study was to analyse and compare the effect of various configurations and Reynolds number on the mixing performance and residence time of the flow.

## METHODOLOGY

The simulation model development of this study was approached in a similar manner to previous researchers that concerned with mixing in microchannels particularly (Cieslicki and Piechna 2009, Naher et al. 2011, Rudyak and Minakov 2014). The previous researchers considered a most basic mixing channel (T or Y junction) that forces two fluids into a tight chamber were tested initially, prior to retrofitting the chambers in a manner that the mixing performance would be anticipated to improve and reprocess them under the same model conditions in order to validate the response and the performances, analyze and compare the effect of various configurations, and evaluate the differences and the causes.

During preprocessing, the configurations geometries were designed, built, meshed and the boundaries were specified in accordance with the volume of fluid (VOF) model requirements using GAMBIT. The type of mesh used throughout this study was quadrilateral at an interval size of 0.25. The diameter of all the configurations was intended to be one millimetre and the total length (inlet to outlet) was intended to be 18 millimetres. A total number of mesh cells to process in each geometry ranged between 300 and 450. Steady state implicit VOF model with three Eulerian phases (air, water, salt) was set in FLUENT. The boundary conditions were set as desired and the simulations took place using the PISO pressure-velocity coupling scheme, in addition to PRESTO! as the pressure interpolation scheme and first order momentum discretization scheme, whereas, the QUICK VOF discretization scheme was selected. The simulation was carried out for a total number of 500 iterations; however, all the solutions converged after approximately 200 iterations.

In this study, the fluids were assumed to be fed continuously at a steady state laminar flow with Reynolds number less than 2300. Negligible gravitational effect and injection pressure, therefore, the only fluid characteristic acting as the driving force would be considered to be the velocity. Moreover, the microchannels were assumed to be operating at room pressure (1 atm) and temperature. The fluids were considered to enter the channel from atmospheric conditions and escape to atmospheric conditions. The denser fluid was assumed to be (salt-NaCl) (100 percent sodium chloride solution) and was modelled to be a fluid (liquid) at room temperature and pressure (1 atm). The density of liquid NaCl was assumed to be equivalent to that of solid phase NaCl (2160 kg/m$^3$). The viscosity of NaCl was assumed by interpolating the viscosity of a 100 percent brine solution. Surface tension effect between the fluids and the air was neglected. However, NaCl was assumed to increase $H_2O$ surface tension since due to its solubility. The microchannel was not a subject to any external forces or sources of energy (heat or pressure), therefore, any source of mixing was considered static. The mass transfer and diffusion were considered to take place in the absence of a chemical reaction. Velocity, density, viscosity were considered the only fluid characteristics that affected static mixing performance. A total of four phases/fluids were considered to occupy the configurations at a point or another.

## RESULT AND DISCUSSION

Initially, the simulations response, the grid type and grid size chosen were verified in terms of stability, accuracy and resolution by performing grid independence analysis in processing step. Moreover, upon proceeding with the next step, the simulation solutions were obtained for the first set of geometries (configurations in **Figure 1**), initially the response was monitored by visualizing all profiles of interest (velocity, Reynolds number, density, compositions, pressure) and the prescribed tolerance was examined and appeared to be attained which served as another response verification step. For instance, initial conditions set for the model and at

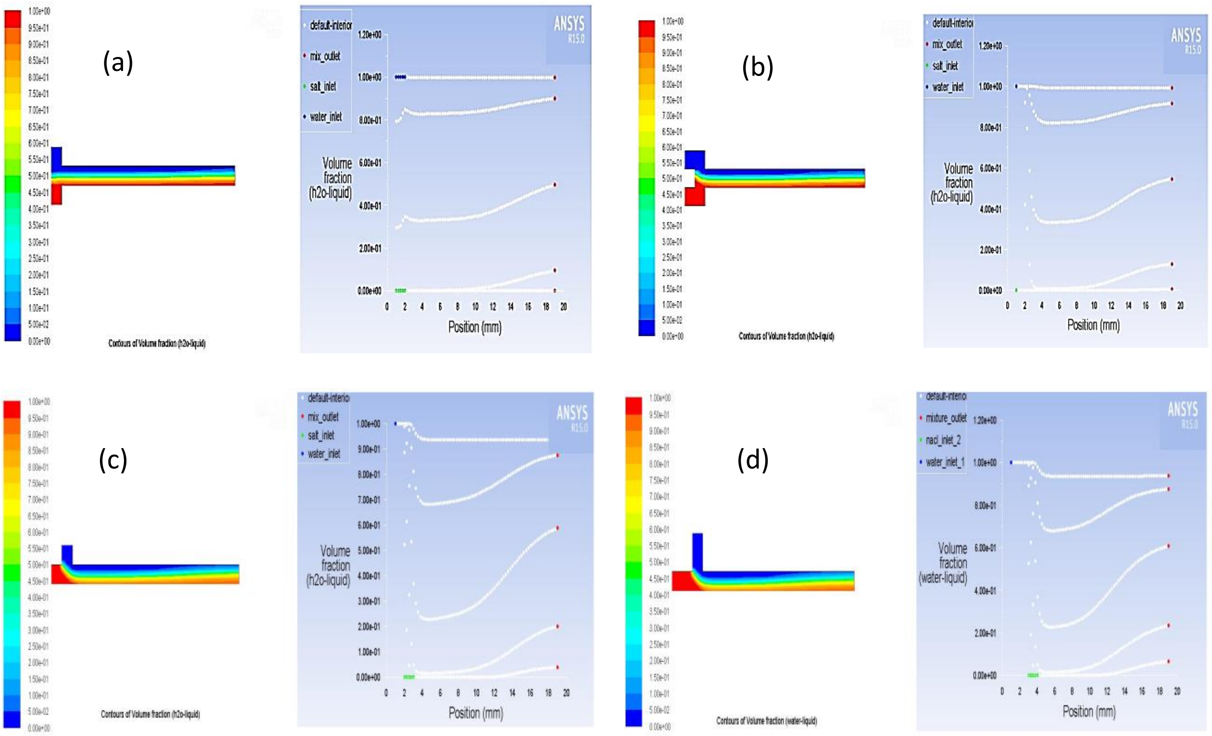

**Fig. 1:** Contour plots and X-Y plots – volume fraction of $H_2O$ profiles for basic microchannel configurations: (a) Capital T-inlet (b) U-inlet (c) Normal T-inlet 1 mm (d) Normal T-inlet 2 mm.

boundaries such as steady state, inlet velocities and compositions, initial pressure, and outlet pressure magnitudes, fluids densities and viscosities. Performing such steps in addition to trial and error are critical in CFD analysis as it helps in detecting uncertainties, errors, bugs related to the software, responsive and non-responsive variable and sensitive parameters.

Using the VOF model set in this study, it was possible to evaluate and analyze the mixing performance of the solutions using various profiles such as density, velocity, composition or viscosity, however, since the compositions profiles appeared to be highly detailed and were meant to represent the results in terms of volume of, therefore, the mixing performance was evaluated based on the compositions at the outlet. The first set of final solutions shown in Figure 1, were initially evaluated and analysed individually, then compared with each other and other studies for further validation and the system appeared to be working adequately in most of the criteria of interest. For example, the mixing performance at the outlet in Figures 1(c) and 1(d), were anticipated to lead better mixing due to the focusing of the denser fluid inlet (blue) which would promote the existence of a horizontal interface for diffusion to take place at regions near the walls (where the fluids do not seem to contact at all in Figures 1(a) and 1(b)). Nonetheless, in all cases in Figure 1, the mixing was not anticipated to occur at any better rate than it was predicted from the simulations since the fluids were expected to mix well

**Table 1.** Mixing performance analysis of basic configurations of microchannel

| **Configuration** | **U-inlet** | **Capital T-inlet** | **Normal T-inlet (1 mm)** | **Normal T-inlet (2 mm)** |
|---|---|---|---|---|
| Type | Basic | Basic | Basic | Basic |
| Number of inlets | Two | Two | Two | Two |
| $H_2O$ (volume fraction) at outlet | 1, 0.9, 0.5, 0.1, 0 | 1, 0.9, 0.5, 0.1, 0 | 0.95, 0.85, 0.6, 0.15, 0.05 | 0.95, 0.85, 0.6, 0.15, 0.05 |
| NaCl (volume fraction) at outlet | 0, 0.1, 0.5, 0.9, 1 | 0, 0.1, 0.5, 0.9, 1 | 0.05, 0.15, 0.4, 0.85, 0.95 | 0.05, 0.15, 0.4, 0.85, 0.95 |
| Diffusion interface | Vertical | Vertical | Vertical/Horizontal | Vertical/Horizontal |
| Mixing base | Inlet Focusing | Inlet Focusing | Inlet Focusing | Inlet Focusing |

at regions near the interface only.

Moreover, for those initial solutions, the effects of various basic configurations on the overall mixing performance was analyzed and tabulated as shown in **Table 1**. However, due to the close similarities in the configurations in terms of the overall design, it was not yet validated that the mixing performance and overall response was reliable, therefore, based on the results obtained and further research on adoptable modification ways concerned with mixing fluids in microchannels, the configurations geometries were further retrofitted. In addition to further analyse and compare the solutions of various configurations and evaluate the effects they have on the mixing performance.

Upon monitoring the contours and plots, it was visible how those geometries had a very high impact on the overall mixing performance, yet, appeared to be following similar responses which further validated the solution setup carried out. Furthermore, the retrofitted and complex configurations performed as anticipated and highly enhanced the mixing performance in some cases as shown in **Figure 2(d)**, whereas, in other cases, **Figures 2(a)**, **2(b)**, and **2(c)**, it was enhanced at regions near the walls (far from the interface) in comparison with previous basic configurations (Figure 1) due to the distribution of the compositions strategically along the microchannel as in Figures 2(b) and 2(c) causing more diffusion interfaces to promote, whereas, in Figure 2(a) the obstacles acted as static mixing elements that promote stretching and folding in addition to diffusion interfaces promotion as well. Furthermore, in Figure 2(d), the fluids appeared to fluctuate intensively through the U-inlet complex structure of the microchannel which is embedded with walls serving as obstacles and mixing elements which promoted horizontal and vertical diffusion along with stretching and folding, which lead to the fluids mixing efficiently and exiting the microchannel as a highly concentrated mixture (VOF composition of 0.5 for each fluid at the outlet). The effects of various retrofitted and complex configurations designed in this study on the overall mixing performance were analysed and tabulated

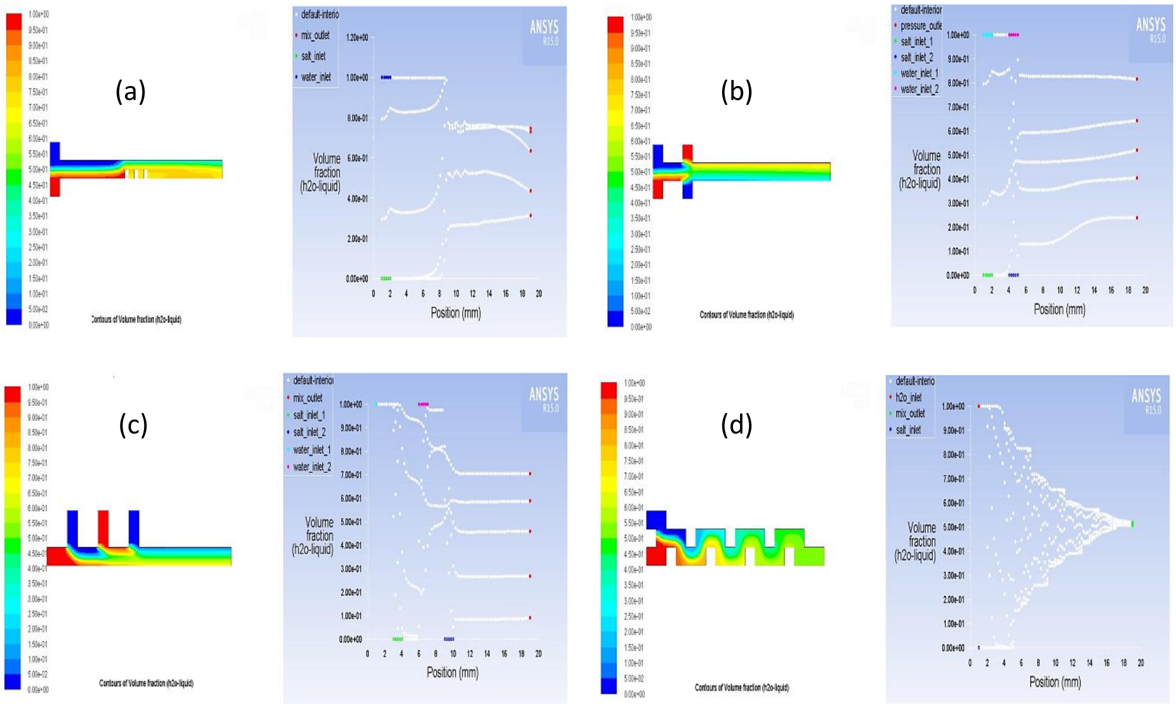

**Fig. 2:** Contour plots and X-Y plots – volume fraction of $H_2O$ profiles for retrofitted and complex microchannel configurations: (a) Retrofitted capital T with obstacles (b) Retrofitted capital T with the co-current flow (c) Retrofitted normal T with additional inlets (d) Wavy complex configuration.

**Table 2.** Mixing performance analysis of basic configurations of microchannel

| **Configuration** | **Capital-T (obstacles)** | **Capital T-inlet (multiple inlets with co-current flows)** | **Normal T-inlet (2 mm multiple inlets)** | **Wavy** |
|---|---|---|---|---|
| Type | Retrofitted | Retrofitted | Retrofitted | Complex |
| Number of inlets | Two | Four | Four | Two |
| $H_2O$ (volume fraction) at outlet | 0.75, 0.7, 0.6, 0.4, 0.3 | 0.8, 0.6, 0.5, 0.4, 0.25 | 0.7, 0.6, 0.45, 0.3, 0.1 | 0.5 |
| NaCl (volume fraction) at outlet | 0.25, 0.3, 0.4, 0.6, 7 | 0.2, 0.4, 0.5, 0.6, 0.75 | 0.3, 0.4, 0.55, 0.7, 0.9 | 0.5 |
| Diffusion interface | Vertical | Vertical | Vertical/Horizontal | Vertical/Horizontal |
| Mixing base | Inlet Focusing | Inlet Focusing | Inlet Focusing | Inlet Focusing |
| Inlet focusing | Available | Available | Available | Available |
| Mixing element/ chaos advection | Available | Not available | Not available | Available |
| Stretching and folding | Available | Not available | Not available | Available |
| Strategic composition distribution | Not available | Available | Available | Not available |

as shown in **Table 2**.

Throughout processing and post-processing all the configurations in the previous sections and stages the velocity, density and viscosity of the fluids in addition to the diameter and overall

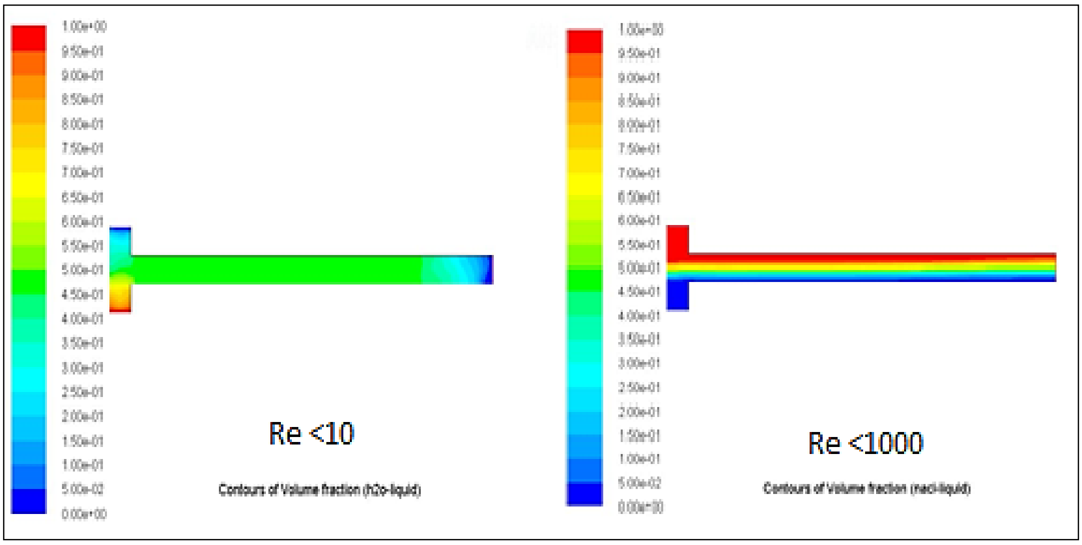

**Fig. 3:** Effect of various Reynold's number on overall mixing performance.

length (except for cases where the diameter fluctuated at some regions in the microchannel structure) of the microchannels were set constant, therefore, the residence time for all the configurations was assumed to be quite equivalent since the microchannel dimensions (diameter and length) and the velocity that are considered the main factors affecting it were approximately equivalent in all cases. Moreover, other factors that could also affect the residence time (since it's associated with Reynold's number) include the fluids viscosities and density, however, it was not possible to change the characteristics of the fluid to examine the effects of Reynold's number on the system since that would fundamentally change the system, similarly to the microchannel configurations. Hence, it appeared that the main factor driving Reynold's number in this study was the velocity which in turn means that the residence time would be highly dependent on the velocity only, apart from the configurations. Therefore, since the retrofitted (Figure 2(a)) and the complex configurations (Figure 2(d)), appear to naturally enhance the residence time due to obstacles and fluctuations, the velocity was manipulated in the basic microchannels in attempt to examine the effect of Reynold's number on the mixing performance and the residence time.

Initially at a velocity of 1 m/s Reynold's number had reached a total of approximately 700. It was said by Cieslicki and Piechna (2009) in their CFD mixing analysis that low Reynold's number that less than 1 lead to longer residence time and eventually earlier mixing appeared to take place. The same approach was followed in this study, the velocity was manipulated at this stage to 0.001 m/s in an attempt to reduce Reynold's number to less than 1 and examine whether the system responds accordingly and further compare and validate the results prior to concluding the effect of the velocity on the residence time and mixing performance in turn from **Figure 3**. Moreover, at the outlet it appeared that some air was still trapped in the microchannel which may correspond to the fluids reaching a stagnant point where Reynold's number dropped further since the fluids mixed and gained densities, their tendency to flow and push the air out of the microchannel appeared to decrease since the velocity was the main driving force. Therefore, by comparing the responses, it appeared that Reynold's number (velocity) can be further manipulated and optimised in the range of 10 to 1000 in order to achieve the desired output with an optimal mixing and residence time.

## CONCLUSION

The simulation of flow in various microchannel configurations was carried out, it appeared that static mixing would be possible to achieve in various microchannels. However, the simulation results predicted that it appeared to be more efficient in complex and retrofitted microchannels that enhance chaotic advection, compositions distributions, residence time and diffusivity than basic microchannels that are mostly dependent only on the injection focus. Moreover, in basic configurations, the Reynolds number modelled appeared to directly influence the residence time which reflects directly on the mixing performance. The conclusion agreed with work by Cieslicki and Piechna (2009) that the lower Reynold's number, the slower the injection and the flow which leads to longer the residence time. Therefore, the mixing would be achieved at earlier stages. The higher Reynold's number quickly forces the fluids towards the outlet which leads to shorter residence time and settling time which in turn leads to less mixing taking place and the requirement of longer, more complex, and retrofitted configurations. Moreover, in all cases, Reynold's number appeared to play a very important factor in the mixing performance in microchannel beside the configurations and can be similarly optimised to enhance mixing in all types of configuration.

## REFERENCES

1. Bajus, M. (2012). Microchannel-technologies, *Pet. Coal, 54 (3),* 294-300.
2. Cieslicki, K. and Piechna, A. (2009). Investigations of mixing process in microfluidic manifold designed according to biomimetic rule, *Lab Chip, 9 (5)*, 726-732.
3. Kee, R., J. (2011). The design, fabrication and evaluation of a ceramic counter-flow micro-channel heat exchanger, *Appl. Therm. Eng., 31 (17-18)*, 2004-2012.
4. Naher, S., Orpen, D., Brabazon, D., Poulsen, C. R. and Morshed, M. M. (2011). Effect of micro-channel geometry on fluid flow and mixing. *Simul. Model. Pract. Th., 19*, 1088-1095.
5. Rudyak, V., and Minakov, A. (2014). Modeling and optimization of Y-Type micromixers. *Micromachines, 5*, 886-912.
6. Stankiewicz, A. I., and Moulijn, J. A. (2000). Process intensification: transferring chemical engineering, *Chem. Eng. Prog.,* 41-49.
7. Stankiewicz, A. I., and Moulijn, J. A.

(2004). *Re-Engineering the chemical processing plant: process intensification,* Marcel Dekker: New York, pg 1-30, pg 167-177.

8. Watts, P., and Wiles, C. (2007). Recent advances in synthetic micro reaction technology, *Chem. Commun.,* 443-467.