MIXING IN MICROCHANNEL PATTERNED WITH SUPERHYDROPHOBIC SURFACES

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Declaration

I hereby to acknowledge that the work in this thesis is on my own except for citations and summaries which have been duly acknowledged by citing references. I solemnly declare that to the part of my knowledge, no part of this report has been submitted elsewhere in a previous application for the award of a degree. I hereby give consent for my thesis, if accepted, to be available for photocopying for interlibrary loan, and for the title and summary to be made available outside organization.

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List of Abbreviations

- **Re** Reynolds Number
- μ Viscosity
- ρ Density of fluid
- **u** Velocity of fluid
- A Area of inlet
- **c** Relative concentration
- **D** Diffusion coefficient of fluid
- **D**_h Wetted diameter of inlet
- **p** Wetted perimeter of the inlet
- \mathbf{c}_{∞} Final concentration of fluid
- $\boldsymbol{\tau}$ Shear Stress
- Pe Peclet Number
- L Characteristic length
- Θ Contact angle
- \overline{I} Average intensity
- **b** Slip Length
- **m**_{eff} Mixing efficiency
- w Channel Width
- **c**₀ Initial concentration
- **H** Channel Height
- r Radius
- **k** Boltzmann constant

Abstract (BM)

Secara umumnya, saluran mikro boleh ditakrifkan sebagai saluran yang mempunyai dimensi dalam julat 1 µm hingga 1mm. Aliran bendalir dalam saluran dimensi melebihi 1mm akan mempamerkan tingkah laku yang serupa dengan aliran dalam dimensi makroskopik. Aliran melalui rangkaian saluran mikro menggunakan mekanisma penyebaran dan laminar secaranya dominan. Pencampuran dalam saluran mikro tidak dapat dijalankan oleh aliran cecair secara bergolak untuk mempertingkatkan prestasinya adunan kerana nombor Re adalah biasanya di bawah nilai kritikal bagi peralihan kepada pergolakan. Oleh itu, ia menjadi cabaran bagi pencampur mikro pasif untuk mencampur cecair berbeza spesies dalam lingkungan yang dikehendaki dengan syarat ketiadaan teknik campuran yang mahir.

Dalam aplikasi mikrofluidik, pencampuran yang efisien telah difahami sebagai salah satu isu yang paling penting dan sukar untuk dicapai. Kajian mencampurkan cecair dalam saluran mikro yang dilapis dengan permukaan hidrofobik adalah penting kerana terdapat keinginan industri untuk mengurangkan ruang saluran dan masa yang diperlukan untuk mencampurkan cecair sepenuhnya, terutamanya dalam aplikasi bioperubatan. T-jenis pengadun akan digunakan sepanjang kajian ini dan simulasi menunjukkan bahawa keberkesanan adunan diturun apabila kelajuan bendalir ditingkatkan.

Untuk mendapatkan keberkesanan yang tinggi dalam proses pencampuran cecair, ruang dalaman saluran mikro hendaklah ditambahkan bagi mengizinkan aliran bendalir yang berbeza spesies untuk bercampur. Simulasi komputasi dinamik bendalir akan digunakan untuk menentukan kerberkesanan pencampuran cecair dalam pelbagai rekaan saluran mikro dan syarat operasi sepanjang kajian ini.

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Abstract (BI)

Generally, microchannels can be defined as channels having dimensions in the range of 1 μ m to 1mm. The fluid flow will exhibit behaviors similar to macroscopic flows when it flows in channels of dimension more than 1mm. The flow through a microchannel network of a lab-on-a-chip device is diffusion dominant and is laminar. Mixing in microchannel cannot be carried out by exciting the liquid streams in turbulent flow to enhance its mixing performance because the Reynolds number (Re) is typically below the critical value where transition to turbulence would occur. Thus, it becomes a challenging problem for passive micromixers to mix fluids of different species within the desired range of mixing channel length in the absence of enhanced mixing techniques.

In microfluidic applications, efficient mixing has been understood as one of the most fundamental and difficult-to-achieve issue. The study of mixing of fluids in microchannel laminated with superhydrophobic surface is important because there is an industrial desire to reduce the channel length and time needed for mixing of fluids for the beneficiary, especially in biomedical applications. T-type mixer is employed throughout the study and simulations show that effective mixing length increases with the fluid speed, depicted by Re number.

In order to obtain efficient mixing of fluids in short residence times and mixing length, contact area for the churning of higher and lower species concentrations needs to be highly increased. Computational fluid dynamics simulations are used to determine the mixing of fluids for various microchannel designs and operating conditions during this study.

Chapter 1: Introduction

1.1 Research Background

Two-fluid mixing is an essential process in many microfluidic devices. For example, various biomedical and biochemical processes involve the mixing of two fluids, including DNA purification, polymerase chain reaction (PCR), enzyme reaction, and protein folding. The performance of such processes relies on effective and rapid mixing of samples and reagents. Many microfluidic mixing applications involve chemical reactions where, most often, the fluid diffusivity is very low so that without the help of chaotic advection, the reaction time can be extremely long.[22] Thus far, many mixers have been developed and proposed for use in various areas of applications such as bio-, nano-, and environmental technologies to aid in the increase of mixing efficiency.

Generally, there are two types of mixing processes, known as active mixing and passive mixing. In active mixing, energy is introduced into the microfluidic device through the use of a magnetic field, an electric field, a thermodynamic medium, variable pumping, or a combination of some or all of these effects.[7] Passive mixing utilises no energy input except the mechanism of diffusion and convection to drive the fluid flow at a constant rate. In active mixers, mixing efficiency can be adjusted by changing the input energy, while in passive micromixers mixing is dependent upon mixer geometry or flow parameters such as velocity of fluid.[12] For a typical microfluidic device, the length scale is too large for a rapid diffusion and too small to include mechanical agitation. It is well known that the mixing of two fluid streams in a microchannel relies mainly on diffusion. [21]

Flows in microscale devices differ from their macroscopic counterparts for two reasons: the small scale makes molecular effects such as wall slip more important, and it amplifies the magnitudes of certain ordinary continuum effects to extreme levels.[14] In flows of microscale devices, diffusion is the main mechanism for fluid mixing. Mixing at low Reynolds number is controlled by molecular diffusion, inducing the growth of vortices or flow patterns which stretch and fold fluid elements can bring the two fluids to be mixed closer together, thereby significantly reducing the time and the channel length required to attain perfect mixing. [7]

Diffusion is a slow process. Initially, the interface between 2 fluids is very sharp because no permeation of fluid molecules has taken place. The continuing diffusion causes gradual distribution of the liquid species across the interface. In dilute species transport, the flux of one species diffusing through the interface is proportional to the gradient of the concentration of the species, given called Fick's law, and the proportional constant is defined as molecular diffusivity.[22]

Many researchers have investigated ways to improve mixing in microfluidic devices, dynamically or statically. Due to difficulties in fabricating and implement dynamic micro-mixers, a high performance static passive mixing strategy needs to be introduced. Due to the small size of the device, pressure-driven flows in simple channels (i.e. with smooth walls) are laminar and mostly uniaxial, so that confluencing liquids tend to flow side by side. In the mixing of microchannel, laminar drag reduction is achieved through the reduced effective surface area of the solid in contact with the flowing fluid where the ultrahydrophobic surface is silanized with microridges and shear-free air-water interface that will aid in fluid drag reduction. At the lowest Reynolds numbers, 0.01 < Re < 1, viscous forces in the fluid dominate inertial forces, and fluid velocities in a channel cross section are essentially two-dimensional.

Any real fluids moving along a solid boundary will incur a shear stress at that boundary. The no-slip condition dictates that the speed of the fluid at the boundary is zero; although at some height from the boundary the flow speed must equal that of the fluid. For all Newtonian fluids in laminar flow, the shear stress (τ) is proportional to the strain rate in the fluid, where the viscosity is the constant of proportionality and its equation is given by

$$\tau(y=0) = \mu \frac{\partial u}{\partial y}$$

where μ is the dynamic viscosity of the flow; u is the average flow velocity along the mixing channel and y is vertical direction.

The boundary condition for the fluid in contact with the microposts remains no slip, however, the air–water interfaces supported between microposts is shear-free, assumed to be perfectly flat and cannot resist the flow. The no-slip condition is treated as velocity of fluid is zero, u=0 near the surface of the wall of microchannel, while the shear-free

condition can be approximated as $\frac{du}{dy} = 0$ at the surface of the wall. The no-slip condition is almost universally accepted as the proper boundary condition to impose along a solid–liquid interface. In actuality, no-slip is an accurate approximation only at macroscopic length scales. For reasons that can be largely explained by molecular chemistry, fluids actually do slip at a wall. However, the slip effect is on the order of molecular sizes and is only important in devices that operate at extremely small length scales.

Microchannels offer advantages of high surface-to-volume ratio and their small volumes. The large surface-to-volume ratio leads to high rate of heat and mass transfer, making microdevices excellent tools for compact heat exchangers. An application of microchannels is in the area of MEMS devices for biological and chemical analysis. In the biological field, microscale devices offer good compatibility with the scale of biological structures and the potential for placing multiple functions for chemical analysis on a small area; that is, the concept of a chemistry laboratory on a chip. Microchannels are used to transport biological materials such as proteins, DNA, cells, and embryos or to transport chemical samples and analytes. [14]

Several geometries of microchannel for passive mixing have been developed and studied concerning its mixing performances, including T-type mixers, serpentine channels, square mixer and straight channel. The simplest one consists of a T-shaped micromixer. T-shaped micromixers have been investigated extensively in recent years, as they are quite suitable to carry out fundamental studies to understand mixing at the microscale. Most of the investigators have confined themselves to the mixing of two identical liquids, assuming that in one of them a dilute solute is dissolved.[11]

The microchannel's geometry is often designed for three-dimensional flow, which can stretch and fold the fluid elements to be mixed. The microchannel's geometry which is silanized with ultrahydrophobic surfaces, are fabricated from silicon wafers using photolithography and are designed to incorporate precise patterns of microridges which are made hydrophobic through a chemical reaction with an organosilane. Passive mixing by geometrical variations in microchannel were designed to improve the lateral convection so that the dispersion of solute were not only contributed by diffusion. The mechanism for obstacles to enhance mixing was to create convective effects. [2] The dimensionless Peclet number expresses the relative weight of diffusion to convection in a moving fluid channel. At small Peclet number, diffusion dominates over convection and mixing occurs largely within the T junction while at high Peclet number a significant amount of mixing takes place in mixing channel at cost of large mixing length. The Peclet number is defined as

$$Pe = \frac{Lu}{D}$$

where L, u, and D are characteristic length, velocity, and diffusion coefficient scales respectively. A large Peclet number (Pe> 1) indicates that convection dominates in a fluid flow. A small Peclet number (Pe< 1) indicates that diffusion dominates the solution.

The biggest limitation of this project is the unavailability to conduct experiments to verify the results of simulations done with ANSYS FLUENT. It is due to the high fabrication costs of developing the internal structure of microchannel and high costs using in examination of mixing of fluid flow like the methodology of using pressure drop measurement or μ PIV (microparticle image velocimetry) measurement.

1.2 Problem Statement

The problem statement presented in this study is to increase the mixing efficiency of fluids in passive micro-mixers by utilising the mechanism of diffusion and convection to drive fluid flow.

1.3 Objectives

This paper will present the improvement of mixing efficiency in T-channel passive micromixer having a rectangular channel, where two fluid streams of different concentrations are flowing parallel to each other. For this study, attentions were focused to gain insight on the various effects of different flow parameters on mixing efficiency i.e., inlet flow velocity, period of superhydrophobic surfaces, symmetrical and unsymmetrical alignment of superhydrophobic surfaces in microchannel. The mixing efficiency was deduced according to the mixing length required to achieve complete mixing, indicating that the shorter the mixing length required for complete mixing, the higher the mixing efficiency. These analyses focused on the concentration distribution of 2 fluid streams having same density, viscosity, and diffusion coefficient flowing at different flow and geometric conditions.

Chapter 2: Literature Review

Numerous methods for enhancing the mixing process to ultimately shorten the mixing length and the mixing time have been proposed, among which can be mentioned the geometry effect, hydrodynamic focusing, alternate injection, electrokinetic method, droplet mixing, and stirring by particles. The simplest approach is based on the geometric effect. The mixing length can be shortened by modifying the geometry of the microfluidic channel.[15]

Suppose there are two different kind of fluids in contact with each other, random motion of the liquid molecules occurs everywhere, it produces no apparent change in the bulk of each liquid far from the interface, because all the molecules in a specific liquid have the same properties. However in the region near the interface, molecules on both sides have different properties, and so random molecular motion results in permeation of molecules from one side to the other. Such apparent permeation is called diffusion.[22]

A typical diffusion coefficient for a molecule in the gas phase is in the range of 10^{-6} to 10^{-5} m²s⁻¹. By contrast, the diffusion for molecules dissolved in liquids is far slower. In an aqueous (water) solution, typical diffusion coefficient is in the range of 10^{-10} to 10^{-9} m²s⁻¹. As a result, diffusion in liquids is very slow over everyday length scales. In order to compute the diffusion coefficient of fluid, the Stokes-Einstein equation can be applied.

$$D = \frac{kT}{6\mu r\pi}$$

where k is the Boltzmann constant, μ is the viscosity, and r is the radius of the diffusing particle. This equation is derived on the assumption that the particles obey Stokes' law for drag, such that the drag exerted on diffusing molecules, by the solvent molecules, can be computed.

It is known that the flow inside microchannels is usually laminar with Re < 25 and limited by molecular diffusion. Such flows cannot be made turbulent by placing obstacles inside the microchannel. In addition, the mechanical stirring methods usually employed in macromixers cannot be implemented in microchannels due to size limitations and fabrication difficulties. In the mixing of fluids in microchannel, as the Schmidt number (i.e. the ratio v/D between kinematic viscosity and molecular diffusivity) is typically very large, the Peclet number is large, that is $Pe = U \cdot D_h /D$, where U is the mean fluid velocity, and D_h the hydraulic diameter.[11] In laminar flows, the effect of slip only becomes important in macroscopic flows when the slip length is comparable to the length scale of the flow geometry. A 20% decrease in the drag requires a slip length of b= h/ 15. Thus, for a simple fluid flowing over a smooth hydrophobic surface, where b=40 nm, a significant drag reduction should only be observed for flow geometries smaller than h=600 nm

Superhydrophobic surfaces were originally inspired by the unique water-repellent properties of the lotus leaf. Recent synthetic surfaces have been developed that are capable of obtaining contact angles that can approach 180°. Superhydrophobic surfaces are rough with micrometer-sized protrusions coming out of the surface. The superhydrophobic surface can be constructed using lithographically etched silanized silicon surfaces with precisely controlled microsurface topology consisting of regular arrays of microposts aligned in the flow direction. Common KOH anisotropic etching techniques were used to fabricate the microstructures.

The standard measurement of the hydrophobicity of the salient surface is the angle formed from a liquid droplet resting on the hydrophobic surface. Clean glass is highly hydrophilic and has an equilibrium contact angle with water close to Θ =0°.Dimethyldichlorosilane, which is relatively easy to deposit on a surface, has a contact angle with water close to Θ =100°. Originally inspired by the unique water repellent properties of the lotus leaf. Superhydrophobic surfaces have recently been developed which are capable of obtaining contact angles with water as high as Θ =177.24°.[6] These extremely large contact angles result in water droplets that are nearly spherical.

Microchannels can be fabricated in many materials — glass, polymers, silicon, metals by using various processes including surface micromachining, bulk micromachining, molding, embossing, and conventional machining with microcutters. The silicon surfaces were patterned with regular arrays of microposts and the receding, and advancing contact angles were measured as the cross sectional geometry, height, and spacing of the microposts were systematically varied. The results of Öner and McCarthy show that for microposts between 10 μ m to 40 μ m across, the contact angle is nearly independent of cross-sectional geometry, post height (only heights greater than 20 μ m were tested), and the surface chemistry. However, Öner and McCarthy found that a significant deterioration of the ultrahydrophobic properties of the surface occurs as the spacing between microposts is increased beyond about 64 μ m.

For Newtonian fluids such as water, fluid slip at the solid boundary is ordinarily negligible, and it is well known that the calculated result obtained under the no-slip boundary condition agrees well with the theory, v=0. Newtonian fluid is the simplest type of viscous fluid, the Newtonian model of fluid response is based on three assumptions: (i) shear stress is proportional to the rate of shear strain in a fluid particle, and it indicates that (ii) shear stress is zero when the rate of shear strain is zero. (iii) the stress to rate-of-strain relation is isotropic—that is, there is no preferred orientation in the fluid.[19]

Stroock et al.'s studies showed that increasing the depth or frequency of microridges increased the strength of the helical flow and the rate of mixing [5]. Additionally, Stroock et al. demonstrated that mixing could be significantly improved if the design of the microridges was modified to a herringbone pattern in order to generate chaotic flow [9]. In order to maximize the strength of the secondary flow generated by the surface patterning of the type used by Johnson et al. and Stroock et al., Stroock et al. demonstrated that one needs to maximize the difference between the drags perpendicular to and parallel to the direction of the microridge.[7] The velocity distributions across the mixing channel are different between the situation of both hydrophilic walls, both hydrophobic walls and one hydrophobic while the other hydrophilic walls and the mixing lengths are found to be same ($\pm 0.25\%$) when flow-rates kept constant.[17] Due to low velocity and small channel size, Reynolds number is assumed to be very low(< 25), because of which viscosity plays a dominant role rather than inertia effects in mixing channel.[9]

Most previous experimental studies on two-fluid mixing in microfluidic devices have used flow visualization to probe the mixing performance. Koch et al. used red and green inks dissolved in ethanol to test a lateral micromixer[23]. Liu et al.[25] and Beebe et al.[24] used solutions of phenolphthalein and sodium hydroxide dissolved in ethyl alcohol to test the mixing performance of a three-dimensional serpentine mixer.Through this, the colour change of the phenolphthalein from colourless to red can be quantified by measuring the intensity of red in the microchannel after the mixing process. For this research study, solutions of concentrated sodium hydroxide will be used to mix with phenolphthalein to quantify its mixing performance in a microchannel by evaluating the intensity of colour change of phenolphthalein.[5] The intensity of red integrated over a window image is proportional to the amount of reacted phenolphthalein in the imaged volume. This intensity is given by $I = \sum_{i=1}^{N} I_i$, where I_i is the intensity of red in pixel i and N is the total number of pixels in the window range image. Since the cross-sectional area of each viewing window may be slightly different, the pixel-averaged intensity $\overline{I} = I / N$ is used for comparison purpose.

Lee et al. and Stroock et al. used distinct streams of a fluorescent and a clear solution to test the mixing performance of an active mixer with a pressure source/sink system and of a staggered herringbone mixer.[2]. At very low Reynolds numbers, the 3D serpentine channel was found to enhance the rate of mixing to more than 16 times than that of a straight channel, and to 1.6 times that of a 2D serpentine channel..

One stream contains phenolphthalein dissolved in 99% ethyl alcohol with a concentration of approximately 0.31mol/L. The second stream contains 98.3% sodium hydroxide pellets dissolved in 99% ethyl alcohol with a concentration of approximately 0.33 mol/L, which gives a pH of approximately. This high concentration of NaOH was used to obtain a large color change in the phenolphthalein. Despite the high pH value, no reactions were observed between the sodium hydroxide stream and the silicon wafer.

Mixing efficiency was used to evaluate the performance of the fluids in the mixers.

$$m_{eff} = \left(1 - \frac{\int_0^w |c - c_\infty| \, dx}{\int_0^w |c_0 - c_\infty| \, dx}\right) \times 100\%$$

where,

meff is the mixing efficiency,

c is the mass concentration distribution across the transverse direction at the outlet,

 c_{∞} is the concentration of a complete mixing and

c₀ is the initial distribution of the concentration before any mixing,

w is the width of the channel.

Mixing in these channels can also be evaluated by considering the uniformity of the intensity in the imaged fluid volume. The uniformity can be quantified by calculating the deviation of the pixel intensity values I_i in a given image from the maximum intensity value.

$$D_{I} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (I_{i} - I_{max})^{2}}$$

Analysis shows that with the increase of diffusion coefficient, mixing concentration efficiency increases and required mixing length decreases to a considerable extent. Increasing of inlet velocity leads to an increase in Reynolds number and with the increase of inlet velocity, mixing efficiency of fluid decreased, requiring higher mixing length to complete the mixing. This is due to the decrease in residence time of fluid, which consequently leads to a high Peclet Number. But in case of high diffusion coefficient, capability of molecular mixing of both the fluid streams is increased and even at high velocity, there is a considerable increase in mixing efficiency within available mixing length.[12] At low Reynolds number, due to the concentration of analyte diffusing into the interior from very slow moving laminae near the walls the overall fluid concentration is high as compare to high Reynolds number. At low Reynolds number, there is a sufficient time for interior portion of the channel to receive a significant amount of analyte from the wall region. And when the fluid velocity reaches to zero this phenomenon become singularity because there is an infinite amount of time for such exchange. Based upon the above-mentioned analysis, it can be concluded that diffusion coefficients and inlet fluid velocity variation lead to a considerable variation in Reynolds number and Peclet number which consequently affects the mixing of fluids and improves the mixing in case of low Reynolds number and Peclet number.

Chapter 3: Research Methodology

3.1: Governing Equations

The relevant governing equations in the generalized form consist of conservation of species, mass, and momentum in the form of partial differential equations. The mixing phenomena are governed by species transport equation given by [18]

$$\frac{\partial c}{\partial t} + \nabla . \left(\mathbf{u} c \right) = \nabla . \left(D \nabla c \right) \ (1)$$

where c and D are relative concentration and diffusion coefficient of fluid respectively. Equation (1) is the transport equation for the scalar species concentration in an incompressible flow field. Furthermore, the mass and momentum transport are derived by assuming the fluid belongs to Newtonian type are

$$\nabla \cdot \mathbf{u} = 0 \quad (2)$$
$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla P + \nabla \cdot [\mu(\nabla \mathbf{u} + \nabla \mathbf{u})^T] \quad (3)$$

where ρ , **u** and μ are density, velocity, and viscosity respectively. Here, the flow is assumed to be incompressible and its fluid properties like temperature and density are assumed to be steady, i.e. these properties do not vary with time. Newtonian fluid is a type of fluid where its viscous stresses are linearly proportional to the local strain rate.

Equation (2) is the continuity equation and it represents the conservation of mass of species flowing through the channel. Equation (3) is the Navier-Stokes equation derived from an incompressible Newtonian fluid. This equation can be derived from a more general statement of linear momentum of balance. The Navier- Stokes equation represent the conservation of momentum of fluid. The first task in modeling the mixing of fluid is to solve the fluid flow equations. There are multiple ways to solve the incompressible Navier-Stokes equations, whether for 2-D or 3-D.

Assuming that the concentration distribution is in a steady state and the fluid velocity is uniform over the channel, u = U, v = 0, an approximate formula of transport equation for the diffusive mixing can be derived, where diffusion along the main-stream direction is neglected.

$$U\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial y^2} \quad (4)$$

3.2: Project Methodology

T-shaped micromixer with rectangular cross sections is chosen to perform simulations. Firstly, a 3-D hydrophilic smooth T-channel is constructed using ANSYS Fluent as shown in Figure 3.1. Here, a water stream having mass fraction $m_a = 1$ is admitted through the upper inlet and another water stream with mass fraction $m_b = 0$ is admitted through the lower inlet. The net transport of species at inlets consists of both convection and diffusion components. These liquids flow parallel to each other at the inlet and meet at the entrance of the mixing channel thus passing through its length of 2mm before reaching the outlet. Both the liquids penetrate to the other half through the contact surface solely by diffusion. Further, the mixing of co-fluent fluid streams progress along the length of the channel and the gradients in concentration between two liquids diminish gradually. The 2 inlet streams are injected at the temperature equilibrium with the microchannel, so the process is isothermal, model and equations governing heat transfer can be ignored. The inlet streams velocity profile is assumed to be fully developed.

The boundary condition of the wall of microchannel is set to no-slip. After inputting correct model, parameters along with appropriate boundary conditions after proper meshing, the mixing concentration of fluid at each node of T-channel is obtained. The channel height, H is set to 200 μ m and the flow rate is maintained such that Re varies from 1 to 25. All the relevant fluid properties such as density and viscosity are taken from that of water, where $\rho = 1000 \text{ kg/m}^3$ and $\mu = 0.001$ Pa.s. Furthermore, it is assumed that the constituent species is dilute and the diffusion coefficient of fluid is D= 1 ×10⁻⁵ m² s⁻¹. Simulations were typically considered converging when the normalized residuals for velocities were stationary with iterations and fell below 1×10⁻⁶, although smaller residuals were favoured.



Figure 3.1: T microchannel

The 3-D contour of velocity and concentration profile of fluid flowing through are displayed to verify the boundary conditions imposed are fulfilled correctly, e.g. the initial concentrations of fluid at both inlets and the velocity of fluid near the channel wall must be verified to be u=0 before further validation.



Figure 3.3: Mixing concentration of 3-D contour

The data obtained from ANSYS is used in post-processing by Matlab to obtain the mixing length required for complete mixing.

After that, the efficient mixing length of Re=10 is plotted to validate its result deviation in accordance with a published paper.[12]



Figure 3.4: Validation of simulation result with reference paper

As can be seen in the above figure, it is concluded that the deviation between the simulation data and the reference data is insignificant.

The formula to calculate the Reynolds number of fluid flowing through the inlet microchannel is

$$Re = \frac{\rho u D_h}{\mu}$$
Where $D_h = \frac{4A}{p}$

Subsequently, the meshing independence test is conducted to further validate that the efficient mixing length of fluid is unaffected by the number of mesh elements imposed on the geometry.



Figure 3.5: Meshing Independence Test

In the figure above, it is known that the efficient mixing length reaches asymptote after 160,000 meshing elements are imposed along the mixing channel. In the study, approximately 200,000 meshing elements is used to impose on the mixing channel because there was not enough confidence in using number around 150,000 and overuse of meshing elements on the geometry will sacrifice resources and computational time.

The geometry of the channel is varied by imposing superhydrophobic surfaces on the upper surface and lower surface of the mixing channel accordingly to obtain the results for further discussion. These micro-mixers are constructed by alternatively repeating hydrophilic and hydrophobic patches having lengths L_{ns} and L_s respectively with a periodicity $L_p = L_{ns} + L_s$ along the length of the mixing channel. The boundary condition of microposts salinized on superhydrophobic surfaces is set to no slip while the boundary condition of the air-water interface supported between adjacent microposts is set to shear-free since there is no acting shear from the air molecules towards the fluid molecules.

The periodicity of superhydrophobic surfaces, L_p ranging from 50µm to 100µm is varied to study the effective length required for proper mixing. As the periodicity decreases the numbers of transition regions available in the mixer increases. For

instance, a channel with L_p /H = 0.25 has 80 interfaces along the inlet and outlet. Subsequently, the effect of arrangements of mixing channel decorated with superhydrophobic surfaces in symmetric and non-symmetric arrangement is examined. The MATLAB code used to determine the efficient mixing length of fluid and to compute the 2-D velocity contour profile of mixing channel is depicted in Figure 3.9 and Figure 3.10 respectively in the Appendix section.



Figure 3.8: Mixing channel with symmetric hydrophobic surfaces



Figure 3.9: Mixing channel with non-symmetric superhydrophobic surfaces