

Numerical Study of Water Droplet Dynamics in Proton Exchange Membrane Fuel Cells

A dissertation submitted to The University of Manchester for the degree of MSc Mechanical Engineering Design in the Faculty of Science and Engineering



2016

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Word Count:14090

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Nomenclature

PEMFC	Proton exchange membrane fuel cell
GDL	Gas diffusion layer
H^+	Hydrogen ion
e^-	Electron
CFD	Computational Fluid Dynamics
NMR	Nuclear Magnetic Resonance
VOF	Volume of Fluid
v	Velocity of air
u	Velocity of water
θ	Static Contact Angle
θ_A	Advancing Contact Angle
θ_R	Receding Contact Angle
PTFE	Polytetrafluoroethylene (produced by DuPont as Teflon)
α_i	Phase content variable (of phase i)
ρ	Density
μ	Dynamic viscosity
CSF	Continuum Surface Force
F_σ	Surface Tension Force
$\vec{F}_{vol}$	Volume Force
σ	Surface Tension
K	Surface Curvature
R	Radius
Re	Reynolds Number

Abstract

Water management is an important topic which affects the performance and durability of PEMFCs and it plays a significant role to increase the performance of PEMFCs. Principally, a certain amount of the existing water is desired to be in the polymer electrolyte membrane to improve the proton conductivity, whereas excessive water than desired causes the blockage of the microporous on the gas diffusion layer and arises flooding on the fuel cell. Although, several studies have been performed to observe water droplet dynamics in the flow channels, these phenomena cannot be understood clearly.

In this study, numerical simulations have been used to investigate the water behaviours in the gas flow channel at cathode side. The procedure implemented for the numerical simulation of two-phase flow is the volume of fluid (VOF) technique. Equations of this method are solved by STAR CCM+. In the first case, effects of different static contact angles, various air inlet velocities and various dimensions of flow channel on water droplet, which occurs in the gas diffusion layer, have been examined. Water volume fraction and pressure drop in the gas flow channel have been determined and compared with existing studies. Results show that hydrophilic surfaces are helpful for removing water and increasing velocity favours water detachment but causes pressure drop in the channel.

In the second case, two u-shaped micro channels, one with rectangular bend and the other with semi-circular bend, have been used in order to obtain water behaviour in the channels. Only changing shape of the channel corner effects have been investigated on water behaviours. Pressure drop, water distribution in the channel have been analysed and especially, water accumulation at the bend have been compared between the two geometries. The results show that the channel with rectangular bend is characterised by faster water removal than the channel with semi-circular bend.

Declaration

I, Enes ASLAN, declared that no portion of the work referred to in the dissertation has been submitted in support of an application for another degree or qualification of this or any other university or other institute of learning.



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Acknowledgements

First of all, I am grateful to God, for providing me this opportunity and giving me the possibility to proceed successfully.

I would like to thank my thesis supervisor Dr. Andrea Bottacin Busolin, who has supported me at each and every point of my research project with patience and enthusiasm. His invaluable support and guidance makes this project easier. The door to Dr. Busolin office was always open whenever I ran into a trouble spot or had a question about my project. He consistently allowed this paper to be my own work, but steered me in the right the direction whenever he thought I needed it.

A special thanks to my family. Words cannot express how grateful I am to my father, mother and sister and also my girlfriend for providing me with unfailing support and continuous encouragement throughout the year of study and through the process of researching and writing this thesis. I would like to thank all of my friends who supported and motivated me to strive towards my goal.

Finally, I would also like thank to Republic of Turkey Ministry of National Education (MEB) for the financial sponsorship of my master study at The University of Manchester.

1. Introduction

The development of new technologies can help improve people's lives but can, at the same time, lead to an increased energy demand. The consumption of energy is rising day by day all over the world in response to the increasing adoption of technological devices such as smartphones, computers and cars, which not only consume energy to function but also require energy to produce. Today fossil fuels are still widely used to satisfy the energy needs of the society. However, fossil fuels do not represent a long-term solution and also have detrimental effects on the environment. Reducing the reliance on fossil fuels requires a shift towards clean and renewable energy systems. Fuel cells represent a promising technology in the field of clean and sustainable energy which characterised by low emissions and high efficiencies. Fuel cells are categorised on the basis of the electrolyte type. One of these is the Polymer Electrolyte Membrane Fuel Cell (PEMFCs), which transforms chemical energy, in the form of Gibbs free energy between oxygen and hydrogen into electrical energy by means of chemical reaction [1]. Fuel cells are used in many commercial applications such as portable, mobile, and stationary power systems, vehicles and combined heat and power generation units [2, 3, 4, 5]. Transportation applications are most common; many famous vehicles manufacturers such as Ford, Toyota, Nissan, Honda, and Hyundai produce and develop engines powered by PEM fuel cells [6]. PEMFCs consist of three main parts, including anode, electrolyte and cathode. A schematic illustration of a PEMFC is shown in Figure 1. At the anode side, pure hydrogen is supplied as fuel from a storage tank and flows through anode channel in gas form. Hydrogen divides into protons and electrons at the anode membrane surface. Protons (H^+) can pass through the electrolyte membrane, whereas electrons (e^-) cannot pass from the anode to the cathode and are transported through an external circuit, thus producing electric current. At the cathode side, air flows through the cathode channel, and when oxygen in the air comes across the protons and electrons, liquid water and heat are produced. The liquid water may cause flooding of the fuel cell, which is an undesirable

situation. The amount of water accumulated in the channels of the cathode bipolar plate is an obstacle for oxygen transit to the catalyst layer. On the contrary, water shortage causes dehydration of the membrane, which produces a decrease in the ionic conductivity of the membrane and affects negatively the overall performance of PEMFC [1]. Both these situations have significant effects on the PEM fuel cells, affecting their efficiency and durability. An effective water management is therefore necessary to ensure that acceptable amounts of liquid water are found in the cell at any time during its operation. Water droplet dynamics is a major area of interest within the field of the water management. For understanding the complexity of water droplet dynamics, scientists have conducted several numerical and experimental studies. These will be described in the next sections.

As abovementioned several types of research have been done about water droplet dynamic by using of numerical methods but it was difficult because of the complex equations. Moreover, internal quantities of PEMFC cannot be measured easily due to the spatial dimensions of PEMFC [11]. The developments of hardware systems over the past two decades have made it possible to simulate fuel cell processes with a computer within acceptable times. In addition to this, a flow can be visualised on a computer by means of computational fluid dynamics (CFD) simulations. This means that the motion of water droplets can be simulated on a computer and the associated dynamics can be analysed in detail. It is the mathematical bases of CFD simulations is given by the the Navier-Stokes equations, expressing mass and momentum conservation for the fluid. These can be coupled with energy and chemical reaction equations when thermodynamic and chemical processes need to be taken into account. The equations are solved using numerical methods and computational algorithms. 2D and 3D simulations of fluid flows can be done with commercially available software packages such as Ansys Fluent, Star CCM+. One of these will be used in this project to simulate the water droplet dynamics on the channel surface in the cathode side of a PEMFC.

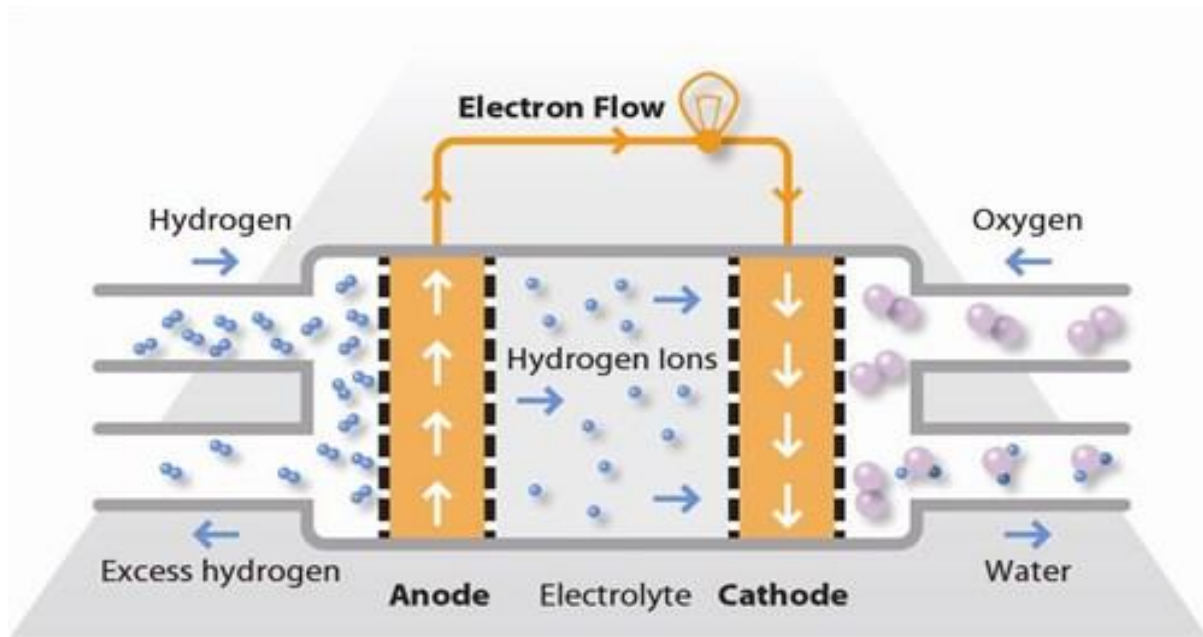


Figure 1: Schematic of a PEM Fuel Cell [From 7]

1.1 Aims and Objectives

Water management in PEM fuel cells is a problem of major concern because excessive amount of water in the gas diffusion layer on the cathode side can prevent oxygen reaching the catalyst layer and reduce the life of the cell. This project will specifically investigate the dynamics of water droplets in the air flow channel on the cathode side of a PEMFC and analyse the effect of different channel geometries on the accumulation and removal of water from the GDL surface.

In particular, the project aims to:

- Review the existing literature on PEMFCs and water management on the PEMFCs and identify the main modelling approaches used to investigate water droplet dynamics on PEMFCs.
- Perform CFD simulations of water droplet dynamics for different geometries of the air flow channels.
- Determine removing time the water droplet from the GDL and cathode channel surfaces as well as the accumulative water ratio on these surfaces.

- Analyse the effect of velocity and hydrophobicity of the channel surfaces on the removal of water droplets.
- Compare the results of the numerical simulations with other numerical and experimental results from the existing literature. The results will be compared in terms of air velocity, channel geometry, coverage rate, surface tension, contact angle and pressure drop.

2. Literature Review

2.1 PEM Fuel Cells

First studies about fuel cells start in the early 1800s, and then 1950s General Electric invented the proton exchange membrane fuel cell. Following this development on the fuel cell, NASA initiated a study to use this technology for space missions in 1960. Over the last 30 years large stationary and fuel cells were developed for commercial and industrial locations. In the last decade fuel cells started to be sold commercially to people as auxiliary power units, car companies started to manufacture cars with this technology, and portable battery chargers have become commercially available [8].

Besides the commercial improvements on PEMFCs many studies have been conducted in the academia. In the early 1990s, Springer et al. [9, 10] published fundamental PEMFC models depend on phosphoric acid fuel cell investigations and experimental studies. In these studies, transport, water addition and removal, cathode flooding was examined [11]. Much of the literature since the mid-1990s have investigated PEMFC models ranging from one-dimensional, single-component to complete three-dimensional. In a comprehensive literature review of modelling, one-dimensional, two-dimensional and three-dimensional model approaches, modelling strategies and commonly used assumptions has been discussed by Siegel [11].

Generally, the model accounts for mass dynamics in five control volumes: the gas flow channels, the gas diffusion layers and the membrane, as well as thermal dynamics.

Almost every paper that has been written on PEMFC modelling includes a section relating to making assumptions and simplification, by the reason of complex simulations. For instance, two-dimensional heat and water transport models that clarify alteration in temperature and membrane hydration along the flow channels were established by Nguyen and White [12]. They assumed that a well-mixed concentration flow in the channels. Another example is that during Yi and Nguyen evaluated the two-dimensional hydrodynamics in the only cathode, the width of the channel was neglected [13]. Dutta et al. used some assumptions in their study [13], the flow is steady state, isothermal and single phase, when modelling three dimensional numerical simulation of straight channel PEM fuel cells.

2.2 Fundamentals of PEMFC

The processes occurring in PEM fuel cell operation are complex; account they include, in particular, heat and mass transfer, multi-phase flows, current transport and electrochemical reactions. These circumstances appear in the following components, catalyst layers, membrane, gas diffusion layer and micro-porous layer, gas flow channels and bipolar plates [6]. In order to investigate the transportation mechanism, fundamental models have been developed based on the laws of conservation of mass, momentum, energy, species and charges and the multi-phase mixture formulation [11, 15, 16]. The rest of this section explains the fundamental components of PEM fuel cells.

2.2.1 Membrane

Membrane can be defined as polymer film which conducts protons from the anode to the cathode. The following necessary characteristics of a membrane provide; high ionic conductivity, impermeability to fuel gas or liquid, mechanically robust, thermally stable

during the operating temperatures high oxidative and hydrolytic stability in the actual fuel cell environment [6,18]. Present membranes are based on the perfluorosulfonic acid, the most outstanding of which, Nafion, is discovered in the late 1960s by Walther Grot of DuPont. Furthermore, Neosepta-FTM (Tokuyama), Gore-SelectTM (W.L. Gore and Associates, Inc.), FlemionTM (Asahi Glass Company), AsiplexTM (Asahi Chemical Industry) are the known other materials which are approved for PEM fuel cell applications [6,18]. Proton and water transport are two major events occurred in the membranes. A great numbers of investigations have been done by the scientists in order to observe proton-conductivity and water content in the membranes. One of the most prevalently known proton-conductivity model is developed by Springer et al [9]. A correlation was introduced by Bernardi and Vergrugge, and Buchi and Srinivasan so as to examine proportional water content of the membrane [6].

2.2.2 Catalyst Layers

There are two catalyst layers in a single fuel cell where are located in the anode side and the cathode side. The catalyst layer is mostly very thin. Hydrogen oxidation reaction takes place in the catalyst layer at the anode side whereas oxygen reduction reaction occurs at the cathode side. Hence the catalyst plays a vital role of reducing the reaction activation barrier [6]. The catalyst usually consists of platinum or platinum alloys (Pt-Co, Pt-Ni, Pt-Fe, Pt-V, Pt-Mn and Pt-Cr). Several academic works have exhibited that platinum and platinum alloys have good catalyst kinetic [6]. For instance, Pt-Co alloy was used in order to evaluate the durability of PtCo/C cathode catalyst in a dynamic fuel cell environment with continuous water fluxing on the cathode [19]. Also the catalyst layer has an important role for the water management in the PEM fuel cells especially at the cathode side. Because of the oxygen reduction reaction water is produced, which may cause flooding on the catalyst layers. The water content of the cathode catalyst directly affects the protonic conductivity in this domain and thus the overall performance of PEM fuel cell.

2.2.3 Gas diffusion layers

The gas diffusion layers have a crucial mission to aid the reactions on the catalyst layer by diffusing the reactants from the flow channels to reach the active sites on the catalyst [17]. Moreover, it provides electronic connection between the bipolar plate with channel-land structure and supports to the membrane electrode assembly mechanically as well as preserves the catalyst layer from corrosion or erosion caused by flows or other factors [6].

2.2.4 Gas flow channels and bipolar plates

The single fuel cell system consist of hydrogen and air supply channels where are at the anode side and cathode side, respectively. They are significant components, which carry oxygen and hydrogen, as well as water produced by chemical reactions, for PEM fuel cells. These are characterised by parallel or serpentine channels with square, rectangular or trapezoid cross-sections and their dimension changing from 0.1 to 1 mm [20]. Over the last two decades various configurations have been defined and analysed such as such as serpentine, parallel, pin-type and interdigitated flow fields [20]. Typical flow fields of PEM fuel cells are illustrated in Figure 2.

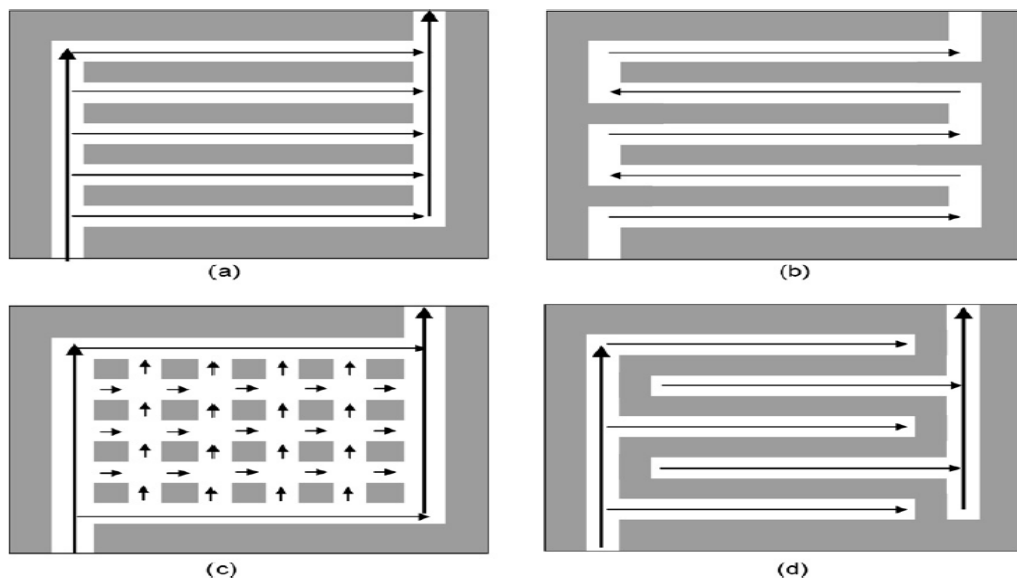


Figure 2: Typical flow fields of PEM FCs. (a) Parallel flow field; (b) serpentine flow field; (c) pin-type flow field; (d) interdigitated flow field. (From [20])

The channels are embedded in the bipolar plates with a typical cross-section dimension of around 1 mm. The bipolar plates provide conductive passages for both heat and electron transport, as well as support structure over the gas diffusion layers [6]. They are produced with the gas flow channels together. Metal plate corrosion and graphite crack may cause the bipolar plates degradation, because of this reason fuel cell life time decreases.

2.3 Water Management in PEMFCs

One of the most important issues in the operation of PEMFCs is water management which has a crucial role in the PEM fuel cell applications. Effective water management brings some benefits such as durability and performance increase in the PEM fuel cell. This operation depends on many factors like membrane material, porosity on the gas diffusion layers, as well as hydrophobic or hydrophilic surfaces. Water droplets are created at the gas diffusion layer surfaces in the gas flow channels of PEMFCs when the PEM fuel cell operation is proceeding [21, 22]. There are two sources for producing water in the system. First and foremost is that the electrochemical reaction in the catalyst layer generates liquid water. The second source of liquid water is from condensation: when the vapour partial pressure arrives at the saturation point, redundant water in the vapour phase condenses to liquid water [21]. Principally, a certain amount of the existing water is desired to be in the polymer electrolyte membrane to improve the proton conductivity, whereas excessive water than desired causes the blockage of the microporous on the gas diffusion layer and arises flooding on the fuel cell. In order to avoid those undesirable situations the excess water must be removed from the gas diffusion layer and the gas flow channels [23].

The most common method used for removing water from the surfaces is to increase the gas flow rate. As a result, the liquid water is expected to leave from the cell as form of water droplets [22]. However, it may cause other problems such as membrane hydration and low reactant utilisation [22].

Naturally, this has some disadvantages for efficiency and performance of PEM fuel cell. In order to prevent and find new solutions for these unfavourable events, many investigations have been carried out to examine water droplet dynamics. There are many studies in the literature to visualize the motion of a water droplet, but during the operation of PEM fuel cell visualization of water transport is a challenging phenomenon because of the opacity of bipolar plates and gas diffusion layers [23].

2.3.1 Experimental and Numerical approaches

Bazylak has reviewed experimental methods to visualize water in his report [23]. These techniques include nuclear magnetic resonance (NMR) imaging, beam interrogation and direct optical photography. In addition, other significant techniques are available in the literature such as real time gas analysis, ionic resistance, infrared absorption and residence time distribution [23]. Beam interrogation techniques are classified into three ways neutron imaging, electron microscopy, and X-ray techniques which were used in many academic researches. These techniques are separated into each other in terms of temporal and spatial resolution. For example, the direct optical visualization of liquid water in PEM fuel cells is able to show high temporal and spatial resolution information about water transport in the gas flow channels and upper layers of the gas diffusion layer [23]. When Liu et al. [25] have studied water flooding and two-phase flow and Carton et al. [26] have examined the water droplet accumulation and motion in the cathode channels of PEMFC by using direct optical visualization techniques. Bazylak have summarized the reported state-of-the-art spatial and temporal resolutions of the methods in his review report [24] with merits and challenges of liquid water visualization, which are shown in Table 1.

Method	Spatial Resolution	Temporal Resolution	Merits	Challenges
NMR	50 μ m	50 s	Compatible with operating fuel cell; can detect water under land areas	Incompatible with carbon materials; limited spatial and temporal resolutions
Neutron imaging	25 μ m	5.4 s	Compatible with operating fuel cell and carbon materials	Limited spatial and temporal resolutions; limited availability
Synchrotron X-ray	3-7 μ m	4.8 s	Compatible with operating fuel cell and carbon materials; signal intensity can be correlated to through-plane water content	Limited temporal resolution; limited availability
Microtomography	10 μ m	0.07 s	Through-plane resolution available	Has yet to be demonstrated with an operating fuel cell; vulnerable to artifacts; limited sensitivity to wat
Optical photography	10 μ m	0.06 s	Compatible with operating fuel cell; high temporal and spatial resolution	Transparent window requires substitution materials for operating fuel cell
Fluorescence microscopy	5.38 μ m	0.3 s	High spatial and temporal resolutions; signal intensity can be correlated to through-plane water content	Has yet to be demonstrated with an operating fuel cell

Table 1: Resolution capabilities are shown for liquid water visualization (From [24]).

Although experimental methods are useful to visualize the behaviour of PEM fuel cells, obtaining quantitative information, such as gas diffusion layer (GDL) water coverage ratio and liquid water volume fraction, is quite difficult from current visualization techniques [27]. Due to the complication of conducting experimental studies to specify actual dynamics of liquid water in PEMFCs, numerous scientists tend have used computational modelling and simulation to achieve qualitative insight into the physics of the two-phase flow and its implications [27]. In addition to this, other important features are the followings: the numerical simulations are less expensive, and also the values of the input data may be easily changed, obtaining results quicker than experimental methods.

In order to examine the formation and motion of liquid water a variety of methods have been used in many studies. These methods include: the Lattice Boltzmann, the pore-network, the level set and the volume of fluid (VOF) method [27, 28]. The Lattice Boltzmann method is based on macroscopic models and kinetic equations. The fluid is considered as an aggregation of pseudo-particles, and the method simulates consecutive propagation and collision processes over a discrete lattice mesh [27]. The pore network model represents the void space of a porous medium by a lattice of wide pores linked by narrower throats [27, 29]. These methods are not suitable for simulating macro scale two-phase flow in the gas channels of PEMFCs [30]. Hence, these approaches have been used for studying micro-scale transport in the porous media of the cell. The other two techniques mentioned above, namely the level set and the VOF methods, are employed for the macroscopic scale, from tens of micrometres to meters based on the conservation laws [27]. The level set model can perform numerical computations involving curves and surfaces on a fixed Cartesian grid. Topological changes and complex interfacial shapes can be solved. Nevertheless, it is not enough accurate for mass conservation. The VOF method is most commonly used for fluid analysis in the PEM fuel cells. This method has been accepted to simulate two or more time dependent immiscible liquids. The position of the interface between the fluids of interest is designed in the VOF method by applying a surface-tracking technique to a fixed Eulerian mesh [26, 28]. Surface tension and wall adhesion effects can be taken into account with this method. Furthermore, the VOF method is integrated in several commercial computational fluid dynamics (CFD) software packages, such as ANSYS Fluent, GERRIS Flow solver, and STAR-CCM [27]. Ferreira et al. [27] has published a review report, like that of Bazylak [24], about the numerical simulations of two-phase flow in PEM fuel cells using the VOF method.

2.3.2 Water Droplet Dynamics

Water accumulation effects were discussed in the previous sections; here, studies about water droplet dynamics will be reviewed. As aforementioned, water droplets are generated on the gas diffusion layer at the cathode side via electrochemical reaction as illustrated in Figure 3 which shows a water droplet resting on the gas diffusion layer. H (droplet height) is the distance from the gas diffusion layer to the top of the droplet and θ is the contact angle which the air/water interface forms with the surface of contact on the gas diffusion layer [31].

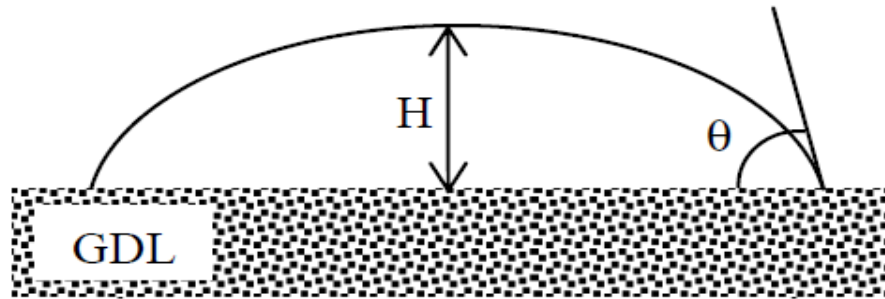


Figure 3: Droplet Height, Contact Angle (From [31])

If there are no external forces on the droplet, the contact angle is constant the entire droplet and is called static contact angle. Otherwise, under forces such as a drag force and a surface adhesion force, the shape of droplet changes and so two angles occur on the gas diffusion layer, namely an advancing (θ_A) and a receding (θ_R) angle (Figure 4) [31]. These angles are defined as dynamic contact angles.

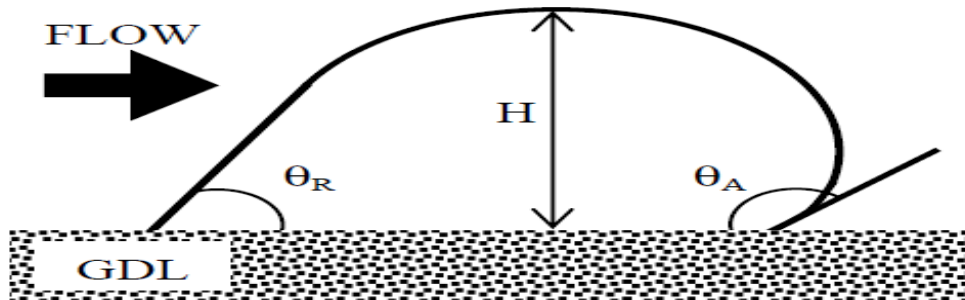


Figure 4: Dynamic Contact Angles for a Droplet Experiencing a Shear Flow (From [31])

Wettability characteristic of a solid surface, by liquid droplets, can be identified by using of the contact angle. Mortazavi and Tajiri have taken into account the behaviour of the surfaces in terms of the contact angle when they examining effect of the wettability on two-phase flow pressure drop. They also mentioned that surface wettability affects the water transport mechanism [32]. Furthermore, the hydrophilic or hydrophobic nature of the surface can be determined according to the contact angle. More specifically, when the contact angle is greater than 90° the surface is hydrophobic, which implies that water slips easily and quickly from the surface and beads up on it, whereas when the contact angle is less than 90° the surface is hydrophilic, in which case water spreads on the surface. In parallel with this, two forces such as a drag force and a surface adhesion force must be considered in order to characterise the detachment of a droplet from the surface [31]. Generally, water droplets detach from the surface when the drag force exerted by the shear flow, is greater than surface adhesion force [31, 32].

Besides the contact angle, there are many parameters which affect the water detachment, including channel geometry, water delivery rate, materials of membrane and channels, pore size on the membranes etc.

2.3.3 Numerical studies on Water Droplets Dynamics

Golpaygan and Ashgriz [33] have studied deformation and detachment of water droplets adhering to the surfaces of the cathode in PEM fuel cells. They illustrated the formation of droplets in the gas flow channels at the cathode side in a PEM fuel cell in Figure 5. They have modelled numerically by using of Navier-Stokes equations for Newtonian fluids in the channel. Furthermore, the effects of interfacial forces have been investigated and the deformation of free surfaces has been determined by using of the VOF method. They have made some assumptions in their numerical model:

- Incompressible Newtonian fluid is considered.
- The droplet is semi-circular shape at the beginning.
- The top and bottom boundaries are no-slip boundaries.
- The inlet boundary has a parabolic velocity profile.
- The outlet boundary, an outflow (no- gradient) boundary condition

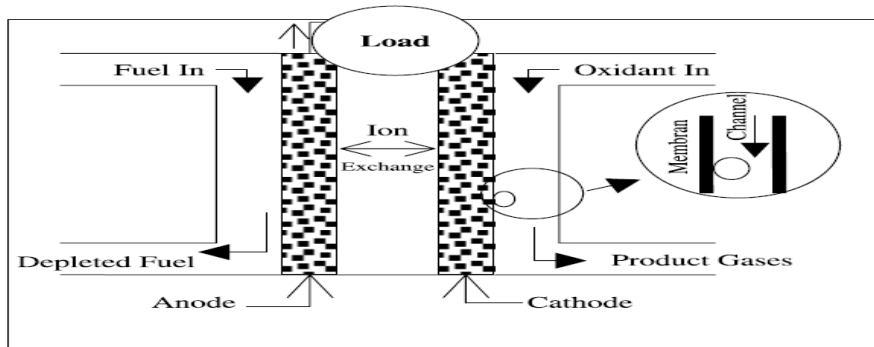


Figure 5: Formation of droplets in the channels of a PEM fuel (From [33])

The water droplet motion has been examined, when a fluid is forced to pass an inactive water droplet in their study. They have investigated as follows; droplet characteristic length, the effects of surface tension and viscosity, inertia of channels, the effects of droplet and channel flow properties, channel geometry, the flow velocity and break-up for the droplet.

Another numerical study of water management in the air flow channel at the cathode side in a PEMFC has been conducted by Quan and Lai [34]. They also used the VOF method with the CFD package FLUENT with the air-water two-phase flow simulated under different operating conditions. In their study, they accounted for the effects of channel surface hydrophilicity, channel geometry, and air inlet velocity on water behaviour, water content inside the channel, and two-phase pressure drop. They considered a U-shaped air flow channel (1mm×0.5mm×23mm) with a gas diffusion layer of 0.2 mm thickness, as illustrated in Figure 6. Their simplified model can be useful for understanding flow dynamics in the air flow channel, providing useful information for bipolar plate design and optimization.

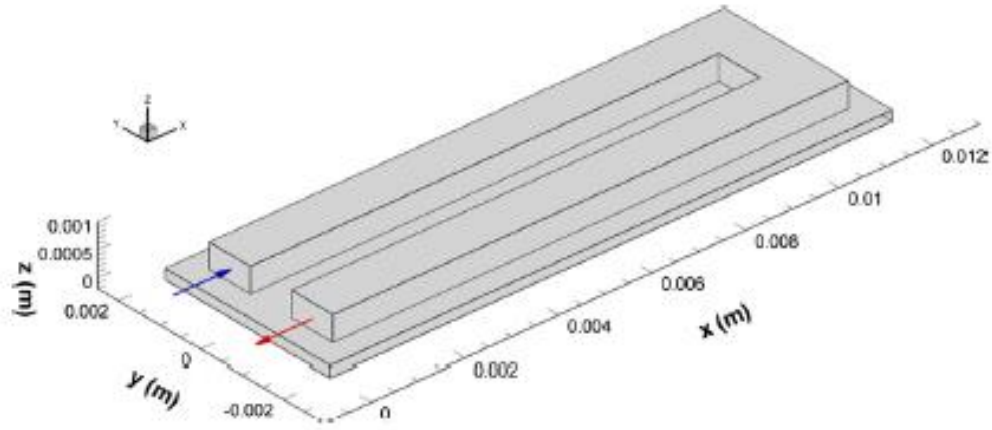


Figure 6: Computation domain: a U-shaped gas flow channel with sharp corners attached to a porous GDL (From [34])

Their assumptions are as follows:

- Isothermal condition
- Electrochemical reactions are not considered in detail.
- product water generated through electrochemical reactions and the water transported from membrane are at liquid phase and the total water flux is assumed constant
- There is no water phase change
- The gas diffusion layer has homogenous porous media.
- No-slip boundary condition was applied to all the three interior walls of the channel.

Quan and Lai [34] examined five simulation cases for the U-shaped channel (sharp corner) with varying hydrophilicity, two simulation cases for the U-shaped channel with round corners and four simulation cases for the U-shaped channel with sharp corners at higher air inlet velocity. In total, eleven cases were considered and leading to the following conclusions:

- Hydrophilic surfaces have advantages for the transport of reactants to the reaction sites.
- When the wall adhesion is not considered water content in the flow channel is at the highest, yet increasing air velocity decreases its amount.

- Water management strategy is managed easily on the hydrophilic channel surfaces, on the other hand hydrophilic channel surfaces cause higher pressure drop.
- A sharp channel could be a better design option.
- Increasing inlet velocity could make the water distribution inside the channel reasonably good in term of water management. The corresponding pressure drop increases almost linearly, which is similar to a single-phase laminar case.

In [21], droplet contact angle was measured on two different surfaces made of carbon paper and carbon cloth. In order to examine the contact angle, an experiment was conducted. Subsequently, a three dimensional model based on the VOF method was developed. Emergence, growing and detachment of a water droplet was simulated. The results showed that at low velocity, the wall adhesion is sufficient to keep the droplet still on the surface. As the gas flow rate increases, the drag force increases rapidly and eventually overcomes the adhesion force and removes the droplet from the surface. Droplet shape is affected by the air velocity. Friess [35] et al. examines and compares two different flow fields according to the surface properties of a hydrophilic gold flow channel and a hydrophilic graphite flow channel. In addition to this, compare three different hydrophilic flow channel architectures: an open gold parallel flow channel, an aluminium foam filled parallel flow channel, and a woven wick filled parallel flow channel.

The flooding condition was observed in terms of using materials of channels (i.e. graphite and gold) with GDL and without GDL. In the gold flow channel (hydrophilic), the limiting current is 0.21 Acm^{-2} for flooding regime without GDL, whereas this value is 0.24 Acm^{-2} for the flooding regime with GDL. When observing the graphite flow channel (hydrophobic) under same conditions, these values are 0.1 Acm^{-2} and 0.17 Acm^{-2} , respectively. Accordingly, the graphite channel design has a greater voltage drop at medium current densities and reaches the flooding regime much earlier than when the gold channel is used.

The second part of the analysis focuses on the effect that architecture of the flow channels have on the performance of fuel cell. For this section three flow channels were discussed: a gold open channel, a gold aluminium foam filled channel, and a gold woven wick filled channel. Their aim was to observe the relation of the current density with power and voltage, separately. As result observations, the aluminium foam filled channel has the best performing architecture and the second is open gold flow channel. Finally, the woven wick filled channel provides the worst power output among the three architectures. These results showed that if the pore size of the material is so small the power performance decreases, because water blocks the pores and the access of the reactant gas to the reactant sites. Therefore, better cell performance can be provided with larger pore size of the material. Pore size of the materials, woven wick and aluminium foam used in this study, can be seen in the Figure 7.

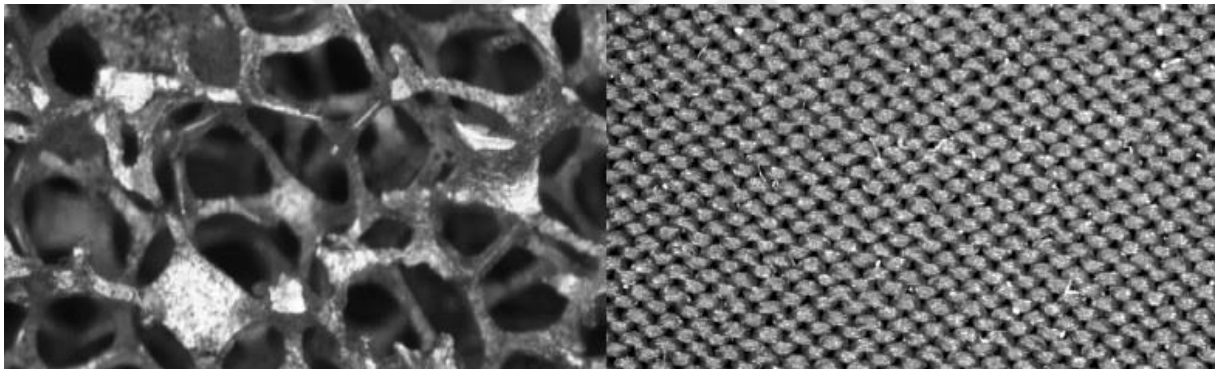


Figure 7: Aluminium foam and woven wick sample, respectively. (From [35])

In the work of Jo and Kim [5], water droplet dynamics were examined in a right angle, as seen Figure 8. The gas channel has a $250 \times 250 \mu\text{m}$ square cross section, $1000 \times 1000 \mu\text{m}$ lengths in the x and z coordinate directions, and a GDL surface on the bottom. There are 3 micro pores on the gas diffusion layers in order to inject water from the back surface of the porous layer. Two of them are close the sides and one of them is in the middle of the others. Water droplets are injected from these pores with different angles (by changing the PTFE content of the GDL) and considering different positions of the pores.

The resulting behaviour of the water coverage ratio on the top wall and the side wall is investigated as a function of time. The numerical simulations are based on the VOF method implemented in the software ANSYS FLUENT. Furthermore, effect of air inlet velocity and water injection velocity are examined. Similar findings were presented in [34]. Water that has emerged from the middle pore hits and expands on the side wall at the front at certain intervals whereas water that has emerged from other two pores climbs up the side walls and moves along the upper edges of the channel toward the channel outlet. As the hydrophobicity of the side and top walls in-creases, water droplets move along the channel without staying in the edge or corner regions. When the air inlet velocity increases, the moving speed of the water increases and so the water content in the gas channel decreases.

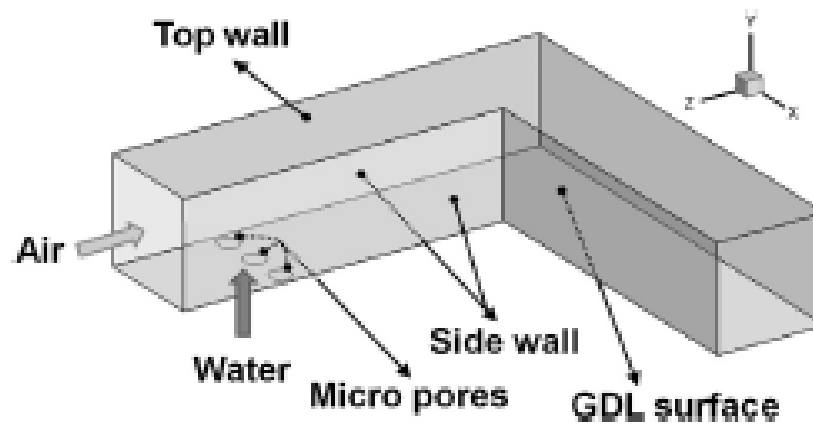


Figure 8: A right angel channel model having a micro pore on the bottom GDL surface. (From [5])

3. Research Methodology

The importance of proton exchange membrane fuel cells has been mentioned in the previous sections. These systems are available with a huge range of applications such as power source for mobile phones, computers and boats and domestic systems that need a few kilowatts as well as cars and buses. The structure of the PEMFCs, used in these types of systems, is more or less similar in terms of the electrolyte used, which is the most well-known and well-established of this is Nafion [2], and the electrode structure and catalyst which are described in section 2. Apart from these, other significant aspects of a PEMFC design must be taken into account; these are [2]

- ❖ Water management (is the most important one)
- ❖ The design of bipolar plates.
- ❖ The way of cooling the fuel cell.
- ❖ The cells connection method.
- ❖ Operating conditions (pressure, temperature, etc.)
- ❖ Another important issue is availability and usability of the reactants (hydrogen and oxygen).

In this study, some of the major design parameters for water management will be investigated. As it is understood above, and also from previous sections, it has a vital role in the operation of PEMFCs. That is important because the percentage of water content affects two crucial aspects in the PEMFCs such as proton conductivity and blockage of the pores in the electrodes or the gas diffusion layer. In other words, the amount of water is necessary for transmission of the proton, from the anode side to the cathode side, whereas increasing level of water causes the electrolyte flood. So, the balance of benefits must be provided when doing a design of PEMFC.

The result of the literature search, it can be seen clearly that a large amount of water is produced by chemical reactions. The chemical reactions and passing direction of H^+ ions in a PEMFC structure are indicated in figure 9. Furthermore, when the partial pressure of the water vapour is greater than the saturated vapour pressure, water droplets occurs. This situation is another reason for generating water. The droplets can be observed on the wall of the channels in figure 10. In the several papers, latter is assumed negligible when analysing the water droplet dynamics.

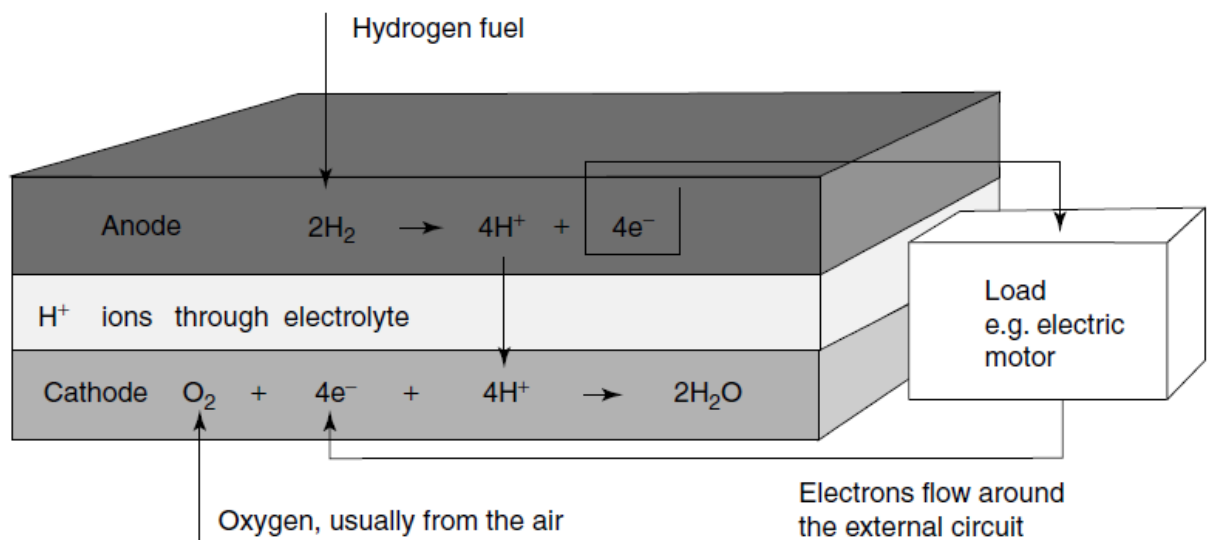


Figure 9 : The chemical reactions in anode and cathode side [From 36]

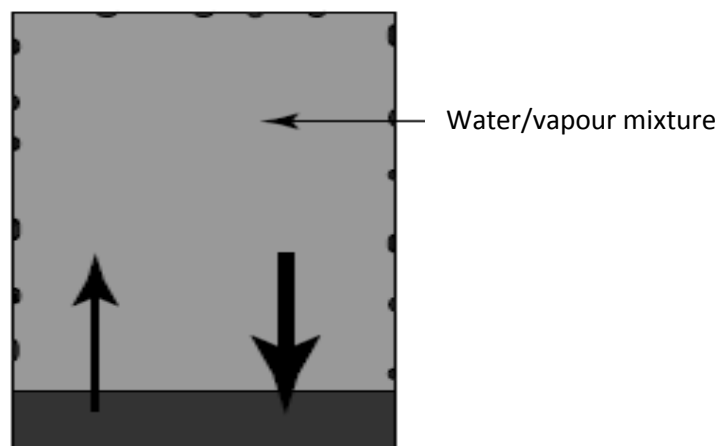


Figure 10 : Occurrence of water droplet from the condensation [From 36]

Various experimental works have been conducted to understand the water dynamics and to find the best way for the removal of the liquid water from the flow channels. Some researchers have focused on the contact angle that is the angle between water droplet and gas diffusion surface layer. As mentioned the previous sections, when the contact angle increases the removal of liquid is easier. Additionally, the increase of the contact angle causes the reduction of the contact area (between the GDL and water droplet) and so, it provides the lower surface tension. In order to create a surface like that, the hydrophobic coatings consisting of PTFE (Polytetrafluoroethylene produced by DuPont as Teflon) have been used. However, this application shrinks the pore size, which affects unfavourably the reactant flow in the gas diffusion layer. Moreover, physical parameters such as air velocity, channel geometry, have been changed to observe the water removal in the GDL in the experimental and numerical studies.

3.1 Channels Geometry

In the present study, three different flow channels are analysed, including a straight channel and a u-shape channel with rectangular bend and circular bend with rectangular cross section, as illustrated in figure 11. The straight channel was used in this study correspond to a microchannel with 0.3 mm x 0.3 mm square cross section and 1.5 mm length. For the u-shape channels; the length is 30 mm with round-trip, have 0.75 mm x 0.75 mm cross section through all channel. Water droplet dynamics were analysed by using of STAR CCM+ which is the simulation and CFD solver software. In our case, there are two time dependent immiscible fluids which are air and water. In order to determine the relation of these fluids each other and the GDL surface, many numerical methods, as it has been mentioned earlier, have been used. Nevertheless, the most convenient method was defined as the volume-of-fluid (VOF) method to observe the liquid water actions in the gas channels [36].

Therefore, existing VOF method in the STAR CCM+ was used in this study. Effects of the air velocity, water velocity, static contact angle and pressure drops have been analysed in 3D models.

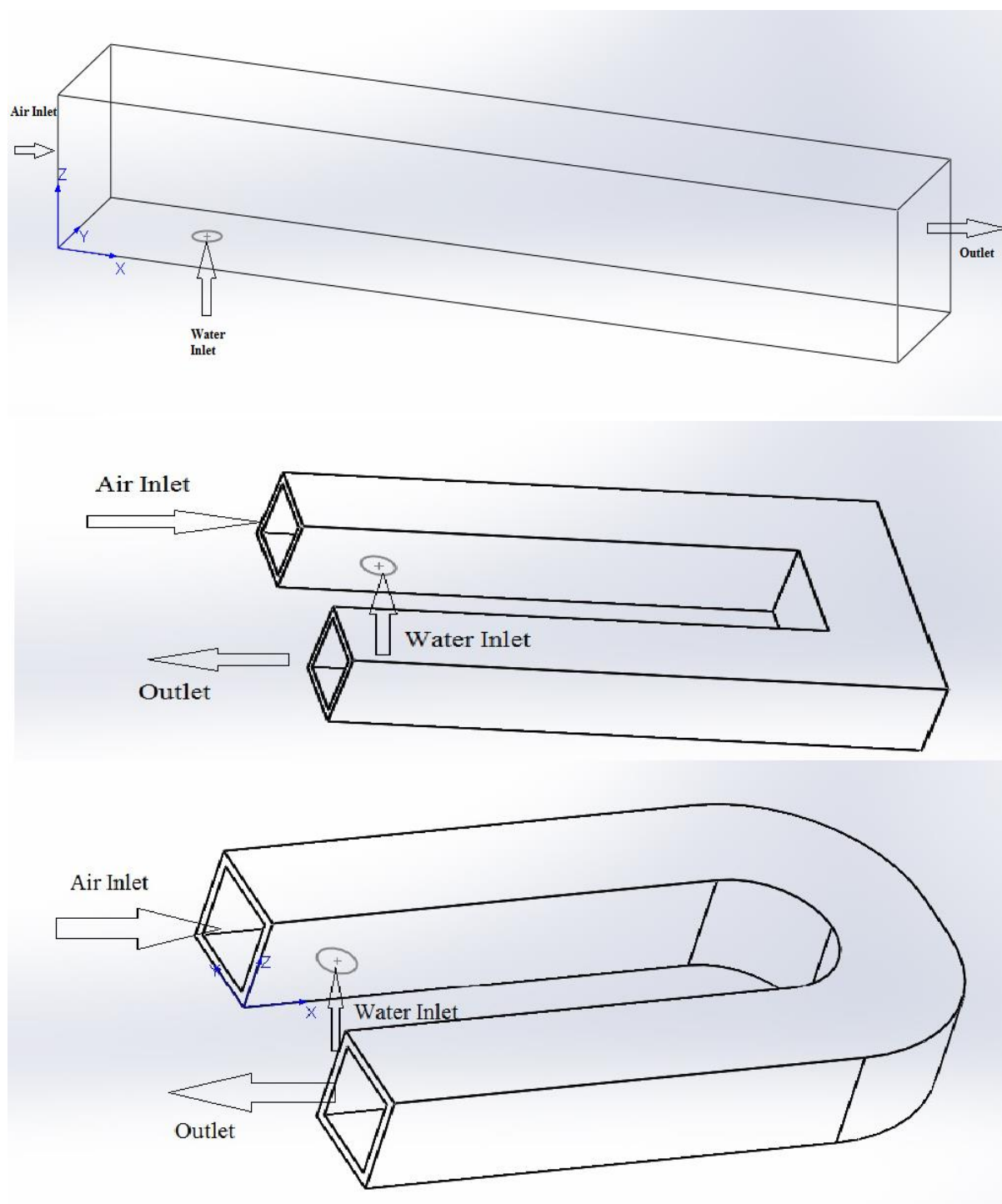


Figure 11: Rectangular, cylindrical and triangular channel models

3.2 Problem Set-up

The volume of fluid procedure is used for simulating the physical behaviour of the interface of two immiscible fluids such as water-air, water-oil, and oil-air or more fluids. This method was used only for single-phase free surface flows in the past [37]. In 1980s this technique was first developed by Hirt and Nichols [36, 38], although it can be used for two fluids or more at the present time. It is a simple and efficient numerical simulation method which calculates the surface tension using the volume fraction approach, has and also has the capacity of tracking immiscible interfaces [36]. The VOF technique has become popular in CFD studies of two phase flows, due to several advantages compared to other techniques.

3.2.1 Mass and Momentum Equations

In fluid dynamics, the continuity equation states as follow:

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

A single momentum equation is solved throughout the domain, and the resulting velocity field is shared among the phases. The momentum equation, shown below, is dependent on the volume fractions.[39] In this study there was no change on the temperature, so energy conservation equation was not taken into account. In other words, the flow is isothermal.

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

where p is the static pressure, $\vec{F}$ a momentum source term stems from surface tension, and ρ & μ are the volume averaged density and dynamic viscosity, respectively. When two-phase system analysed, these variables (ρ & μ) are calculated to account for the variable volume fractions of the air-water flow.

3.2.2 Volume of Fluid Method and Formulations

As mentioned above volume of fluid is a basic multiphase model. This technique is suitable for simulating streams of a few immiscible fluids on numerical grids fit for determining the interface between the phases of the mixture [40]. For two-phase flows using the VOF model, unsuitable grids (a) and suitable grids (b) are shown in the figure 12. Large contact area between phases provides better numerical results rather than small contact area. Sloshing flow in a water tank is a good example for the large contact area where the free surface is routinely smooth [40]. This method needs a fine mesh to reduce the modelling errors for example each droplet have to represent at least three cells.

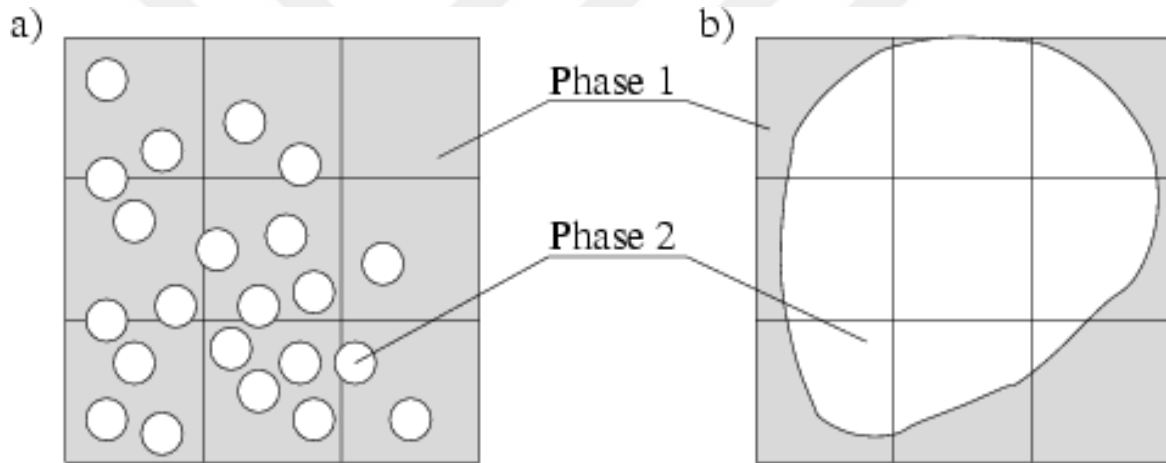


Figure 12 : Unsuitable and suitable grids for two phase flows [From 40]

Volume fraction can be defined as the spatial distribution of each phase at a given time. In order to calculate these types of distributions, a transport equation is solved for volume fraction of the phases using VOF model equations [40]. These fractions of all phases constitute a union in every control volume. The interface between phases is followed for each computational cell along the domain by calculating the volume fraction for the specific fluid. For instance, if the i^{th} fluid's volume fraction in the cell is specified as α_i , then the following three possible conditions occur [39]:

$\alpha_i = 0 \quad \rightarrow \quad \text{The cell is empty of the } i^{\text{th}} \text{ fluid}$

$\alpha_i = 1 \quad \rightarrow \quad \text{The cell is full of the } i^{\text{th}} \text{ fluid} \quad (1)$

$0 < \alpha_i < 1 \quad \rightarrow \quad \text{The cell involves the interface between } i^{\text{th}} \text{ fluid and another fluid}$

For all phases, the sum of the volume fraction function is equal to 1 [38], it is indicated as follows:

$$\sum_{i=1}^n \alpha_i = 1 \quad (\text{For } n \text{ phases}) \quad (2)$$

The volume fraction equation, available in [39], is solved for each computational cell by using of the volume fraction function α_i .

$$\frac{\partial}{\partial t}(\alpha_i \rho_i) + \nabla \cdot (\alpha_i \rho_i \vec{v}_i) = 0 \quad (3)$$

After that, the Navier-Stokes equation, which is based on the volume fractions of whole phases throughout the fluid properties ρ & μ , is used when the two-phase fluid flows in the microchannel are modelled.

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot [\mu(\nabla \vec{v} + \nabla \vec{v}^T)] + \rho \vec{g} + \vec{F} \quad (4)$$

where p is the static pressure, $\vec{F}$ a momentum source term stems from surface tension, and ρ & μ are the volume averaged density and dynamic viscosity, respectively. When two-phase system analysed, these variables (ρ & μ) are calculated to account for the variable volume fractions of the air-water flow.

Formulation is shown below:

$$\rho = \rho_a + \alpha_w(\rho_w - \rho_a) \quad (5)$$

$$\mu = \mu_a + \alpha_w(\mu_w - \mu_a) \quad (6)$$

3.2.3 Surface Tension Formulation

The surface tension force can be defined as a tensile force which is tangential to the interface dividing two fluids. This force is an interfacial force, which tries to hold together the fluid molecules at the free surface. The surface tension is modelled as a volumetric force using the Continuum Surface Force (CSF) approach of Brackbill and others [40].

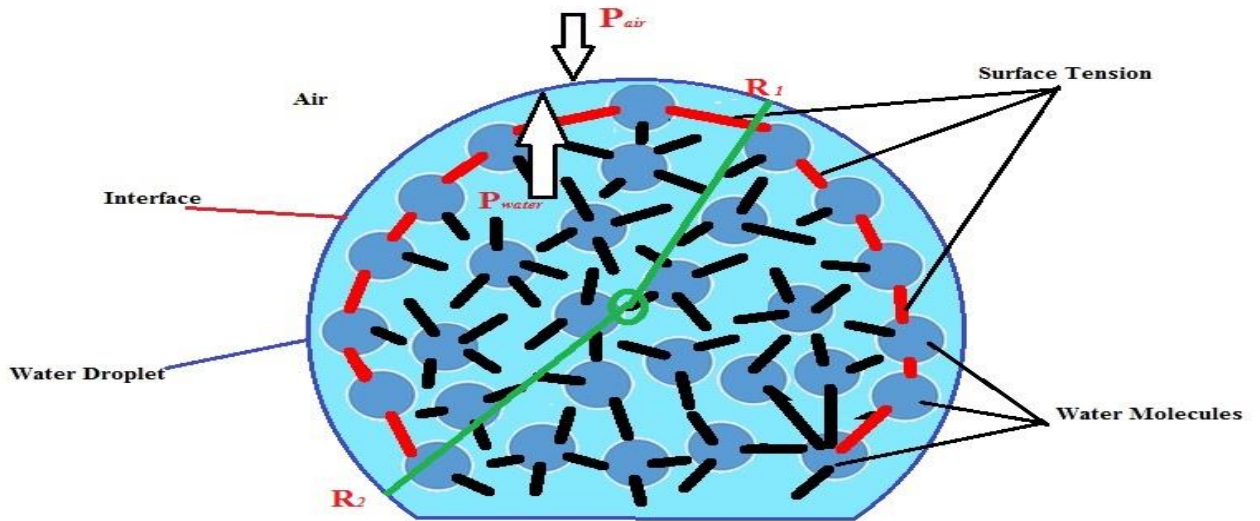


Figure 13 : An illustration of surface tension, interface and pressures

The value of the surface tension relies principally on the nature of the fluid and on temperature. For a curved interface, the surface tension force $\vec{F}_\sigma$ can be written into two components as below [40]:

$$\vec{F}_\sigma = \vec{F}_{\sigma,n} + \vec{F}_{\sigma,t} \quad (7)$$

where:

$$\vec{F}_{\sigma,n} = \sigma K \vec{n} \quad (8)$$

$$\vec{F}_{\sigma,t} = \frac{\partial \sigma}{\partial t} \vec{t} \quad (9)$$

Here, σ is the surface tension coefficient. $\vec{n}$ is the unit vector normal to the free surface and directed from liquid to gas. $\vec{t}$ is the unit vector in the tangential direction to the free surface. K is the mean curvature of the free surface.

When the surface tension coefficient has a constant value, there is not a tangential force; it becomes 0, as well as due to constant the surface tension along the surface, temperature differences do not occur. So, tangential part vanishes in the equation (7) and the surface tension results in a force normal to the interface ($\vec{F}_\sigma = \vec{F}_{\sigma,n}$). In this case, this force can be shown that the pressure drop across the surface depends upon the surface tension coefficient, σ , and the surface curvature K as taken by two radii in orthogonal directions, R_1 & R_2 (in figure 13) [39], ($P_{water} - P_{air}$ on either side of the interface can be seen in Figure 13) :

$$P_{water} - P_{air} = \sigma \left(\frac{1}{R_1} + \frac{1}{R_2} \right) \quad (10)$$

In the STAR-CCM+, continuum surface force (CSF) model is used when the surface tension force is calculated. That is, it uses the smooth field of the phase volume fraction to calculate a vector normal to the interface [40]:

$$\vec{n} = \nabla \alpha_i \quad (11)$$

The curvature of the interface is defined in terms of the divergence of the unit normal, $\vec{n}$ [40]:

$$K = - \nabla \cdot \frac{\nabla \alpha_i}{|\nabla \alpha_i|} \quad (12)$$

When a cell contains only two phases, the volume force in the momentum equation to account for the surface tension can be expressed as:

$$\vec{F}_{vol} = \sigma K \frac{\rho \nabla \alpha_i}{\frac{1}{2}(\rho_a + \rho_w)} \quad (13)$$

where ρ is the volume-averaged density computed as follows:

$$\rho = \sum \alpha_i \rho_i \quad (14)$$

3.2.4 Contact Angle

The angle between the liquid surface and the outline of the solid surface that contact with the present liquid is described as the contact angle (θ). The rate of wettability of the solid surface can be determined using the contact angle as mentioned in the section (2.3.2). By default, STAR-CCM+ uses a static value of contact angle for calculating the surface tension [41]. However, a static contact angle can generate impractical free surface shapes when implemented some applications, so definition of a dynamic contact angle is required. In the software, Kistler function [40] can be used to define a dynamic contact angle, but in the current study only static contact angle was considered.

In other words, in the present study, the wettability of the surface was determined by changing the contact angle where it was calculated from the liquid side. More specifically, when the contact angle is greater than 90° the surface is hydrophobic, which implies that water slips easily and quickly from the surface and beads up on it, whereas when the contact angle is less than 90° the surface is hydrophilic, in which case water spreads on the surface. An illustration of these surfaces can be seen in figure 14.

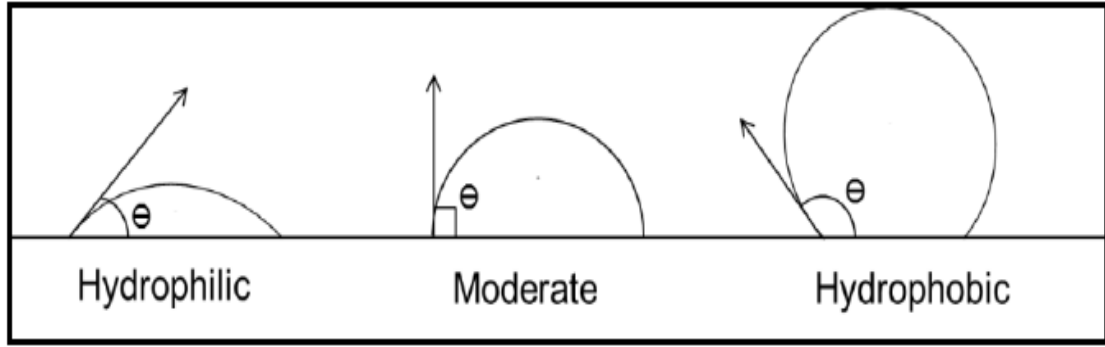


Figure 14 : Static contact angles between the solid surface and liquid surface [From 37]

3.3 Numerical Model

Three different channel geometries were utilised in this study as illustrated in figure 11. The u-shaped channel models are typically used within the serpentine flow channels in the PEM fuel cells. When these domains are modelled as three dimensional, some assumptions are necessary to complete the numerical simulation. These are: the flow is laminar and isothermal for air and water in the channel. Three dimensional models provide a complete description of the liquid gas interface and also the assumption of the isothermal flow reduces the complexity of the two phase flow. The flow is laminar because of the channel dimensions which correspond to microchannel. Reynold number ($Re = \frac{\rho u L}{\mu}$), is a dimensionless quantity for determining the fluid flow situations and if Re is less than 2000 the flow is described as a laminar flow. Where $\rho = 1.18415 \text{ kg/m}^3$, $u = 10 \text{ m/s}$, $L = 0.3 \times 10^{-3} \text{ m}$ and $\mu = 1.85508 \text{E-}5 \text{ Pa-s}$, so Re was calculated as 192 in this study as a reference value.

The numerical simulation was implemented using STAR CCM+. The Eulerian multiphase model was solved with VOF model in this software. For the phase interaction, water-air in this study, in the model a constant surface tension (σ) coefficient was used. Its value is 0.07199 N/m at the room temperature according to [41]. The information about the dimensions of the models and corresponding mesh will be given in the results section.

3.3.1 Initial and Boundary Conditions

Three dimensional two-phase flow (air-water) inside the micro-channel is modelled. No-slip boundary condition is imposed to all interior walls. There is no heat transfer between the phases. A uniform velocity was imposed at the air inlet and a mass flow rate was determined for the water inlet on the GDL. Water injection ratio was determined as 0.00202 ml/min for the whole cases, whereas air velocity could be varied.

At the beginning, water content does not exist, only air with an initial velocity as 10 m/s becomes in the channel. The domain is under normal the atmospheric conditions, therefore pressure at the inlet and outlet is constant. The type of boundary of the outlet surface condition is set as a pressure outlet boundary. Various contact angles were utilised for the bottom wall, while side and top wall have a constant contact angle value, 45° . The surface tension (σ) is 0.07199 N/m, which becomes dominant over viscous force and gravitational forces, so the effects of these forces are negligible. Figure 15 represents the boundary conditions of the straight channel.

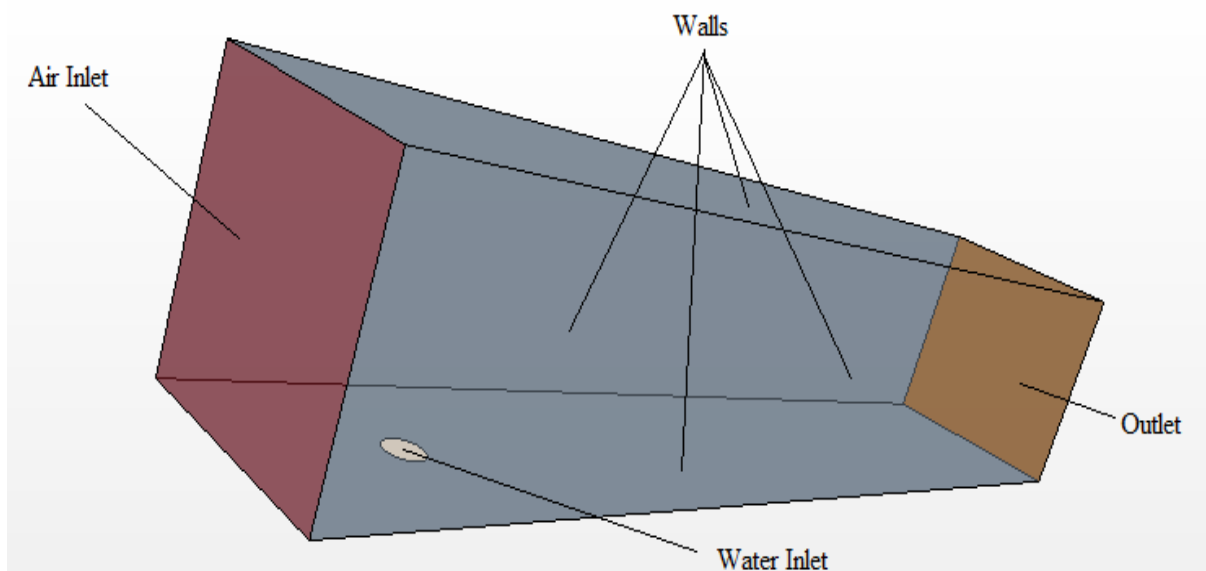


Figure 15 : Boundary Conditions

3.3.2 Mesh Sensitivity Analysis

In order to obtain accurate results with experimental data, mesh size plays a significant role in the numerical simulations. Therefore, before starting the analysis, a mesh refinement study was conducted. A structural tetrahedral computational mesh was used with 9 μm base size. The following approach was conducted for the mesh refinement study.

Firstly, the reference cell size was chosen as 11 μm and then this length reduced to 7.5 μm one by one. A decrease of the length of the mesh size causes the increase of the number of computational cells. Whereas this situation provides better and expected results, it takes a long time for the solution. For this reason, it is necessary to find a minimum and appropriate characteristic length for the mesh. Figure 16 shows water droplet formation in terms of the length of the mesh size at the time of 0.2 s.

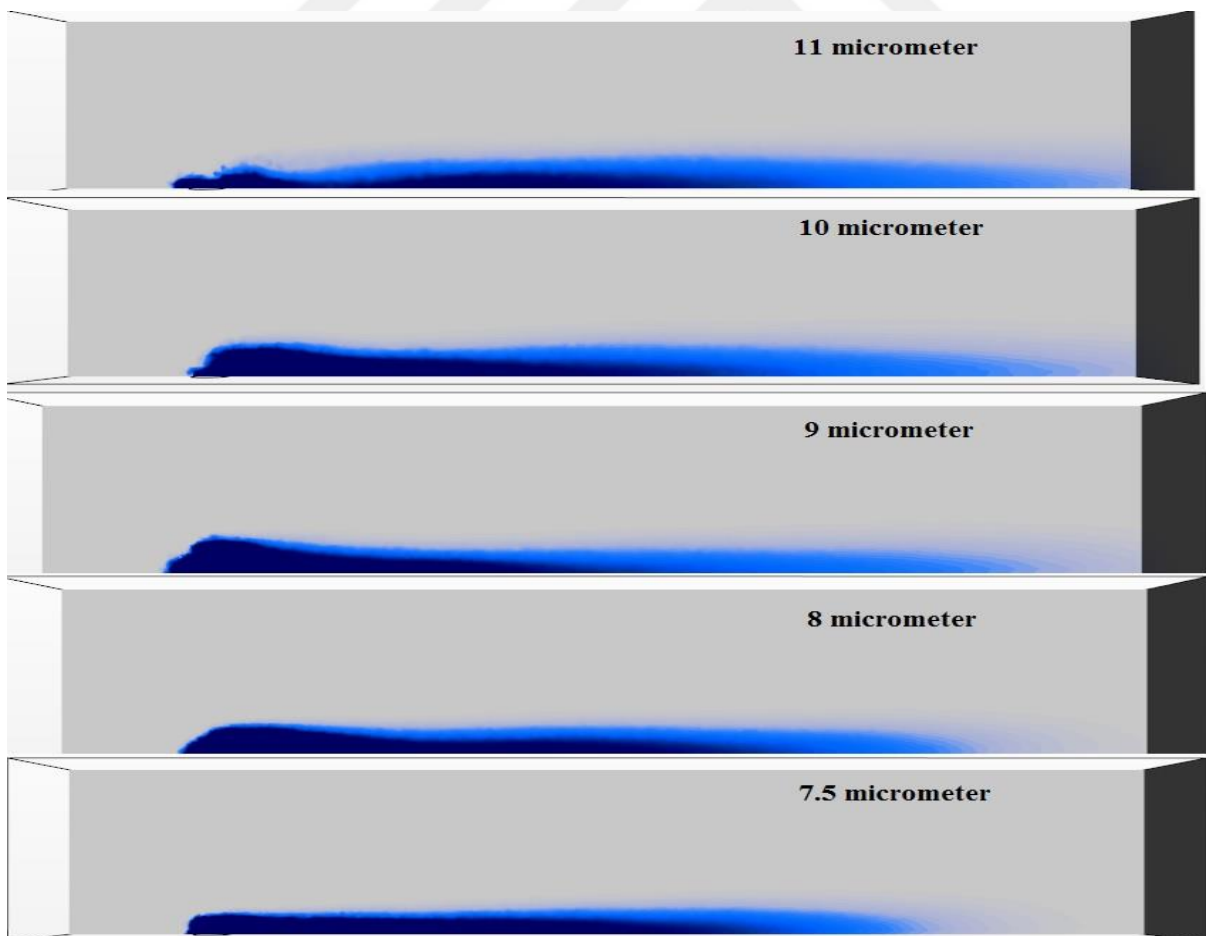


Figure 16: Formation of the water droplet for different mesh sizes after 0.2 s from the injection.

The mesh sensitivity test was conducted under the 10 m/s air velocity and 0.00202 ml/min water injection rate and the static contact angle of the gas diffusion layer was set as 140° , others were set as 45° which are baseline conditions. The dimension of the channel in this study correspond to a microchannel with $0.3 \text{ mm} \times 0.3 \text{ mm}$ square cross section and length with 1.5 mm a pore of radius $R=0.025 \text{ mm}$ at 0.2 mm away from the entrance of the channel in the GDL surface. Water mass flow rate at outlet of the channel was used with different mesh size for the determination of the averaged value. Figure 17 was obtained using five different characteristic mesh sizes.

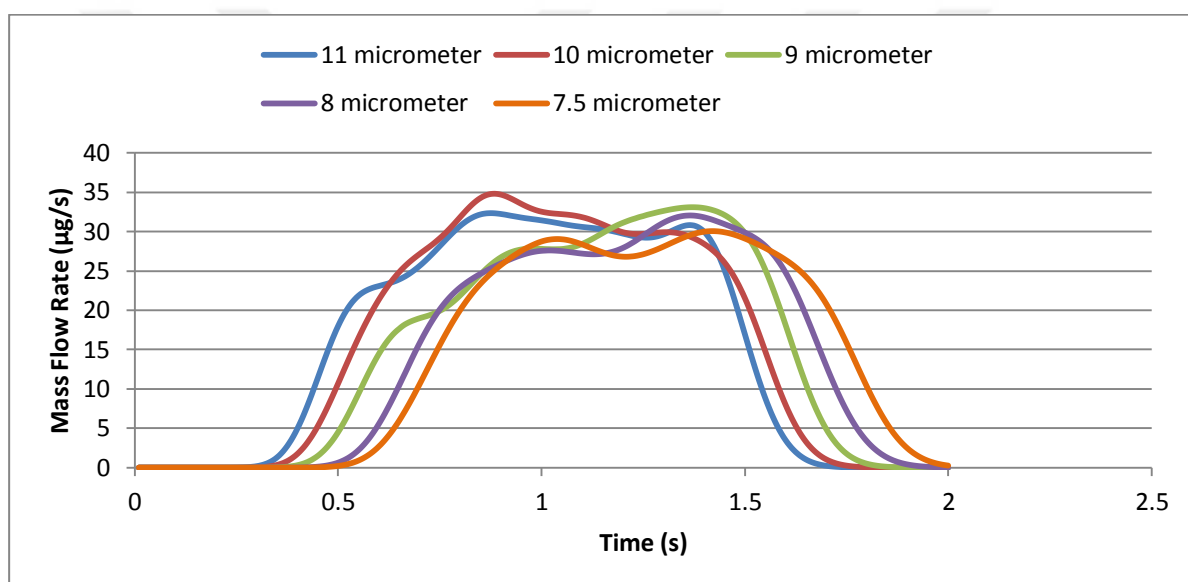


Figure 17 : Mass flow rate of water at outlet for different the mesh sizes

In figure 17, although characteristic lengths of 11 and 10 μm have a similar behaviour, the mass flow rate at the channel outlet is significantly different from that obtained with smaller mesh sizes of 9, 8, 7.5 μm . Among these three values 9 μm was selected for the mesh size and so approximately 950,000 cells were created and a computer that has Intel Core i7-3610QM @2.30GHz 2.30GHz with 8 GB RAM have been used. . A schematic illustration of the three-dimensional computational domain and the corresponding mesh can be seen in the figure 18.

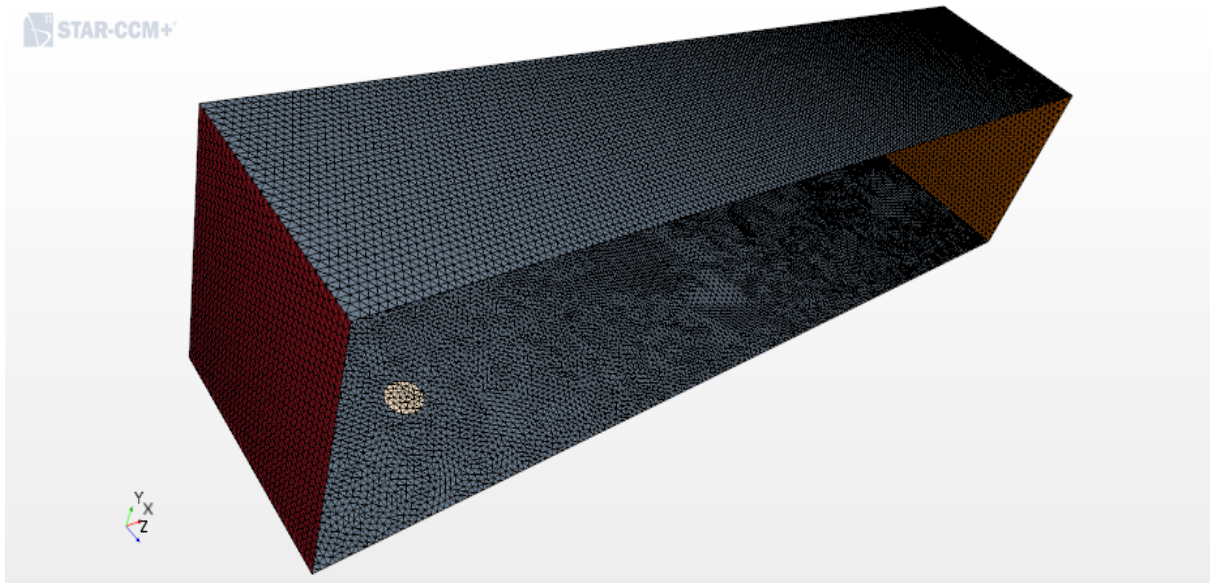


Figure 18 : An illustration of the computational domain mesh with base size $9\ \mu\text{m}$

For the time sensitivity analysis, volume fraction of water in the channel was observed by altering the time step. Initially, the time step was set equal to 0.01 seconds. Subsequently, the time step was increased to 0.1, but the trend of the volume fraction of water was found to be significantly different, whereas for a smaller time step of 0.001 seconds, a similar trend was obtained. This is demonstrated in figure 19, which shows the volume fraction of water in the channel for a time interval of 0.05 s. Thus, the time step of 0.01 seconds has been used for the all calculations.

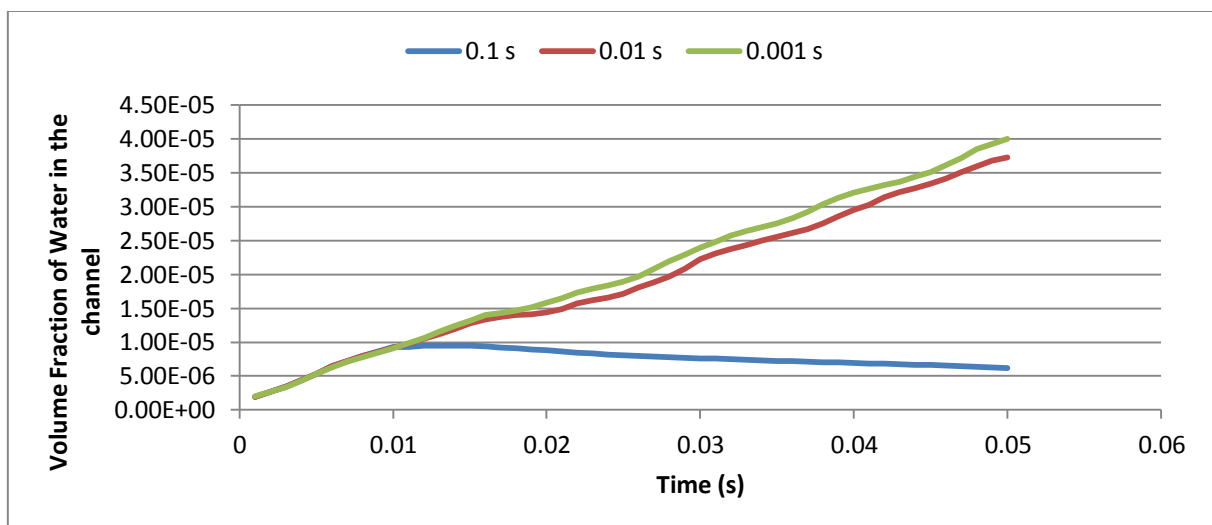


Figure 19 : Time sensitivity analysis

4. Results and Discussions

In this section, results of the all simulations are showed and discussed after the calculations were done in the STAR CCM+. Surface tension has an important role analysing the water droplet dynamics in the micro gas channel. The ratio of the surface tension to the other forces can be represented by some dimensionless numbers which are the capillary number ($Ca = \frac{\mu u}{\sigma}$), Weber number ($We = \frac{\rho u^2 d}{\sigma}$), and Bond number ($Bo = \frac{\rho g d^2}{\sigma}$). For baseline conditions in this study, $Ca = 0.21 \times 10^{-3}$, $We = 2 \times 10^{-3}$ and $Bo = 0.34 \times 10^{-3}$, d is the injection pore diameter and ρ, μ, σ are the density, viscosity, and surface tension coefficient of water ,respectively. In our case velocity of water, u , is calculated by using $\dot{m} = \rho u A$ where A is the area of the water injection pore. The small Ca and Bo numbers show that viscous force and gravitational force are negligible when compared to the surface tension force.

4.1 Analysis of a Straight Channel

The dimensions of the channel shown in the figure 20 was utilised to examine the effects of the contact angle, air velocity and aspect ratio of the channel over the water droplet. All tests in this section were conducted under a constant value of water injection rate and surface tension 0.00202 ml/min and 0.07199 N/m, respectively. Water injection was started after 0.2 seconds and continued during 1 second.

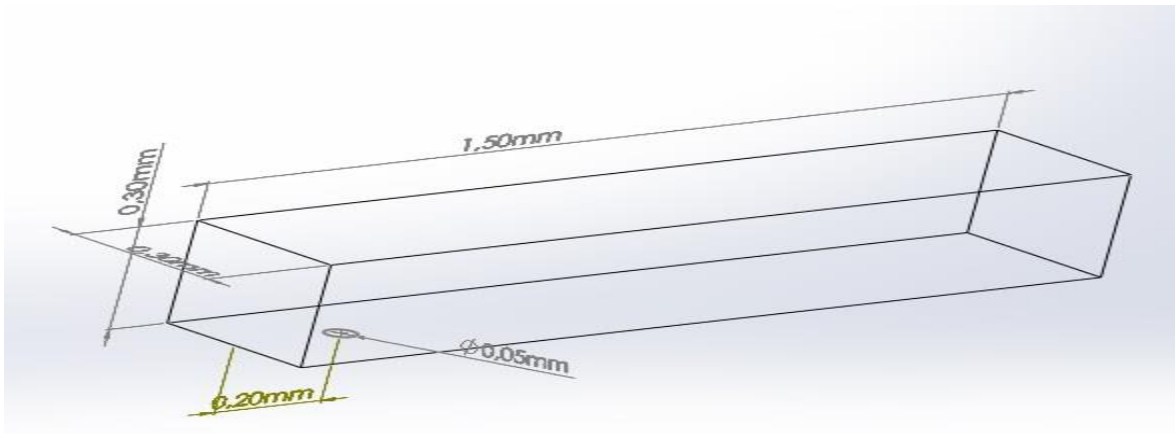


Figure 20 : Dimensions of the straight channel

4.1.1 Effects of the Static Contact Angle

In a typical PEM fuel cell gas microchannel, the surface of the GDL is important in terms of the water droplet dynamics. It is formed teflonated carbon paper or carbon cloth. The other three interior walls compose of a bipolar plate made of treated carbon-based or metallic materials [28]. The contact angle between gas diffusion layer and water droplet depends on the materials of the GDL, so the wettability of the GDL surface is related to PTFE content.

In the present study, different static contact angles have been implemented to GDL in the model to examine the formation of water droplet and wettability of the GDL. Only the static contact angle of the bottom wall (GDL) was changed, other three walls set a constant value as 45° . These static contact angle values of the GDL surface are 45° , 60° , 90° , 140° and 160° . As mentioned earlier, if the contact angle less than 90° this surface named hydrophilic surface. According to this definition, it is expected that water droplet must tighten step by step from 45° to 160° . In order to understand and observe this fact, the results of the research conducted shows the water droplet has large area at the small contact angles. Firstly, the simulations have been performed for each static contact angle during 0.2 seconds. At the same time, some images were taken from the domain at 0.2s and showed that the largest and widest water droplet occurs at the static contact angle of the surface is 45° . Neutrally, the smallest droplet takes places at 160° . Figure 21 indicates a top view of the GDL surface with water droplet formation toward the channel outlet. It can be seen clearly that, an increase of the static contact angle leads a decrease of the transverse length of the water droplet at the 0.25 mm away from water injection pore. The lengths have been measured as 0.1854 mm, 0.1797 mm, 0.1686 mm, 0.1623 mm and 0.1588 mm from 45° to 160° , respectively. Moreover, although there were so little water particles in the channel, almost all the water content in the channel surface removed at the end of the 2.5 seconds.

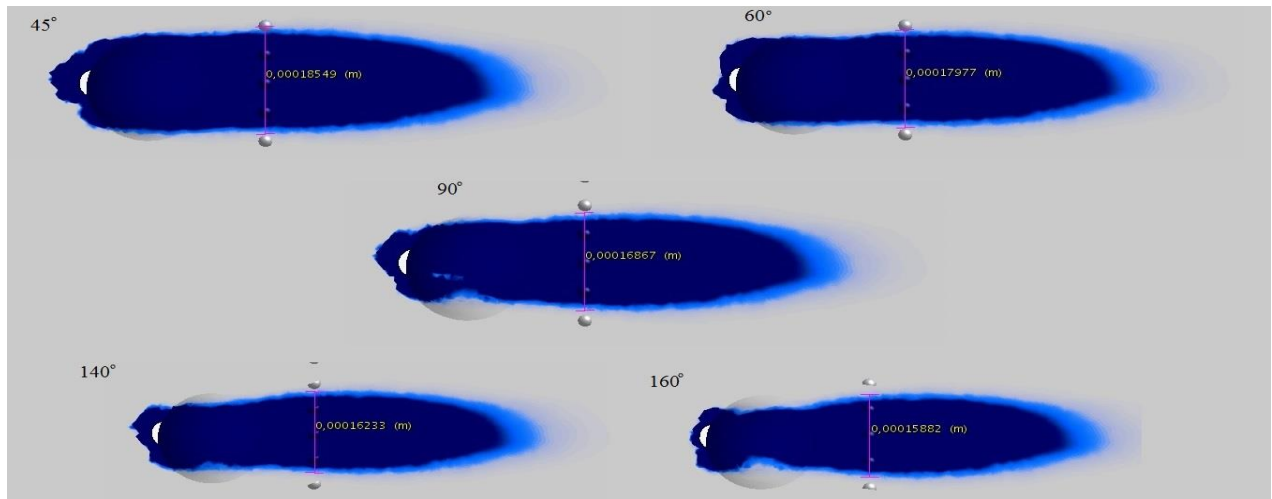


Figure 21 : A top view of the transverse length of the water droplet at different static contact angles

The percentage of wettability of the channel rises as the static contact angle decreases; it can be seen in the figure 22. Therefore, water droplet expands in the GDL and occupies more of the channel before being removed. Water fills the channel nearly similar rate at close static contact angles. At the end of the water injection, water occupies about 0.4 ‰ of the total volume of the channel for the highest contact angle, whereas it occupies the channel nearly 0.6‰ at the lowest contact angle. Normally, water volume in the channel expects the same level, although due to high velocity there are some differences among the water volume values in the channel.

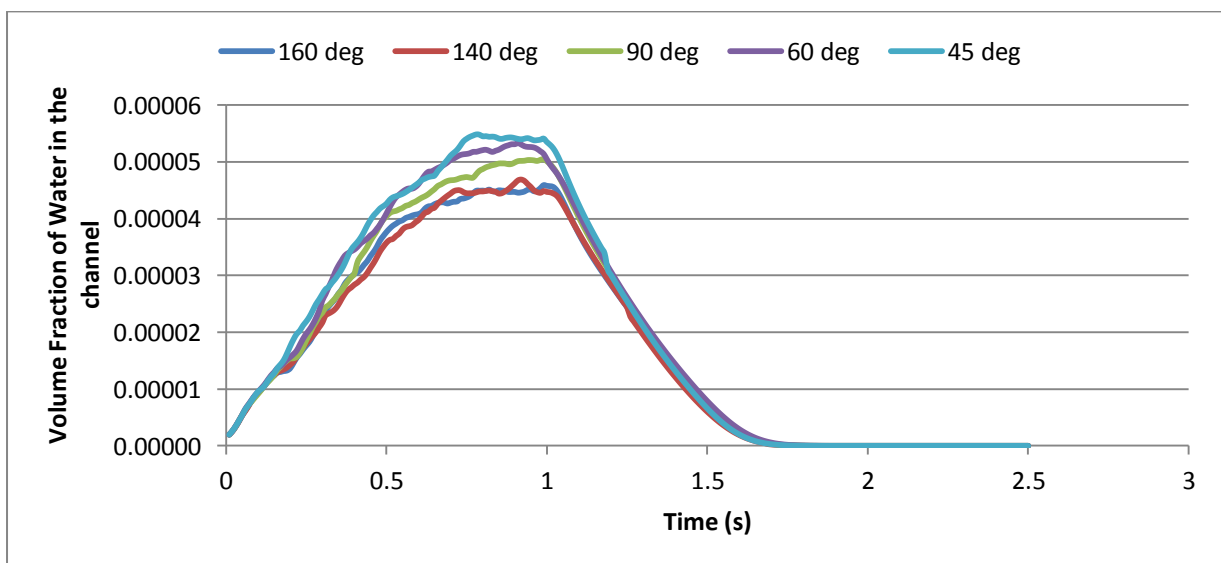


Figure 22 : Water occupying the channel

Similarly, the surface of the gas diffusion layer is covered by water at the highest rate by the value of 6 % for the lowest contact angle, as indicated in figure 23. So it can be said that the wettability of the GDL increase by decreasing the static contact angle.

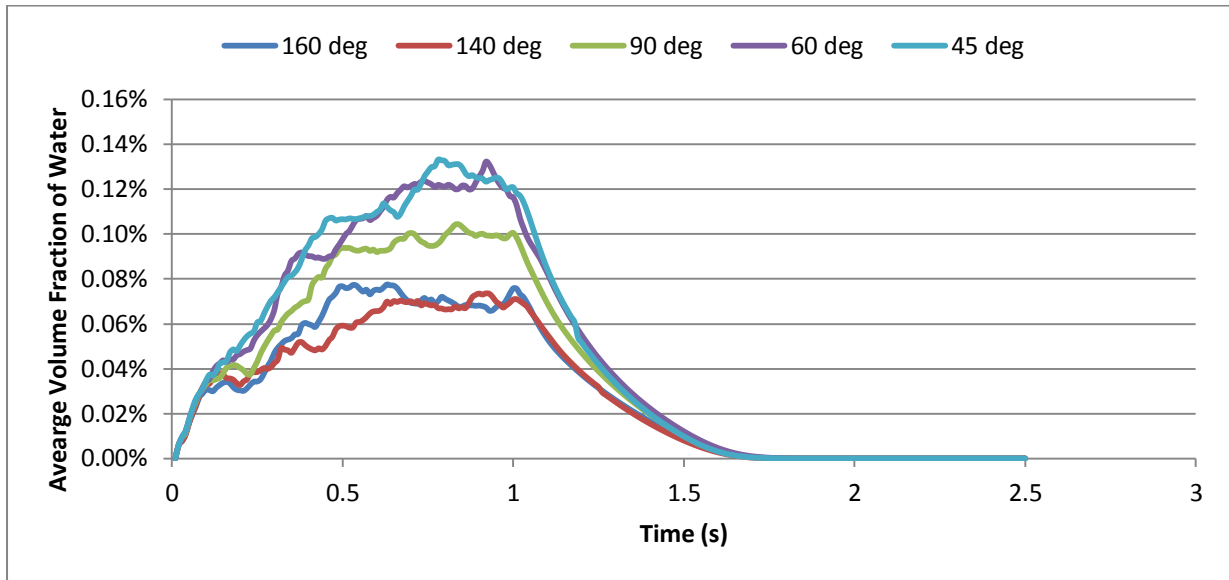


Figure 23 : Average Volume Fraction of Water in the GDL

4.1.2 Effects of the Air Inlet Velocity

Air inlet velocity is another important parameter for the water management in the gas flow channel. In this stage, the impact of the air inlet velocity to water droplet was examined using varying air inlet velocities; 3 m/s, 6 m/s, 10 m/s, 12 m/s. While altering the air inlet velocities static contact angle of the walls set as constant 140° for the GDL surface, 45° for the other three interior walls as well as the water injection rate is maintained constant. Compared the results for each air inlet velocities were investigated that the height of the water droplet is the maximum at the lowest air inlet velocity. In other words, water droplets have a fine condition to grow up under the lowest air inlet velocities. This situation occurs because of the weaker pressure forces and shear stress. As a result in the low velocities, stronger surface tension occurs due to the longer three phase contact line and larger coverage area. This strong surface tension forces provides the stabile shape for the water droplet. Then, first detachment becomes when the water droplet reach enough size at 0.3 s, as shown in figure 24.

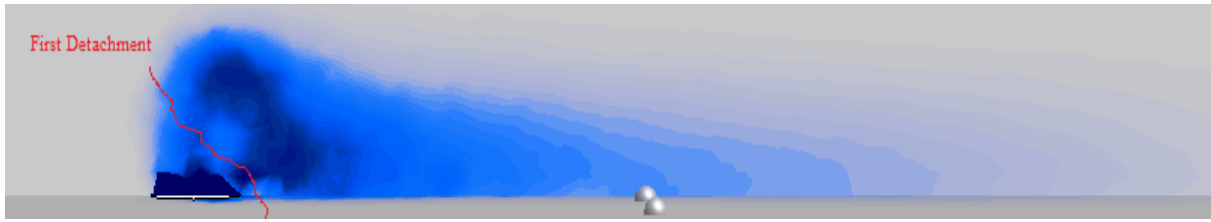


Figure 24 : Detachment of water droplet from the main part

In all simulation cases shows that the water droplet deforms downstream. Neutrally, this deformation has been fast by increasing the air inlet velocity. Therefore, the height of the droplet decreases from low to high velocities. For instance, the highest height of the droplet is 0.052 mm when the air inlet velocity as 3 m/s, whereas the minimum water droplet height is 0.012 mm when the air inlet velocity as 12 m/s. This shows that effects of the surface tension forces are less at high velocities than low velocities. Figure 25 illustrates the water droplet motion and heights under the different velocities at 0.2 s.

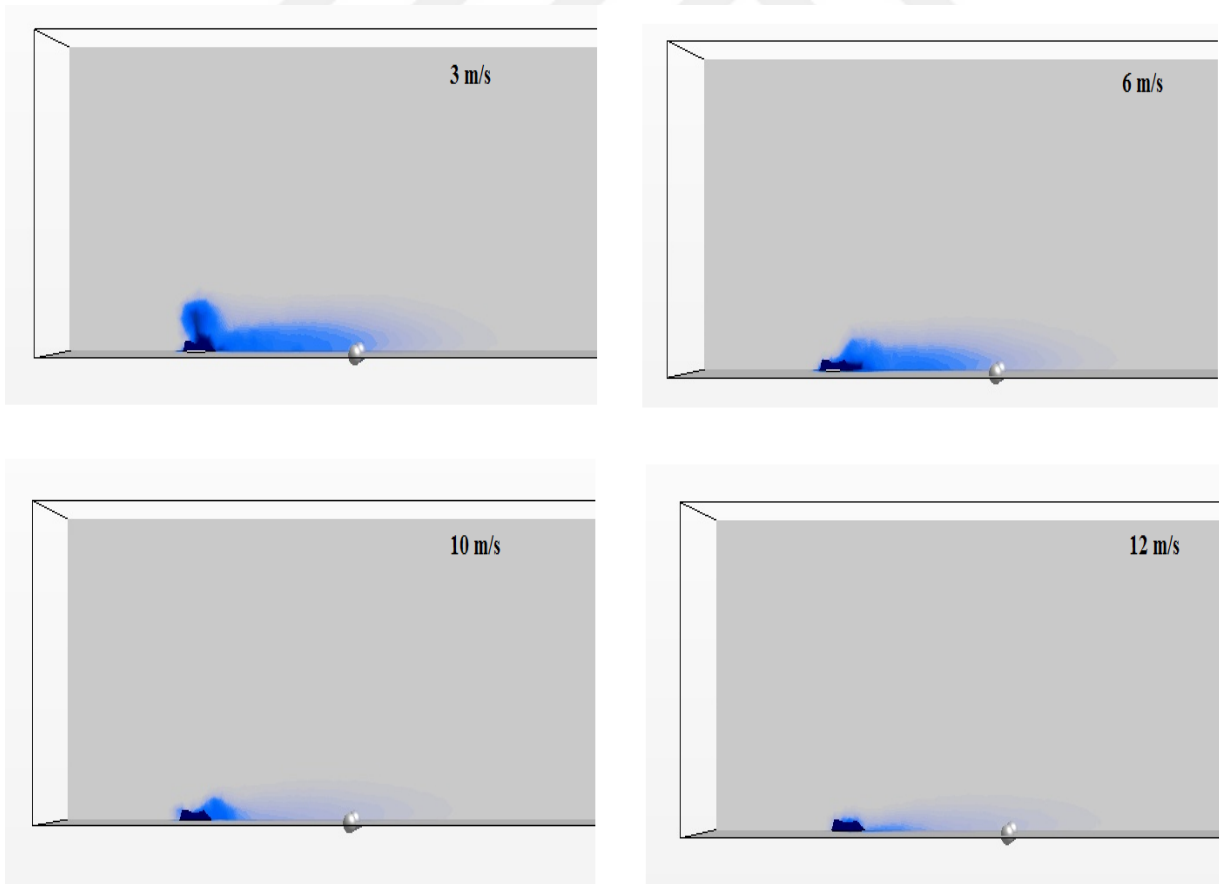


Figure 25: Water droplet formation under different velocities

Following results were obtained when examining the alteration of the water volume fraction in the channel and on the gas diffusion layer at different air inlet velocities. As it is expected, the downstream on the droplet is strong at higher velocities, so the percentage of water coverage reduces with increasing air velocities. As it can be seen clearly below the graph (figure 26), the maximum volume fraction of water is 0.00012 at 3 m/s, whereas this value is minimum, approximately 0.00004 at the highest velocity as 12 m/s.

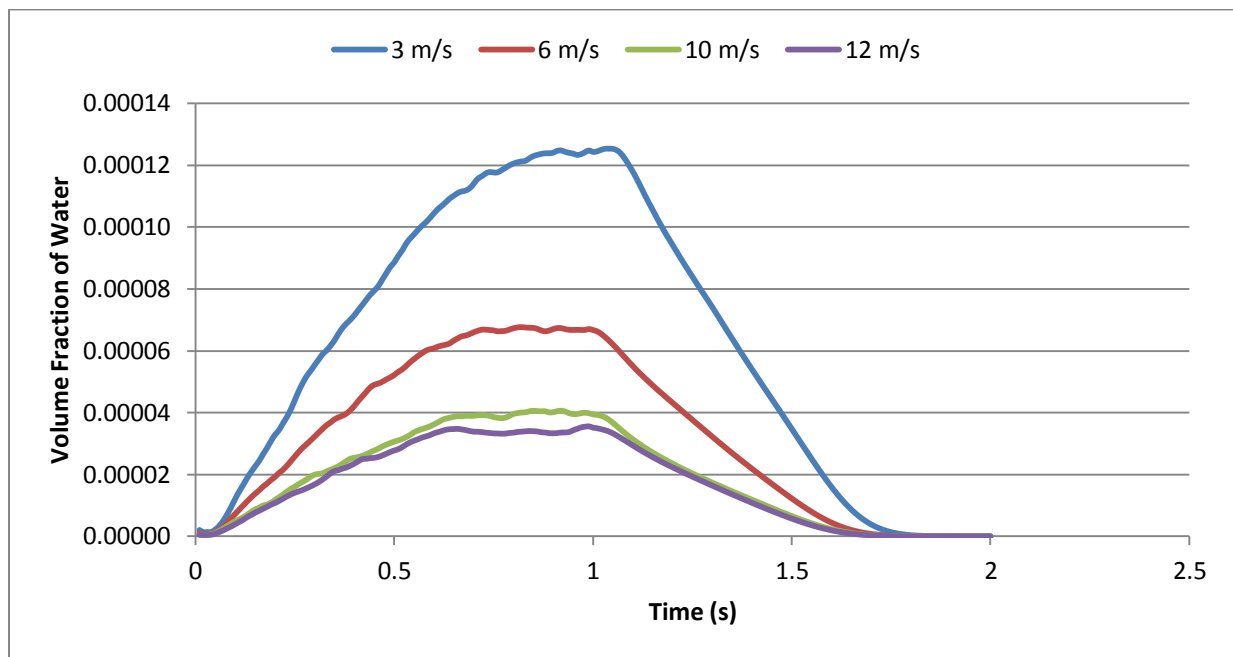


Figure 26 : Volume fraction of water in the channel under the different velocities

In addition to this, although there were so little water particles in the channel, almost all the water content in the channel surface removed at the end of the 2 seconds. According to analyses water stays in the channel for a long time at 3m/s, which leaves at 1.98 s, whereas for the air velocity of 12 m/s this time decreases to 1.88 s. As a result it can be said that low air inlet velocities causes the blockage of the GDL surface.

4.1.3 Effects of the Channel Dimension Alterations

The dimension and geometry of the flow channels have a significant role in terms of the performance of the fuel cells. Channel dimensions play an important role on the pressure drop. In this section, pressure drop in the channel and water amount in the GDL were investigated changing the width and height of the channel. The length of the channel was not changed during all tests. Furthermore, air inlet velocity and static contact angle of the GDL was kept constant as 10 m/s and 140° , respectively. The static contact angle of the other walls set as 45° . Tests were conducted using the following channel dimensions 0.2mmx0.2mmx1.5mm, 0.3mmx0.3mmx1.5mm, 0.5mmx0.5mmx1.5mm, 1mmx1mmx1.5mm. Figure 27 shows the water droplet behaviour at 0.1 s, as top view and side view. It can be seen here water droplet is faster in high size channels, so its speed increase while increasing the dimension of the channel. In other words, as seen in figure 28 and 30, water quits the highest size channel completely at 1.42 s, quicker than others.

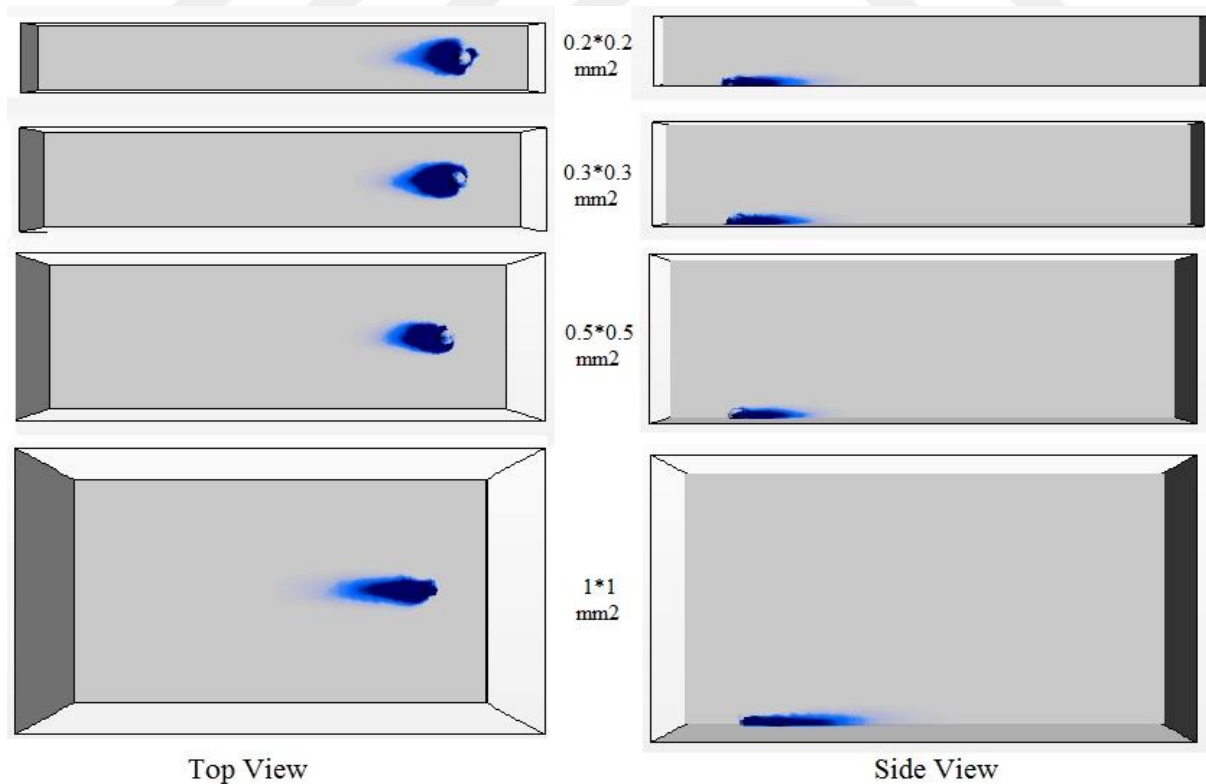


Figure 27 : The water droplet behaviour at 0.1 s in channels of different size.

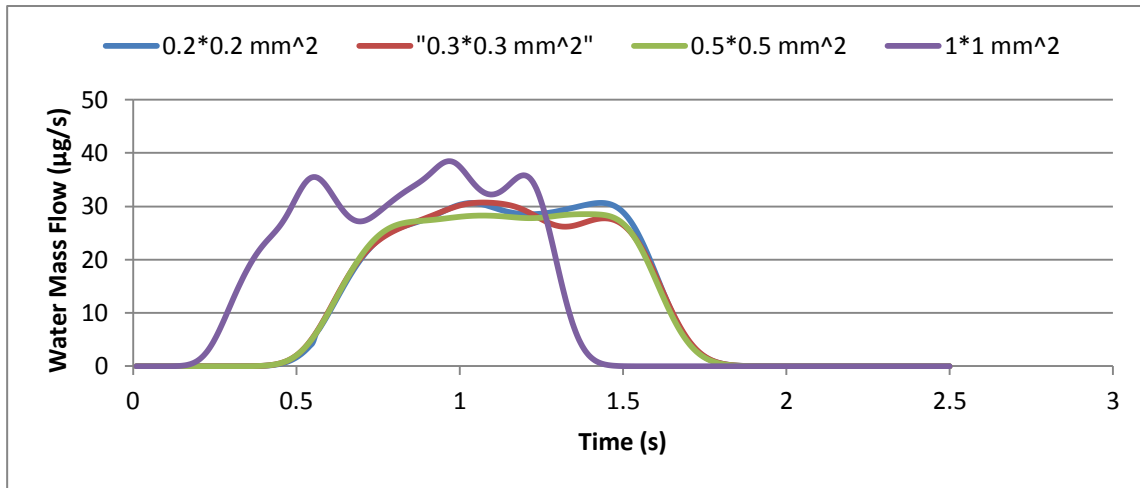


Figure 28 : Water mass flow at outlet

As mentioned above, pressure drop is an important parameter that depends on the dimension of the channels. When the distance between water droplet and channel walls is reduced, a strong shear stress and pressure gradient on the water droplet occur. This situation is forced into removing the droplet from the pore immediately so the droplet cannot grow in the small channels. Pressure variations in channels that have different dimensions can be seen in figure 29. For example, the greatest channel (1mmx1mmx1.5mm) has the minimum pressure drop values as about 128 *Pa* whereas the smallest channel (0.2mmx02mmx1.5mm) has the maximum value as approximately 1172 *Pa*.

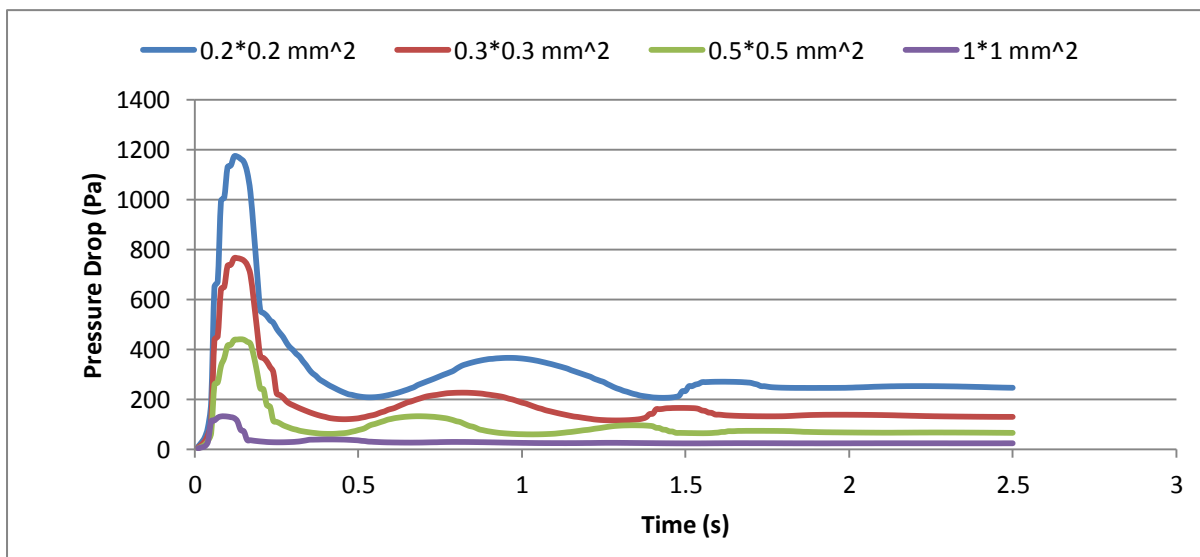


Figure 29 : Pressure Drop in different channels

When water coverage rate was examined in this section, it was seen that area covered by the water is smaller in larger channel. Inherently, larger channel provides more space for the water droplet to grow up as well as the air flow field is more uniform. In parallel with this fact volume fraction of water in the GDL increases by decreasing dimensions of the channel, as shown in figure 30. Average volume fraction was found that each volume fraction value was divided by the total surface area of GDL for each channel dimensions, so water volume fraction was calculated per unit area. It can be seen clearly in the figure 30 water is removed faster from the highest size channel than others. It seems clear that the larger the surface, the smaller the average volume fraction.

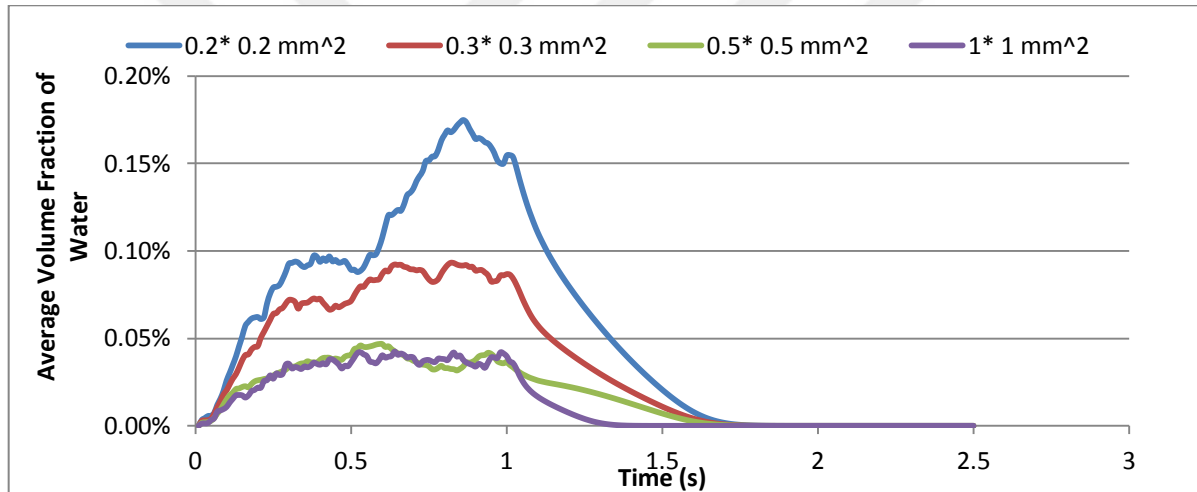


Figure 30 : Average Volume Fraction of Water on the GDL under different channel dimensions

4.1.4 Comparison of the Results for Straight Channel Model

In order to validate the model and compare the results a study [28] has been used. The researchers have investigated dynamic behaviour of liquid water droplet in the gas flow channel in terms of the different static contact angles and different air inlet velocities. Although different contact angles and water flow rate were used from each other in these studies, there is a similarity when comparing the present results to this study's results. For example, alterations of the water volume fraction versus static contact angle have the same trend in the both studies. It can be seen in figure 31.

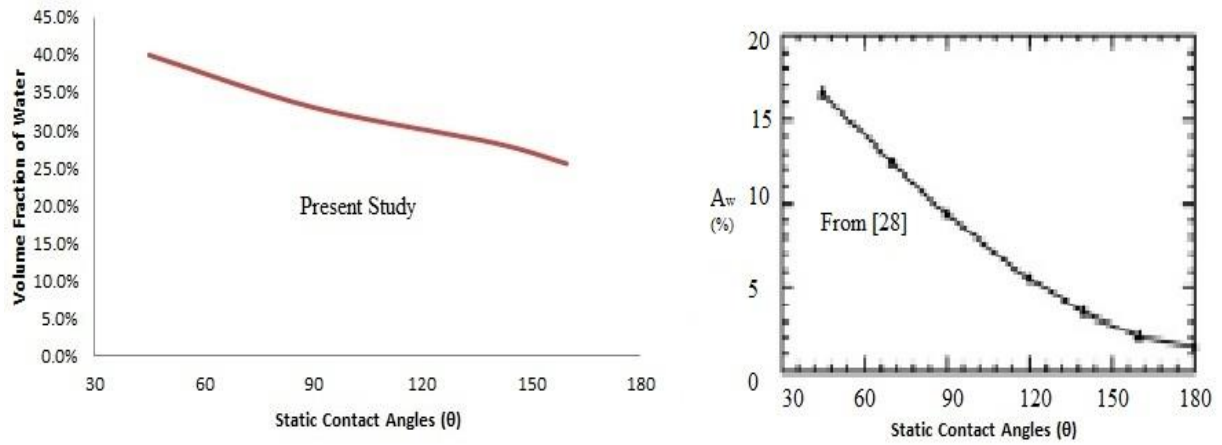


Figure 31: Comparison of contact angles versus volume fraction of water in the present study and in the work of [28]

In addition to this, effects of channel size on water behaviour were examined in [38] and they reached the result that water droplet can grow easily in the higher size channel, so their results also are similar with the present study. Moreover, when comparing the velocity effects on water content in the channel with [34], similar trend was obtained in the both study. Even though air inlet velocities and water injection rate are different from each other, the main finding is that increasing velocity reduces the water content in the channel, as can be seen in figure 32. In order to define average water content, volume fraction of water in the channel was observed for a time which is between water injects in the channel and leaves from the channel. Using this time history average water content was determined.

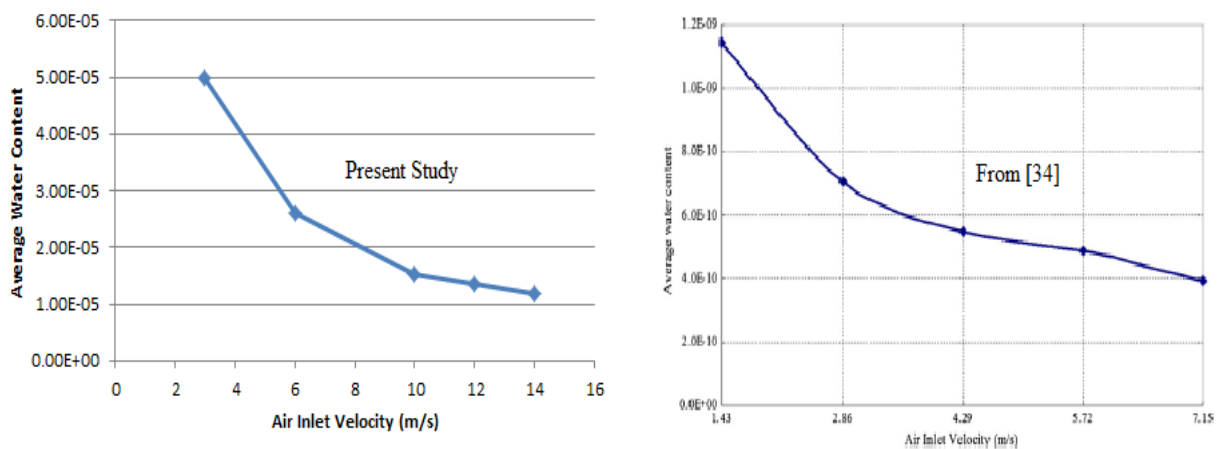


Figure 32 : Comparison air inlet velocity average water content in the present study and in the work of [28]

4.2 U- Shaped Sharp Corner Channel and Bended Channel

In this part of the study two u-shaped micro channels were used in order to obtain water behaviour in the channels. One of them has the sharp corner channel, while another has a bended corner; they are seen in figure 33 with the boundary of water inlet, air inlet and outlet. Channels length is 30 mm with round-trip, have 0.75 mm x0.75 mm cross section through all channel with a pore of radius $R=0.025\text{mm}$ at 2 mm away from the entrance of the channel in GDL surface.

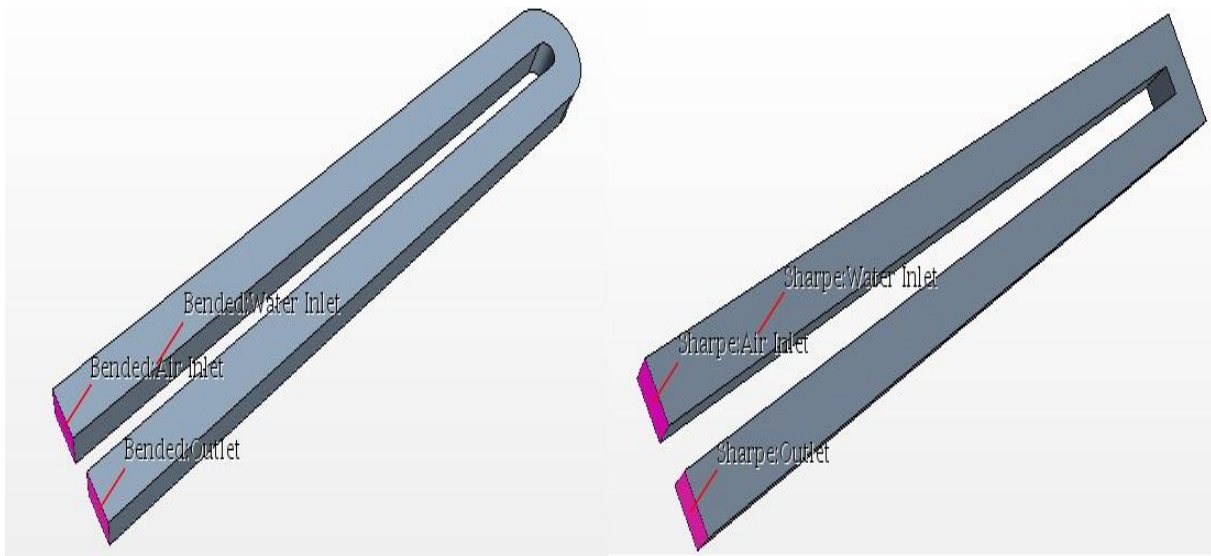


Figure 33 : U shape channels with the boundary conditions

4.2.1 The U- shape Domain Mesh

Because of the channel dimensions, when used the 9 micro meters for the base size for meshing operation, a huge number of cells required describing the domain and so it causes loss of time. In order to prevent this undesired situation and also obtain consistent results, different mesh sizes were used for the corner and water inlet from other boundaries. 9 micro meters base size was used for these two surfaces, whereas 0.1 mm was used for others, so approximately 650,000 cells were created. This difference and the computational domain mesh for the both shape is indicated in figure 34.

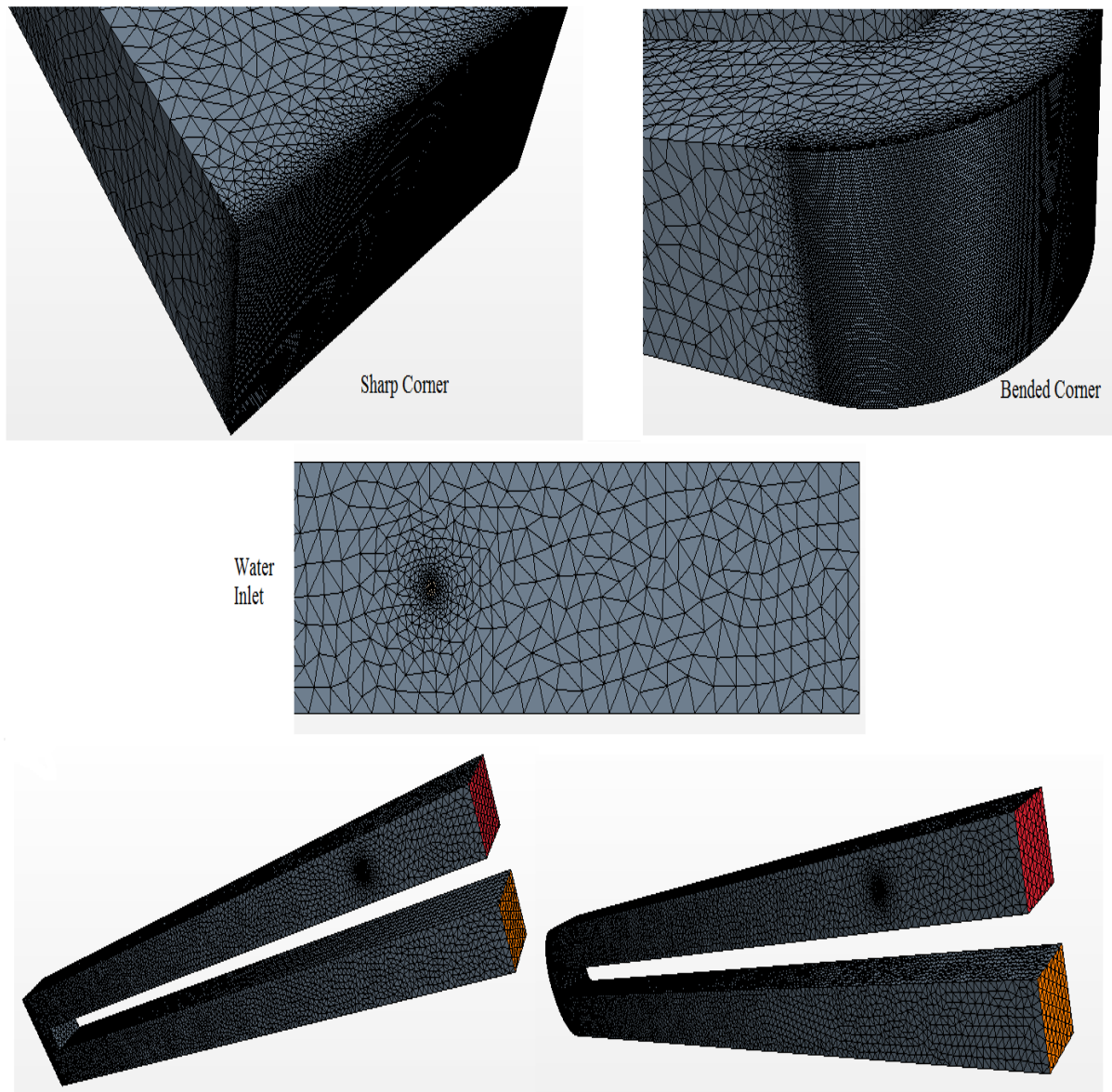


Figure 34 : The U-Shape computational domain mesh

4.2.2 Water Behaviour in Sharp Corner Channel and Bended Channel

Volume fraction of water, its behaviour and pressure drop were examined in the channels and on the gas diffusion layer. Tests were performed with STAR CCM+, water injection rate, surface tension value was the same as previous tests but air inlet velocity was set as 5 m/s and 45° was used for the static angle value to determine phase interaction for the walls. In addition, uniform air velocity field can be obtained after 0.2 seconds so after that time water injection was started and continued during 1 second.

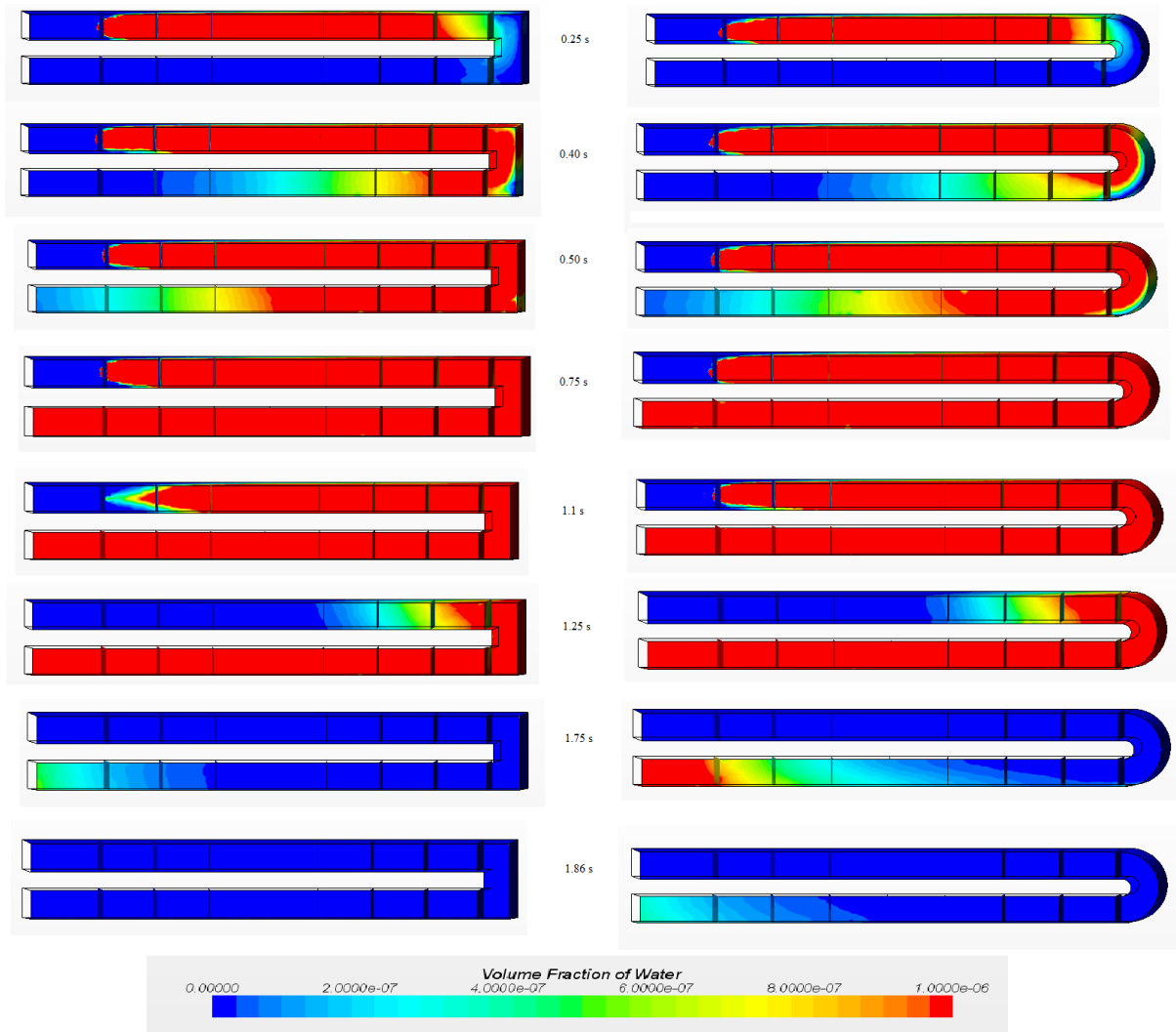


Figure 35 : Water distribution in two channels

Figure 35 shows the water distribution on gas diffusion layer with time in two different channels. As it can be seen here, until water arrive the corner of channel its distribution exhibited same behaviour for both channels. After the corner, water content moved slower in the bended channel than the sharp corner channel. The reason for this is that the bended corner keeps more water than sharp-cornered channel on its surface. It means that a large quantity of water is accumulated inside the bend area so most of the GDL was covered by the liquid water, as shown in figure 37. It causes to increase the blockage of the GDL layer by comparing the sharp corner channel. Figure 36 shows the average volume fraction in the bend area for both channel geometry.

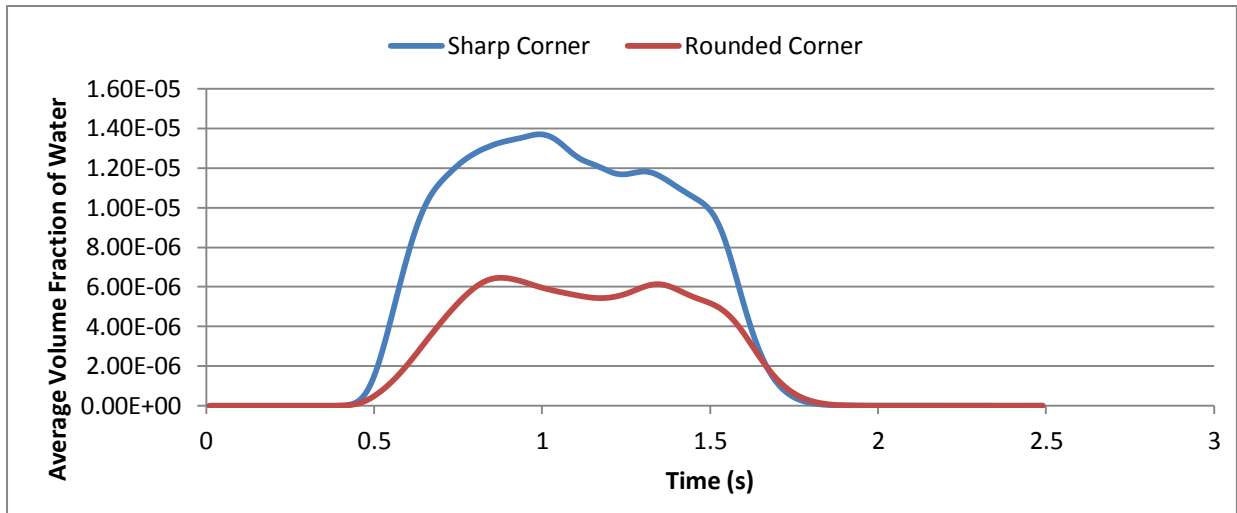


Figure 36 : Average Volume fraction of water in the bend of the channels

Furthermore, water leaves from the sharp corner channel at 1.86 seconds, while it leaves at 1.97 seconds from the bended corner channel completely. Because it was slower in the bended corner, the GDL was occupied by the water for a longer time. Another advantage of the sharp channel is that path of the water goes to upper surface of the channel under favour the edges, whereas water moves in the GDL in the bended channel. Figure 37 shows the path of the water at both corners.

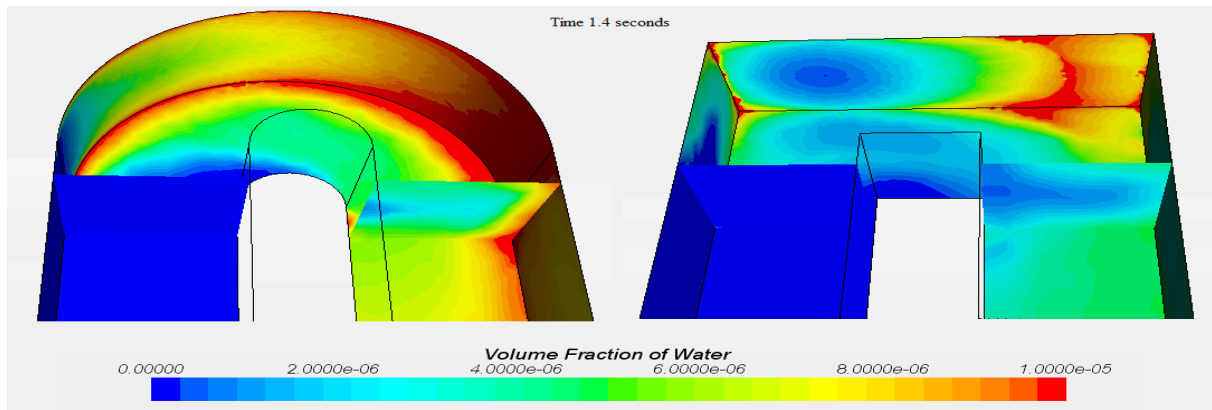


Figure 37 : Volume fraction of water on the corners at 1.4 s

Small quantities of water exist in the corners either sharp or bended channel but the amount of water is more in sharp corner channel than in the rounded case, as seen in the figure 38 and 36. These small quantities can be negligible when the water injects from one pore during 1 second, whereas in the real systems these small quantities may be a problem cause of the

continuing water injection into channel. Therefore, these phenomena must be taken a consideration when designing a gas flow channel.

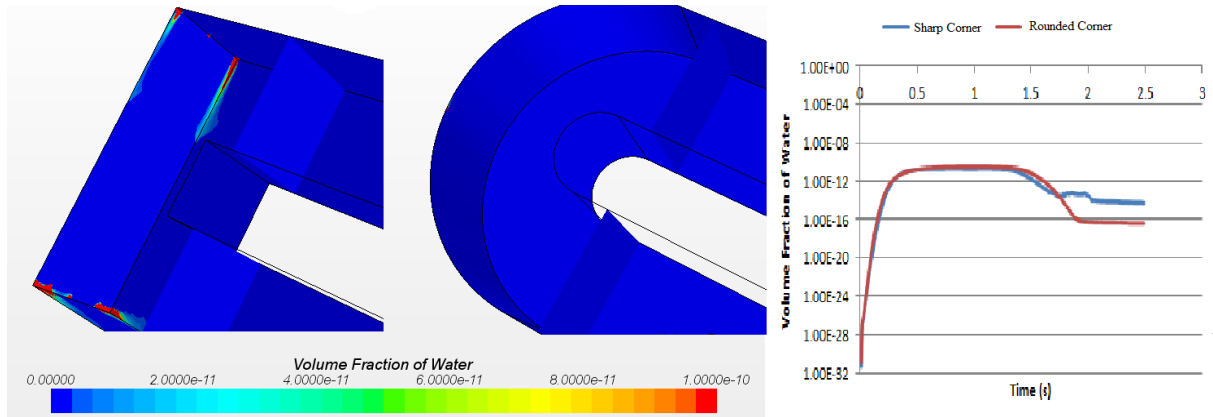


Figure 38 : Water content in the corner of the channels after 2 seconds

When observing of the pressure drop for the two channels, there is not any significant difference between each of them. Only beginning of the water injection starts, pressure drop for the sharp corner case is slightly higher than for the bended corner case.

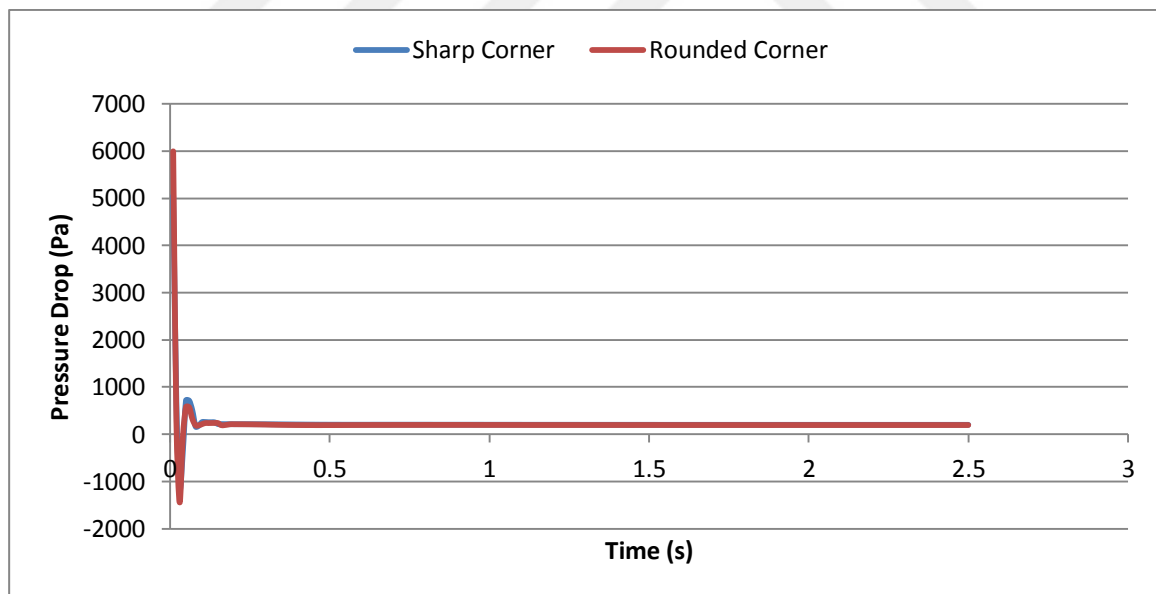


Figure 39 : Pressure drop in the sharp corner and bended corner channel

As a result, when designing a gas flow channel sharp corners may have some benefits for water management. As mentioned above, sharp corner channel provides paths for the liquid water to the upper surface. In this way, more usable GDL surface area can be obtained for reactant transport.

5. Conclusion

Some papers about PEM fuel cells and water management at the cathode side in PEMFCs have been reviewed in the first two sections of this report. Basic components of PEMFCs have been explained in the four stages in the literature review section. In the present study, different channel geometries have been used for the representation of gas flow channel in the PEMFCs in order to investigate and understand of water droplet dynamics on the gas diffusion layer. In order to explain these dynamics two phase flow has been analysed with the volume of fluid method. The model equations have been solved using STAR CCM+.

Firstly, straight gas flow channel has been modelled in STAR CCM+ software. Using different static contact angles, various air inlet velocities and various dimensions of the channel under the same water injection rate and constant surface tension, water behaviour has been investigated. Pressure drops in the channel, water volume fraction and water coverage ratio in the GDL has been observed.

Secondly, two u-shaped micro channels were analysed, including one with sharp corner and one with rounded corner. Pressure drop, water distribution in the channel were analysed as a function of channel geometry and especially, water accumulation at the channel bend were compared between the two geometries.

From the numerical results produced for different test cases, the following insights were obtained.

- Static contact angle is one of the main parameters controlling water droplet behaviours. The type of carbon cloth used in the real PEMFC systems specifies the contact angle. The surface of the gas diffusion layer is covered by water at all angles, but the wettability of the GDL increases for decreasing static contact angles.

- Air inlet velocity has considerable effects on water droplet dynamics. High velocities are helpful for removing water from GDL, as well as for water detachment, but cause pressure drop in the channel.
- Volume fraction of water was examined for channels of different dimensions, showing that the proportion of area covered by the water is smaller in larger channel. Inherently, larger channels provide more space for the water droplet to spread, and the air flow field is more uniform. In addition, the volume fraction of water in the GDL increases for decreasing dimensions of the channel.
- Sharp channel design for a gas flow channel is better than rounded corners. Water accumulation on GDL surface of the rounded corner channels is more than sharp corners, so this situation makes difficult transportation of reactants compared to sharp corner channels.

This project have specifically investigated the dynamics of water droplets in the air flow channel on the cathode side of a PEMFC and analyse the effect of different channel geometries on the accumulation and removal of water from the GDL surface by means of numerical simulation methods. The results of the numerical simulations have been discussed. All in all, water management is one of the most important parameters for the PEMFCs in terms of the increasing the efficiency of the system. So, it needs more investigation to understand what happening in a PEMFC clearly.

For the future works, water behaviours can be investigated in the u-shaped models under different air velocities or different static contact angles. Different cross section models can be used for the channels such as trapezoid, concave or semi-circle to analyse. Furthermore, double cross section model can be performed for investigation of water droplet dynamics. Lastly, the surface roughness model can be used to understand effect of the static contact angles; it can provide a closer approximation to the random nature of the gas diffusion layer.

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