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Multiphase Flow in Hydrogen Generation

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Abstract

This study examined the laminar-multiphase characteristics in hydrogen production processes by utilizing the simulation software, "COMSOL 5.3 multiphysics simulation software". The study's objective enhanced the evaluation of the multiphase flow operations involved in hydrogen generation, and determined the key contributors to the multiphase flow in the production of hydrogen. The methodology of the study also involved the design and simulation of the multiphase flow operations involved in hydrogen production and showed the analysis of the flow properties, including pressure profile, velocity profile, concentration profile, and shear rate profile, thereby insights into the multiphase flow interactions. Additionally, the research results enabled an improved understanding of the multiphase flow interactions in hydrogen production and led to an improvement in the process operational conditions for the system. The inference of the study was based on the quantifiable results obtained from the simulation which provided a comprehensive analysis of the multiphase flow characteristics in hydrogen production. More importantly, the shear stress for water-hydrogen system and hydrogen were shown with the shear rate describing the gradient in velocity and the pressure profile, shear rate profile, and velocity profile were calculated for a 2D profile versus the arc length for each of these variables. Thereafter, the results of this research simulation demonstrated that high velocity profile for hydrogen flow was observed within the reactor; with the highest velocity observed in the reactor within the length of (0.5 – 6.5)m, hence indicating optimum length of the water-split reactor for maximum velocity flow. The results further indicated that the profile of water-hydrogen and hydrogen pressure becomes uniform at a distance of 1mm from the entrance and the maximum pressure flow for water-hydrogen and hydrogen fluids pressure are 17.8Pa and 238.27Pa which shows a sufficiently higher pressure of hydrogen.

Keywords: multiphase flow, hydrogen production, pressure profile, velocity profile, flow interaction

1. Introduction

Energy is a crucial component of global energy improvement. Hydrogen is an energy carrier that is expected to play a significant role in the world's future energy systems as it addresses the challenges global warming that are related to the use of fossil fuels and are caused by man-made carbon dioxide (CO2) emissions (Zarghami, Deen, & Vreman, 2020). Hydrogen generation is usually accompanied by several processes, and "multiphase flow during hydrogen production" is one crucial phenomenon that occurs in the value chain of large-scale hydrogen production even based on the fact that at the point of usage, it only emits water.

More importantly, using hydrogen as a source of energy is projected playing a significant part in energy systems of the future because hydrogen is largely gaining high utilization and acceptability across various industries, specifically in the renewable energy sector and the power sector, where it might be blended with CO emissions or natural gas to synthetize syngas. These processes and interactions during hydrogen production gives rise to multiphase flow. The high acceptance of hydrogen can be attributed to the rise in energy prices brought on by the dwindling oil supplies, production, and reserves, as well as concerns over climate change and global warming brought on by human emissions of CO_2 (Zarghami et al., 2020) linked to the usage of fossil fuels (McGlade, 2012).

In addition to this, hydrogen energy used by various sectors is rapidly growing and therefore based on the vast industries that are utilizing hydrogen, and with the available large-scale consumption across multiple sectors (transport sector, low-carbon transportation using fuel-cell electric vehicles, as well as buildings and the power sector, where it might be coupled with natural gas or CO2 emissions to create syngas, which gives rise to multiphase flow), large scale hydrogen production is the most critical way to make hydrogen available for large scale industries. However, hydrogen production on a large scale involves multiphase flow interactions, even when using the water electrolysis method, which is a well-established technique that produces hydrogen in one of the simplest ways possible with the benefit of being exceptionally pure (> 99.9%).

Therefore, based on this, multiphase flow plays a critical role in hydrogen production because, for hydrogen production, the Alkaline electrolyzers work by transferring hydroxide ions (OH-) from the cathode to the anode through the electrolyte, where the cathode produces hydrogen bubbles and the anode produces oxygen bubbles (Norby & Luo, 2004). Research has further shown that the hydrodynamic properties of the gas-liquid flow in each cell play an important role in how well an alkaline-water electrolyzer functions. Local turbulence, which bubbles are known to produce, is known to be particularly effective at mixing and distributing species locally. However, as the bubbles rise, the electrolyte flow close to the electrode likewise picks up speed, signaling the convective movement of species that are electrochemically active. It is obvious that the efficiency of an electrolysis cell can be significantly impacted by the two-phase flow's hydrodynamic behavior, which stresses the importance of multiphase flow in the creation of hydrogen.

An essential operation parameter affecting the performance of the cell in multiphase flow in hydrogen production is bubble coverage, or the percentage of the electrode surface covered by adherent bubbles. As a matter of fact, when bubbles cling to an electrode surface, they insulate a portion of the surface, rendering it inactive in the electrochemical reaction, increasing the current density and surface overpotential at the portion of the surface that is bubble-free if the total current is kept constant (Norby et al., 2004). For a better understanding of the mechanism and to improve the efficiency of an electrochemical cell, which is essential for producing hydrogen, additional research into bubble dynamics, phase interactions, and gas hold-up is required. Due to the high gas percentage in electrochemical cells, research has also concentrated on employing computational fluid dynamics to explore complex multiphase flow (Li, Yang, Yu, Mo, Li, Xie*, et al.*, 2021).This is because optical approaches are unable to capture many important aspects of the multiphase flow field. The confirmation of CFD results (such is the width of a cell's gas hold-up and the volume proportion of hydrogen) with analogous experimental data, despite the abundance of intriguing CFD research accessible in the literature, is surprisingly uncommon.

There isn't agreement on the best and most appropriate way to simulate the flow of gas and liquid in an electrolyzer as a result. In this way, a key criterion for the model's accuracy and dependability is its capacity to anticipate the width of the hydrogen bubbles curtain, a crucial aspect of the flow. The goals in the study paper (Li, *et al.*, 2021). included developing a CFD model to predict multiphase flow in an alkaline-water electrolysis cell and contrasting the output with experimental data. The width of the bubble curtain in a cell and the gas fraction were the subjects of particularly detailed research. To determine how each parameter would affect the flow pattern, the effects of drag and turbulent dispersion forces acting on the bubbles were examined.

More particular, numerical results were compared to experimental data to confirm his modeling technique. Investigations into the impact of interphase forces on the CFD model's accuracy and stability as well as the outcomes of simulations were also conducted (Yang, Zhao & Ye, 2005) The package known as ANSYS Fluent 19.1 is used to simulate the multiphase flow in the creation of hydrogen, and most research has shown and assumed that the flow is Newtonian, viscous, incompressible, and isothermal since the physical characteristics of the phases remain constant. Additionally, experimental data was utilized for validation when designing the CFD model performed by (Yang et al., 2005.) Compartments for cathodic and anodic ions made up the two compartments of the experimental setup, which were divided by a diaphragm. Ten electrode pairs installed in the electrolyser's upper section were used to develop the gases. The specific governing equations for the forces of drag, turbulence dispersion, buoyancy, and bubble size were examined. Accordingly, the study's flow visualizations have demonstrated that bubble coalescence only takes place in the area around the electrodes, and that it mostly occurs among bubbles that haven't yet disengaged from the surface. The relevance of this phenomena is known to be constrained by electrolyte solutions' high ionic strength, which is a gauge of the overall concentration of ions in solution. For instance, it has been seen that a considerable proportion of bubbles keep their original modest size and do not merge. As a result, the phenomena are extremely rare, and we think that bubble coalescence and break-up do not occur (Li, et al., 2019). According to the study's findings, there are no appreciable differences between the outcomes of the chosen strategy and those of a strategy with multiple computational domains, each of which contains an electrode with a length equal to the sum of all the active electrodes taken into account.

The parameter, h, reflects the height along the electrode's 40 cm height in the simulation, but h also represents the distance from the lowest active electrode's bottom to the highest active electrode's top in the experiment, where the experimental gas fraction was measured. The slip velocity of bubbles, which controls the transfer of momentum between phases, is one of the significant elements influencing the behavior of multiphase flows. According to the research findings, the pace of the electrochemical reaction is inversely correlated with the current density, thus as the current density grows, so does the rate of gas production, which raises the vacuum fraction percentage at the cathode surface. Increases in current density leads to increases in gas volume fraction because the turbulent dispersion force is proportional to the gas volume percentage. fraction to increase, which in turn causes the gas layer to expand and the bubbles to migrate away from the electrode (Li, et al., 2019).

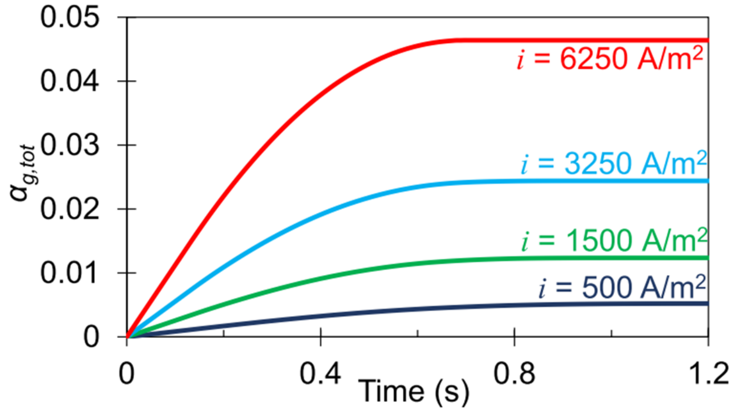

Figure. 1. Effect of current density on total volume fraction of gas in the electrolyzer

The hydrodynamics of the multiphase flow in electrolyzers must therefore be understood in order to make a precise gas volume fraction prediction distribution. Additionally, by factoring in the impacts of the two most significant inter-phase forces, drag and turbulent dispersion forces, the hydrodynamics of gas-liquid flow in an electrolyser may be predicted and validated. In conclusion, it is crucial to consider the turbulence dispersion force when modelling the gas-liquid flow in an electrolyser.

2. Objective of Study

The examination of the generation of hydrogen using a multiphase flow falls under the purview of this research project. The investigation within the multiphase flow characteristics of the production of hydrogen is the primary goal. To achieve this objective of an effective analysis for Multiphase Flow during hydrogen generation process, this research project will utilize the "COMSOL 5.3 simulation software" for the investigation of multiphase flow characteristics of hydrogen production. The developed approach is a methodology for design, simulation, and analysis of the multiphase flow operations in hydrogen production by calculating and producing results that bridges the research gap through the analysis of the flow properties through pressure profile, velocity profile, concentration profile, and shear rate profile, as well as indication of the iteration profile by optimizing process operating conditions. Furthermore, this project work also determines the main contributors to Multiphase Flow in Hydrogen Production and in the process improve the system of Multiphase flow interactions during hydrogen production. The significant aspect of this research exercise is summarized as follows:

a. Modeling of the multiphase hydrogen production utilizing Computation Fluid Dynamics Software, COMSOL 5.3 to improve previous design by researchers.

b. Recent developments in Multiphase flow of Hydrogen production process utilized diverse designs, however, research has consistently shown that there are still many challenges involved the analysis of velocity profile, concentration profile, and pressure profile for a fully constructed mesh with different fluid properties such as density and dynamic viscosity assigned to both water and hydrogen.

c. Designing and development of Iteration profiles for the flow simulation task, illustrating the error profile in relation to the iteration count. To calculate the pressure profile, shear rate profile, and velocity profile for a 2D profile versus the arc length for each of these variables.

3. Literature Review

Multiple applications in the areas of multiphase flow of hydrogen production has been one of the most vital researches in the area. Specifically, the project research by (Li, et al., 2021) focused on the investigation of utilizing two-phase flow phenomena and bubble dynamics to create efficient mass transportation for hydrogen production. This is due to the fact that during the water electrolysis process, a significant amount of gas bubbles will be produced. As a result, inefficient removal of bubbles in the liquid/gas diffusion layer (LGDL) may result in pore blockage and catalyst layer coverage phenomena, which will obstruct liquid water being moved from flow fields to a catalyst layer. and reduce the number of reaction sites and the efficiency of the hydrogen production process (Li, et al., 2021). To comprehensively assess the influence of various operational parameters on multiphase flow in hydrogen production, such as current density and liquid flow rates, several considerations must be taken into account. In their research, (Li, et al.,2021) specifically concentrated on Proton Exchange Membrane Electrolyzer Cells (PEMECs), which have garnered substantial attention over the past decade.

Moreover, the operational mechanism of PEMECs closely resembles that of PEM fuel cells. During the process of water electrolysis, water is introduced to the anode, where it undergoes dissociation, resulting in the formation of gas bubbles, protons, and electrons. The protons traverse the catalyst-coated membrane and reach the porous cathode electrode, where they recombine with electrons to generate hydrogen gas. Subsequently, this hydrogen gas is transported through the liquid gas diffusion layer (LGDL) and flow field towards the cell's outlet. Throughout this procedure, the anode is susceptible to water blockage due to gas accumulation. As water serves as the reactant in an electrolysis cell, it is crucial to ensure its efficient delivery to the active reaction sites within the anode. The presence of by-product oxygen gas can hinder this delivery process if it becomes trapped within the electrode's pores or microchannels. All of these processes vividly demonstrate the complex interactions of multiphase flow during the hydrogen production process. In particular, investigations have been conducted into the dynamics of bubbles in electrolyzers and other electrochemical devices.

(Yang et al., 2005) explored the behavior of CO2 gas bubbles within the anode of a Direct Methanol Fuel Cell (DMFC) and determined that current density, flow velocity, and temperature significantly impact bubble dynamics and cell performance. Likewise, Mo et al. delved into the mechanism behind bubble generation within a PEMEC and ascertained those bubbles exclusively formed at the juncture between the catalyst layer and the liquid gas diffusion layer. This underscores the critical role of a triple-phase boundary in facilitating the electrochemical reaction. To further underscore the significance of multiphase flow in hydrogen production, Li et al. conducted a study on how wettability impacts bubble dynamics and performance in a PEMEC featuring a Ti thin film LGDL. Their findings revealed that wettability had a limited effect on activation and transport over-potential but had a substantial influence on bubble dynamics within a current density range of 0 to 2 A/cm² (Li, et al., 2019). In a related vein, (Selamet et al., 2011) explored two-phase flow and the evolution of gas bubbles within a PEMEC using neutron imaging and a high-resolution camera.

Their investigation unveiled that gravity and buoyancy forces exerted a significant impact on water distribution across the cell, with areas near the anode inlet containing more water (Selamet et al., 2011). Additionally, Dedigama et al. focused on phenomena within a single-channel PEMEC, concluding that bubble diameter increased as flow velocity decreased and potential increased (Majasan, et al., 2018). Selamet et al.'s work was dedicated to examining two-phase flow and bubble dynamics on the anode side of a transparent PEMEC, employing a microscale and high-speed visualization system. This research visualized and discussed various two-phase flow patterns under diverse operating conditions, marking the first time an in-situ investigation of the ultra-fast and micro-scale oxygen bubble detachment process in a PEMEC was conducted. This work significantly advanced the comprehension of bubble detachment and two-phase flow mechanisms in PEMECs, holding promise for enhancing cell performance and efficiency, ultimately contributing to the realm of multiphase interactions in hydrogen generation. In summary, this research centered on comprehending two-phase flow and bubble dynamics across a spectrum of operating conditions. The outcomes provided an extensive understanding of how different operating conditions, particularly current densities of 0.04, 0.2, and 1 A/cm², impact the system.

Furthermore, the research highlighted the pivotal role of the relationship between current density and voltage in PEMEC performance, where lower voltage at a given current density indicated superior performance. At higher current densities, the analysis indicated that increased bubble generation led to higher gas volume fractions in the flow channel, and smaller bubbles were more prone to coalesce into larger ones. Consequently, the bubbly flow within the channel transitioned into slug flow as current density increased, thereby influencing multiphase flow in the hydrogen production process (Selamet et al., 2011). Moreover, different flow velocities could induce changes in two-phase flow patterns. Slug flow phenomena could also manifest at very low flow velocities due to the sluggish movement of gas bubbles leading to their accumulation and eventual formation of slug flow. In general, alterations in the shape, size, and flow patterns of gas bubbles correlated with increasing current density within a single channel. At very low current density (0.04 A/cm²), numerous small, spherical gas bubbles emerged from various locations on the Ti felt surface and channel edge. Two distinct bubble detachment processes were observed:

some detached with the incoming flow, while others were more resistant and merged with adjacent bubbles before detaching at significantly larger diameters (Garcia-Navarro, Schulze, Friedrich, 2019)

As the current density increases, more gas is produced and as the bubbles depart and coalesce with newly formed bubbles along the channel, transition to the slug flow pattern begins, and continual bubble coalescence leads to several slugs occupying sections of the microchannel. In two-phase flow, flow and bubble dynamics changed significantly alongside an increasing anode water flow velocity. The slug flow forms more easily at a low flow velocity. At the relatively low flow velocity of 33 mm/s, bubbles needed more time to detach from the surface and flow to the outlet (Kobayashi, et al., 2014). This can be attributed to the small drag force and large surface tension force (Li, et al., 2019); bubbles had sufficient time to merge with one another at very low flow velocities.

Bubble flow then became dominant alongside an increase in flow velocity (Li, et al., 2018). The two-phase flow patterns in PEMECs is mainly determined by the gas volume fraction. The higher the amount of gas compared to the liquid phase mass flow rate, the easier to form slug or even annular flows in the flow channels. The two-phase flow behavior in the PEMECs are also be impacted by the gas generation rates due to operating current densities and the local pore morphologies of transport layers (Lafmejani, Olesen & Kær, 2017; Larimi, et al., 2019). Summarily the research showed that, the impact of different flow velocities on bubble detachment diameter indicates a certain impact on detachment time. An increase in flow velocity may to some extent have increased bubble detachment frequency during the bubble detachment process. However, it had a small impact on bubble detachment diameter, the increased of the flow velocity from 33 to 67 m/s decreased the bubble detachment diameter from about 170 to 150μm. This can be attributed to the large flow drag force, which can decrease bubble detachment diameter, playing a dominant role during the bubble's invasion behavior during hydrogen production process. In relation to multiphase flow of hydrogen production, the earliest model of PEMWE was proposed by (Onda, et, al., 2022).

They proposed a 2D, non-isothermal PEMFWE model and pointed out that the exothermic heat from overpotentials is almost balanced by the endothermic heat due to entropy change and evaporation. However, their model had extensive simplifications in the thermophysical phenomena of PEMWEs. The results by this research showed that the temperature range of 313K to 353K is optimal and the high-current performance of PEMWE is deteriorated by increasing cathode pressure during hydrogen production process. However, their model did not consider the multiphase flow which yet has a significant effect on PEMWE performance, especially under high current density (Kemppainen et al., 2016) proposed a 2D nanoscale PEMWE model that incorporated the hydrogen evolution reaction on the platinum nanoparticle electrode and the transport of both gaseous and dissolved H_2. They found that increasing the gas volume fraction makes the H_2 surface concentration nonlinearly changes with the current density. Although this study conducted a detailed theoretical description of multiphase flow in PEMWE, the model was 1D without consideration of species transport in the in-plane and flow direction. A 2D computational study was proposed by (Chen, et al., 2020) to investigate the effect of the porous media thickness on liquid saturation and local current density. They found the 100μm thick, porous transport layer shows less than 0.01 liquid saturation at the catalyst-diffusion interface. (Kemppainen et al., 2016) developed a 3D multiphase PEMWE model to analyze the power efficiency of a laboratory-scale PEMWE. However, their model simplified the water transport phenomenon by neglecting the capillary flow in the porous media.

(Qian, Kim, & Jung, 2022) presented a two-phase, 3D model of PEMWE. They studied the effect of the electrolysis temperature and flow direction on the electrolysis performance by treating the two-phase flow in a porous media as a binary diffusion. However, it is known that the two-phase flow is dominated by capillary pressure in a porous media. Summarily the study by (Qian et al., 2022), aimed to model the proton exchange membrane water electrolyzer (PEMWE) process, which is used to produce hydrogen. The research used multiphase and multidimensional modeling to study the fluid dynamics, thermal behavior, and electrochemical performance of PEMWEs. The main insights of the study were that the multiphase, multidimensional modeling approach provides valuable insights into the behavior of PEMWEs, including the flow and mixing of hydrogen and water, heat transfer, and electrolysis reaction kinetics. The study also identified potential research gaps, such as the need for further investigation of the complex interaction between the different phases in PEMWEs and the development of more advanced modelling tools to accurately predict their performance (Qian et al., 2022). Overall, the study highlights the importance of multiphase, multidimensional modeling in understanding the behaviour of PEMWEs and highlights areas for future research to improve the efficiency and performance of hydrogen production processes. Key findings of the study includes that multiphase, multidimensional modeling approach provides valuable insights into the behavior of proton exchange membrane water electrolyzers (PEMWEs). Additionally, the model developed was able to capture the fluid dynamics, thermal behavior, and electrochemical performance of PEMWEs. The model showed the importance of the multiphase flow and mixing of hydrogen and water in PEMWEs.

Furthermore, it also demonstrated the potential of multiphase, multidimensional modelling in improving the understanding of the behavior, efficiency and performance of hydrogen production processes. Although the research was excellent, the research gaps includes that; The study identified a need for further investigation of the complex interaction between the hydrogen and water phases in PEMWEs. In addition to this, the study highlights the need for the development of more advanced modeling tools to accurately predict the performance of PEMWEs, and also suggests a need to further study the multiphase flow behavior of hydrogen and the electrolysis reaction kinetics in PEMWEs. Interestingly, future areas of research includes improving the understanding of the complex interaction between the hydrogen and water phases in PEMWEs, the development of more advanced modeling tools to accurately predict the performance of PEMWEs and a further study of multiphase flow behavior in PEMWEs since the research approach in the study was multiphase, multidimensional modeling, which was used to analyze the behavior of PEMWEs and gain a better understanding of the complex processes involved in hydrogen production (Qian et al., 2022). The study of Hydrogen generation and utilization in a two-phase flow membraneless microfluidic electrolyzer-fuel cell tandem operation for micropower application by (De, et al., 2022), presents some key findings.

The research demonstrates the feasibility of using a two-phase flow membraneless microfluidic electrolyzer-fuel cell tandem system for simultaneous hydrogen generation and power production. The system operates by electrolyzing water into hydrogen and oxygen in the electrolyzer and using hydrogen as fuel and oxygen as oxidant in the fuel cell. The results of the experiments specified that the system has a high conversion efficiency, with a high hydrogen production rate and a high fuel cell performance. The system shows low resistance and high fuel utilization. Additionally, the authors examine the impact of different operating conditions, such as flow rate and current density, on the performance of the system. The results show that the system is capable of producing hydrogen and generating power under different operating conditions. In alignment with the research gaps the authors acknowledge the need for further research to improve the performance, efficiency, cost-effectiveness, scalability, and reliability of the system. They suggest exploring the integration of the system with renewable energy sources to increase sustainability. Additionally, future research could focus on improving the performance and efficiency of the system, exploring alternative materials for the electrodes and catalysts, and developing a low-cost, scalable, and reliable system for hydrogen production and utilization. In conclusion, the study provides evidence of the feasibility of using a two-phase flow membraneless microfluidic electrolyzer-fuel cell tandem system for hydrogen generation and utilization. However, the authors also highlight the need for further research to address the current limitations and improve the system's performance and efficiency (De et al., 2022)

4. Methodology

4.1 Brief Overview of Multiphase Flow

Multiphase flow systems have been the subject of numerous prior research. For instance, (Baker & Tabor, 2010) presented a method for identifying a random packed bed arrangement that is identical to a packed bed. The pressure drop of packed bed vertical flow in multiphase hydrogen production has also been studied by (Pope, Naterer & Wang, 2011) with very small particles, such as microscale diameters, the number of particles within a packed bed is very high, which restricts the use of CFD simulation to packing materials with relatively large diameters, (Pope et, al., 2011). Additionally, in multiphase flow, the fluid travels in very complicated and irregular flow patterns through a packed bed and other process equipment. Due of this, it is challenging to obtain exact solutions and accurate fluid flow representations. The irregularity of the packing material results in highly varied flow routes and significant variations in local and average velocities, which makes the radial fluid velocity important (Atmakidis & Kenig, 2009). The experimental correlation created by (Ergun, 1952) or other similar correlations are typically used to forecast the pressure decrease across a packed bed. Similar methods are employed by the majority of Ergun equation extensions; however, some research also include additional parameters in the course of the hydrogen production involving multiphase flow. However, the Multiphase Hydrogen Production through simulation is the main emphasis of this study. The fluid properties in the areas of pressure profile, velocity profile, concentration profile, and shear rate profile, as well as an indicator of the iteration profile of the simulation process, would be taken into consideration during the simulation using COMSOL 5.3 multiphase simulation.

4.2 Modelling Technique (COMSOL): Multiphase Flow of Hydrogen Production

COMSOL Multiphysics is an all-inclusive simulation software environment with a structured interface that is simple to utilize (Griesmer, 2023). The proposed modelling technique using COMSOL is aimed at simulating the multiphase flow of hydrogen production. This method involves the use of a multiphysics software tool called COMSOL Multiphysics, which is designed for modeling and simulating physical systems involving multiple physical phenomena. The proposed modelling technique using COMSOL involves creating a computational model that can simulate the multiphase flow of hydrogen production which will be based on the fundamental principles of fluid mechanics. Overall, the proposed modelling technique using COMSOL for the multiphase flow of hydrogen production has the potential to provide valuable insights into the behavior of the system and help to improve the efficiency and effectiveness of the hydrogen production process.

4.3 Process Design for Simulation of Multiphase Flow in Hydrogen Production

The simulation approach is the research work's suggested methodology. As was previously said, this effort would adopt the modeling of the multiphase hydrogen production utilizing Computation Fluid Dynamics Software, COMSOL 5.3. Simulation is done in order to replicate or anticipate a real-time process. Normal water-split electrolysis processes would result in typical flow parameters. Water molecules, which split into hydrogen and other molecules throughout the reaction, would be the principal constituents under concern. The materials chosen in the simulation environment are Water and Hydrogen when using the design interface seen in figure 1. For laminar flow, the Multiphysics system is taken into account while considering the movement of diluted species. “Laminar flow” is chosen because there are no eddies and no back mixing in the fluid, which makes the fluid's properties-such as concentration, pressure, and velocity-reliable at this regime. For the water system and hydrogen system at distinct transport layers, a mesh system is created. However, computation of the fluid configuration is done to achieve the multiphase flow properties such as velocity profile, concentration profile, and pressure profile for a fully constructed mesh with different fluid properties such as density and dynamic viscosity assigned to both water and hydrogen, respectively. Iteration profiles are also created for the flow simulation task, illustrating the error profile in relation to the iteration count. In order to calculate the pressure profile, shear rate profile, and velocity profile for a 2D profile versus the arc length for each of these variables, the flow properties are thus further evaluated.

4.4 Technical Gaps Observed for Multiphase Flow in Hydrogen Production

As a justification of the research work, the summary of the observed technical gaps includes the following;

1) Complex interaction between different phases: The various literatures identified a need for further investigation of the complex interaction between the hydrogen and water phases in the water electrolysis process involved in hydrogen production.

2) Multiphase flow behavior: The various research suggests a need to further study the multiphase flow behavior of hydrogen and water in PEMWEs and also a need for further research into the electrolysis reaction kinetics in PEMWEs.

3) Built Mesh for Flow Layers: While advanced meshing algorithms have been developed to handle the complex geometries and flow patterns associated with multiphase flows, there is still a need for further research in this area. For example, it would be valuable to investigate the use of more sophisticated mesh generation techniques, such as adaptive meshing, to improve the accuracy and efficiency of multiphase flow modeling.

4) Concentration Profile: The development of accurate concentration profiles remains a key challenge in multiphase flow modeling. While noteworthy progress has been made in this part, there is still a need for further research to understand the impact of factors such as solubility, diffusion, and convection on the mixing and distribution of the different components in the flow.

5) Pressure Profile: The pressure profile in multiphase flows is influenced by a range of factors, including viscosity, density, and flow rate, as well as the effect of turbulence. Despite significant progress in understanding these factors, there is still a need for further research to improve the accuracy and reliability of pressure profile predictions.

6) Velocity Profile: The velocity profile in multiphase flows is critical for understanding the flow behavior and for predicting potential flow patterns and regions of turbulence. While significant progress has been made in this area, there is still a need for further research to improve the accuracy and reliability of velocity profile predictions. For example, research could focus on developing new methods for modeling the impact of flow rate, pressure gradient, and turbulence intensity on velocity profiles, or on improving the accuracy of velocity profile predictions in complex geometries.

Specifically, these research gaps represent areas where further investigation and development is needed to improve our understanding of multiphase flow in hydrogen production systems. By addressing these gaps, there will be a substantial advancement in the field of multiphase flow as it relates to hydrogen production and there will be the availability of valuable insights into improving hydrogen production systems.

4.5 COMSOL Modeling – Multiphase Flow of Hydrogen Production

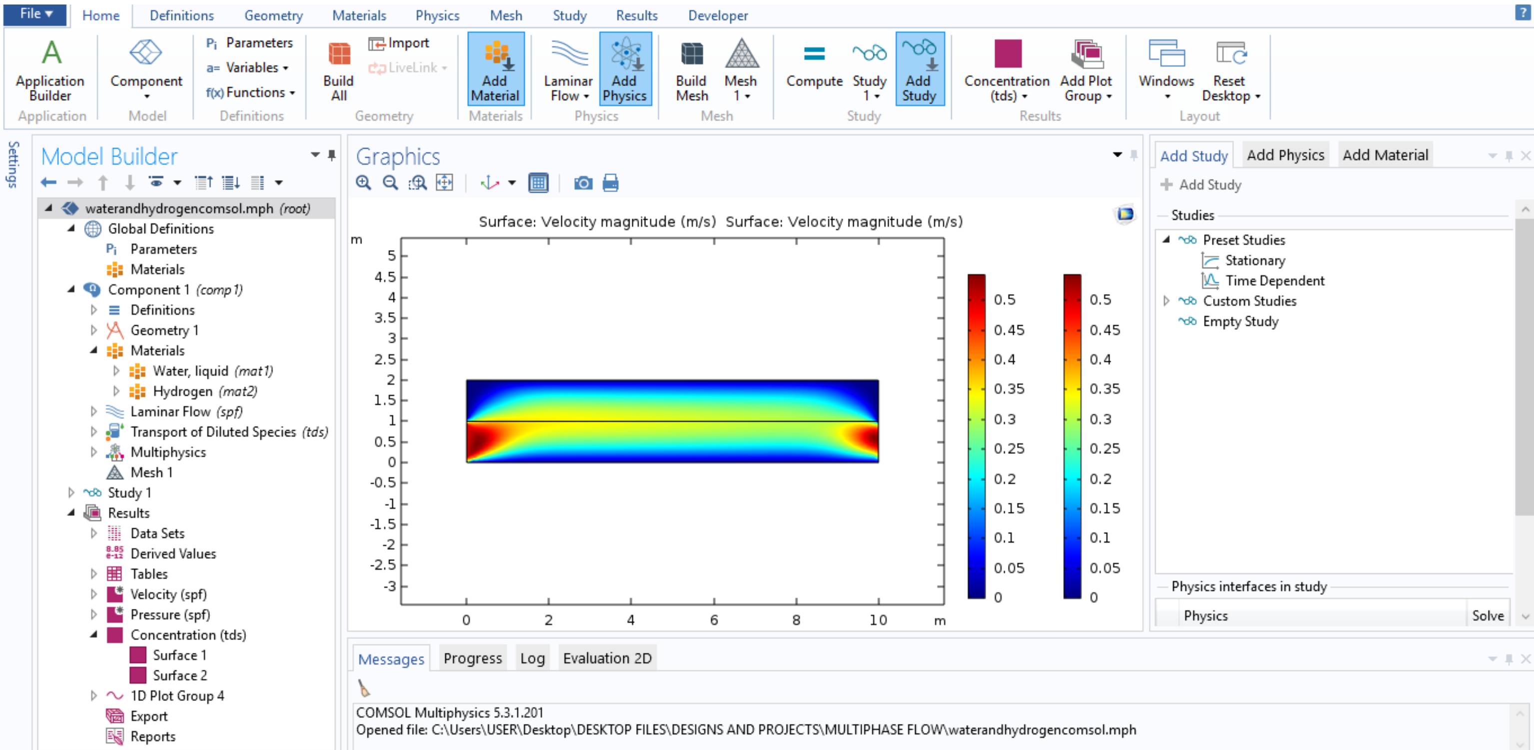

Figure 2. COMSOL design interface for multiphase hydrogen production

4.6 Expected Results for Modeling Multiphase Flow in Hydrogen Production

Multiphase flow modeling in hydrogen production systems is a multifaceted and stimulating task that requires a deep understanding of both the underlying physics and the numerical methods used to simulate such flows. In this section, we will examine the expected results of multiphase flow modeling in hydrogen production, with a focus on the key variables and profiles that must be considered to achieve accurate and reliable results. In order to accurately predict and analyze multiphase flow in hydrogen production, it is important to consider several key variables, including;

a. Built mesh for flow layers.

b. Concentration profile

c. Pressure profile

d. Velocity profile

e. Iteration profile, showing the convergent iteration number.

f. 2D analysis of pressure profile, shear rate profile and velocity profile against the arc length.

a. **Built Mesh for Flow Layers:** The first step in multiphase flow modeling is the construction of an appropriate mesh that represents the flow layers in the hydrogen production system. This mesh must be carefully designed to accurately capture the distribution and flow patterns of the different phases involved, taking into account factors such as porosity, permeability, and flow rate. The mesh would be constructed using advanced meshing algorithms that can handle the complex geometries and flow patterns associated with multiphase flows. This is in addition to the fact that the simulation results would reflect the expected flow behavior in the real-world system.

b. **Concentration Profile:** The concentration profile is an important factor to consider when modeling multiphase flow in hydrogen production. This profile provides information about the distribution of the different components in the flow and helps to predict how these components will interact and mix with each other. In order to accurately represent the concentration profile, it is necessary to consider factors such as solubility, diffusion, and convection as well as the effect of turbulence on mixing.

c. **Pressure Profile:** The pressure profile is another key factor to consider when modeling multiphase flow in hydrogen production. This profile provides information about the pressure distribution throughout the flow, and can help to predict how pressure changes will impact the flow behavior. In order to accurately represent the pressure profile, we will consider factors such as viscosity, density, and flow rate as well as the effect of turbulence on pressure distribution.

d. **Velocity Profile:** The velocity profile is an important factor to consider when modeling multiphase flow in hydrogen production, as it provides information about the flow velocity throughout the flow. This profile can help to predict how changes in velocity will impact the flow behavior and can also help to identify potential flow patterns and regions of turbulence. In order to accurately represent the velocity profile, it is necessary to consider factors such as flow rate, pressure gradient, and turbulence intensity.

e. **Iteration Profile:** The iteration profile is an important aspect of modeling multiphase flow in hydrogen production, as it provides information about the number of iterations required for the simulation to converge. This profile is important for ensuring that the simulation results are accurate and can also help to identify potential issues or areas for improvement. In order to accurately represent the iteration profile, it is necessary to consider factors such as the numerical method used, the convergence criteria, and the stability of the simulation.

f. **2D Analysis of Pressure Profile, Shear Rate Profile, and Velocity Profile against the Arc length:** Finally, a 2D analysis of the pressure profile, shear rate profile, and velocity profile against the arc length is a valuable tool for understanding the flow behavior in hydrogen production systems. This analysis can help to identify regions of high or low pressure, shear rate, or velocity, and can also help to predict how these factors will impact the flow behavior. To perform this analysis accurately, it is necessary to consider factors such as the spatial distribution of the flow, the flow rate, and the turbulence intensity. Therefore, multiphase flow modeling in hydrogen production systems is a complex and challenging task that requires a deep understanding of both the underlying physics and the numerical methods used to simulate such flows. By carefully considering the key variables and profiles discussed above, it is possible to achieve accurate and reliable results that provide valuable insights into the behavior of hydrogen production systems.

5. Method Analysis

The simulation approach is the research work's suggested methodology. As was previously said, this effort would adopt the modeling of the multiphase hydrogen production utilizing Computation Fluid Dynamics Software, COMSOL 5.3. Simulation is done in order to replicate or anticipate a real-time process. Normal water-split electrolysis processes would result in typical flow parameters. Water molecules, which split into hydrogen and other molecules throughout the reaction, would be the principal constituents under concern. The materials chosen in the simulation environment are Water and Hydrogen when using the design interface seen in figure 1. For laminar flow, the Multiphysics system is taken into account while considering the movement of diluted species. Laminar flow is chosen because there are no eddies and no back mixing in the fluid, which makes the fluid's properties—such as concentration, pressure, and velocity—reliable at this regime. For the water system and hydrogen system at distinct transport layers, a mesh system is created. However, computation of the fluid configuration is done to achieve the multiphase flow properties such as velocity profile, concentration profile, and pressure profile for a fully constructed mesh with different fluid properties such as density and dynamic viscosity assigned to both water and hydrogen, respectively. Iteration profiles are also created for the flow simulation task, illustrating the error profile in relation to the iteration count. In order to calculate the pressure profile, shear rate profile, and velocity profile for a 2D profile versus the arc length for each of these variables, the flow properties are further evaluated.

6. Results and Discussion

The overall results of this research progressively tackled the technical gaps. In this regard, figure 2 shows the entire CFD fluid domain that includes the hydrogen, represented in the rectangular shape at the top and the water, represented in the rectangular shape at the bottom. Specifically, Fig 3 gives a well-detailed 3D Plots of the Surface: Concentration (mol/m3) and surface: Velocity Magnitude (m/s) of the hydrogen production process. This 3D plot of the concentration and velocity magnitude is fully developed by utilizing the COMSOL Multiphysics simulation tool. This figure shows that the concentration of hydrogen increases adjacent to the membrane reactor because of the increase in reaction rate and the production rate of hydrogen that is continuous. As observed following the certain length in the reactor, the concentration of the hydrogen is reduced in the reaction side due to the fact that the diffusivity of hydrogen is high through the permeable membrane. Figures 5 and 6 are the multiphase diagrams representing the fluid domains for the water-hydrogen system, without mesh and with built mesh, respectively. The former represents the fluid domain where the water and hydrogen in the fluid flow independently. However, the latter represents the fluid domain where the water and hydrogen co-exists in the fluid flow dynamics. Here, the simulation study covers the multiphase fluid flow properties for the water-hydrogen co-existence and multiphase fluid flow properties for the independent hydrogen flow. Fig 3 and 4 also gives a similar analysis of the 3D Plots of the Surface: Concentration (mol/m3) and surface: Velocity Magnitude (m/s) and Mesh for Hydrogen Flow with Arrow Line: Velocity Field showing grid mesh, with specific focus on Mesh for Hydrogen Flow, which is highlighted in a green net-mesh colouration.

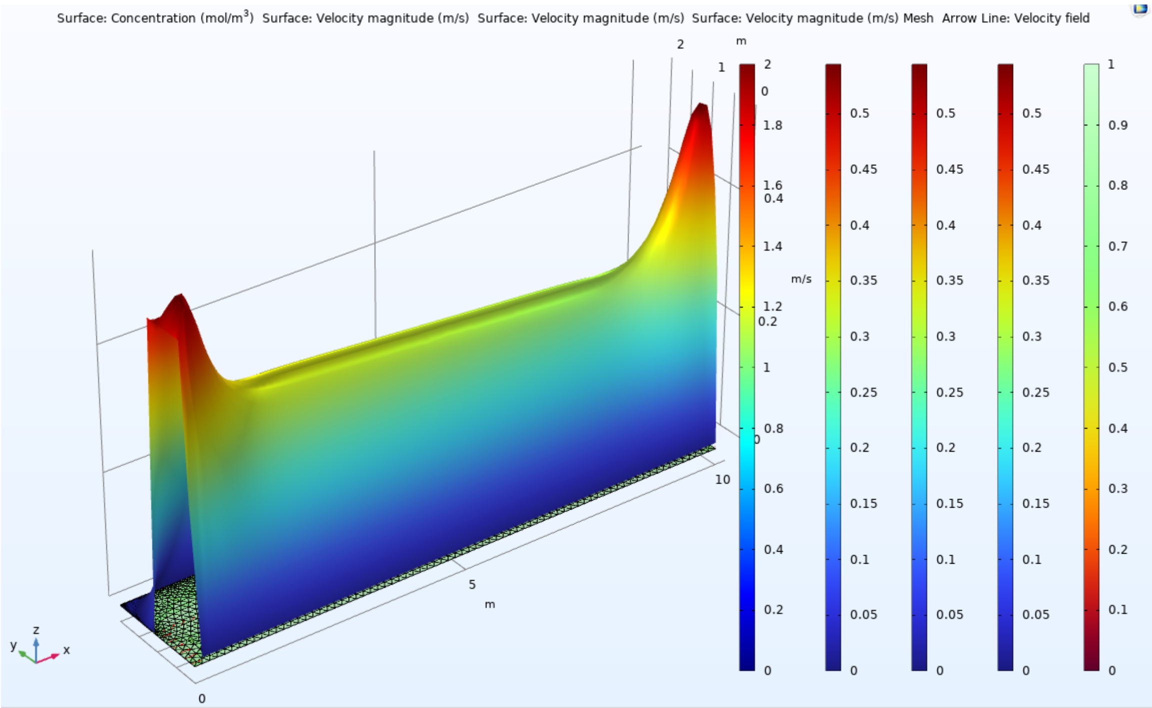

Figure 3. 3D Plots of the surface: Concentration (mol/m^3) and surface: Velocity magnitude (m/s)

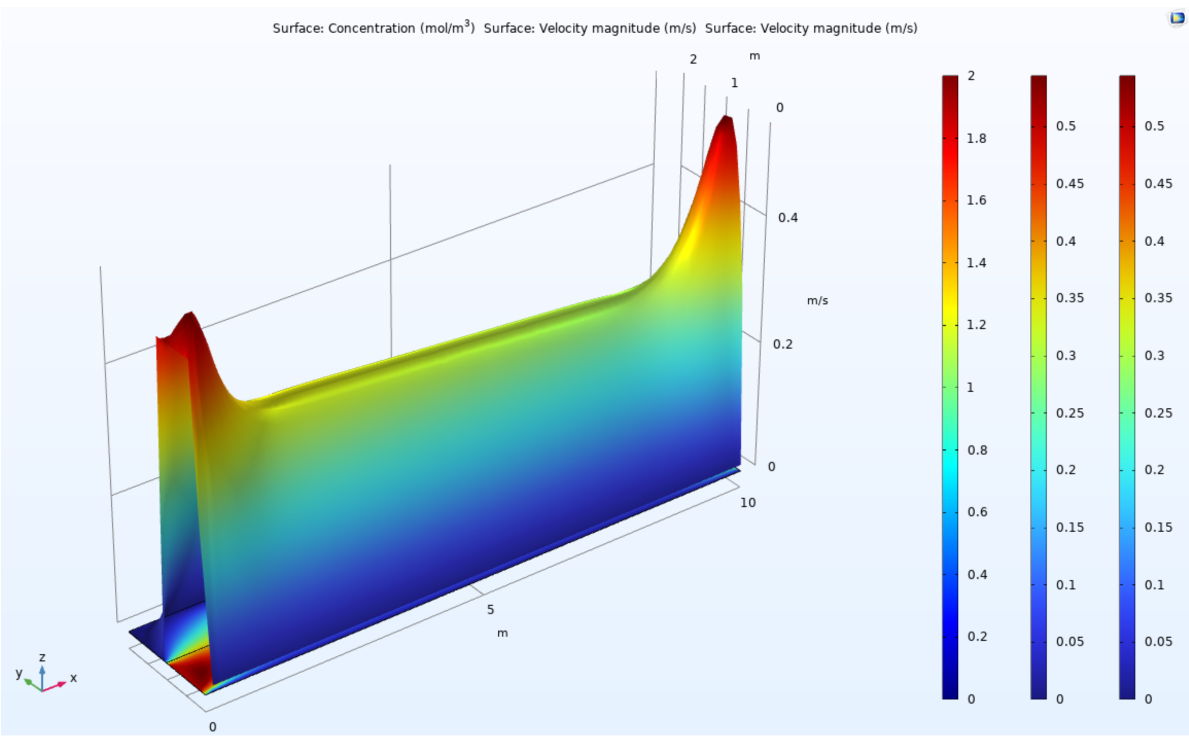

Figure 4. 3D plots of the surface: Concentration (mol/m^3) and surface: Velocity magnitude (m/s) and mesh for hydrogen flow with arrow line: Velocity field showing grid mesh

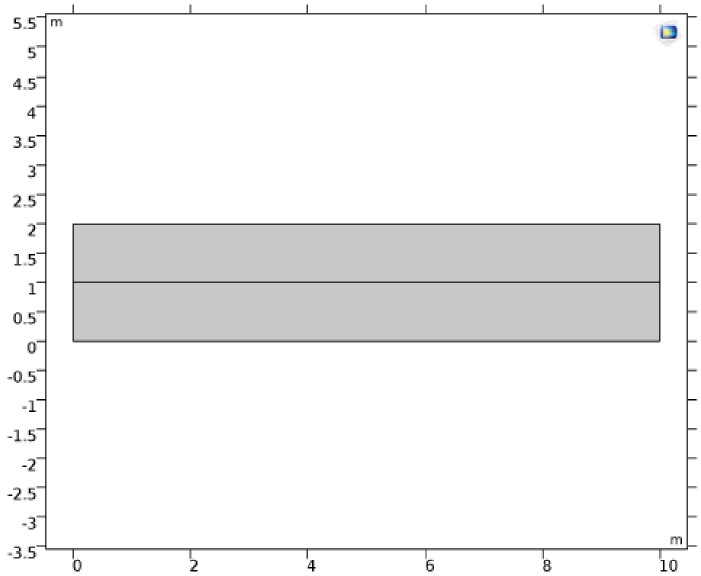

Figure 5. CFD fluid domain for water- hydrogen system without mesh

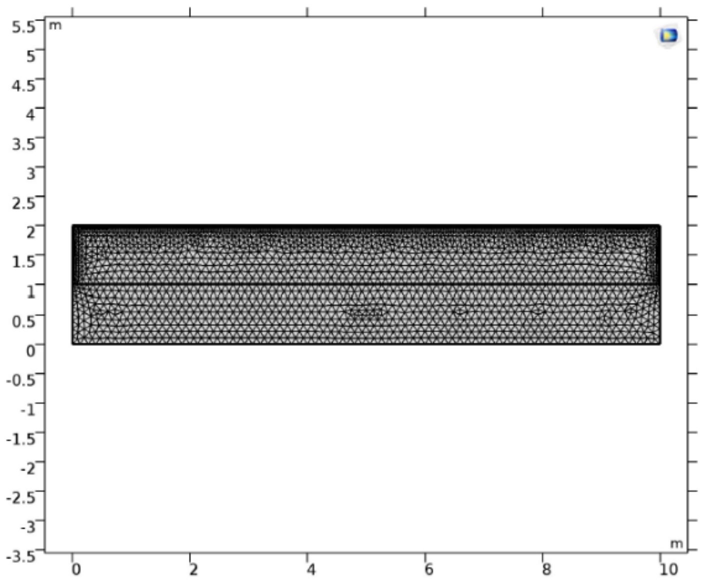

Figure 6. Built mesh for water- hydrogen

Furthermore, figures 5 and 6 provide a visual representation of the fluid domains for the water-hydrogen system, with and without a built mesh, respectively. The diagrams illustrate the differences between the fluid domains when considering the co-existence of water and hydrogen versus independent hydrogen flow. In Figure 5, the fluid domain without a built mesh represents the flow of water and hydrogen independently, where each phase flows separately. The simulation study covers the multiphase fluid flow properties for the independent hydrogen flow. This includes properties such as pressure, velocity, and concentration profiles, which can be used to analyze the behavior of the system and identify areas where improvements can be made. In contrast, Figure 6 represents the fluid domain with a built mesh, where the water and hydrogen co-exist in the fluid flow dynamics. In this case, the simulation study covers the multiphase fluid flow properties for the water-hydrogen co-existence. One advantage of using a built mesh for multiphase flow simulations is that it allows for a more accurate representation of the fluid behavior, particularly in complex geometries. The mesh discretizes the fluid domain into smaller cells or elements, which can be used to solve the governing equations of the system. This allows for a more detailed analysis of the behavior of the system and can provide more accurate results than simulations without a mesh. Hydrogen is the main product of water-split process. The scatter surface for the velocity magnitude water-hydrogen system is given in Fig 7. Higher velocity magnitudes of water-hydrogen system is observed at the inlet and outlet points, and are far away from the reactor wall. However, high velocity profile for hydrogen flow is observed within the reactor; with the highest velocity observed in the reactor within the length of 0.5 m – 6.5 m, hence indicating optimum length of the water-split reactor for maximum velocity flow. Also, these point of maximum velocity profile indicates decrease in velocity profile as the water- hydrogen fluid system transverses the reactor, and uniform fluid velocity flow is observed from 6.5 m to the exit.

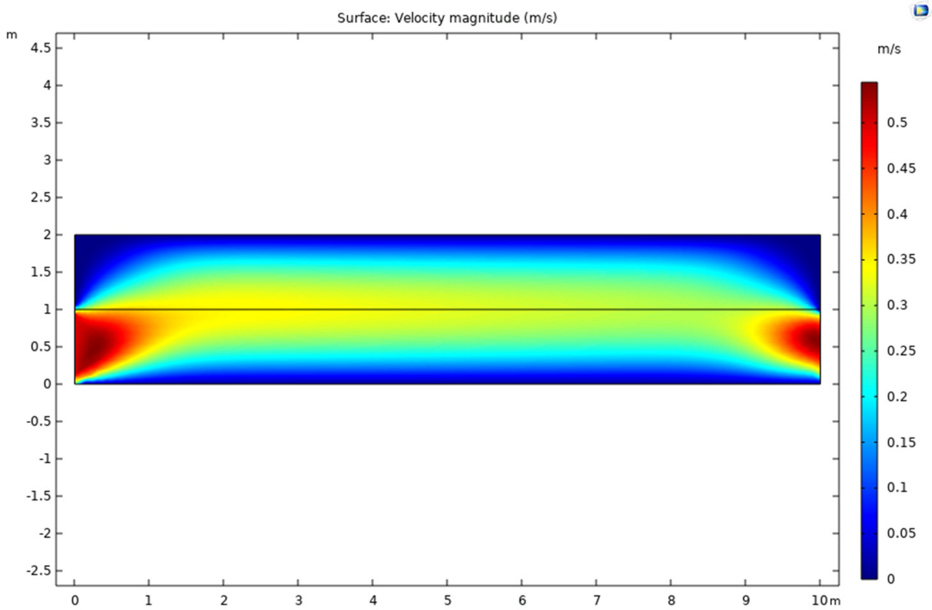

Figure 7. Scatter surface for velocity magnitude water- hydrogen system

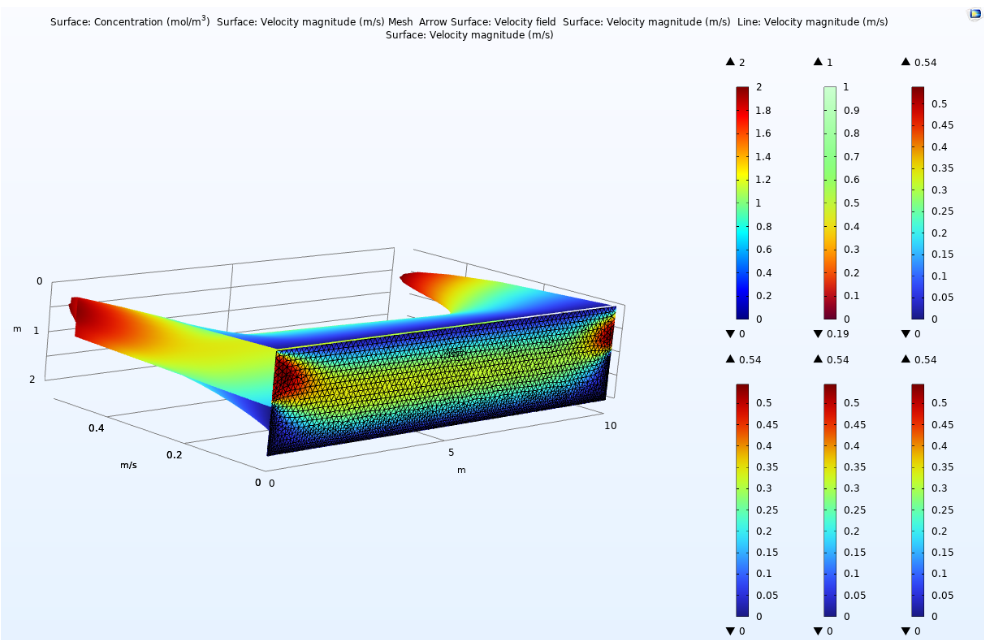

Figure 8. 3D plots of the surface: Concentration (mol/m^3), velocity magnitude (m/s) mesh; arrow surface: Velocity field surface: Velocity magnitude (m/s), line: Velocity magnitude (m/s)

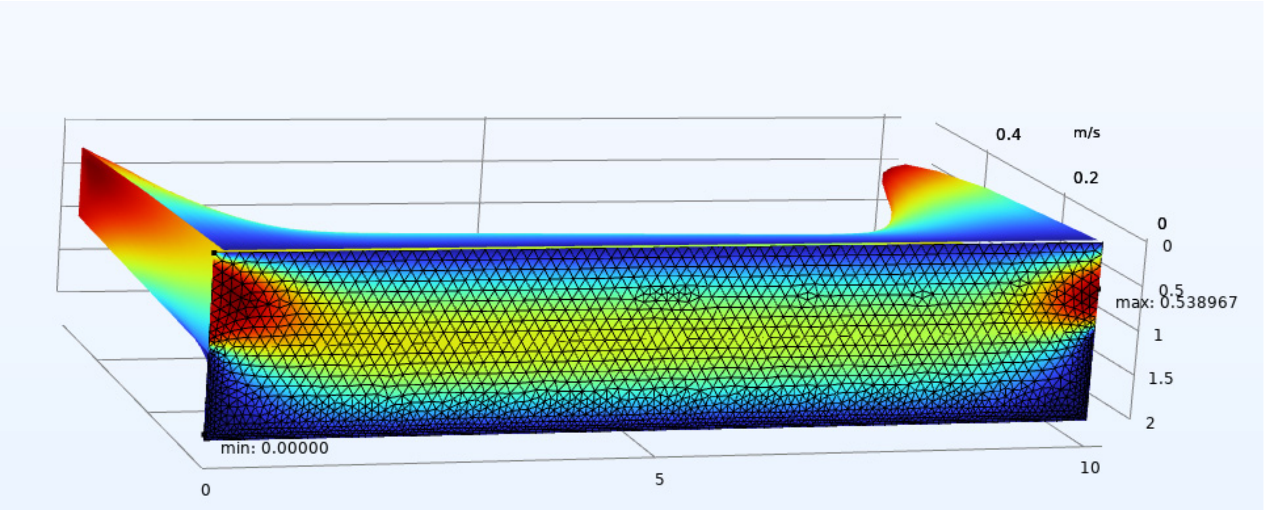

Figure 9. Backend view of the mesh of the 3D plots of the surface: Concentration (mol/m^3), velocity magnitude (m/s) mesh; arrow surface: Velocity field surface: Velocity magnitude (m/s), line: Velocity magnitude (m/s)

The 3D plot showing the backend view of the mesh of the concentration and velocity magnitude in mol/m3 and m/s, respectively, is a crucial component of the simulation study of the multiphase fluid flow properties for the water-hydrogen system. The mesh of the 3D plots provides a detailed view of the system's geometry, enabling a more comprehensive analysis of the behavior of the system.

The concentration plot shows the distribution of the hydrogen and water molecules in the fluid domain, providing insights into the behavior of the system and how the hydrogen production process can be optimized. The velocity magnitude plot, on the other hand, displays the fluid flow dynamics, providing information on the speed and direction of the fluid flow. The arrow surface in the velocity field surface plot provides a visual representation of the fluid flow direction and magnitude, while the line on the velocity magnitude plot displays the variation in the fluid flow velocity along a specific line or path.

The backend view of the mesh in the 3D plots provides additional insights into the geometry of the system and how the fluid flow is affected by the presence of different components in the fluid domain. This information is crucial for the accurate simulation of fluid flow behavior and optimizing the hydrogen production process. Overall, the 3D plots with backend view mesh provide a comprehensive visualization of the fluid flow behavior and concentration distribution in the water-hydrogen system. By analyzing the concentration and velocity magnitude plots and the arrow and line surfaces, we can gain insights into the behavior of the system and optimize the hydrogen production process for maximum efficiency and sustainability.

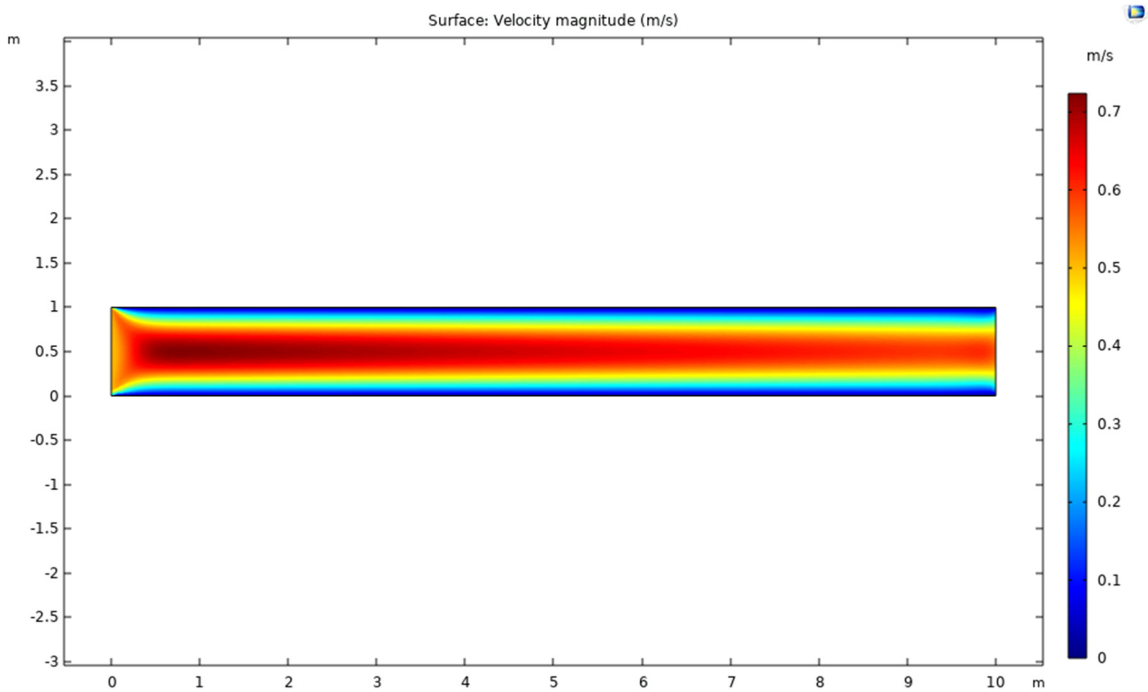

Figure 10. Scatter surface for velocity magnitude hydrogen

The contour plots of water-hydrogen system and hydrogen fluid flow pressure are given in figures 11 and 12, respectively. The profile of water-hydrogen and hydrogen pressure becomes uniform at a distance of 1 mm from the entrance. However, the maximum pressure flow for water-hydrogen and hydrogen fluids pressure are 17.8 Pa and 238.27Pa. This reveals that sufficiently higher pressure of hydrogen is observed.

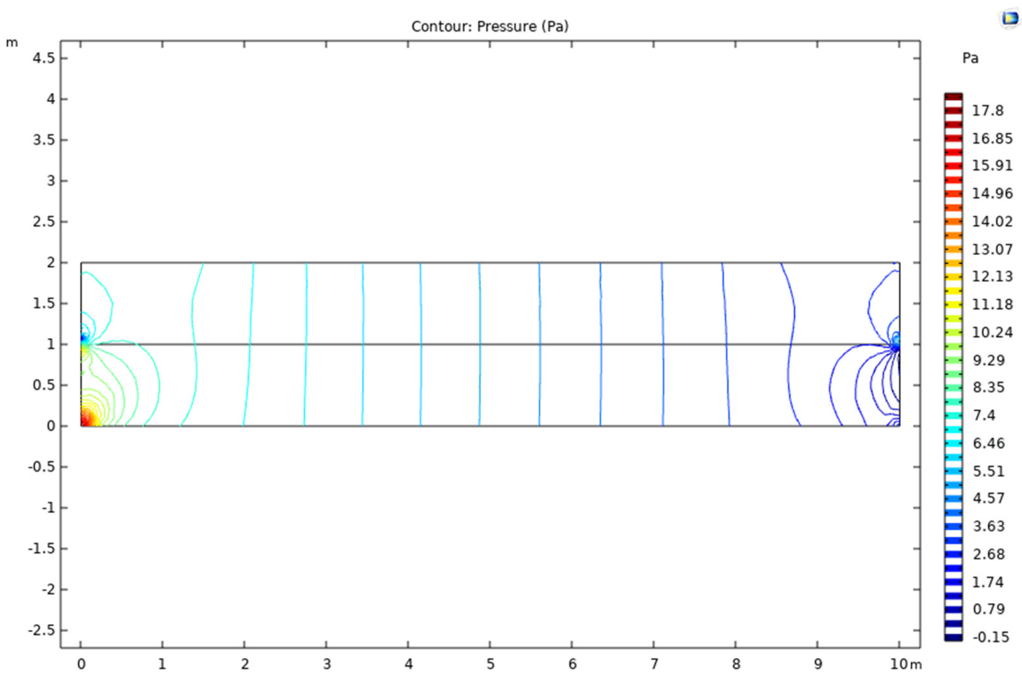

Figure 11. The contour plots of water-hydrogen system and hydrogen fluid flow pressure

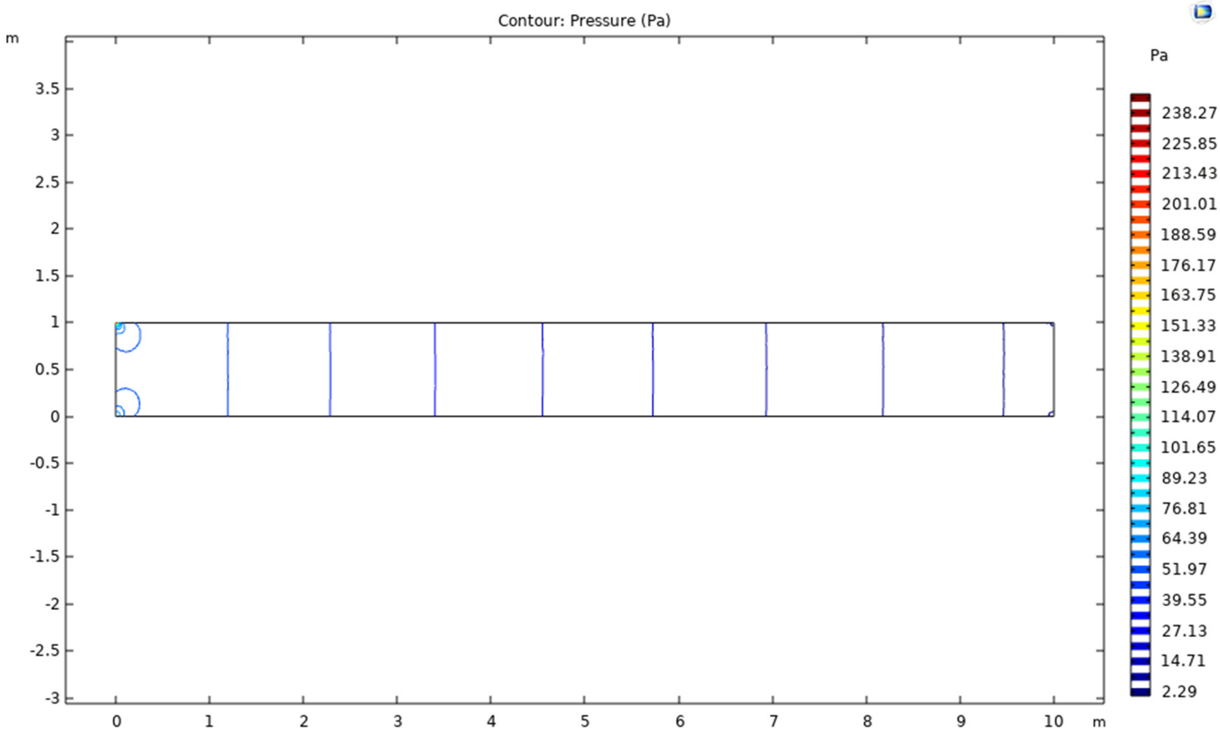

Figure 12. Scatter surface for pressure hydrogen

The contour plots of water-hydrogen system and hydrogen fluid flow concentrations are given in figures 11and 12, respectively. The results reveal maximum obtainable concentration of the water-hydrogen system and hydrogen are 2 $molm^{-3}$ and 1 $molm^{-3}$, respectively. However, the feasibility of hydrogen concentration attaining 1 $molm^{-3}$ was found at all distances as shown in figures 13.

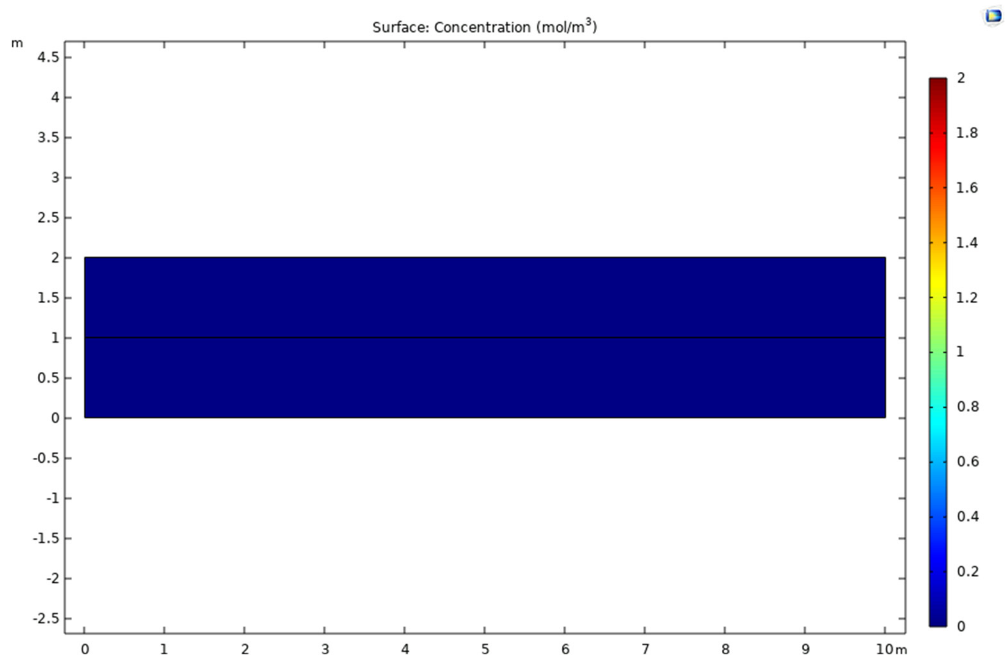

Figure 13. Scatter surface for concentration: Water-hydrogen system

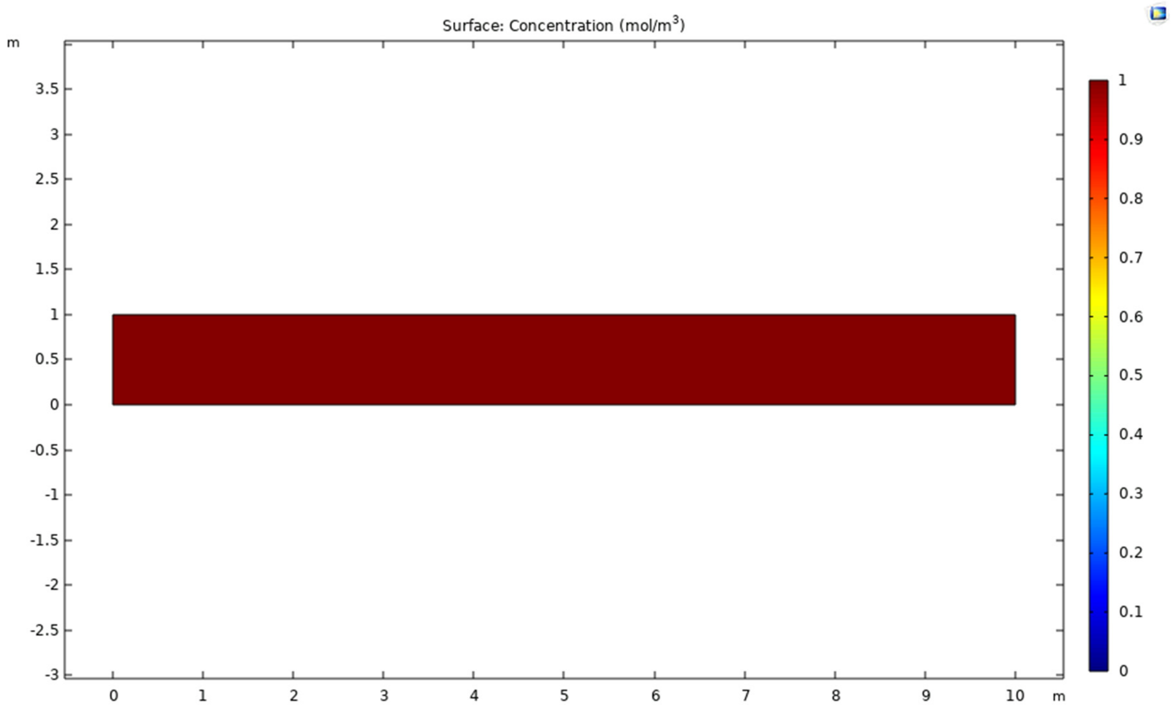

Figure 14. Scatter surface for concentration hydrogen

Figures 15 and 16 represent the convergence points. This reveals the profiles are similar and as applicable to the simulation work, the error value initially at epoch number (iteration number) of 1 decreases from 100% to 0% at iteration number of 4. Hence revealing the validity and reliance of the COMSOL simulation work.

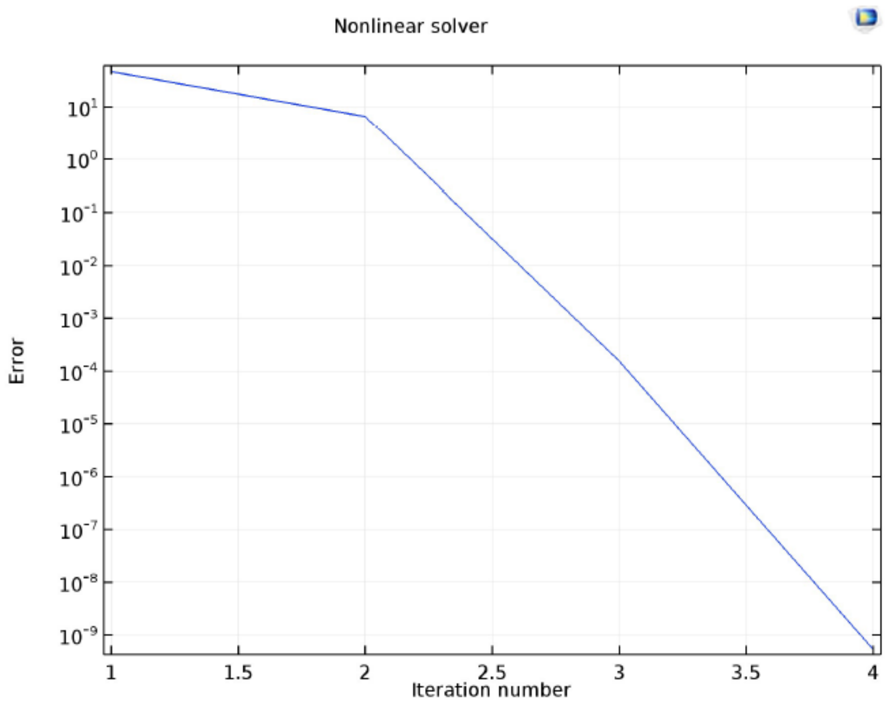

Figure 15. Convergence point for water-hydrogen system iteration

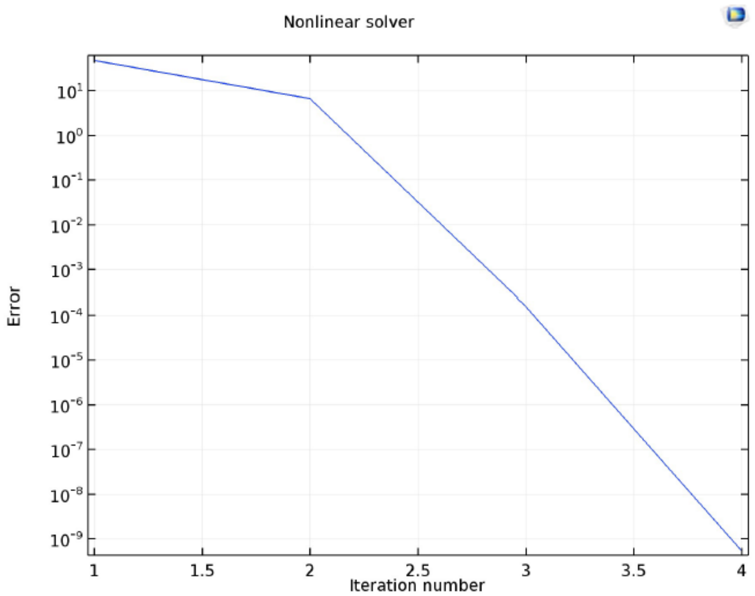

Figure 16. Convergence point for hydrogen iteration

Assessing the line plots for this process, figure 16 reveals drastic decrease in the pressure, however, a sharp pressure increase was observed from 0 – 0.05 m as observed in figure 18, brief decrease from 0.015 - 0.175, and drastic pressure decrease from 0.175 to 0.4, the exit of the water-split reactor system. Figure 17 and 18 below shows the plots of the pressure versus arc length for the water-hydrogen system and the pressure versus arc length for the hydrogen system. The line graph interactions shows diverse response, for both systems with a sharp line graph increase for the hydrogen system from 51.95(pa) to 52.8(pa).

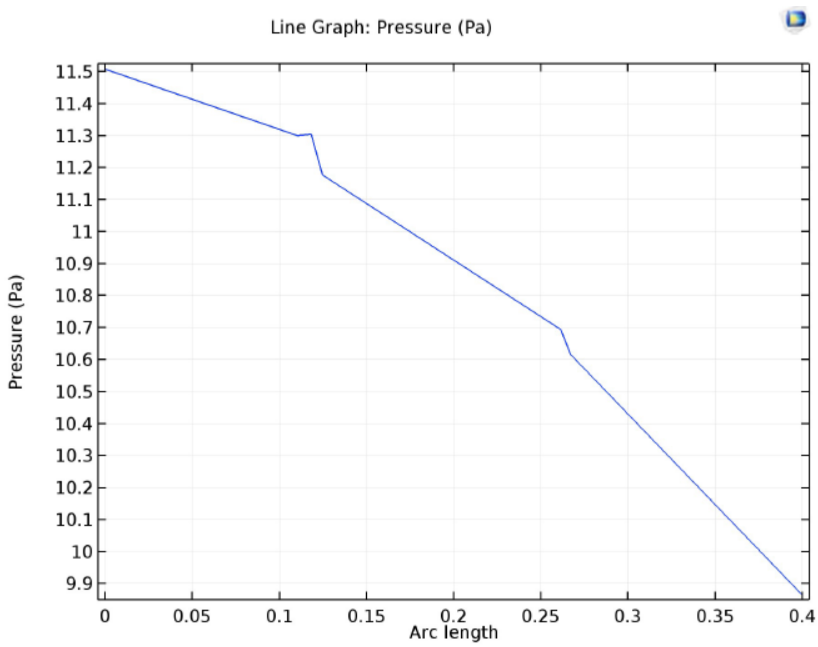

Figure 17. Pressure versus arc length for water-hydrogen system

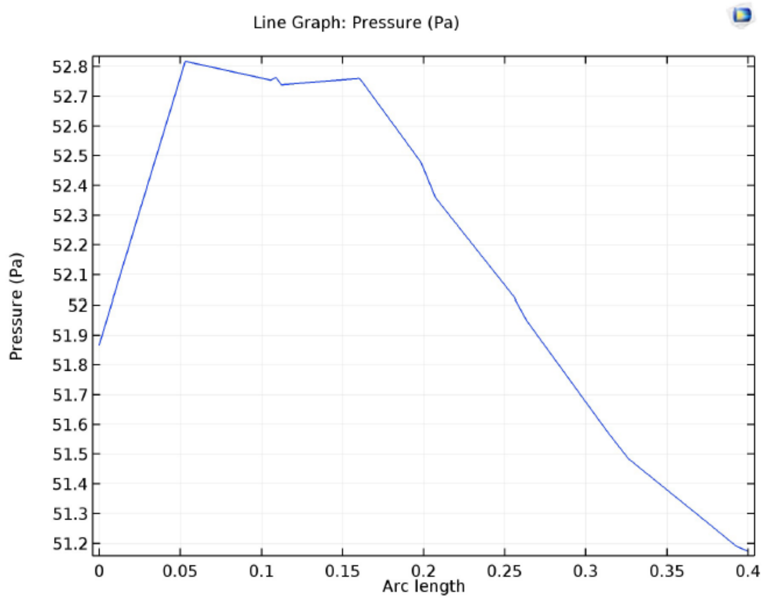

Figure 18. Pressure versus arc length for hydrogen

The shear stress for water-hydrogen system and hydrogen are shown in figures 19 and 20, respectively. The shear rate describes the gradient in velocity and also describes the differences in velocity between the surfaces containing the fluid, divided by the distance between them. From figure 19, a sharp increase is observed from 0 – 0.12, then constant shear rate at this point, before a further decrease to 0.265 and then increase to 0.27 with the share rate (0.3 s^{-1}) at this point to exit. However, haphazard decrease in the shear rate of hydrogen is strongly observed, with decrease from (4.5 – 1.1) s^{-1}.

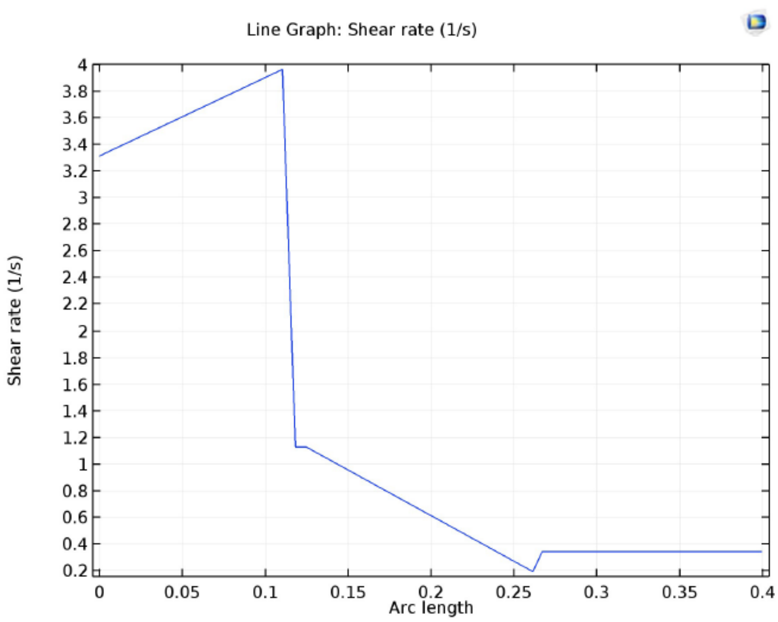

Figure 19. Shear rate versus arc length water hydrogen system

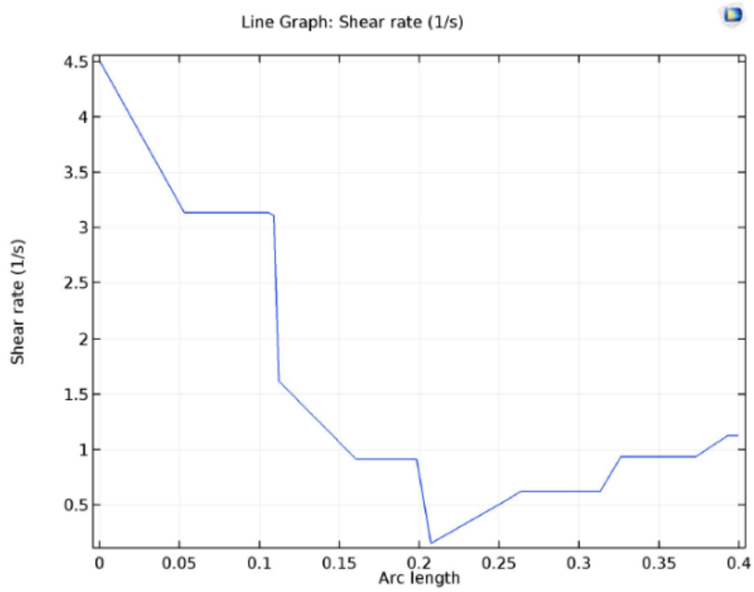

Figure 20. Shear rate versus arc length for water-for water hydrogen system

7. Conclusion

Moreover, the simulation results reveal that the profiles of water-hydrogen and hydrogen pressure become uniform at a distance of 1 mm from the entrance. The uniformity in pressure profile indicates a steady state of the fluid flow, which is crucial for ensuring consistent hydrogen production. The maximum pressure flow for water-hydrogen and hydrogen fluids is 17.8Pa and 238.27Pa, respectively, which are high enough to maintain the flow of the fluids through the reactor, while minimizing the pressure drop. Furthermore, the maximum achievable concentration of the water-hydrogen system and hydrogen are found to be 2 $molm^{-3}$ and 1 $molm^{-3}$, respectively.

These results suggest that the water-split reactor can produce hydrogen at high concentration levels, which is essential for meeting the demand for clean energy sources. The feasibility of attaining a hydrogen concentration of 1 $molm^{-3}$ is observed at all distances, which demonstrates the efficiency of the reactor in producing hydrogen with high purity. In addition, the simulation results also illustrate the shear stress for water-hydrogen system and hydrogen. The shear rate is used to describe the gradient in velocity and the differences in velocity between the surfaces containing the fluid, divided by the distance between them.

Specifically, Figure 19 displays a sharp increase in the shear rate from 0 to 0.12 of the arc length, followed by a constant shear rate at this point, before a further decrease to 0.265 and then an increase to 0.27 with the shear rate (0.3 s^{-1}) at the exit. The shear stress and shear rate are critical parameters in understanding the flow behavior of the fluids and designing the hydrogen production process to optimize mass transfer rates and improve production efficiency.

Overall, these findings provide crucial insights into the multiphase flow behavior of hydrogen production in the water-split reactor, which is essential for optimizing the reactor design and improving hydrogen production efficiency on a large scale. The results highlight the importance of understanding the flow behavior of the fluids and the role of critical parameters such as velocity, pressure, concentration, and shear stress in enhancing efficiency.

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Authors contributions

Wilson Ekpotu contributed to investigation, methodology, conceptualization, and writing – original draft. Joseph Akintola performed investigation, conceptualization, writing – original draft, Martins Obialor contributed to writing – review & editing, simulation analysis, and review. Udom Philemon participated in investigation and visualization and Imo-Obong contributed to research analysis, review, and project administration. All authors have thoroughly read and given their approval for the final manuscript to be published.

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Competing interests

The authors confirm that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Informed consent

Obtained.

Ethics approval

The Publication Ethics Committee of the Canadian Center of Science and Education.

The journal's policies adhere to the Core Practices established by the Committee on Publication Ethics (COPE).

Provenance and peer review

Not commissioned; externally double-blind peer reviewed.

Data availability statement

The data that support the findings of this study are available on request from the corresponding author. The data are not publicly available due to privacy or ethical restrictions.

Data sharing statement

No additional data are available.