

Full-scale Modeling of PEM Water Electrolyzer: Effect of Geometrical Parameters

by

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Author's Declaration

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Abstract

The transition to a low-carbon energy system has intensified interest in green hydrogen as a clean energy carrier. Proton Exchange Membrane Water Electrolyzers (PEMWE), powered by renewable electricity, offer a promising pathway for hydrogen production. The performance of PEMWE is essentially affected by operating conditions and geometrical parameters. However, a full-scale model is seldomly considered for numerical simulations, which requires investigation for better performance of PEMWE. This study develops a 3D full-scale model of A numerical simulation that has been conducted in this study to analyze the effects of PEMWE geometrical parameters, including porous transport layer (PTL) thickness, channel width and cell length, on hydrogen production rate and temperature distribution. Cell length was analyzed as a sensitive factor for hydrogen production rate while all three parameters were sensitive factors for temperature distribution. The results reveal that longer cell lengths and thinner PTL contribute positively to hydrogen output. The channel width demonstrated parabolic trend across different ranges and can be optimized for maximum efficiency. Additionally, both the average temperature and the temperature variance within the catalyst layer rise with increasing PTL thickness, channel width and cell length. The model was further optimized with respect to three geometrical parameters, aiming to maximize the hydrogen production rate while minimizing the operating temperature. This study provides an evaluation of geometrical design of PEMWE in a full-scale numerical model, offering practical guidance for the design of advanced electrolyzer systems with improved performance.

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List of Abbreviations

PEMWE	Proton exchange membrane water electrolyzer
SMR	Steam methane reforming
CCUS	Carbon capture, utilization and storage
CAPEX	Capital expenditure
AWE	Alkaline water electrolyzer
SOEC	Solid oxide electrolysis cell
AEMWE	Anion exchange membrane water electrolyzer
PCCEL	Proton conducting ceramic electrolyzer
BPP	Bipolar plate
PTL	Porous transport layer
CL	Catalyst layer
PEM	Proton exchange membrane
HER	Hydrogen evolution reaction
OER	Oxygen evolution reaction
PSD	Pore size distribution
CCM	Catalyst-coated membrane
GA	Genetic algorithm
VOF	Volume of fluid
TSFF	Triple serpentine flow field
PFF	Parallel flow field
SWFF	Sinusoidal wave flow field
ICFF	Intercepted flow field
AM	Additive manufacturing
MEA	Membrane-electrode assembly
CCM	Catalyst-coated membrane
RSM	Response surface method

List of Symbols

Symbol	Unit	Description
ρ	$kg \cdot m^{-3}$	Density of the species
$\mathbf{u}$	$m \cdot s^{-1}$	Velocity profile
S	-	Source term
μ	$Pa \cdot s$	Dynamic viscosity
R	$J \cdot mol^{-1} \cdot K^{-1}$	Gas constant
T	K	Temperature
x_l	-	Mole fraction of liquid
t_{lg}	-	Coefficient for viscosity calculation
ω_l	-	Mass fraction of liquid
M_l	$g \cdot mol^{-1}$	Molar mass of liquid
ε	-	Porosity
ε^{eff}	-	Effective porosity
s	-	Saturation
H_p	m	Pressure head
p	Pa	Pressure
g	$m^2 \cdot s^{-1}$	Gravitational acceleration
i	$A \cdot cm^{-2}$	Current density
$i_{v,tot}$	$A \cdot cm^{-3}$	Volumetric current density
φ	V	Electric potential
σ	$S \cdot m^{-1}$	Electric conductivity
p_{sat}	Pa	Saturated pressure
i_0	$A \cdot cm^{-2}$	Exchange current density
α_a	-	Anodic (forward) charge transfer coefficient
α_c	-	Cathodic (backward) charge transfer coefficient
n	mol^{-1}	Number of charge transfer per mole

F	$C \cdot mol^{-1}$	Faraday's constant
$i_{0,a}$	$A \cdot cm^{-2}$	Anodic exchange current density
$i_{0,c}$	$A \cdot cm^{-2}$	Cathodic exchange current density
$i_{ref,a}$	$A \cdot cm^{-2}$	Anodic reference exchange current density
$i_{ref,c}$	$A \cdot cm^{-2}$	Cathodic reference exchange current density
$E_{act,a}$	$J \cdot mol^{-1}$	Anodic activation energy
$E_{act,c}$	$J \cdot mol^{-1}$	Cathodic activation energy
T_{ref}	K	Reference temperature
η	V	Overpotential
φ_s	V	Electrode potential
φ_l	V	Electrolyte potential
E_{eq}	V	Equilibrium potential
$E_{eq,ref}$	V	Reference equilibrium potential
c_{H_2}	$mol \cdot m^{-3}$	Concentration of hydrogen
c_{O_2}	$mol \cdot m^{-3}$	Concentration of oxygen
D_{gl}	$m^2 \cdot s^{-1}$	Binary diffusivity
R_g	$kg \cdot m^{-3} \cdot s^{-1}$	Mass source
v	m^3	Atomic diffusion volume
A_V	m^{-1}	Reactive surface area density
Y_g	-	Stoichiometric coefficient of gas in the reaction
Q_{Joule}	$W \cdot m^{-3}$	Heat source due to Joule heating
Q_{chr}	$W \cdot m^{-3}$	Heat source due to electrochemical heating
q	$W \cdot m^{-2}$	Heat flux
C_p	$J \cdot K^{-1}$	Heat capacity
$C_{p,eff}$	$J \cdot K^{-1}$	Effective heat capacity
ΔH_r	$kJ \cdot mol^{-1}$	Enthalpy change per mole reaction

k_{eff}	$W \cdot m^{-1} \cdot K^{-1}$	Effective thermal conductivity
$C_{p,g}$	$J \cdot K^{-1}$	Heat capacity of gas phase
$C_{p,l}$	$J \cdot K^{-1}$	Heat capacity of liquid phase
$C_{p,s}$	$J \cdot K^{-1}$	Heat capacity of solid phase
k_g	$W \cdot m^{-1} \cdot K^{-1}$	Thermal conductivity of gas phase
k_l	$W \cdot m^{-1} \cdot K^{-1}$	Thermal conductivity of liquid phase
k_s	$W \cdot m^{-1} \cdot K^{-1}$	Thermal conductivity of solid phase
γ_g	-	Volume fraction of gas phase
γ_l	-	Volume fraction of liquid phase
γ_s	-	Volume fraction of solid phase
St	-	Stoichiometric factor of water
$\dot{m}_{H_2O}$	$kg \cdot s^{-1}$	Water feed rate
A	cm^2	Active area
M	-	Number of computational fields
N_j	-	Number of degrees of freedom in field j
$W_{i,j}$	-	Current approximation to the true solution vector
$E_{i,j}$	-	Estimated error

1. Introduction

1.1 Background

Paris Agreement defined a long-term target of limiting the global average temperature rise to well below 2 °C for Canada and 194 other countries [1], [2], [3]. The goal proposed to the new carbon emissions reduction challenges the world. Burning of fossil fuels results in high carbon emissions, especially CO₂ and CH₄ [4], [5]. Hydrogen is a promising solution for reducing the carbon emissions [6]. It has the advantages of high energy density, versatility, scalability, security and zero emissions, which is the most essential [7], [8]. Hydrogen is differentiated to various colors by different generation methods from green to pink [9]. For example, Grey Hydrogen is produced from Steam Methane Reforming (SMR) without Carbon Capture, Utilization and Storage (CCUS). Blue Hydrogen is produced from SMR with CCUS [10]. These two production methods both use SMR which results in carbon emission. Green Hydrogen is produced from green energy like solar/wind and electrolysis which has zero carbon emission [11], [12]. The hydrogen production reached 97 Mt in 2023 [13] and the amount that produced by technology and region is shown in Figure 1.

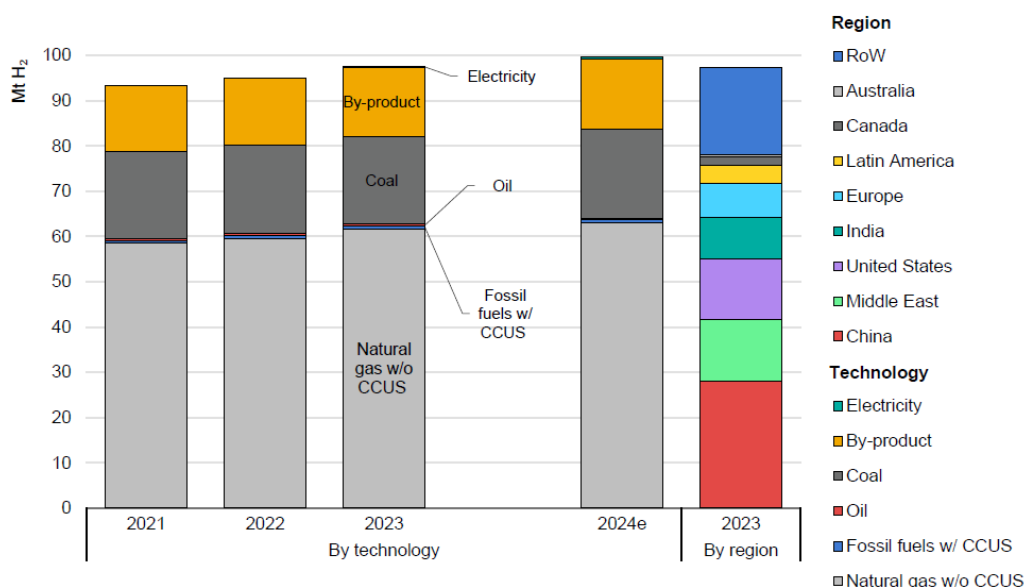


Figure 1. Hydrogen production by technology and by region, 2021-2024 [13]

China accounts for almost 30% global total hydrogen production which is the most massive amount of hydrogen production, followed by the United States and Middle East, which

account for 14% each. Unabated fossil fuels are the dominant method of hydrogen production until 2023. Also, more than 15% of hydrogen is produced as a by-product in refineries. Furthermore, the percentage of low-emission hydrogen production which refers to fossil fuels with CCUS and electrolysis is less than 1%. The amount of hydrogen produced by electrolysis is below 100 kt and primarily in China, Europe and the United States in 2023.

Green hydrogen is an attractive and popular research topic which is a feasible solution to reducing carbon emissions in sectors that are hard to decarbonize through electrolysis alone [14], [15]. The biggest advantage of green hydrogen is that it emits zero CO₂ during the production process [16]. Electrolysis is a fundamental process in green hydrogen production, [17] with electrolyzers serving as the primary devices for hydrogen generation [18], [19]. For green hydrogen production by electrolysis, the high utilizations of the electrolyzers reduces the high Capital expenditure (CAPEX) in the total cost of hydrogen production, [13] which expend the feasibility of electrolyzer reaches the stage of Final investment decision and development.

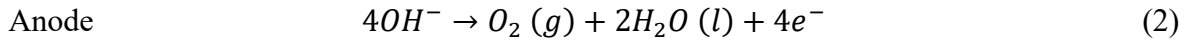
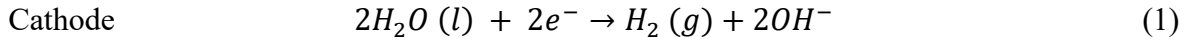
Currently, there are several types of water electrolyzers that can achieve the goal of green hydrogen production [20]. Alkaline water electrolyzer (AWE) uses an alkaline solution as the electrolyte. AWE is a low-temperature water electrolyzer with operating temperature 50-90°C and the efficiency of it is around 60-80% [21]. Proton exchange membrane water electrolyzer (PEMWE) uses solid polymer membrane as the electrolyte, with 50-80°C operating temperature. The maximum efficiency can approach 85%. PEMWE is much more expensive because of the high cost of its catalysts [22]. Solid oxide electrolysis cell (SOEC) is a high-temperature water electrolyzer which has a 500-850°C operating temperature. The efficiency range of SOE is 80-90% [23]. The details of drawbacks and advantages of the three different water electrolyzers are listed in Table 1 below.

Table 1. Comparison of different water electrolyzers [20]

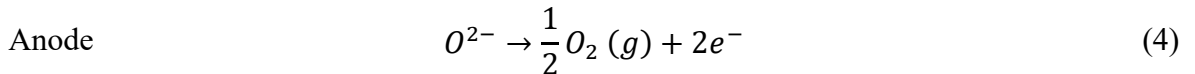
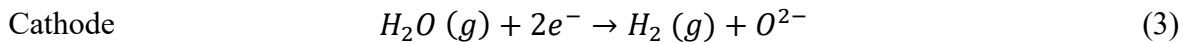
Type	Advantages	Disadvantages
AWE	Low capital cost, mature technology, scalable for large production	Corrosion challenges, lower efficiency and current density

PEMWE	High efficiency and current density, high-purity hydrogen	High capital costs, expensive materials, lower scalability
SOEC	Highest efficiency, non-noble electro catalysts	High temperature operation, material degradation, not yet mature

Each of technology has distinct advantages and limitations. AWE is the most commercially mature, offering low-cost operation, long durability, and the use of non-noble metal catalysts, though it suffers from limited dynamic response and lower hydrogen purity, making it less suitable for intermittent renewable integration [21], [24], [25], [26]. Liquid water gains electrons at cathode side to generate hydrogen and hydroxyl. Hydroxyl transfers from cathode to anode, loses electrons and splits to oxygen and liquid water.



PEMWE provides high-purity hydrogen, fast response times, and compact system design, which enable effective coupling with fluctuating power sources. A lower operational temperature also reduces the extra energy consumption; however, the reliance on expensive noble metal catalysts and membrane degradation issues contribute to higher system costs [22], [27]. SOEC operates at elevated temperatures and achieves high efficiency, especially when integrated with industrial heat sources, yet challenges related to thermal stability, material degradation, and slow start-up constrain its deployment in flexible and decentralized applications [28], [29]. SOEC splits water into hydrogen O^{2-} at cathode side. O^{2-} transfers from the electrolyte to the anode side, loses electrons and generates oxygen. The half reactions are listed below.



Except these three main types of water electrolyzer, Anion exchange membrane water electrolyzer (AEMWE) and Proton conducting ceramic electrolyzer (PCCCL) are also investigated by many researchers. AEMWE has the same half reactions as AWE. AEMWE has

a membrane which allows hydroxyl to pass while AWE uses liquid alkaline solution as a replacement. The application of the non-porous membrane can reduce the internal resistance and increase anionic conductivity, also allows a higher operation pressure [30]. Alkaline also allows a great variety of catalyst material selection, like non-platinum or non-precious metal-based catalysts. On the other hand, the high operation pressure creates challenges to the design of AEMs. The hydrogen cross-permeation through the membrane and mechanical failure potential should be considered. PCCEL is another high temperature electrolyzer which operated around 500 °C. Water is supplied to the anode side and pure hydrogen is generated at the cathode side. The higher operation temperature brings advantages in economy, for example, lower electrical energy demands since portion of the supplied energy is in the form of thermal energy [30]. The schematics of the five main types of water electrolyzers are shown below.

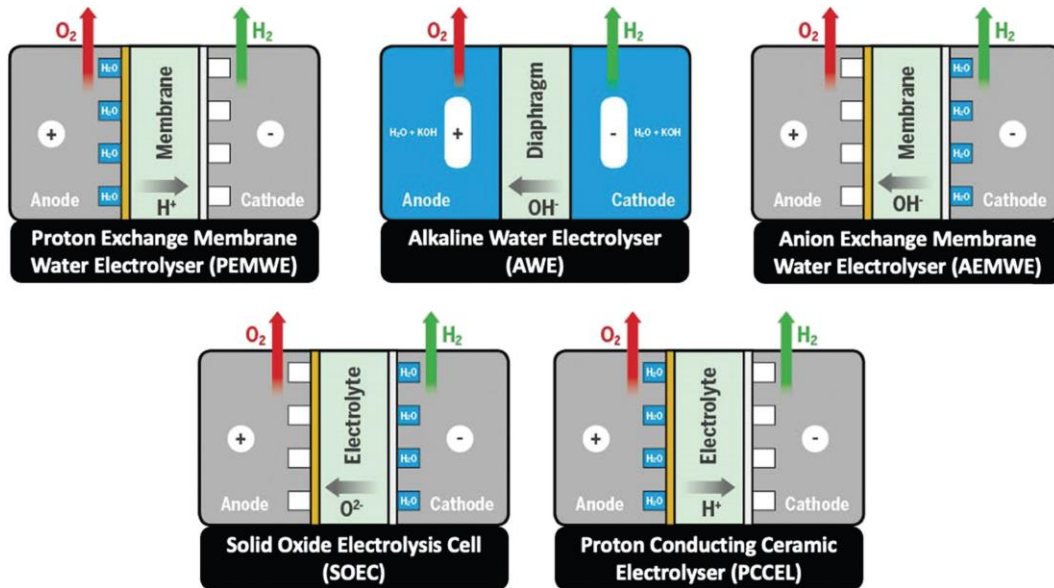


Figure 2. Schematics of the five types of water electrolyzers [30]

The capacity of installed water electrolyzer reached 1.4 GW until 2023 with China accounted for approximately 80% [13]. Alkaline technology (ALK in Figure 3) keeps dominating the hydrogen production since 2020, followed by PEM water electrolysis which accounted for 22% of the whole hydrogen production in 2023. With the increasing hydrogen production in the world, the capacity of electrolysis is also enhanced.

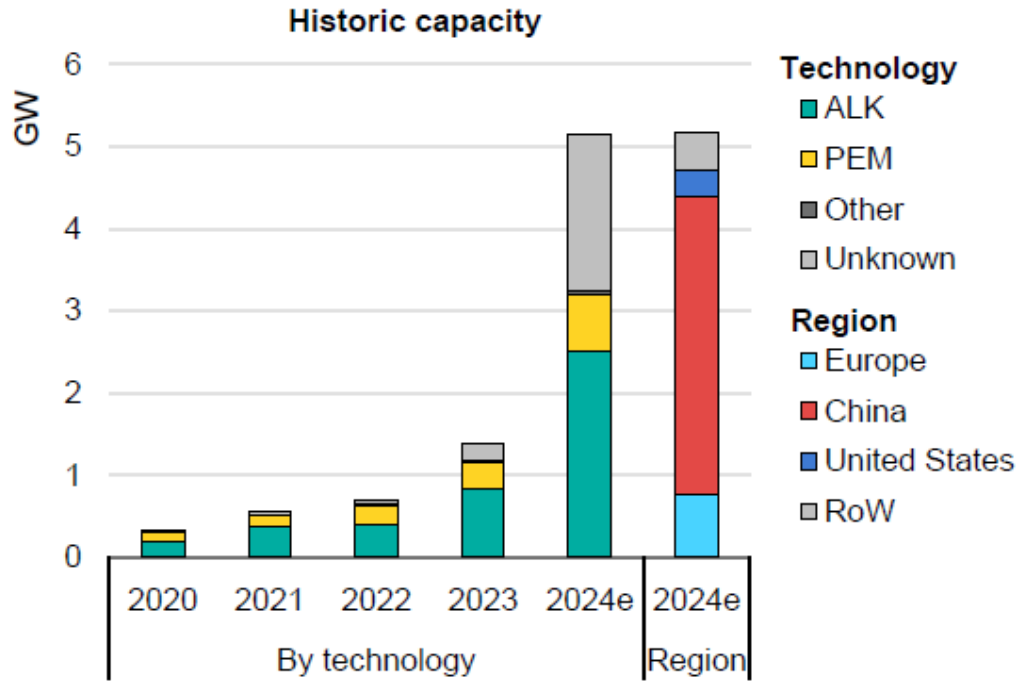


Figure 3. Installed electrolyzer capacity by technology and region, 2021-2024 [13]

Among the various types, PEMWE has been more extensively investigated due to its higher efficiency, faster dynamic response, and greater technological maturity [20]. It can produce pure hydrogen and operate with a lower temperature range [31]. These advantages make PEMWE a feasible solution for green hydrogen production. However, the evaluation of PEMWE performance is still a challenge for PEMWE design and optimization. A schematic of PEMWE system is shown in the following figure. The system includes the electrolyzer stack, gas/liquid separators, circulation loop for water, pressure control valves, transformer, and rectifier for power-conditioning. The gas/liquid separators are used for both hydrogen and oxygen, to produce pure hydrogen/oxygen. A control system including safety devices is applied for the rectifier.

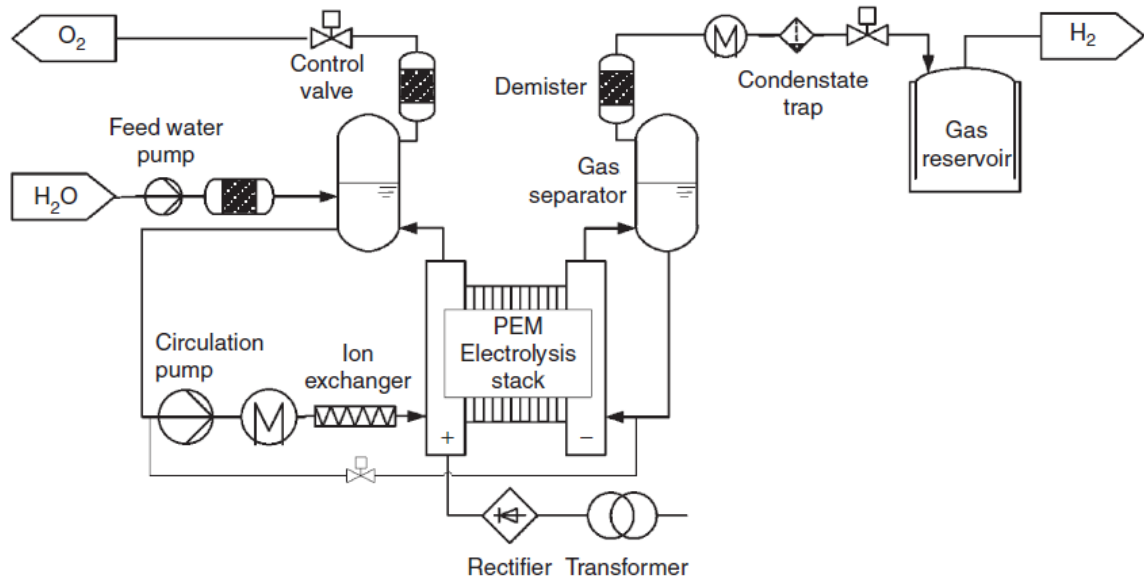


Figure 4. Typical layout of a proton exchange membrane water electrolyzer unit. [32]

The average power consumption of the stacks is 4.2 ± 0.3 kWh N m⁻³ hydrogen, while the stack efficiency is in a range of 67-77%. Figure 5 demonstrates the correlation between power consumption and the hydrogen production rate.

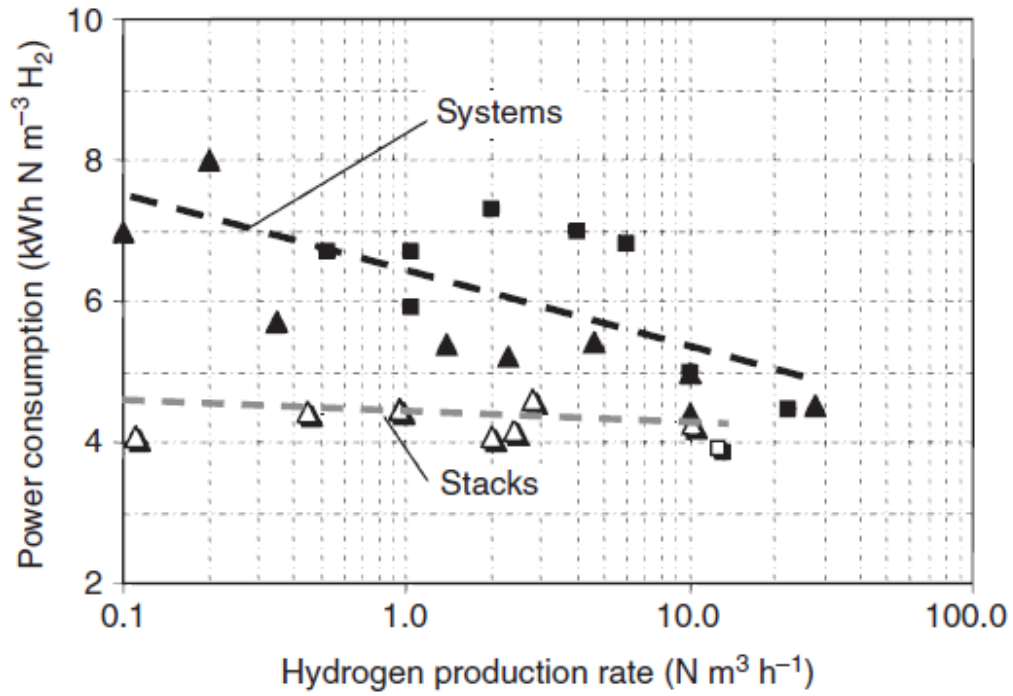


Figure 5. Power consumption of different proton exchange membrane water electrolyzer stacks and systems as a function of the hydrogen production rate (Dark square for commercial systems; dark triangle for systems under development; blank square for commercial stacks; blank triangle for stacks under development). [32]

With the high-speed development of Fuel Cell industry, water electrolyzers will also attract more attention in the future. Especially, PEMWEs offer pure hydrogen in small, highly efficient units that will be more suitable for distributed operation. Therefore, PEMWEs are considered as an essential component for renewable energy industry development [32].

1.2 Principle of Proton Exchange Membrane Water Electrolyzer (PEMWE)

PEMWE is one of the main equipment for green hydrogen production, which operates based on the electrochemical conversion from electricity into hydrogen and oxygen. It was first developed with a concept of solid polymer electrolyte in 1960s [33]. The concept was further idealized by Grubb [34], [35]. In his study, a solid sulfonated polystyrene membrane was used as an electrolyte, which refers to the Proton Exchange Membrane. The schematic of a PEMWE single cell is shown in Figure 6.

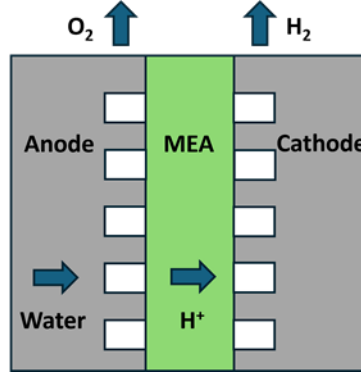


Figure 6. Schematics of single proton exchange membrane water electrolyzer (PEMWE) cell

The PEMWE cell stack consists of multiple units and each unit containing multiple flow channels [36], [37]. For each unit, the main part is the proton exchange membrane which only allows the passing of protons. The end plates are the end of the PEMWE stack, which provide the functions such as compaction and support [38]. The current collectors are attaching to the end plates and bipolar plates to conduct the electrons. Bipolar plates and porous transport layers are the two components that from the flow field, also conduct the electrons from the catalyst layers. The membrane electrode assembly (MEA) always contains porous transport layers, catalysts and membrane. The porous transport layers are porous material which can both separate the water from flow field to the catalyst also collect the current [39]. Catalyst layers are the components where the reactions happen. For this study one unit of PEMWE cell is investigated. PEMWE converts electricity into chemical energy by splitting water into oxygen at the anode and hydrogen at the cathode. The overall reaction of a PEMWE is shown in Equation (5) [40].



The oxygen evolution reaction (OER) on the anode side split water into protons and electrons, while generating oxygen simultaneously. The generated oxygen at anode flows out by water flow. The electrons are transferring from the external circuit to reach cathode side because of the lower electric potential. The protons transfer through the membrane which only allows proton to pass through [41]. The hydrogen evolution reaction (HER) at cathode side combines

the protons and electrons from different paths to hydrogen [41]. There are four major components of a PEMWE: bipolar plates (BPP), porous transport layer (PTL), catalyst layer (CL) and proton exchange membrane (PEM) [42], [43]. BPPs and PTL form the flow channels that facilitate water entry the PEMWE at the anode side. Both the PTL and CL are designed as porous media to facilitate this process. As water passes through the PTL, it interacts with the catalyst in the CL, resulting in the generation of oxygen and protons. The MEA within the system is selectively permeable, allowing only protons to pass through. Consequently, the protons produced at the anode migrate through the membrane to the cathode side, while the electrons released during the anodic reaction traverse an external circuit to reach the cathode. At the cathode, these protons and electrons react within the CL to produce hydrogen [22], [27].

PEMWE can be operated with much higher current densities ($>2 \text{ A cm}^{-2}$) which reduces the costs of operation [22]. The low gas crossover rate of the membrane improves the purity of the generated hydrogen also reduces the cost of purifying hydrogen. This also results in a wider operational range of power input. The use of solid electrolyte allows stronger system design with higher operational pressure [44]. The higher operating pressure also reduce the energy demand for compression and storage [22]. The increasing pressure also reduces the expansion and dehydration of the membrane [45]. On the contrary, the acidic operation environment limits the lifespan of the catalysts and other components, the protons that generated from OER results in a lower pH value in the PEMWE. The higher cost of the catalysts is another restriction of the PEMWE development.

The improvement of PEMWE efficiency is always a topic that is investigated by researchers. The losses of PEMWE efficiency come from three types of overpotential, including activation polarization, ohmic polarization and concentration polarization [46]. Activation polarization refers to the electrochemical phenomenon in which an applied overpotential drives the electrochemical cell away from its equilibrium state during current flow. A positive overpotential facilitates the progression of oxidation reactions at the electrode surface [22], [47]. Ohmic polarization is caused by the resistance of the material when the electric current through the electrochemical cell [48, p. 1]. The ohmic polarization is influenced by the electric current, electrolyte conductivity and the distance between two electrodes.

Concentration polarization denotes the loss due to the mass transfer within the water electrolyzer, which is described as the sum of cathode and anode concentration overpotential [49].

1.3 Geometrical Parameters of PEMWE

Importantly, the geometrical parameters of PEMWE components, such as PTL thickness, cell length, and the width of BPP channels and ribs, have profound influences in current density and temperature distribution [22], [50], [51], [52], [53]. As the indicator for hydrogen production capacity, current density can be improved through proper geometrical designs. In addition, even temperature distribution avoids the formation of hotspots to protect the components from thermal damage and to maintain the activity of catalysts, leading to improved lifespan of PEMWE. Therefore, the geometrical parameters of PEMWE components are important in terms of improving performance and durability.

To evaluate the effects of geometrical designs on PEMWE performance, the preceding geometrical parameters of PEMWE components are widely studied. Numerical modeling is widely adopted to simulate physical and electrochemical processes in PEMWE, [50], [54], [55], [56], [57], [58], allowing a cost-effective and reliable evaluation of PEMWE performance. For example, Zhou et al. [59] developed a three-dimensional, two-phase, one-channel PEMWE model, investigated the effect of anode PTL porosity and membrane thickness on PEMWE performance. Their results show that current density has a parabolic trend with increasing anode PTL porosity, while higher membrane thickness results in higher current density but higher temperature. In addition, Hassan et al. [60] numerically studied the geometrical designs of flow channel, reporting that one-path serpentine pattern provides the most uniform flow and temperature distribution in PEMWE. Furthermore, Zhuang et al. [51] investigated the influence of flow channel height and width using a non-isothermal PEMWE single-channel model. Their results indicate higher channel height results in higher hydrogen mole fraction; increasing channel width leads to lower pressure drop. Han et al. [61] built an 1D model of BPP, PTL, CL and PEM with ohmic loss to evaluate the current density of PEMWE under various electrode thicknesses. Increasing electrode thickness results in decreasing current density due to higher diffusion and ohmic losses. Moreover, Olesen et al. [62] developed a

three-dimensional anode model of PEMWE to predict current density and heat maldistribution. These existing studies indicate that numerical modeling is a powerful tool to evaluate PEMWE geometrical designs in terms of performance and durability.

1.4 Objectives and Scope of Thesis Research

Hydrogen production plays an essential role in hydrogen economic development. In this study, a comprehensive PEMWE evaluation model is considered as the method of hydrogen production.

Specifically, the objectives of this thesis research are:

- To develop a 3D numerical model for the evaluation of a PEMWE unit. With consideration of flow field, electrochemical reaction, charge transport, heat transport, and mass transport in the numerical model.
- To develop a simulation framework to consider the effects of geometrical parameters, including PTL thickness, channel width and cell length on the performance of PEMWE unit, especially hydrogen production rate and temperature distribution are analyzed to compare the difference between various cases.
- To optimize the geometrical design of the PEMWE unit by sensitivity analysis and Response Surface Method (RSM). Specify the significant geometrical parameters within the designed ranges.

To achieve the above objectives, this thesis focuses on establishing a 3D non-isothermal simulation model with parallel flow field to evaluate the performance of a PEMWE unit, especially hydrogen production rate and temperature distribution. This research also involves the optimization of geometrical parameters by Genetic Algorithm (GA). This study will provide insights into PEMWE design which is beneficial for water electrolyzer development.

2. Literature Review

PEMWE is a promising technology for sustainable hydrogen production due to their high efficiency, compact design, and ability to operate at high current densities with pure water feed [63]. In PEMWE systems, overall performance - encompassing hydrogen production rate, energy efficiency, durability, and scalability - is governed by complex interactions between electrochemical reactions, mass transport, heat transfer, charge transport and multi-phase flow phenomena [64]. Among the key factors influencing these coupled processes, cell geometry and component design play a critical role. Geometrical parameters - including the PTL thickness, porosity, and tortuosity; flow field channel width, depth, rib width, and rib/channel ratio; as well as the overall cell length - strongly affect water distribution, gas removal, ionic and electronic transport, and thermal gradients within the cell [39], [65], [66]. Given the essential role of geometrical parameters in determining PEMWE performance, understanding and optimizing cell design is crucial for advancing the development of efficient and scalable electrolyzer systems. This section reviews the current state of knowledge on how geometrical factors influence PEMWE operation.

A typical PEMWE consists of several key components, each of which has geometrical characteristics that directly impact cell performance. The core of the PEMWE is the catalyst-coated membrane (CCM), which includes a PEM and CL on both the anode and cathode sides [64]. Flanking the CCM are PTL, which serve to distribute water to the CL, facilitate gas evacuation, and provide electronic and thermal conductivity [67], [68]. The PTL is defined by geometrical parameters such as thickness, porosity, pore size distribution, and tortuosity, all of which influence mass transport and heat management within the cell [67], [69]. The flow channels, which are formed with BPP and PTL, govern the in-plane distribution of water and the removal of produced gases, while also influencing the pressure drop and flow uniformity [70], [71]. Critical geometrical parameters of flow channels include channel width, channel height, rib width, and number of channels. In addition, the overall cell dimensions have gained increasing attention, as they control gradients in temperature, pressure, and reactant concentration, which can limit scale-up and impact membrane hydration and durability.

Careful selection and optimization of these geometrical parameters are therefore essential to achieving high-performance, durable, and scalable PEMWE systems.

The PEM serves as the core functional component of a PEMWE, providing proton conductivity while acting as an electronic insulator simultaneously. Zhou et al. [72] found decreasing membrane thickness results in the enhancement of the PEMWE performance depends on the polarization curves since the thinner PEM thickness reduces the ohmic resistance. On the other hand, the reduction of PEM thickness leads to decrease of hydrogen permeability and impair the mechanical stability. Han et al. [73] built an ohmic loss model of PEMWE to evaluate the performance of PEMWE under various operating conditions and design parameters. Key factors that influence its performance include exchange current density, temperature, pressure, and the properties of the electrode and membrane. The equivalent resistance model is shown in Figure 7. Lower electrode thickness and PEM thickness lead to better PEMWE performance. The ohmic loss and diffusion overpotential are directly related with the PEM conductivity and thickness. Additionally, it is observed that there is a significant increase in overpotential with the increase of PEM thickness from 50 to 200 micros. On the other hand, the PEM ohmic loss comprises 63.6% of the total loss for a 178 micros thick PEM that operated under 1.5 A cm^{-2} current density

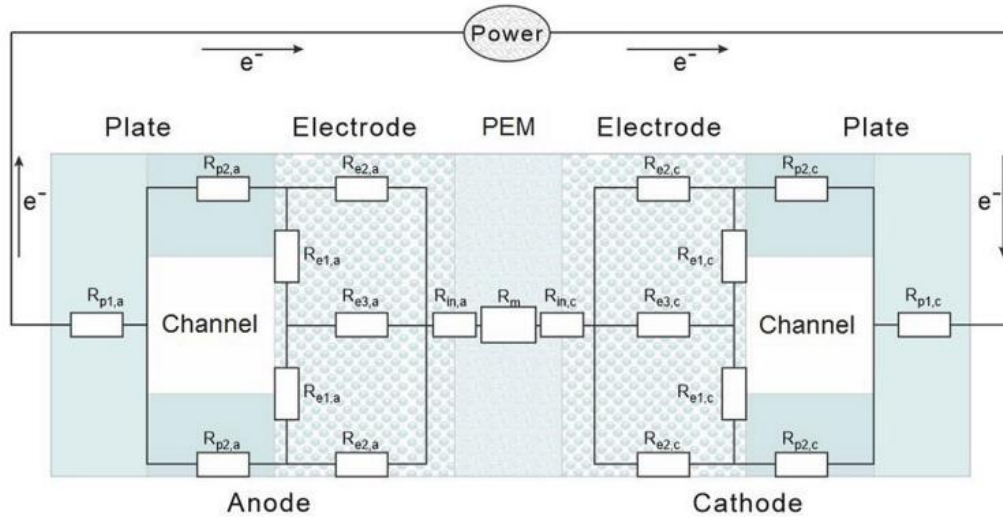


Figure 7. Equivalent resistance model of a PEM electrolyzer cell. [73]

Afshari et al. [74] examined the effect of membrane thickness on the hydrogen crossover by establishing a mathematical model of PEMWE. The results indicate that increasing membrane thickness improves the PEMWE performance due to reducing the amount of hydrogen crossover from cathode to anode. In addition, higher membrane thickness results in an increment, increasing diffusion loss and ionic resistance, which causes the reduction of electro-osmotic drag. Furthermore, thicker membrane prevents the membrane water passage due to differential concentration. Therefore, a thinner membrane is recommended by this study, but the strength and stability issues should also be considered.

The CL facilitates electrochemical water splitting reactions at both anode and cathode, thereby directly determining the reaction kinetics, and overall performance of the PEMWE. Li et al. [75] indicates that the current density is decreasing with lower catalyst utilization near the CL-PEM interface, since this region is more sensitive to mass transportation rather than the reaction kinetics. Moore et al. [76] established a 2-D, finite element simulation model to investigate the effect of pore size distribution (PSD) of anode catalyst layer, which is shown in Figure 8. The results indicate that the IrO_x catalyst doesn't show significant change for different pore sizes since the hydrophilic volume fraction is nearly similar among different PSDs. However, a noticeable difference is observed for larger PSD of Ir catalyst, which indicates the model is sensitive to the mass transport loss. In addition, a significant lower pressure is observed with medium PSD of Ir catalyst, since larger PSDs are more permeable to gas.

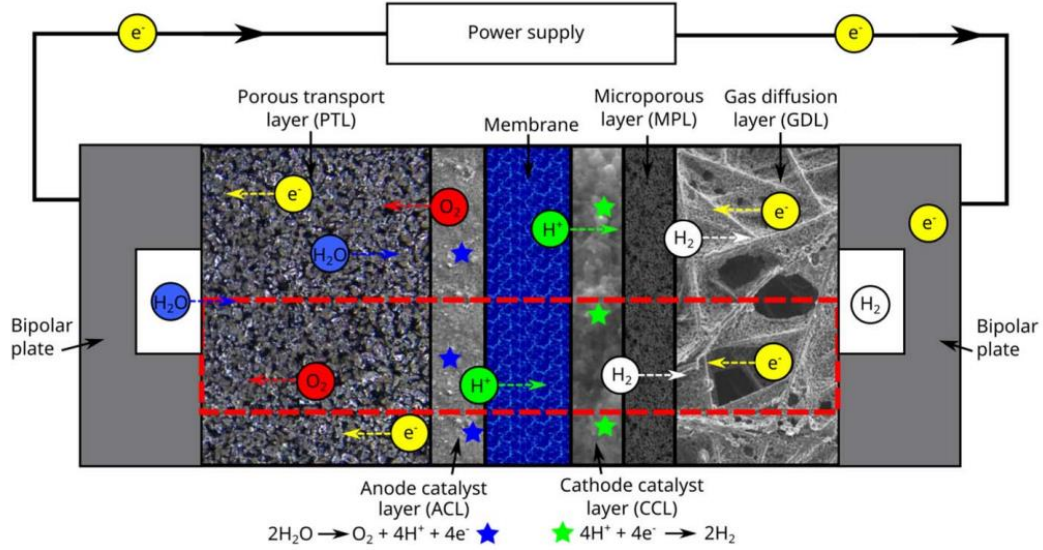


Figure 8. Transport processes within the cell, the computational domain is shown in red dash line. [76]

Wang et al. [77] investigate the impact of CL structures and conductivities between PEM and CL by establishing a mathematical model of PEMWE. The electrolysis voltage and power consumption are both decreasing rapidly and then tending to unchanged with the decrease of CL thickness. Moreover, the anode activation overvoltage is increasing with the decrease of CL thickness since decreasing the CL thickness results in reduction of CL porosity. In addition, it is observed that increasing CL porosity leads to higher electrolysis voltage and power consumption. However, this trend is only reported for CL porosity, which is higher than 0.5, no obvious differences are reported for CL porosity under 0.4. Ma et al. [78] established a 2D single-phase model to investigate the characteristics of in-plane and through-plane directions of the CL and the interface between CL and PTL. The computational domain is shown in Figure 9. A lower catalyst utilization is observed with the increased electrode potential and pore size at the PTL and anode CL interface, since the inhomogeneity results to the increases of hot spots. Furthermore, electron transport within the pore and at the surfaces of CL are the major reasons that constraints the OER reaction rate. This research suggested closer and higher electrical and ionic conductivity.

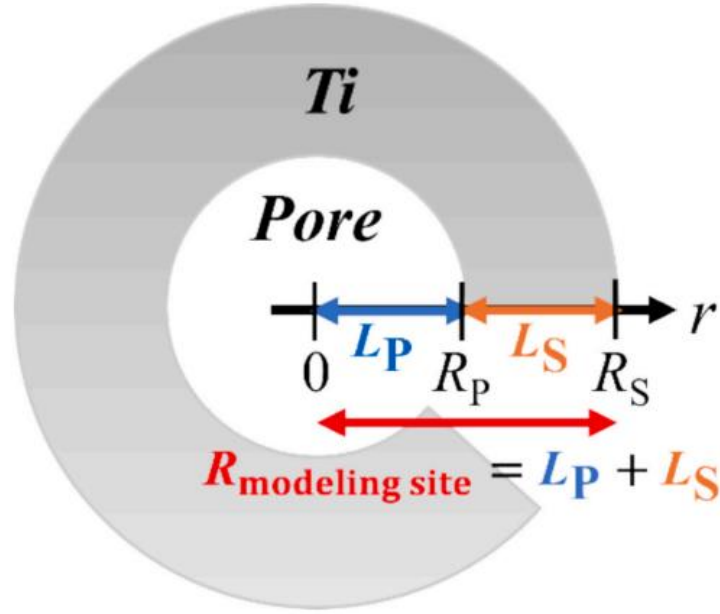


Figure 9. Top view of the computational domain. [78]

Zeng et al. [79] built a macroscale performance model of PEMWE by coupling CL pore network. The CL model of anode and cathode is shown in Figure 10. The results indicate that larger radius of the anode catalyst layer particles results in worse PEMWE performance, since larger particle size reduces the catalyst loading. However, larger particle size improves the conductivity of anode CL by increasing the effective electron transport path. Additionally, it is observed that the hydrogen mole fraction on the cathode side gradually decreases with the increase of anode CL particle size. This is because the increase of particle size impairs the PEMWE performance so less hydrogen is generated. Furthermore, the temperature decreases linearly with the increase of catalyst particle size. On the other hand, the increase of the pore diameter of the anode CL has a negative effect on the PEMWE performance (polarization curve), hydrogen generation and temperature distribution.

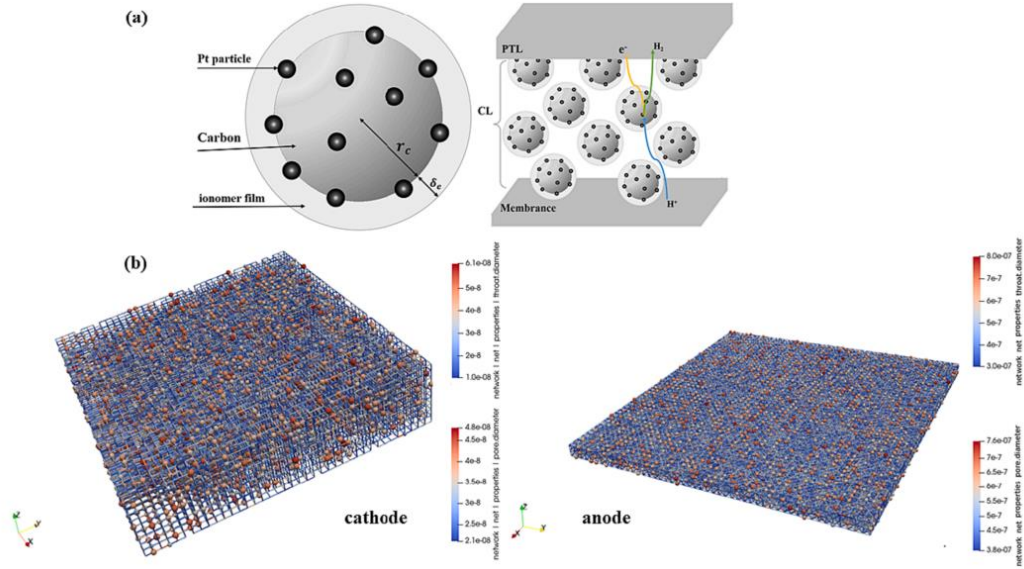


Figure 10. (a) Schematic of the structure model of the cathode CL. (b) Microstructures of the pore network of the cathode/anode CLs. [79]

PTL is a component that is widely investigated by researchers due to its function of mass transport and charge transport in PEMWE. Nouri-Khorasani et al. [80] presents a mathematical model to investigate the formation, growth, and detachment of oxygen bubbles inside the PTL of PEMWE cells. The model shows that a hydrophilic PTL and smaller pore sizes leading to decreasing bubble overpotential in the cell. The decreasing trend of oxygen bubble overpotential and bubble lifetime with increasing PTL contact angle is observed. Wrubel et al. [81] developed a 2D Multiphysics model to simulate the multiphase transport in a PEMWE cell with thin foil PTL as Figure 11. The results indicate that larger pores are beneficial to both the oxygen evolution reaction and the membrane hydration due to the improved access of water to the anode catalyst layer. It prevents water flow through the membrane and decreases the reaction rate of oxygen evolution reaction. It also enhanced the oxygen gas transport in catalyst layer. In addition, a nonuniform water distribution is reported through the membrane because of the anisotropic periodic structure of the PTL pore array.

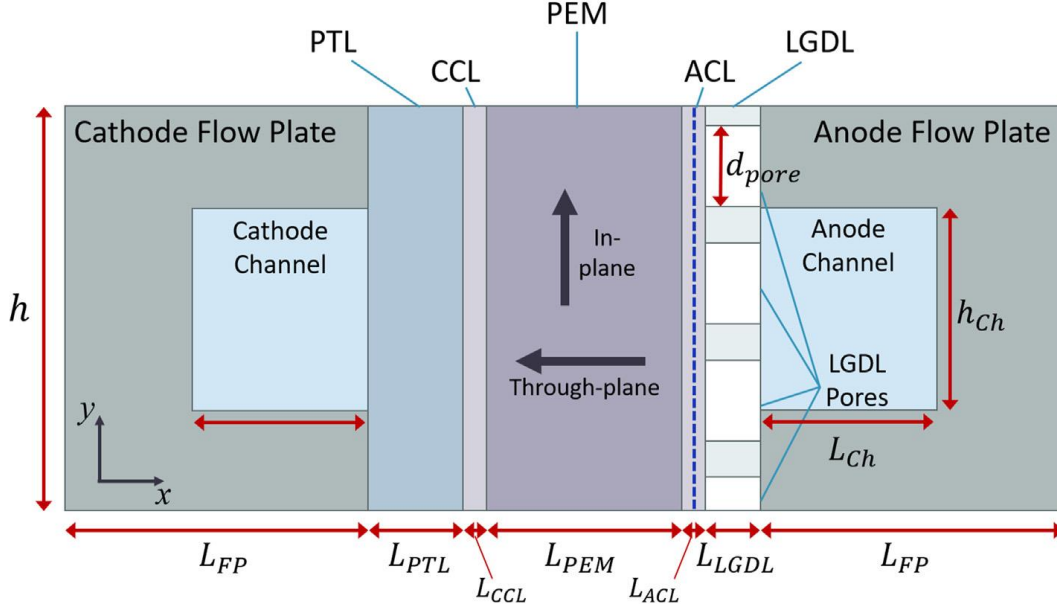


Figure 11. Geometric sketch of the components modeled in the 2D cell sandwich. [81]

Lee et al. [82] explored the effects of PTL-catalyst coated membrane (CCM) contact, pore and throat sizes and porosity on two phase transport by applied pore network modelling to PEM water electrolyzer. Figure 12 shows the schematics of contact between PTL and CCM and the inlet pores. Higher oxygen saturation is observed with increasing sizes of pores and throats. Higher porosity of PTL results in lower gas saturations and higher liquid water permeabilities. Additionally, the porosity gradient had essential influence on the two-phase permeabilities. The permeability increases from extremely low porosity (8%), while high gas saturation (85%) occurred at high porosities.

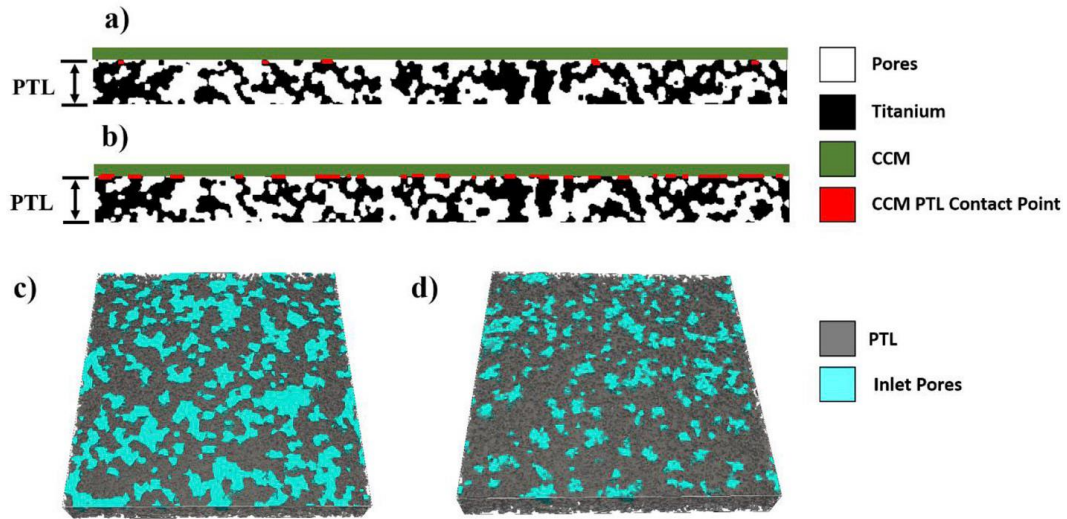


Figure 12. Schematic of contact between the PTL and CCM interface for (a) rough contact PTL, (b) full contact PTL and inlet pores of (c) rough contact PTL, (d) full contact PTL. [82]

Ito et al. [83] tested various titanium-felt substrate with different porosities and pore diameters. Figure 13 indicates the capillary flow porometry (CFP), which is used for pore diameter measurement. The results show that the electrolysis performance was enhanced with decreasing pore diameter when the mean pore diameter of the current collector was larger than 10 μm . On the contrary, the various porosities had no essential influence on cell performance when the porosity exceeded 0.50.

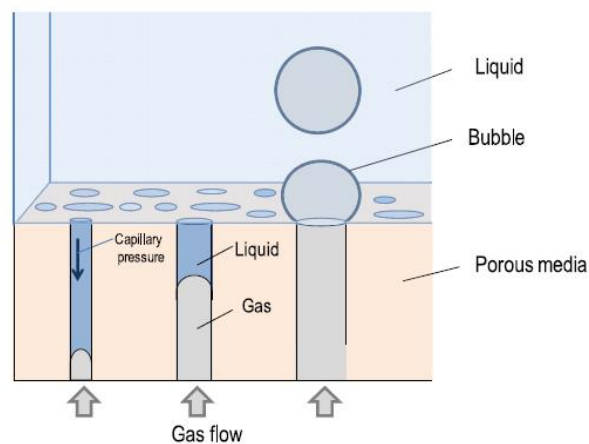


Figure 13. Schematic of capillary flow porometry (CFP) measurement. [83]

Zhou et al. [72] developed a three-dimensional, two-phase, single-channel PEMWE model which specified the bipolar plates, flow channels, gas diffusion layers and membrane, investigated the effect of contact angle and porosity of anode PTL. Figure 14 shows the computational domain and imposed boundary conditions of this study. The results indicate that liquid water saturation is decreasing from 0.75 to 0.57 with the increase of anode PTL contact angle from 20° to 80°, especially at high electric potential. In addition, the increase of anode PTL porosity leads to increasing liquid water saturation in anode CL. The current density and temperature in anode CL show a parabolic trend with the increasing anode PTL porosity, the highest current density can be observed in the porosity range of 0.5 to 0.6.

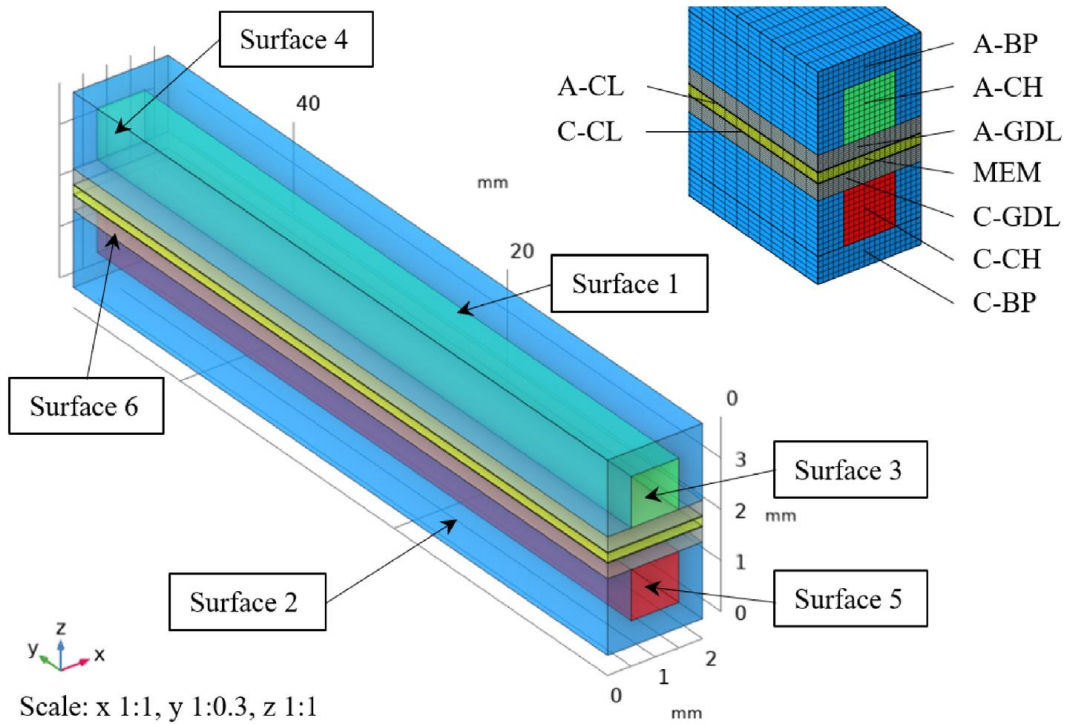


Figure 14. Computational domain and imposed boundary surfaces. [72]

Rakousky et al. [84] investigated the durability of a PEMWE for over 1000 h. A significant degradation rate of 194 $\mu\text{V h}^{-1}$ and 78% of the detectable degradation were observed and explained by the increasing ohmic resistance. The increase of ohmic cell resistance is because of the anode PTL passivation, a Pt-coated PTL was also tested and shown lower degradation rate. Aubras et al. [85] established a 2D stationary PEMWE model to investigate the

relationship between anode two phase flow and cell performance. It demonstrates the water management has significant relationship with the Not Coalesced Bubble regime (NCB regime) and the Coalesced Bubble regime (CB regime). The simulation results indicate that the coalesced phenomenon leads to the improvement of mass transfer, lower ohmic resistance and higher PEMWE efficiency. The study also found the NCB regime and the void fraction in the channel are affected by the anode porous media porosity. A higher porosity will lead to the enhancement of the PEMWE. Han et al. [86] developed a mathematical model to simulate the two-phase flow and performance of a PEMWE by considering the effects of contact angle, porosity and pore size in liquid/gas diffusion layer (PTL). The results indicate that higher porosity and pore size results in enhanced liquid water saturation. In addition, increasing pore size can improve the efficiency of PEMWE and this effect is more obvious under high current density.

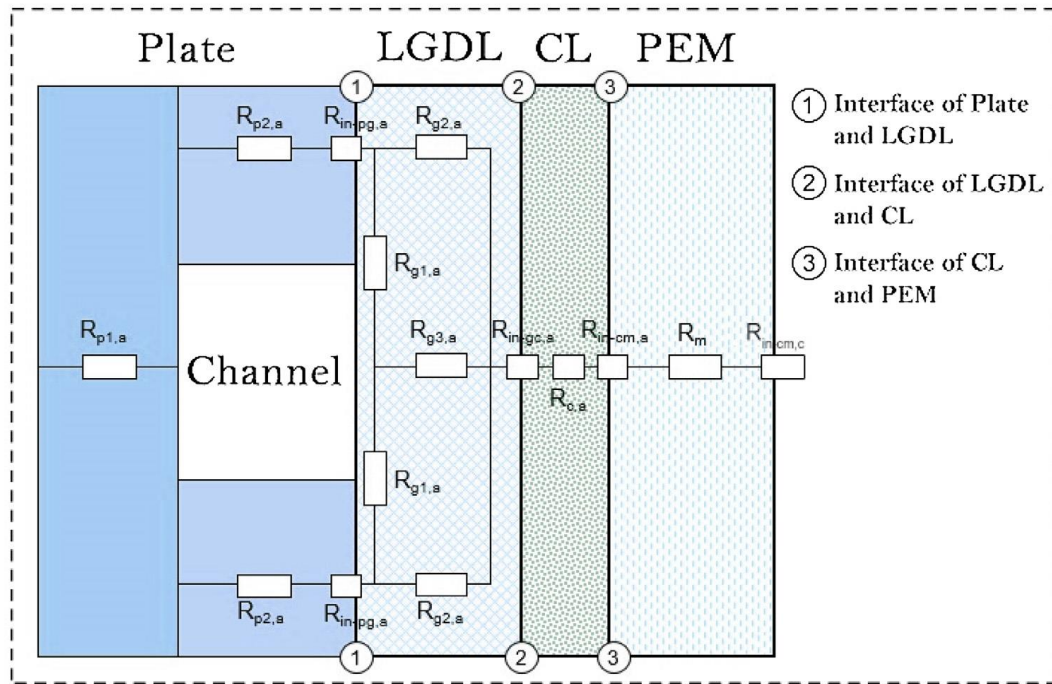


Figure 15. Ohmic loss calculation model of a single PEMWE anode. [86]

Li et al. [87] investigated the micro oxygen bubble dynamic behavior and two-phase flow by using a high-speed camera coupled with a specific PEMWE, which has a liquid/gas diffusion layer with straight-through pores. The results indicate that the bubble growth rate in PTL is

strongly relative to the temperature and current density. In contrast, the effects of flow rate are very limited. In addition, higher temperature and current density also increase the number, growth rate, nucleation site, and slug flow regime of oxygen gas bubbles, which means that it can improve the oxygen production efficiency. Kang et al. [67] built a mathematical model to investigate the effects of ohmic, activation, diffusion and Nernst potential by considering PTL material, structure and wettability. The results indicate that shifting OTL wettability to more hydrophobic leads to the increase of diffusion, ohmic and activation loss, especially diffusion loss. Liu et al [88] tested the PEMWE performance with intentionally incomplete Pt coatings on Titanium PTL. Figure 16 shows the schematic of coating gaps. It is observed that the cell voltages are increasing with the decrease of coated PTL, since the high frequency resistance (HFR) increases while the catalyst utilization decreases. In addition, both narrower gaps in the PTL coating and lower electronic resistance of the CL results in the mitigation of voltage impacts from PTL gaps.

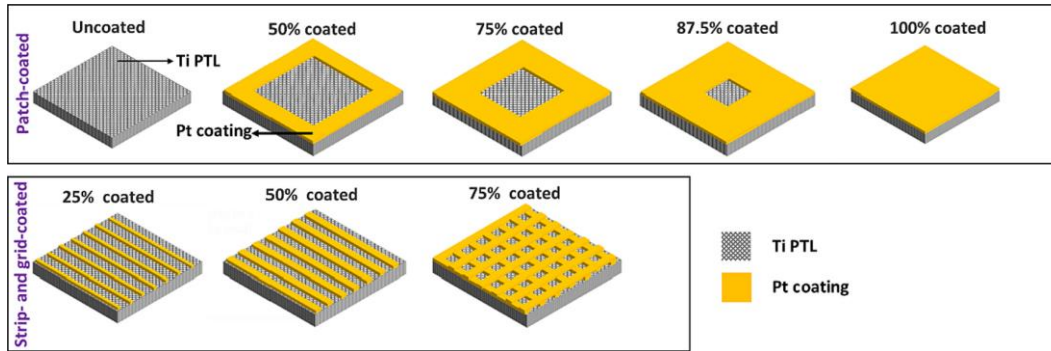


Figure 16. Schematic of coating gaps on the PTL facing to the catalyst coated membrane (CCM) side. [88]

Fu et al. [89] established a numerical framework for PEMWE by incorporating PTL pore structure reconstruction. The results show that it is more effective for permeability enhancement than porosity increase when the fiber diameter is increased. In addition, the two-phase simulations indicate that gas transport efficiency is significantly dominated by the localized pore characteristics. The process of oxygen transport is governed by the number and location of nucleation sites on CL surface, contact angle and pore sizes. Furthermore, the

increase of PTL porosity increases the temperature due to the enhancement of PTL thermal conductivity.

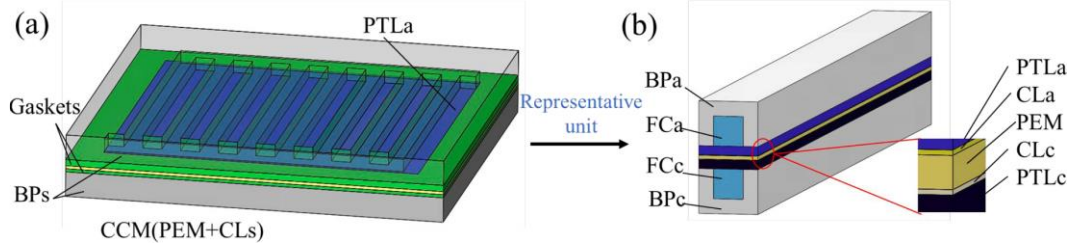


Figure 17. Computational domain of (a) cell model and (b) single channel model. [89]

Kang et al. [90] investigated the effects of interfacial contact properties between PTL and CL on PEMWE performance. The cell is significantly less sensitive to the heat distribution issues if the PTL is coated and the interfacial properties between PTL and CL are optimized, since it mitigates the ohmic loss and heterogenous. Bhaskaran et al. [91] implemented Shan-Chen Lattice Boltzmann method (LBM) to investigate the oxygen invasion of Titanium felt PTL. Higher final overall oxygen saturation is observed for cases which have more homogeneous pore size and porosity distribution. In addition, the saturation profiles are significantly affecting the transport properties. Furthermore, the mass transfer loss can be reduced if the water and oxygen distribution along the height of PTL can be more homogeneous. Xu et al. [92] optimized the structure of PTL to improve the PEMWE performance. The results show that the single-phase permeability of PTL is essentially increased with the reduction of PTL thickness. The transmission flux is improved with the increasing pore size and porosity; however, interface contact is decreased simultaneously.

The flow channels are the space that is provided for fluid including water, oxygen and hydrogen, which have the function of water introduction and gas removal. The investigations of flow channels are mainly focusing on the geometrical parameters and flow patterns. Lin et al. [93] explored the impact of flow field design on PEMWE performance through both numerical simulations and experiments. The study evaluates three flow field structures, which are parallel, serpentine, and point flow fields. The structures of the three different flow fields are shown in Figure 18. The flow velocity, pressure distribution, and electrochemical behavior are analyzed. Results indicate that the parallel flow field provides the best performance due to

its uniform pressure distribution and lower contact impedance, particularly at 60 °C and 0.1 bar anode pressure, where the electrolyzer achieves 2.1 V at 1 A cm⁻². The serpentine flow field enhances mass transfer but suffers from pressure drops and bubble accumulation, while the point flow field has uneven pressure distribution and higher impedance. The study confirms that flow field structure is the most critical factor affecting PEMWE efficiency, more so than operating temperature or water pressure, providing valuable insights for optimizing PEMWE design.

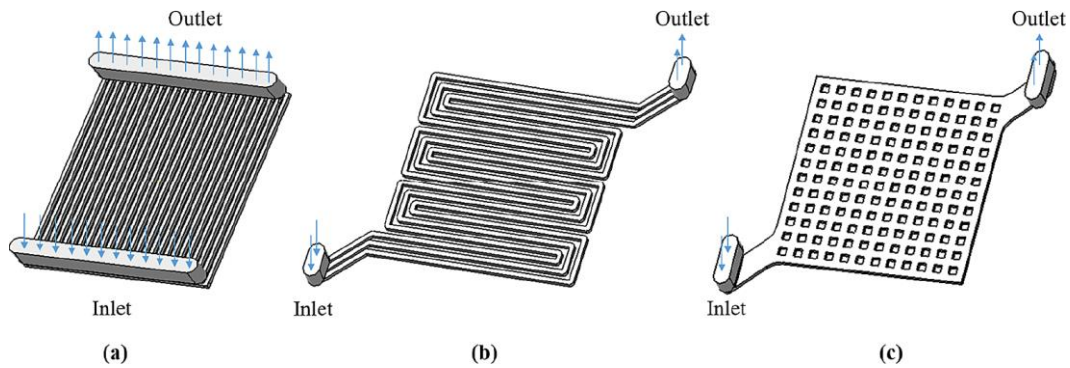


Figure 18. The structure of the three different flow fields (a) parallel flow field; (b) serpentine flow field; (c) point flow field. [93]

Hassan et al. [60] investigated the performance of five different circular-shaped flow field (Figure 19) to optimize the flow pattern with several parameters, such as velocity, pressure, temperature and current density distribution, it also decreases the thermal and enhances the lifespan of PEMWE. The results show the one-path serpentine pattern provides the most superior uniformity and temperature distribution in PEMWE. The uniformity of temperature and current density distribution were enhanced with increasing flow field. The voltage efficiency and polarization performance of the two-path, two-segment, and four-segment serpentine flow patterns demonstrate commendable results, further complemented by favorable pressure drop characteristics. Moreover, the four-segment, two-segment, and two-path serpentine flow patterns yield the most favorable polarization curve performance, achieving a current density that is 7.5% higher than the poorest polarization performance observed at a cell voltage of 2.1 V.

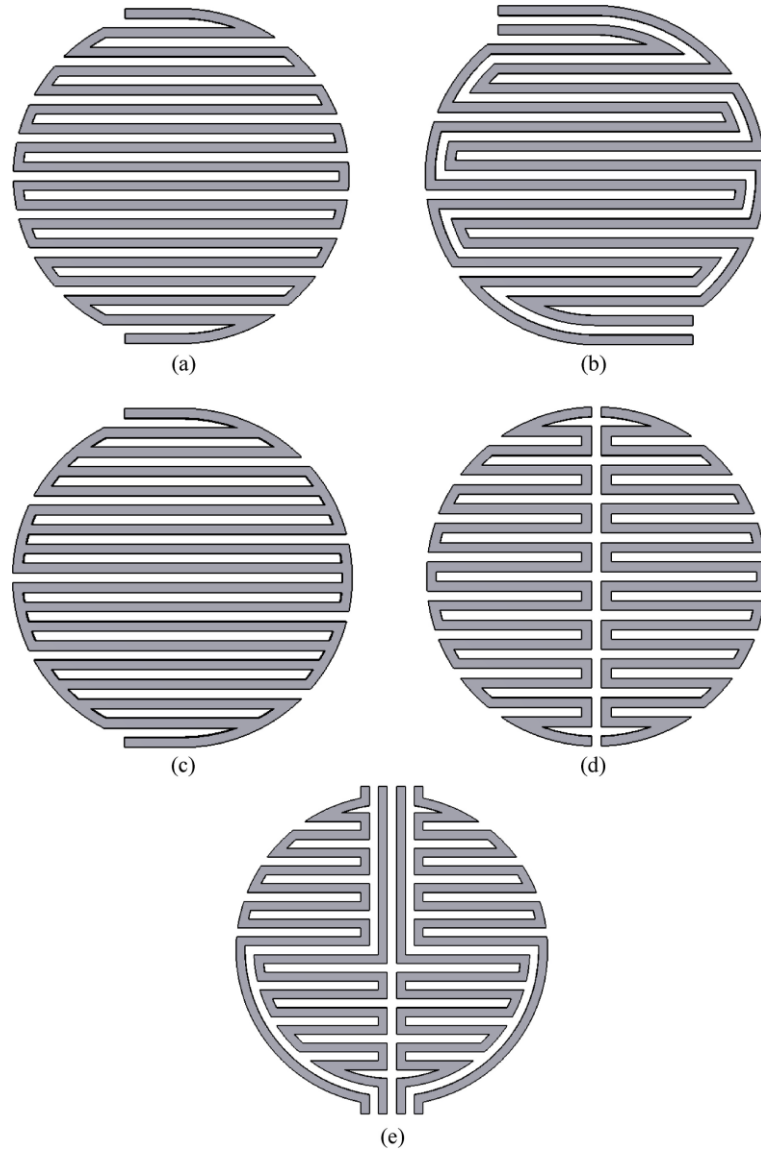


Figure 19. 2D schematics of different flow patterns, including (a) one-path, (b) two path, (c) two-channel, (d) two-segment, and (e) four-segment serpentine flow patterns. [60]

Toghyani et al. [94] developed a three-dimensional model of a PEMWE system incorporating metal foam as a flow distributor (referred to as Model C). The performance of this configuration was compared with three alternative designs: a parallel flow field (Model A), a double-path serpentine flow field (Model B), and a simple channel incorporating metal foam (Model D). Simulation results indicated that Model D exhibited the most favorable

performance, attributed to its lower temperature gradient, improved uniformity in current density, and more consistent hydrogen mass fraction. Moreover, the configurations incorporating metal foam demonstrated superior temperature uniformity compared to those without it.

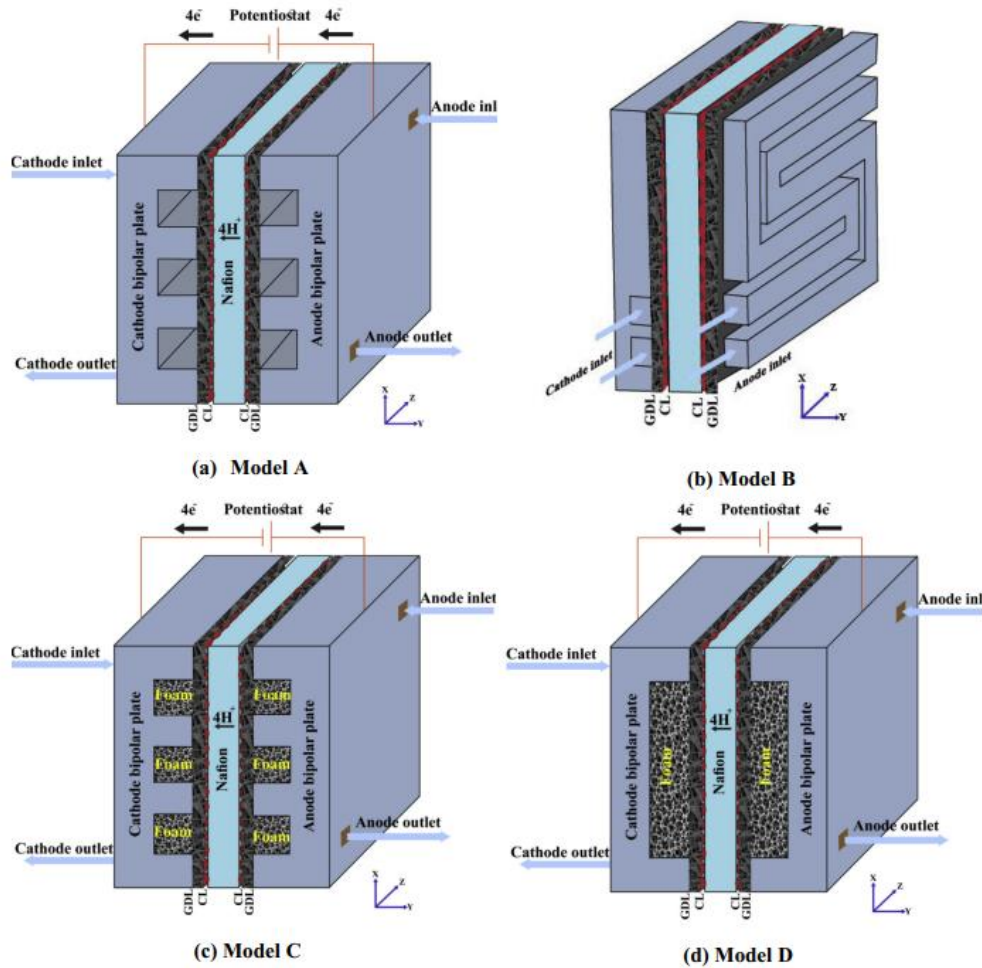


Figure 20. Schematics of different flow patterns (a) parallel flow pattern, (b) dual path serpentine pattern, (c) parallel pattern with nickel foam as flow distributor, and (d) channel with merging ribs and nickel foam as flow distributor. [94]

Zhuang et al. [51] conducted a numerical investigation into the influence of flow channel height and width using a three-dimensional, non-isothermal PEMWE channel model, which is shown in Figure 21. The mole fractions of oxygen and hydrogen are increasing with the increase of channel height from 0.3 mm to 1.5 mm, while the pressure drop in the electrodes

shows an opposite trend. In addition, the increase of channel width from 0.3 mm to 1.5 mm results in the reduction of the mole fractions of oxygen and hydrogen and the flow velocity. Building upon the analysis of a single-channel configuration, a comprehensive PEMWE model comprising five channels was developed. The dimensions of each channel were optimized using a genetic algorithm (GA), with the objective of minimizing pressure drop under low-voltage operating conditions. The study concluded that channel width has a more significant impact on cell voltage compared to channel height. It was also found that increasing both the height and width of the channels led to higher gas fractions and cell voltages, while simultaneously reducing pressure drop. The optimized design achieved a 34.97% reduction in pressure drop under low-voltage conditions.

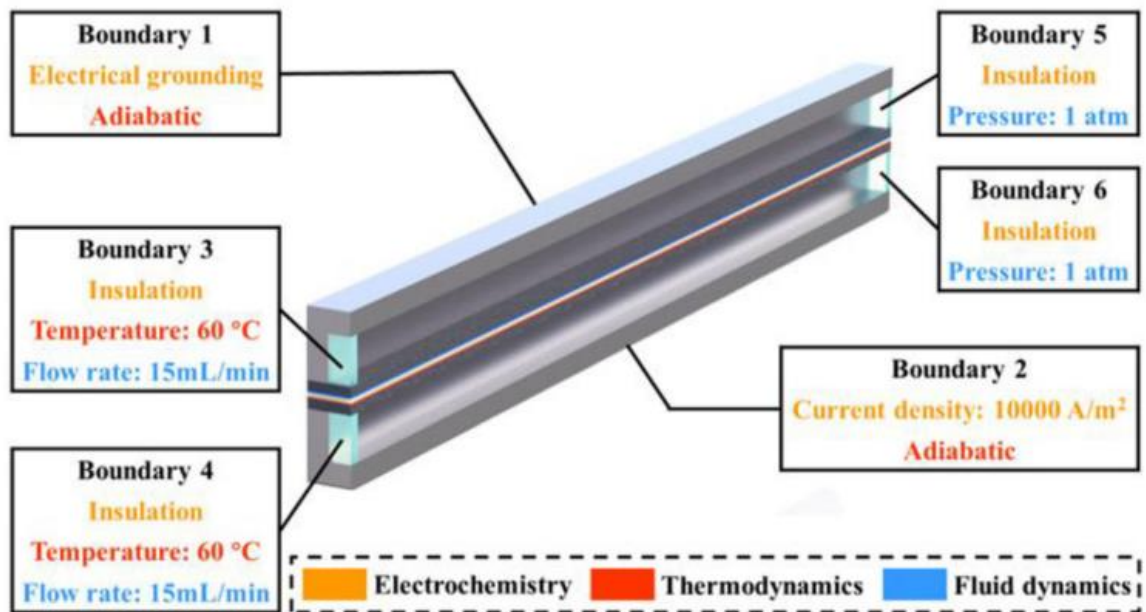


Figure 21. Boundary modifying and corresponding boundary conditions. [51]

Lafmejani et al. [95] investigated gas-liquid two-phase flow behavior within the flow channels of an interdigitated PEMWE using the Volume of Fluid (VOF) method. While the model did not incorporate electrochemical reactions, a stable gas source was introduced at the interface between the anode PTL and the CL to simulate gas generation. The simulation results indicated that the wall film thickness varied along the channel height due to differences in phase

superficial velocities from the bottom to the top of the outlet channel. Moreover, the presence of longer Taylor bubbles contributed to a more uniform distribution of liquid flow within both the channels and the PTL. Olesen et al. [96] investigated the performance of a high-pressure PEMWE with circular-planar, interdigitated anode flow field, which is shown in Figure 22. The results indicate the presence of the gas phase affects the maldistribution in the liquid flow, which leads to the formation of hotspots. In addition, approaching equal in-plane cross sectional land area sizes can reduce the mass flow maldistribution. Moreover, reducing the channel bending can minimize the formation of hotspots around the widest land areas.

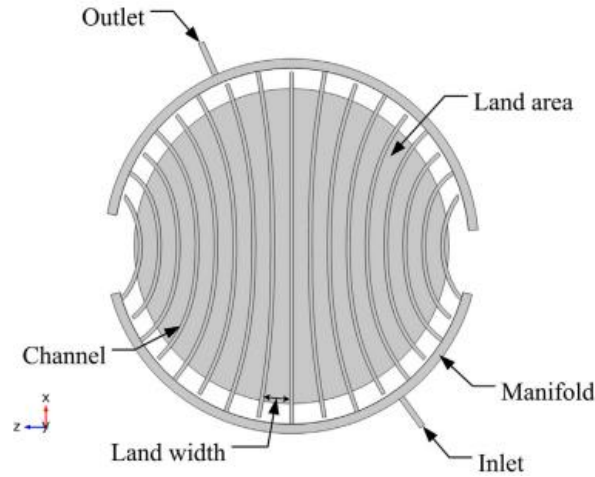


Figure 22. Anode planar-circular flow field. [96]

Chen et al. [97] proposed a new interdigitated-jet hole flow field (JHFF) of PEMWE, while a 3D, two-phase model is developed in this study to simulate this flow field and explore the effects of structural parameters. The application of JHFF on both anode and cathode side results in an increase of temperature uniformity and polarization performance by 41.78% and 16.25%, respectively. A further uniform temperature distribution can be achieved while a greater number of inlet flow channels and counter-flow water supply are applied. The decreasing of jet holes height leads to better normal mass transfer and polarization performance, but it reduces the uniformity of temperature distribution in contrast. The diameter of the jet holes is also found to have influence of the normal mass transfer. Furthermore, 0.2

mm hole height and 0.4 mm hole diameter are recommended by simulations of different structural parameters.

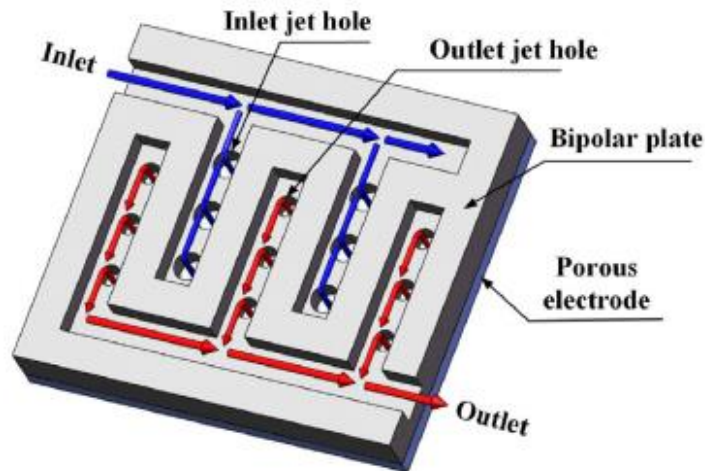


Figure 23. The schematic of the jet hole flow field (JHFF). [97]

Olesen et al. [62] established a 3D anode-side model to investigate the effect of flow field design on heat, mass and charge uniformity. Figure 24 demonstrates the three circular, integrated anode geometries. It is observed that the cell performance in terms of cell voltage and cell current density is not affected by the flow field design; however, the different design results in different irreversible degradation of the PEM due to the temperature variations. Additionally, Case A provides the most uniform temperature distribution and current density within the three designs, while a design of slight bent channels with uneven distribution land area width is recommended.

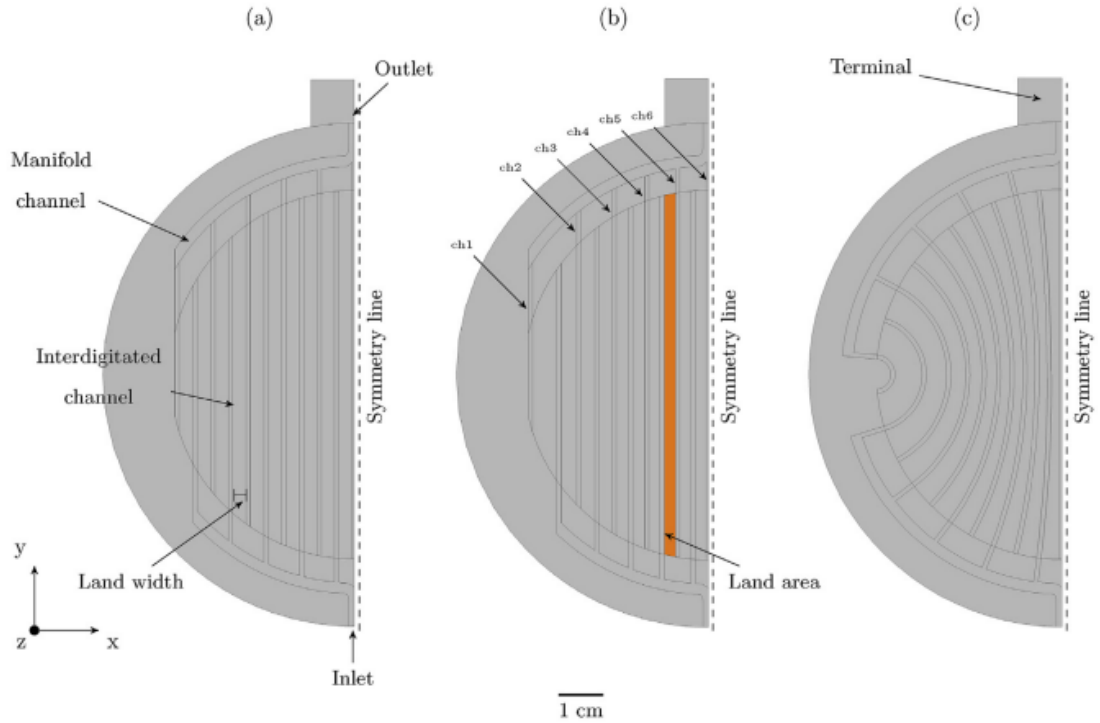


Figure 24. Flow field design of (a) equal land width, (b) equal land area, and (c) equal half area with half the area of case b. [62]

Li et al. [98] tested the effects of different flow-field patterns - serpentine, parallel and cascade – on PEMWE performance under 120 °C high temperature. The results indicate that the cathode flow-field pattern only affects ohmic resistance, while the serpentine flow-field pattern has the lowest ohmic resistance due to the creation of under-rib flow. On the other hand, the anode flow-field pattern essentially affects the overpotential and cascade flow-field pattern reduces the overpotential. Furthermore, a little impact on PEMWE performance is observed for flow configuration variations.

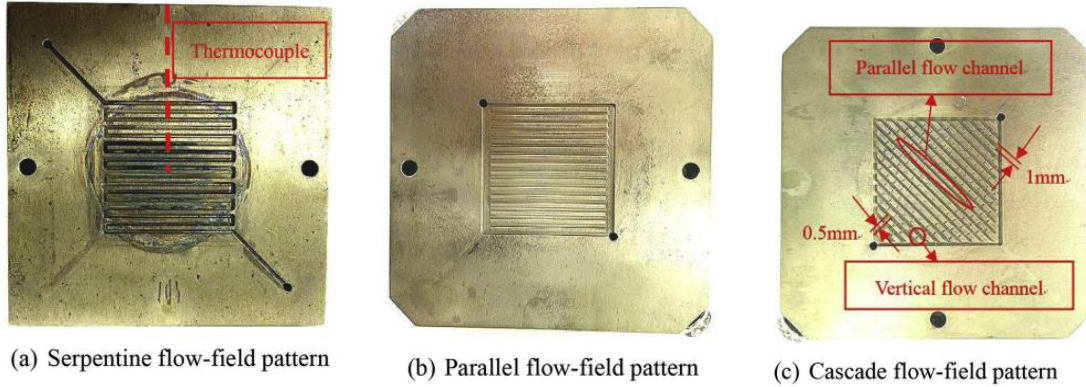


Figure 25. Three conventional flow-field patterns used in this study. [98]

He et al. [99] investigated the difference between triple serpentine flow field (TSFF) and parallel flow field (PFF) by experiments. Based on the polarization curves, PEMWE with PFF has less voltage degradation than TSFF. Additionally, TSFF results in higher ohmic resistance and anodic charge transfer resistance compared to PFF. He et al. [100] evaluated the PEMWE performance and water-gas transport characteristics with different cell structures, including parallel flow field (PFF), sinusoidal wave flow field (SWFF), intercepted flow field (ICFF), and single-serpentine flow field (SSFF). PFF has more nonuniform flow and temperature distribution; however, the higher average temperature of PFF provides a slightly worse polarization curve compared to SWFF and ICFF. The technique for order preference by similarity to ideal solution (TOPSIS) based on entropy weight method indicates the SWFF is the metric that fits the best solution, and following are ICFF, SSFF, while PFF is the worst one.

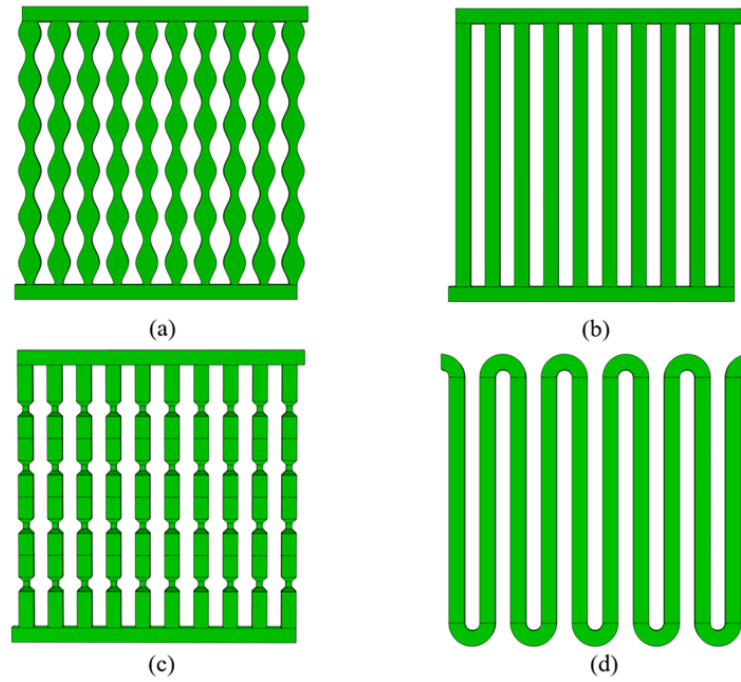


Figure 26. Schematics of (a) sinusoidal wave flow field (SWFF), (b) parallel flow field (PFF), (c) intercepted flow field (ICFF), and (d) single-serpentine flow field (SSFF). [100] Zhou et al. [101] investigated the bubble mitigation behavior and mass transfer capacity with various parameters in PEMWE. The results indicate that the increase of anode flow channel depth results in the decrease of mass transport overpotential. In addition, a hydrophobic anode flow channel wall improves the contact between bubbles and the flow channel upper wall, which leads to less bubble coverage on the bottom wall.

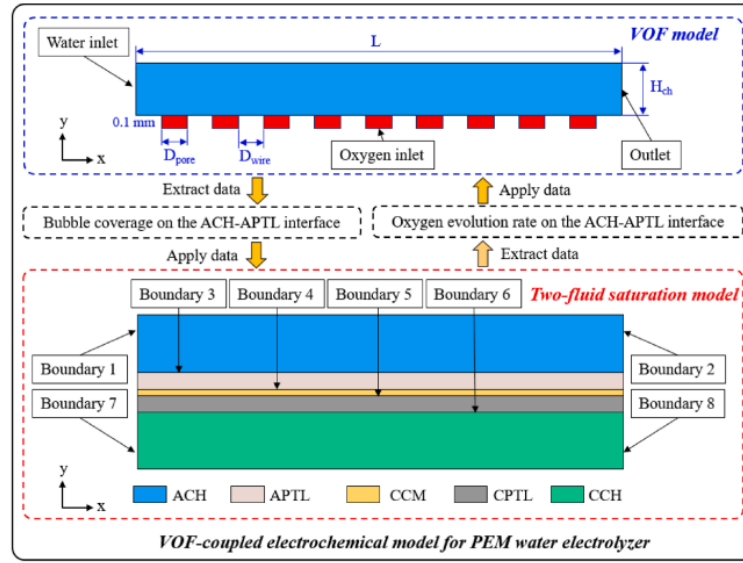


Figure 27. Schematics of the volume of fluid (VOF)-coupled electrochemical model. [101]

BPPs provide mechanical support, enable current collection and distribution, and integrate flow field designs that regulate fluid dynamics and heat transfer, making them indispensable for the structural and functional integrity of PEMWE stacks. Yang et al. [102] proposed an innovation on fundamental material and structure using additive manufacturing (AM), which increase the energy efficiency and reduce the weight of the PEMWE. Four components of a PEMWE (liquid/gas diffusion layer, bipolar plate, gasket and current distributor) were manufactured in a multifunctional AM plate. The characterizations of the cells indicate excellent energy efficiency and high current density, which are up to 86.48% and 2 A cm^{-2} , respectively. The hydrogen production rate also increases by 61.81% against conventional cells. These results demonstrate the feasibility of using AM technology to produce the PEMWE components and improve performance, providing a new solution of green energy development. Gago et al. [103] replaced costly BPP by stainless steel with dense titanium coating, the coatings are produced by vacuum plasma spraying (VPS). Additionally, further surface modification is completed with Ti coating and Pt (8 wt% Pt/Ti) deposited by physical vapor deposition (PVD). The coatings are characterized by several methods. The results show the coatings can protect the substrate well. But the coating with Pt only has the

issue of pitting corrosion since the absence of the thermally sprayed Ti layer. The coatings show great conductive and corrosion-resistant features, also provide a lower thickness.

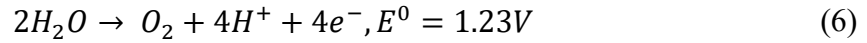
Notably, the preceding studies employ significant simplifications of PEMWE assembly, although their explorations of geometrical parameters are important. These studies either simplify the component dimension to 1D/2D or only focus on the anode side/single flow channel of PEMWE. In practical, a 3D full-scale PEMWE with both cathode and anode introduces complexities arising from spatial transport of heat, mass and momentum on both electrodes, which are essential for evaluating the hydrogen production rate, current density and temperature distribution of PEMWE. Therefore, a full-scale PEMWE model should be developed to better evaluate the effects of geometrical design on performance and durability of PEMWE.

3. Methodology

3.1 Model Formulation

3.1.1 Model Development

Figure 28a shows the physical and electrochemical process within a PEMWE cell. The cell includes both an anodic and cathodic side, partitioned by a PEM. Each of the two electrode sides includes two mechanical components: BPP and PTL. The CCM component consists of a PEM and CL coated on the membrane. During operation, water is introduced to the anode flow channels built on the BPP, and transports through PTL to reach the anode CL. The water generates oxygen, protons and electrons through the oxygen evolution reaction (OER):

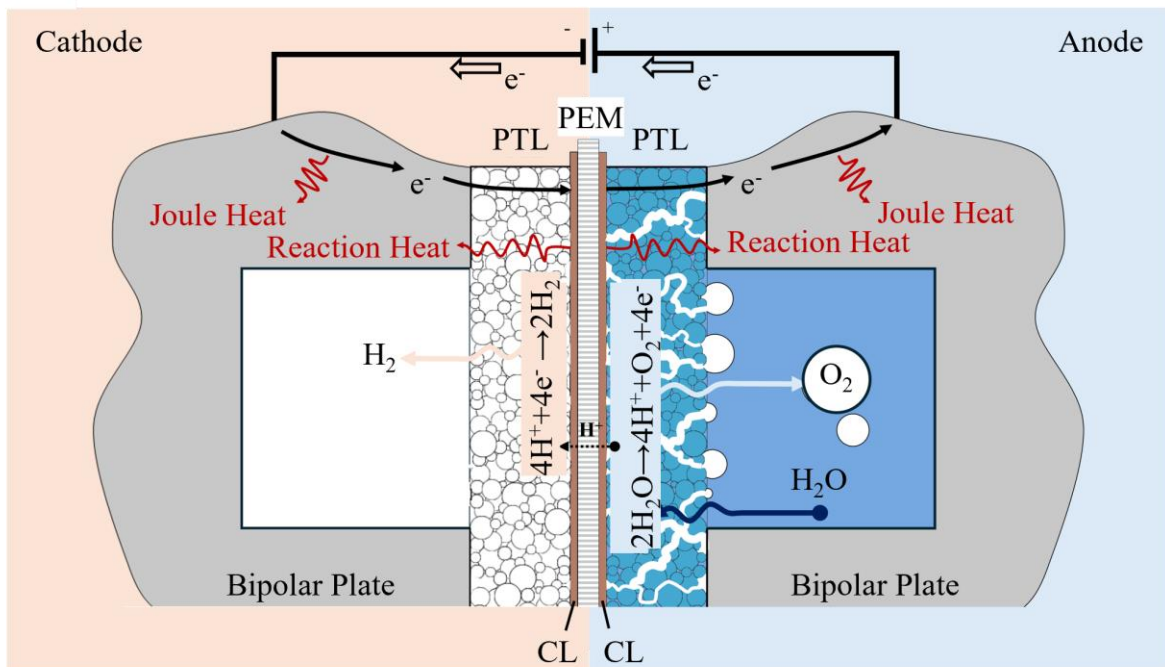


The produced oxygen gas is transported through PTL to form bubbles in the channel, which are then removed by water flow. The proton is transported through PEM, and the electrons transit through the external circuit, passing through anode PTL, anode BPP, power supply, cathode BPP and cathode PTL. The protons and electrons reach the cathode CL, and the hydrogen evolution reaction (HER) occurs:



The produced hydrogen then flows out of cells through the pores of the CL and PTL and then to be collected through the cathode flow channels.

During the preceding process, heat is generated in CL due to electrochemical reactions and in PTL and BPP due to Joule heating. As the PEMWE cell external surfaces are considered as thermally insulated without the existence of cooling systems [104], the generated heat is transported through convection due to fluid flow in BPP channels, which affects the temperature distribution across PEMWE components. In addition, the heating of CL also affects the electrochemical reaction rates through Arrhenius effects. Overall, modeling the above processes is necessary for achieving the objectives of this study, because fluid flow, charge transport, reaction and thermal effects are all important for hydrogen production and temperature distribution.



(a)

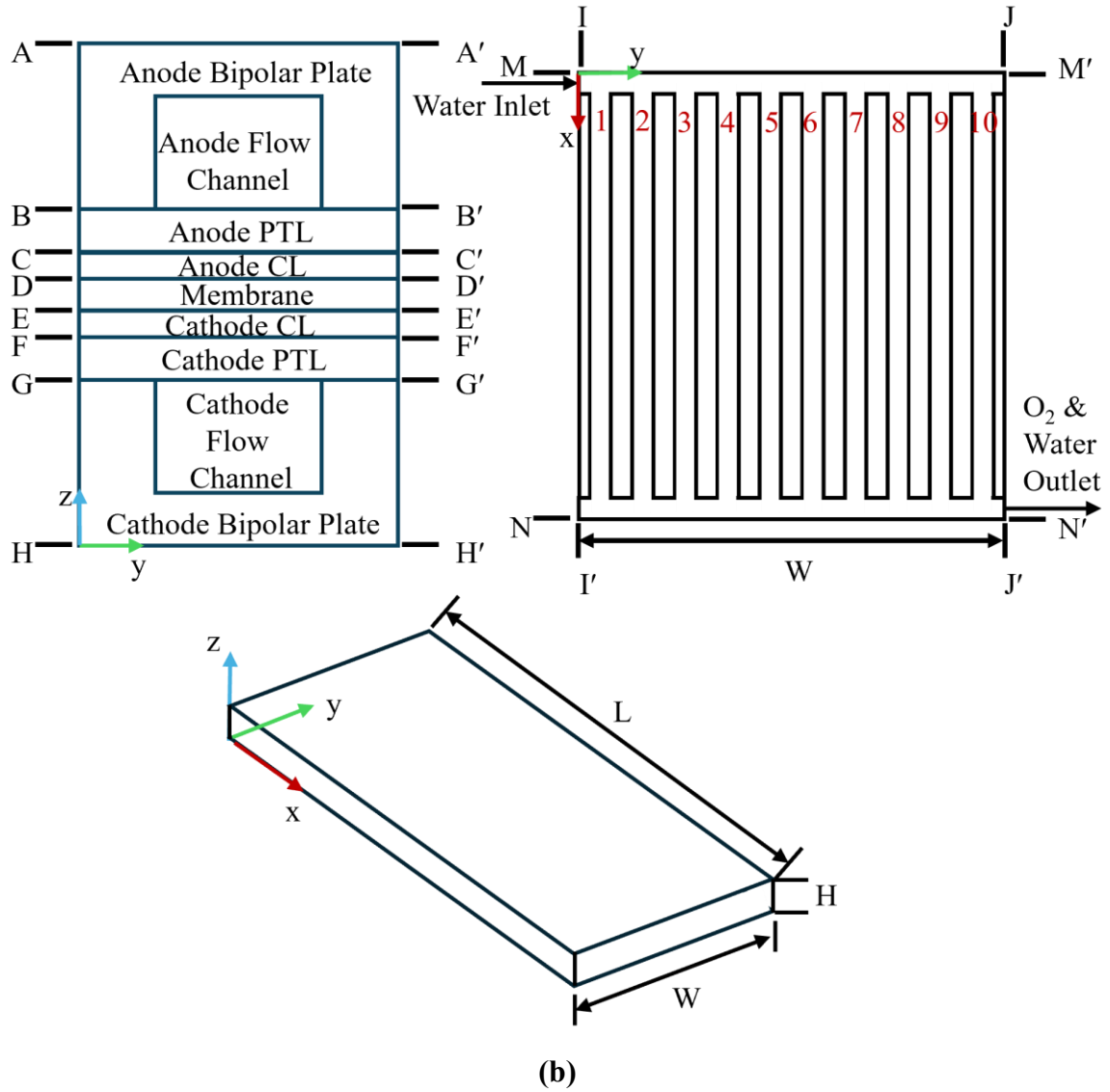


Figure 28. Introduction of proton exchange membrane water electrolyzer (PEMWE). (a) Schematic of PEMWE with mass transport, charge transport and heat transfer. (b) Computational model with cross-sectional views of xy plane ($z=2.818$ mm) and yz plane ($x=1$ mm). PTL denotes porous transport layer and CL denotes catalyst layer.

A physical model is developed to simulate the preceding processes in this study. As shown in Figure 28b, a full-scale PEMWE cell is selected as the computational domain, which includes the BPP, PTL and CL on both the anode and cathode side with the PEM sandwiched in-between. Each of the BPPs has a total of 10 parallel flow channels for fluid distribution, which are

connected to the inlet and outlet headers to receive reactants and discharge products. The rest of the components are placed between the two BPPs to form the single PEMWE cell. The following specific physical fields are considered in the present simulation:

- Fluid flow is considered in flow channels and PTL domains with liquid and gas phases. The two-phase flow on the anode side is considered as a mixture flow with density and viscosity obtained as the volumetric average of the gas and liquid phases. The water inlet is defined as a fully developed flow condition with a defined mass flow rate, and the boundaries of oxygen and water outlet and hydrogen outlet are assigned with fixed static pressures (specified inlet flow and outlet pressure condition). BPP flow channels are non-slip walls. In addition, the flow in PTL domain is simulated as a uniform and homogeneous porous medium without considering microscopic porous structures. The interface between the flow channel and PTL is governed by flow continuity conditions.
- Charge transport is considered in solid subdomains of CL, PEM, PTL and BPP. Specifically, CL, PTL and BPP are electron-conductive, and the contact resistance at their interfaces is neglected. Proton transport is considered across the CL and PEM domains. The interfaces between CL and PEM domains are electron insulated but proton conductive. The BPP are defined as charge conductive, used for electron transport. Other external surfaces are electrically insulated. The surfaces of BPP are specified electric potential and 0V electric ground for anode and cathode, respectively. The charge transport in the fluid phase of PTL and BPP channels is not considered because of the low ionic conductivity of liquid water.
- Mass transport occurs in the CL, PTL and flow channels. Convective mass transfer is modeled using the velocity obtained from the flow field. Diffusive mass transfer is considered based on the local concentrations of species, whereas the diffusivity in porous domains is corrected to include the effect of the porous solid structures. All external boundaries except the inlet and outlet are set to zero diffusive flux. The internal boundaries of the flow channels, PTL, and CL follow the continuity of concentration.
- Electrochemical reaction is considered in the anode and cathode CL. Current density is

used as input to the physical model. The reaction kinetics is modeled using current density from the charge transport. The temperature and concentration dependence of the reaction kinetics is considered based on the physical fields of heat and mass transport. As a result, the variation of chemical species is obtained as a mass source that further affects the mass transfer process.

- Heat transport is considered across all the components. The heat sources are 1) the reaction heat in the CLs, and 2) Joule heat from the PEM, CL, PTL and BPP domains due to electric current. Heat conduction is considered in solid and fluid phases, and heat convection is included in the fluid phases. All external surfaces of the entire computational domain are defined as zero conductive flux (of course, except the flow channel inlets and exits). Temperature continuity is applied to all the internal boundaries since interfacial heat transfer resistance is neglected. Heat convection boundary is introduced to the internal solid-liquid boundaries between BPP, PTL and flow channels.

Clearly multi-physics fields are involved and coupled with the electrochemical reactions within a PEMWE, multi-physics modeling needs to couple the multi-physics variables including velocity, pressure, current density, electric potential, overpotential, mass fraction, and temperatures with the rate of electrochemical reactions. The performance of a PEMWE, i.e., hydrogen production rate and temperature distribution, can then be investigated for various designs and operating conditions.

To formulate the mathematical model for the above described multi-physics fields along with electrochemical reactions in a PEMWE, the following assumptions are made:

1. The liquid/gas flow in the flow channels is laminar and incompressible.
2. Gravitational effects are neglected.
3. All physical fields are in steady states because the present study focuses on the steady output of hydrogen production and temperature distribution.
4. Electrical migration is neglected.

3.1.2 Governing Equations

3.1.2.1 Fluid Flow

The pressure and velocity in the flow channels are calculated using Navier-Stokes equations for 3D incompressible steady flow:

$$\text{Continuity} \quad \rho \nabla \cdot \mathbf{u} = 0 \quad (8)$$

$$\text{Momentum} \quad \rho(\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} \quad (9)$$

where $\mathbf{u}$ is the fluid velocity, p is the pressure. μ and ρ are the density and dynamic viscosity of the mixture fluid, and determined as follows:

$$\rho = \omega_l \rho_l + \omega_g \rho_g \quad (10)$$

where ω_l and ω_g are mass fractions of liquid and gas, respectively. ρ_l and ρ_g are densities of liquid and gas. The dynamic viscosity can be calculated by [105]

$$\mu = \frac{x_l \mu_l}{x_l + x_g t_{lg}} + \frac{x_g \mu_g}{x_g + x_l t_{gl}} \quad (11)$$

where t_{lg} and t_{gl} are coefficients which are defined based on the molar mass of species, the coefficients are defined as [105]

$$t_{lg} = \frac{\left[\frac{4 \cdot M_l \cdot M_g}{(M_l + M_g)^2} \right]^{0.25}}{\sqrt{\frac{M_l}{M_g}}} \left\{ 1 + \frac{\frac{M_l}{M_g} - \left(\frac{M_l}{M_g} \right)^{0.45}}{\left[2 \left(1 + \frac{M_l}{M_g} \right) + \frac{1 + \left(\frac{M_l}{M_g} \right)^{0.45}}{\left(1 + \frac{M_l}{M_g} \right) \sqrt{\left[\frac{4 \cdot M_l \cdot M_g}{(M_l + M_g)^2} \right]^{0.25}}} \right]} \right\} \cdot \sqrt{\frac{\mu_l}{\mu_g}} \quad (12)$$

The relationship between mass fraction and mole fraction can be expressed as:

$$x_1 = \frac{\omega_1}{M_1 \left(\frac{\omega_1}{M_1} + \frac{\omega_g}{M_g} \right)} \quad (13)$$

For the porous domain of CLs and PTLs, the momentum equation is modified to Brinkman equation that describes the two-phase percolation within the porous structures [106]:

$$\rho \nabla \cdot \mathbf{u} = S \quad (14)$$

$$\begin{aligned} \frac{\rho}{\varepsilon^{\text{eff}}} (\mathbf{u} \cdot \nabla) \frac{\mathbf{u}}{\varepsilon^{\text{eff}}} = & -\nabla p + \frac{1}{\varepsilon^{\text{eff}}} \nabla \cdot \left[\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right] \\ & - \left(\frac{\mu}{K_0 k_{rl}} + \frac{S}{(\varepsilon^{\text{eff}})^2} \right) \mathbf{u} \end{aligned} \quad (15)$$

where S is the mass source term due to oxygen generation, which is non-zero for CL and equals to 0 in PTL subdomains. ε^{eff} is the effective porosity of porous medium, which is related to the porosity $\varepsilon^{\text{eff}} = a \cdot \varepsilon^b$ [107]. K_0 is the absolute permeability and k_{rl} is the Corey correlation for water $k_{rl} = s^4$ [108]. s is the saturation of gas, which is defined as the percentage of gas in the pores of the porous media. s is defined based on Van Genuchten equations [109]

$$s = \begin{cases} (1 + |\alpha H_p|^n)^{-m}, & H_p < 0 \\ 1, & H_p \geq 0 \end{cases} \quad (16)$$

where α is the inverse of air entry pressure, n, m are constant and depend on medium type. H_p is the pressure head, defined as $H_p = p/(\rho g)$. It should be noted that gas and liquid phases are calculated separately because of their distinct saturation s that follows $s_l = 1 - s_g$.

3.1.2.2 Charge Transport

The transport of charge follows charge conservation and Ohm's law, which are written as follows:

$$\nabla \cdot (-\sigma \nabla \varphi_s) = -i_{v,\text{tot}} \quad (17)$$

$$\nabla \cdot (-\kappa \nabla \varphi_1) = i_{v,\text{tot}} \quad (18)$$

where σ is the electrode conductivity (S cm^{-1}), φ_s is the electric potential, κ is the ionic conductivity of the electrolyte, φ_1 is the electrolyte potential, and $i_{v,\text{tot}}$ (A cm^{-3}) is the volumetric current density contributions. In addition, φ_s and φ_1 only exist in solid phase and liquid phase, respectively. The conductivity of PTL and CL are corrected by porosity since they are porous medium. For the PEM subdomain, the conductivity is determined as [110], [111]:

$$\kappa = \kappa_{\text{ref}} \times \exp \left[\frac{E_a}{R} \left(\frac{1}{303} - \frac{1}{T} \right) \right] \quad (19)$$

where κ_{ref} is the reference conductivity with the value of 0.1 S cm^{-1} [112], [113], E_a is the activation energy for proton transport with the range of $9\text{-}15 \text{ kJ mol}^{-1}$ [111]. These values are for Nafion 117 membrane. T is the temperature with unit K .

3.1.2.3 Electrochemical Reactions

The preceding charge transport field requires the total volumetric current density $i_{v,\text{tot}}$, which can be calculated by the Butler-Volmer equation.

$$i_{v,\text{tot}} = i_0 A_V \left[\exp \left(\frac{\alpha_a n F \eta}{RT} \right) - \exp \left(- \frac{\alpha_c n F \eta}{RT} \right) \right] \quad (20)$$

where i_0 (A cm^{-2}) is the exchange current density, which is the current density at equilibrium. A_V (m^{-1}) is the reactive surface area density which is defined as actual reactive surface area divided by volume of electrode [114]. α_a and α_c are the forward and backward charge transfer coefficients, which are properties of domain materials. R is the universal gas constant, T is the temperature, η is the overpotential. Specifically, the exchange current density is calculated by mass action law [115]:

$$i_0 = n F k^0 (C_O)^{\alpha_c} (C_R)^{\alpha_a} \quad (21)$$

where n is the number of electrons transferred, k^0 (cm s^{-1}) is the standard rate constant, C_O and C_R are the concentration for oxidant and reductant, respectively. The concentrations can be calculated based on the mass fraction:

$$C_O = \frac{\omega_O \rho}{M_O} \quad (22)$$

where ω_O is the mass fraction of oxidant and M_O is the molar mass of oxidant. The membrane is assumed to be fully hydrated so the concentration of proton is constant, which is around 1300 mol m^{-3} . And E_{act} (J mol^{-1}) is the corresponding activation energy. In addition, the overpotential η is calculated as the difference between the electrode potential, electrolyte potential and equilibrium potential as follows:

$$\eta = \varphi_s - \varphi_l - E_{\text{eq}} \quad (23)$$

where φ_s and φ_l are the potential of the electrode and electrolyte, which are determined according to the charge transport equations [116]. E_{eq} is the equilibrium potential, which is defined by the Nernst equation [117]:

$$E_{\text{eq}} = E_{\text{eq,ref}} - \frac{RT}{nF} \ln \left(\frac{c_{H_2} c_{O_2}^{1/2}}{c_{H_2O}} \right) \quad (24)$$

where c_{H_2} , c_{O_2} and c_{H_2O} are the concentrations of hydrogen, oxygen and water, respectively, obtained from the conservation of species equation.

3.1.2.4 Mass Transport

The mass transport is calculated by the following mass conservation equation with consideration of mass convection and diffusion:

$$-\nabla \cdot D_{\text{gl}} \nabla (\rho \omega_g) + \rho (u \cdot \nabla) \omega_g = R_g \quad (25)$$

where D_{gl} is the binary diffusivity of gas in the surrounding fluid, ω_g is the mass fraction of gas, and R_g is the mass source due to electrochemical reactions for gas. For flow channel subdomains, the diffusivity D_{gl} is calculated according to the Fuller–Schettler–Giddings model [105]:

$$D_{\text{gl}} = \frac{1.01325 \times 10^{-2} T^{1.75} \sqrt{\frac{1}{M_g} + \frac{1}{M_l}}}{P \left[(\sum_g v)^{\frac{1}{3}} + (\sum_l v)^{\frac{1}{3}} \right]^2} \quad (26)$$

where v is the atomic diffusion volume (Fuller diffusion volume) (cm^3). T represents the

temperature with unit K, P is the pressure (Pa), and M is the molar mass (g mol^{-1}). In addition, the mass source term R_g is only non-zero in the CL subdomain and is calculated according to the Faraday's Law of electrochemistry as follows:

$$R_g = Y_g \cdot \frac{i_{v,\text{tot}} M_g}{nF} \quad (27)$$

Y_g is the stoichiometric coefficient of gas, $i_{v,\text{tot}}$ is the volumetric current density from the reaction, n is the number of electrons transferred in the reaction.

3.1.2.5 Heat Transport

The heat transport in all subdomains follows the energy equation:

$$\rho C_{p,\text{eff}} u \cdot \nabla T + \nabla \cdot q = Q_{\text{Joule}} + Q_{\text{chr}} \quad (28)$$

where ρ is the density of the material, u velocity in flow channels and porous medium. q (W m^{-2}) is the conductive heat flux, and Q_{Joule} (W m^{-3}) and Q_{chr} (W m^{-3}) are heat sources due to Joule heating and chemical reactions, respectively. Different components are assumed to be assembled in series. $C_{p,\text{eff}}$ is specific heat capacity calculated by

$$C_{p,\text{eff}} = \gamma_g C_{p,g} + \gamma_l C_{p,l} + \gamma_s C_{p,s} \quad (29)$$

where $C_{p,g}$, $C_{p,l}$ and $C_{p,s}$ are heat capacity of gas phase, liquid phase and solid phase, respectively. γ_g , γ_l and γ_s are volume fractions of gas, liquid and solid phase, respectively.

$$\gamma_g = \frac{\omega_g / \rho_g}{\omega_g / \rho_g + \omega_l / \rho_l + \omega_s / \rho_s} \quad (30)$$

Specifically, the heat flux q is defined by Fourier's law as follows:

$$q = -k_{\text{eff}} \nabla T \quad (31)$$

where k_{eff} is the effective thermal conductivity, which can be calculated by

$$k_{\text{eff}} = \gamma_g k_g + \gamma_l k_l + \gamma_s k_s \quad (32)$$

where k_g , k_l and k_s are thermal conductivity of gas, liquid and solid phase, respectively. In addition, the Joule heat Q_{Joule} is non-zero in the CL, PTL, BPP subdomains and is calculated

using Joule's law:

$$Q_{\text{Joule}} = \frac{i_{v,\text{tot}}^2}{\sigma A_V^2} \quad (33)$$

The heat source due to chemical reaction Q_{chr} is only non-zero in the CL subdomains, and calculated as follows:

$$Q_{\text{chr}} = \Delta H_r \cdot \frac{R_g}{Y_g M_g} \quad (34)$$

where ΔH_r is the enthalpy change per mole reaction of water in OER, while normally $\Delta H_r = 0$ for HER, M_g is the molar mass of gas.

3.1.3 Model Coupling

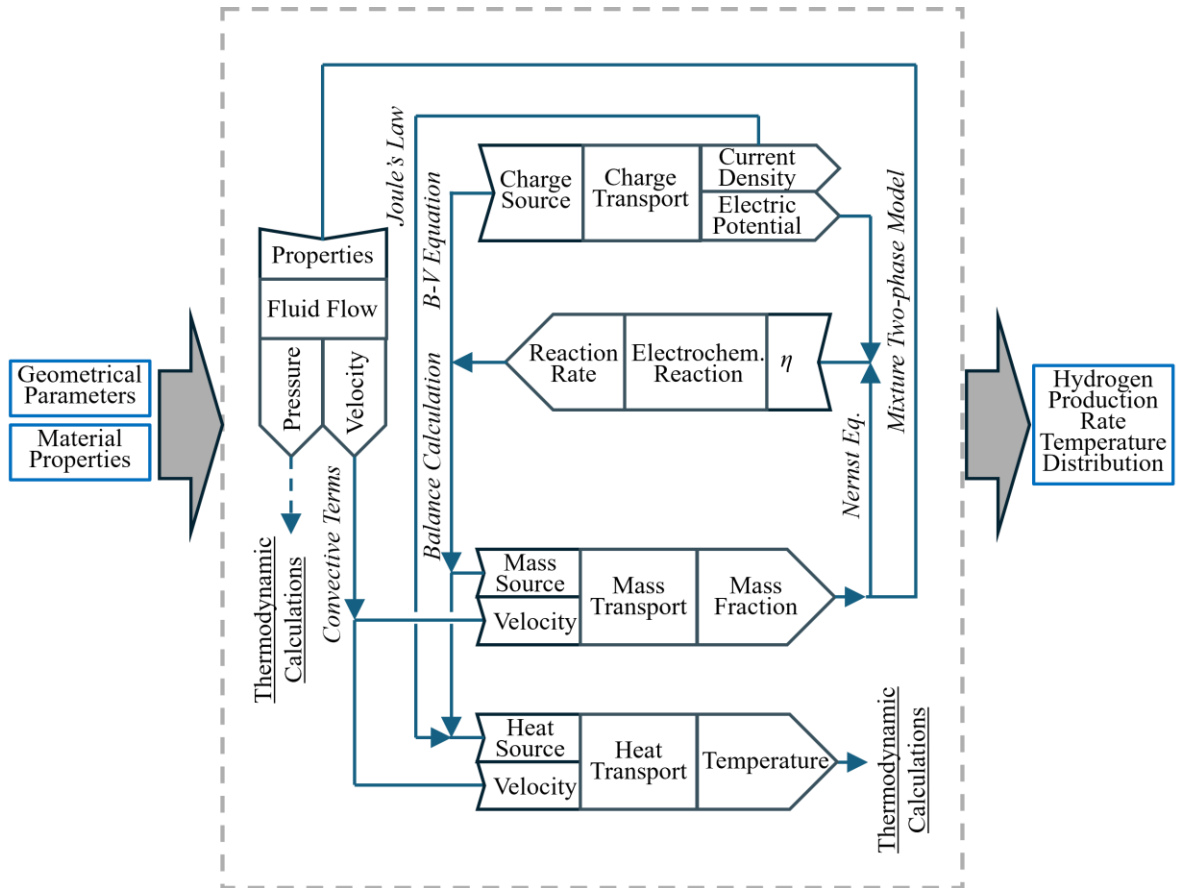


Figure 29. Coupling methods and parameters of computational fields including fluid field, mass transport, heat transport, charge transport and electrochemical reaction. η denotes the overpotential.

Figure 29 shows the coupling framework implemented in the model. The model integrates four primary physical fields – fluid flow, charge transport, mass transport and heat transport, which are coupled with electrochemical reaction. The fluid flow field governs the distribution and movement of the liquid and gaseous species, which directly influences the mass transport by determining local concentration gradients and indirectly affect heat transport via convective contributions. The mass fraction based on mass transport also governs the fluid flow properties in turn. Mass transport supplies reactants and removes products at the reaction site, thus modulating the electrochemical reaction by Nernst Equation. The electrochemical reactions generate local source terms for mass and heat transport via balance calculation, for charge transport through Butler-Volmer Equation. Charge transport determines the electrode potential, which governs the overpotential for electrochemical reactions. Additionally, Joule heating and electrochemical heating act as heat sources, which are determined by current density and electrochemical reactions, respectively. The heat sources are another factor governs the temperature distribution. The temperature field feeds back into the system by influencing species diffusivities, electrolyte conductivity, reaction kinetics, and fluid properties, by thermodynamic calculations. Furthermore, all coupled fields are affected by the geometrical parameters and material properties. This fully coupled framework provides an accurate result of hydrogen production rate and temperature distribution, which are essential factors for PEMWE performance evaluation.

Boundary Conditions

Table 2 shows the boundary conditions of the present model, which are formulated according to descriptions in Section 3.1.1.

Table 2. Boundary conditions of the computational model

Potential	Velocity	Mass Fraction	Temperature	Pressure
-----------	----------	------------------	-------------	----------

A-A'	$\varphi = \varphi_c$	-	-	$n \cdot \nabla T = 0$	-
B-B'	Continuity	Continuity	Continuity	Continuity	Continuity
C-C'	Continuity	Continuity	Continuity	Continuity	Continuity
D-D'	$n \cdot \nabla \varphi = 0$	-	Continuity	Continuity	Continuity
E-E'	$n \cdot \nabla \varphi = 0$	-	Continuity	Continuity	Continuity
F-F'	Continuity	Continuity	Continuity	Continuity	Continuity
G-G'	Continuity	Continuity	Continuity	Continuity	Continuity
H-H'	$\varphi = 0$	-	-	$n \cdot \nabla T = 0$	-
I-I'	$n \cdot \nabla \varphi = 0$	-	-	$n \cdot \nabla T = 0$	-
J-J'	$n \cdot \nabla \varphi = 0$	-	-	$n \cdot \nabla T = 0$	-
M-M'	$n \cdot \nabla \varphi = 0$	-	-	$n \cdot \nabla T = 0$	-
N-N'	$n \cdot \nabla \varphi = 0$	-	-	$n \cdot \nabla T = 0$	-
Cell inlet*	-	$\int (\mathbf{u} \cdot \mathbf{n}) dS$ $= -\dot{m}_{H_2O}/\rho$	$\omega_1 = 1$	$T = T_{ustr}$	-
Cell outlet**	-	-	-	-	$p = p_0$
Non-slip boundaries	-	$\mathbf{u} = 0$	-	q $= h \cdot (T_s - T_f)$	-

* Cell inlet indicates the water inlet on anode side.

** Cell outlet indicates the oxygen and water outlet on anode side and hydrogen outlet on cathode side.

3.1.4 Model Parameters

Table 3 shows the fixed parameters used in the present simulation. The electric potential is selected as 2.105V which is generally used in lab-scale PEMWE tests. [72], [118]. The current density of 1.71 A cm⁻² is selected for the 2.105V cell potential based on existing literatures. [118] The water feed rate can be calculated with cathode reaction rate by

$$\dot{m}_{H_2O} = \frac{i \cdot A \cdot M_{H_2O} \cdot St}{2F} \quad (35)$$

i is the current density selected before, A is the active area of the PEMWE, M_{H_2O} is the molar mass of water and the value is 18 g mol^{-1} . St is the stoichiometric factor of water, which means the ratio of actual water feed rate to theoretical water consumption rate. St of 3 is selected in this study for sufficient water supply. [119] The porosities and permeabilities of PTL and CL are the typical values that has been used in previous studies [72]. The PEM proton conductivity is the properties of the commercial product Nafion 117 [120].

Table 3. Physical parameters used in the present model

Parameters	Units	Values	References
Porosity of PTL at anode & cathode		0.5	[72]
Porosity of CL at anode & cathode		0.25	[72]
Anodic charge transfer coefficient α_a		0.5	[72]
Cathodic charge transfer coefficient α_c		0.5	[72]
Electrical conductivity of PTLs	S m^{-1}	1.19E6	[121]
Electrical conductivity of anode CL	S m^{-1}	1.47E7	[122]
Electrical conductivity of cathode CL	S m^{-1}	7.0725E6	[123]
Electrical conductivity of BPP	S m^{-1}	2.38E6	[121]
Reference exchange current density, hydrogen reaction	A m^{-2}	10000	[72]
Reference exchange current density, oxygen reaction	A m^{-2}	0.1	[72]
Electrode permeability	m^{-2}	1E-10	[110]
PEM proton conductivity	S m^{-1}	16.6	
Anode activation energy	J mol^{-1}	62836	[124]
Cathode activation energy	J mol^{-1}	24359	[124]
Upstream temperature T_{ustr}	K	353.15	
Outlet absolute pressure p_0	atm	1	
Inverse of air entry pressure α	Pa^{-1}	1E-4	[109]
Shape parameter n		2	[109]
Shape parameter m		-0.5	[109]

Enthalpy change of OER	kJ mol ⁻¹	285.83
Enthalpy change of HER	kJ mol ⁻¹	0
Universal gas constant	J mol ⁻¹ K ⁻¹	8.314

3.2 Numerical Implementation

This study is implemented by COMSOL Multiphysics 6.3, on a desktop with 12th Gen Intel® Core™ i7-12700 KF CPU with 128GB RAM. For the formulated model, Parallel Direct Sparse Solver (PARDISO) solver [125], [126], [127] is used for solving fluid dynamics and heat transfer problems in this study. The PARDISO solver works on general systems of the form $Ax = b$. They exploit pipelining parallelism with a combination of left-looking and right-looking supernode techniques [128]. Comparing with other solvers, PARDISO solver has the advantages consists of multicore processors utilization, memory efficiency and higher robustness, which make PARDISO solver more suitable to handle large-scale 3D problems and complex coupled physics. In addition, a relative tolerance of 1E-4 is specified as the convergence criteria for all fields. The computation converges when the computed relative error is lower than the specified relative tolerance, and the relative error can be calculated as follows:

$$err = \sqrt{\frac{1}{M} \sum_{j=1}^M \frac{1}{N_j} \sum_{i=1}^{N_j} \left(\frac{|E_{i,j}|}{W_{i,j}} \right)^2} \quad (36)$$

where M is the number of fields, N_j is the number of degrees of freedom in field j . $W_{i,j} = \max(|U_{i,j}|, S_j)$, $U_{i,j}$ is the current approximation to the true solution vector, while S_j is a scale factor that the solver determines from the scaling method, and $E_{i,j}$ is the estimated error of the degree of freedom of i in field j .

The model mesh is shown in Figure 30, the blue lines highlight the boundaries of flow channels. All components are discretized using the Mapped meshing technique, which generates a structured quadrilateral mesh on boundaries in 3D [129]. The PTL, inlet and outlet headers subdomains are refined. The PTLs, CLs and PEM are meshed with the uniform mesh

distribution. The mesh points on the direction of the cell thickness are 8, 3, 5 for PTL, CL and PEM, respectively. There are 109,080 meshes generated for flow channels. Boundary layers are applied to the meshes of flow channels to make sure the accuracy of velocity field near the wall. There are 10 layers of boundary layers that are generated with a stretching factor of 1.2. The mesh quality is measured by the skewness of the meshes, which can be defined by:

$$skewness = \frac{\theta_{\max} - \theta_{\text{opt}}}{\theta_{\max} - \theta_{\min}} \quad (37)$$

where $\theta_{\max}$ is the largest angle in the element, $\theta_{\min}$ is the smallest angle in the element and θ_{opt} is the angle in the ideal element. The average mesh quality is the arithmetic average of the quality values of all mesh elements in the computational domain. The average mesh quality which is measured by skewness is 0.8177, with 0.4352 minimal mesh quality. This makes sure the accuracy of simulations.

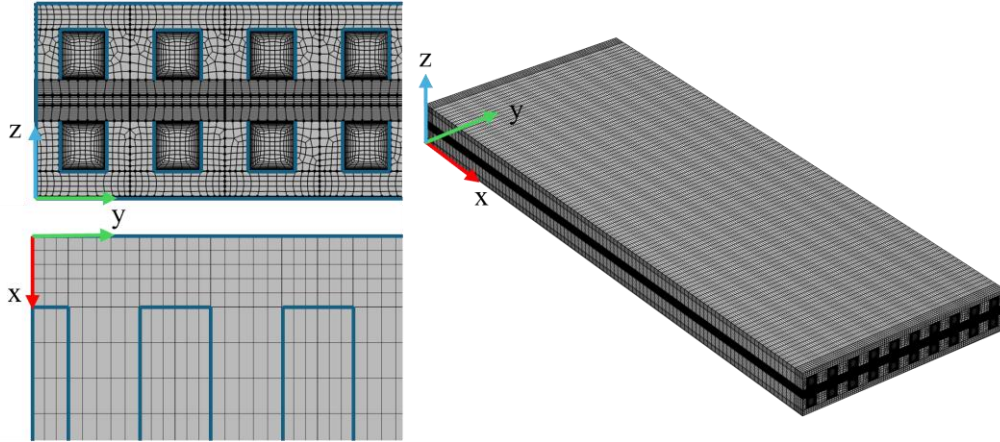


Figure 30. Mesh details of the computational model (right) with cross-sectional view of yz plane (top left) and xy plane (bottom left), the blue lines highlight the boundaries of flow channels.

Figure 31 shows the mesh independence test for the model developed with mesh numbers ranging from 47,400 to 612,000. The surface average current density at the interface of anode CL and PTL is selected as the criteria of grid independence by taking the integrated mean of the current density across CL subdomain. The current density increases with fluctuation when increasing mesh numbers from 47,400 – 349,800 meshes, indicating that the

fineness of the meshes is insufficient within this range. Furthermore, the results become stable for the mesh number larger than 349,800, indicating that further mesh refinement leads to negligible improvements. Therefore, 349,800 are selected for mesh numbers by considering both calculation accuracy and computational expenses.

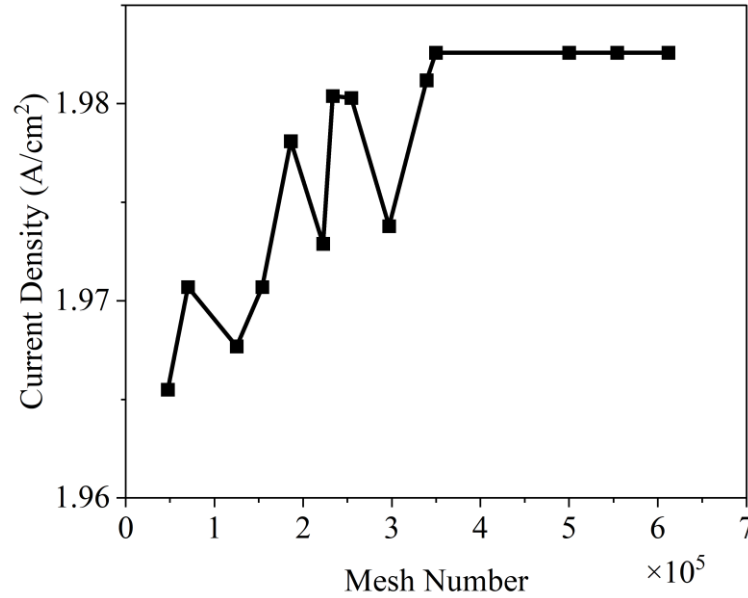


Figure 31. Simulation results of current density at 2.105 V operating voltage and $z=2.018$ mm with various mesh numbers from 47,400 to 612,000.

The model is validated by comparing to a published experiment of PEMWE cell. The referenced experiment is carried out on 3 cm×0.35 cm×0.38 cm PEMWE with operational conditions of 353.15 K, 15 ml min⁻¹ water feed rate and varied electric potential from 1.089-2.420 V [118]. A titanium sinter with 0.35 mm thickness is used for anode PTL, while cathode uses a 0.19 mm-thick carbon paper. The present model is modified according to the reference dimension and operational conditions of the experiment. As shown in Figure 32, the curves show comparison of current density in simulation results and the experiment results. The current density is evaluated with the integrated mean of the current density across CL subdomain. The results indicated a small difference between simulation and experiment results, which ensure the accuracy of the simulation model.

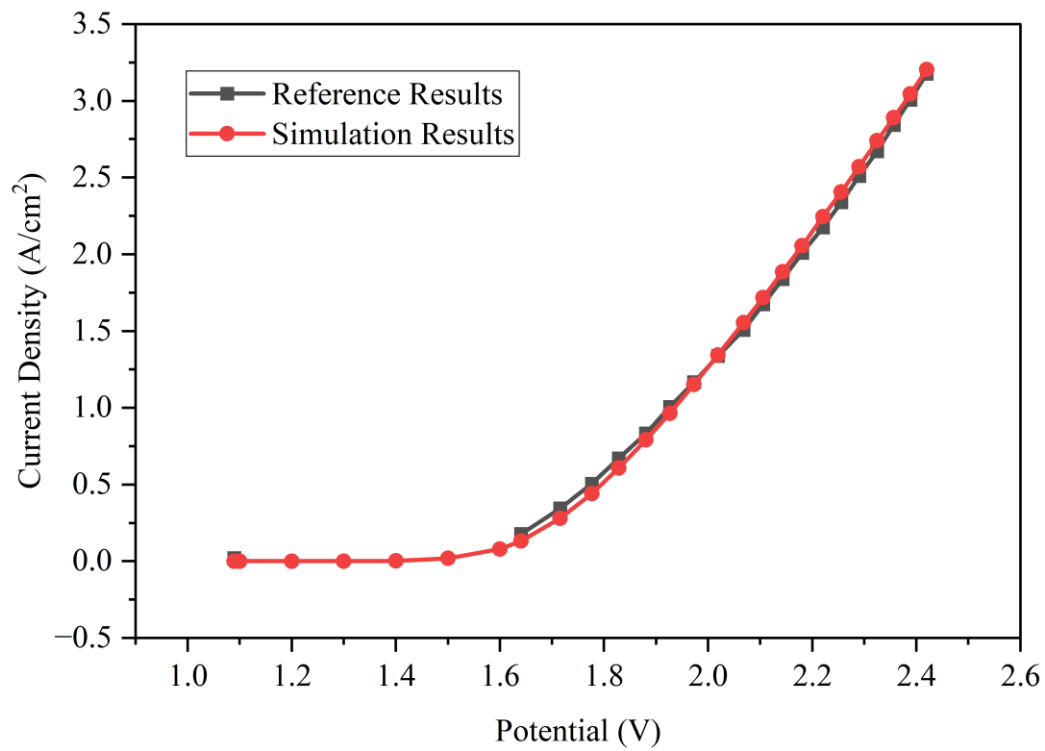


Figure 32. Model validation results by comparison of simulation and experiment results from [118].

4. Results and Discussion

4.1 Water Electrolyzer Geometric Model

This study starts with simulating a PEMWE cell with fixed geometry to show the results of the 3D numerical model with both anode and cathode sides. Table 4 lists the geometrical parameters selected for the study. The PTL thickness, CL thickness cell length, membrane thickness channel height and Channel/Rib width Ratio of 1:1 are obtained from the existing studies [59].

Table 4. Geometry parameters of the computational model

Parameters	Unit	Values
Cell length	mm	50
Cell width	mm	20
Channel width	mm	1
Channel height	mm	1
Rib width	mm	1
PTL thickness	mm	0.3
CL thickness	mm	0.02
PEM thickness (fully hydrated)	mm	0.178

Figure 33 shows the simulation results of outlet hydrogen production rate. The outlet hydrogen production rates are increasing exponentially with the increase of channel numbers from $0.8 \times 10^{-8} \text{ kg s}^{-1}$ to $2.1 \times 10^{-8} \text{ kg s}^{-1}$. The average hydrogen production rate is $1.2 \times 10^{-8} \text{ kg s}^{-1}$. This indicates more hydrogen is produced at channels located further from the inlet than the ones near the inlet.

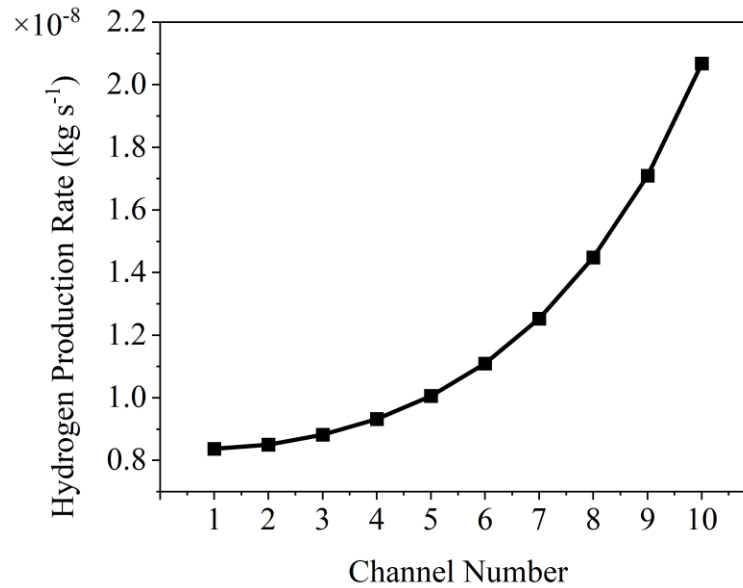


Figure 33. Hydrogen production rates of Channel #1 to #10 outlets

The preceding distribution of hydrogen production rates is explained according to the water flow distribution in BPP channels. As shown in Figure 34, the velocity profile of mixture flow is plotted at the xy plane of the anodic flow channels at $z=2.818$ mm. The results indicate high velocity in the inlet header up to 18.6 m s^{-1} . For each channel, the velocity reduces to the range of 0.8 to 3.0 m s^{-1} due to expanded flow area, and the velocity increases with channel number and peaks in the channel closest to cell outlet. This flow distribution is based on the conversion between dynamic and static pressure inside headers that leads to maximum pressure difference across the channel closed to cell outlet. As a result, the high velocity at large channel numbers lead to increased mass convection and high local reactant concentrations, which further increase the reaction rate and hydrogen production. Therefore, the channels closer to cell outlet generate more hydrogen due to the increased velocity, indicating that the production rate of hydrogen mainly depends on the convective mass transport resulting from flow field inside PEMWE cells.

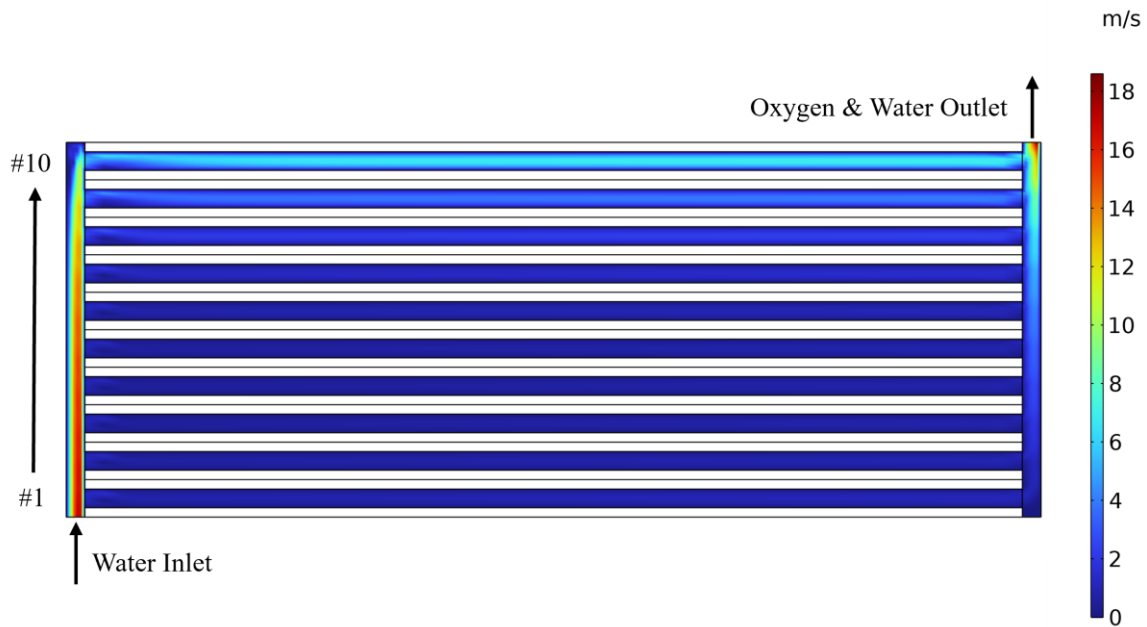
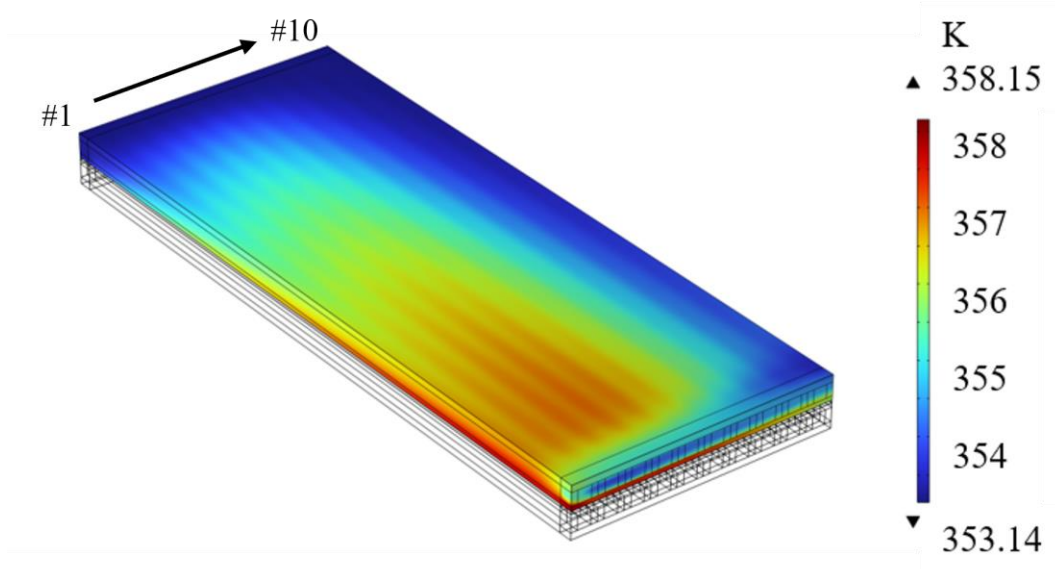


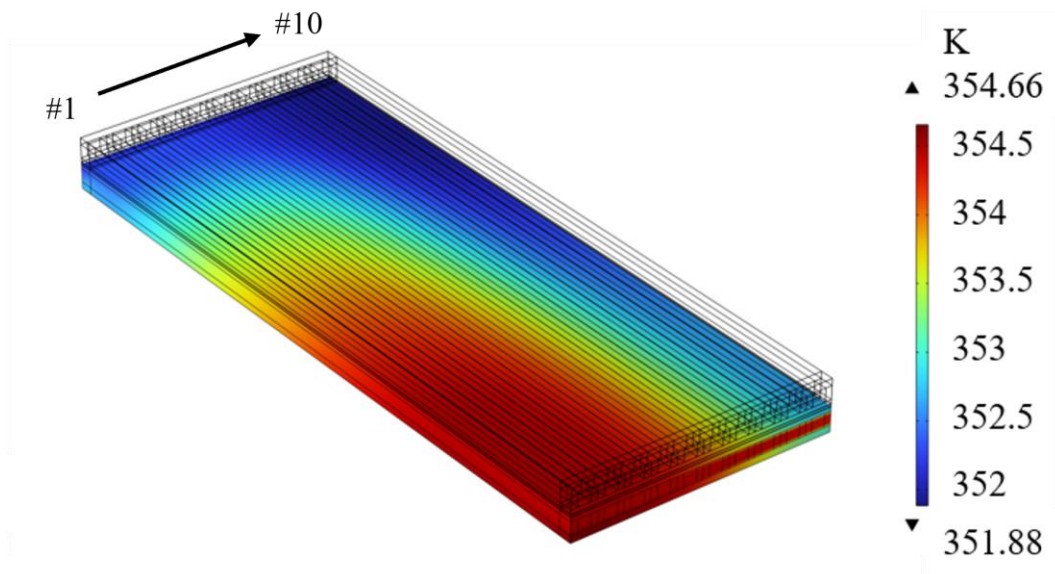
Figure 34. Anode velocity contour of xy plane at $z=2.818$ mm

Figure 35 a and b show the temperature distribution on the anode and cathode domain surfaces. In general, the temperature distribution of anode side is in the range of 353.14 K to 358.15K, which is higher than the cathode side with the temperature range of 351.88K to 354.66 K. This is because the OER reaction at the anode generates $285.83 \text{ kJ mol}^{-1}$ heat to elevate the temperature of the cell, while the HER reaction at the cathode has a zero enthalpy change. In addition, the cooling of solid structure due to fluid flow is observed where a lower temperature at BPP surface near flow channels compared to rib area. For example, the anodic average temperature is 354.30 K for fluids in all flow channels and 355.37 K for the surrounding ribs. This 1.07 K temperature difference suggests the heat convection of anodic fluids that cool solid structures. In contrast, the value of the temperature difference at cathode side is 0.1 K, indicating a weak cooling effect due to the zero reaction heat generation and small heat capacity of gaseous hydrogen. Furthermore, due to the convection cooling, the temperature distribution on the xy plane of the cell is strongly affected by the flow distribution in channels. As discussed, the anode fluid flow exhibits a distribution that flow velocity is higher in channels that are closer to the cell outlet. As a result, the convection cooling is significant in areas with higher flow velocities, which appears as the temperature distribution

in Figure 35. Overall, the temperature distribution across the PEMWE cell is strongly affected by fluid flow in channels and anode/cathode reactions.



(a)



(b)

Figure 35. Visualized simulation contour of Surface temperature distribution on (a) anode and (b) cathode.

Figure 36 shows the simulation results of temperature distribution for different yz

planes, which are perpendicular to the flow direction in the flow channels. The plane of $x=1\text{mm}$ denotes the inlet of 10 channels and $x=51\text{mm}$ denotes the outlet, with an interval of 10 mm between. Plane $x=1\text{mm}$ has the lowest temperature range compared to other planes, since there's no reaction when the water flows into the channels. The higher temperature always occurs near the anode PTL and CL from Channel #1 to #6, especially for $x=31\text{mm}$ and $x=41\text{mm}$. The higher temperature distribution represents higher electrochemical reaction rate and higher current density. In addition, the cooling effect of water is also reflected for lower temperature of Channel #7 to #10, higher water flow rate increases the effect of heat convection and decreases the temperature of these channels.

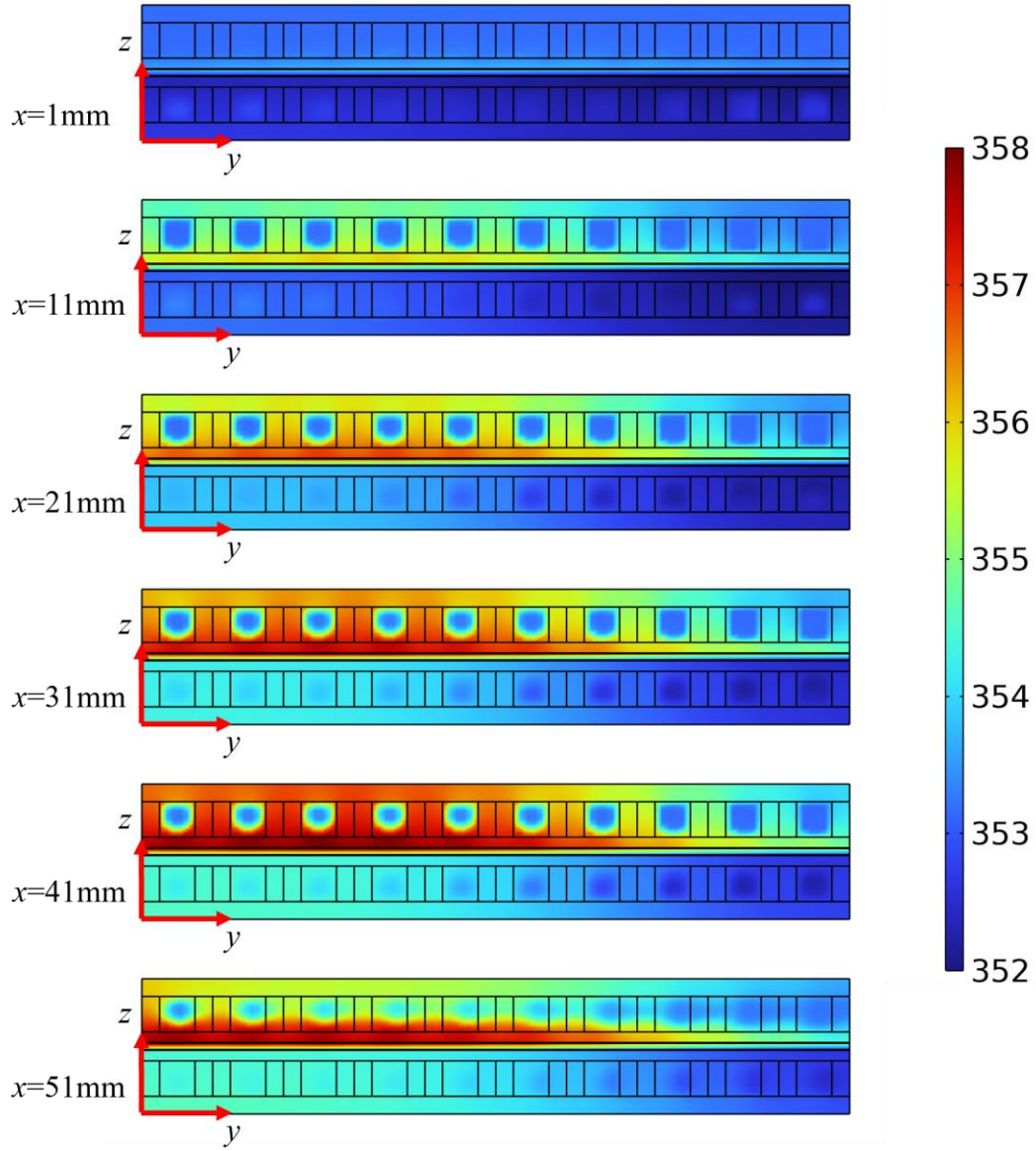


Figure 36. Temperature distribution for different yz plane

Figure 37 indicates the temperature distribution of different xz planes, which are parallel to the flow direction. The five figures correspond to the middle cut plane of Channel #1, #3, #5, #7, #9, respectively. The results show the heat accumulation along the flow direction, especially in anode CL and PTL. Higher percentage of high temperature (357K-358K) is reported for Channel #1, #3 and #5, where have lower water mole fraction, which impair the

cooling effect for these channels.

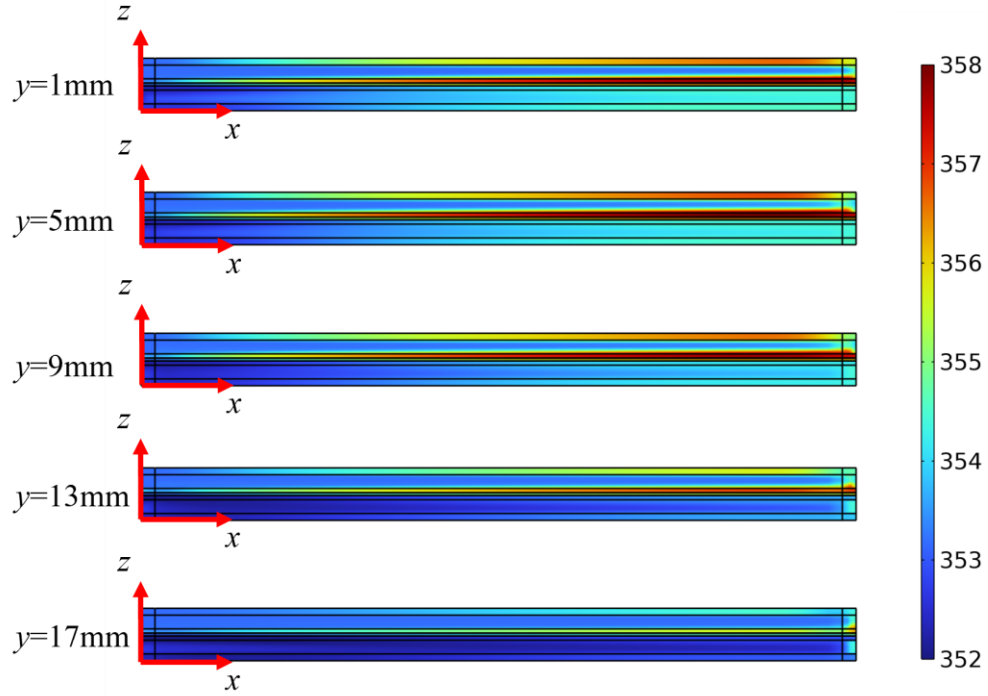


Figure 37. Temperature distribution for different xz plane

4.2 Sensitivity Analysis

4.2.1 Response Surface Method (RSM)

The Response Surface Method (RSM), originally proposed by Box and Wilson [130], is an optimization technique that combines principles of experimental design with mathematical modeling. Initially developed for fitting physical experiments, RSM has since found widespread application across diverse fields, including pharmaceuticals, environmental science, chemical engineering, and mechanical engineering. The method offers several advantages, such as reduced experimental effort, high accuracy in approximating complex systems, and strong predictive capability for output parameters. [130]

A general regression model can be expressed as

$$Y = \beta_0 + \beta_1 X_1 + \dots + \beta_n X_n + \varepsilon \quad (38)$$

where β_i are the estimated coefficients of each input, ε is the error term and X_i are the inputs.

R^2 is the total variation in the response variable is explained by the model. [131]

$$R^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y}_i)^2} \quad (39)$$

where the numerator is the sum of squared errors and the denominator is the total variation. $\hat{y}_i$ is the predicted values, y_i is the actual values and $\bar{y}_i$ is the mean of actual values. Furthermore, there are two more types of R^2 can represent the quality of the predicted model. Adjusted R^2 penalizes the model for using too many predictors.

$$R_{adj}^2 = 1 - \left(\frac{(1 - R^2)(n - 1)}{n - k - 1} \right) \quad (40)$$

where n is the number of observations and k is the number of predictors.

Predicted R^2 measures predictive performance on new data.

$$R_{pred}^2 = 1 - \frac{PRESS}{\sum(y_i - \bar{y}_i)^2} \quad (41)$$

To investigate the influences of different geometrical parameters on PEMWE performance, especially hydrogen production and temperature distribution. The effects of several geometrical parameters on the performance of PEMWE single unit are considered in this study, including PTL thickness, width of flow channel & rib and length of the unit. A simple lab-scale PEMWE has the values of PTL thickness, channel width and cell length for 0.3 mm, 1.0 mm and 50 mm, respectively. [72], [118] Therefore, the ranges are expanded for both lower and higher values of the investigated geometrical parameters to explore the effects of variable parameters on PEMWE performance. The values of selected parameters are shown in Table 5 below.

Table 5. Values of selected parameters

Parameters	Units	Values
PTL thickness	mm	0.1, 0.2, 0.3, 0.4, 0.5
Channel width	mm	0.6, 0.8, 1.0, 1.2, 1.4
Cell length	mm	30, 40, 50, 60, 70

Based on the simulation model that is estimated above, the orthogonal tests are designed and run with the model, the design of orthogonal experiments and results of hydrogen production rate and maximum temperature are listed in Table 6.

Table 6. Orthogonal experiments design and simulation results

Run	PTL thickness (mm)	Channel width (mm)	Cell length (mm)	Hydrogen production rate ($10^{-7} \text{ kg s}^{-1}$)	Maximum temperature (K)
1	0.1	1.4	30	0.74536	358.23
2	0.3	1	30	0.74385	357.27
3	0.3	1	50	1.2096	358.15
4	0.3	0.6	50	1.1906	356.5
5	0.1	0.6	70	1.6676	356.69
6	0.1	0.6	30	0.72083	355.67
7	0.5	1	50	1.2083	358.4
8	0.5	1.4	30	0.74409	358.32
9	0.5	0.6	70	1.6637	357.18
10	0.5	1.4	70	1.6397	360.32
11	0.3	1.4	50	1.193	359.28
12	0.1	1.4	70	1.6423	360.1
13	0.1	1	50	1.2109	358.03
14	0.5	0.6	30	0.71873	356.09
15	0.3	1	70	1.6767	358.81

By analyzing the simulations results, Quadratic model that is more significant for this study is used for establishing the relationship between the inputs and outputs. The RSM equations are

Hydrogen Production Rate

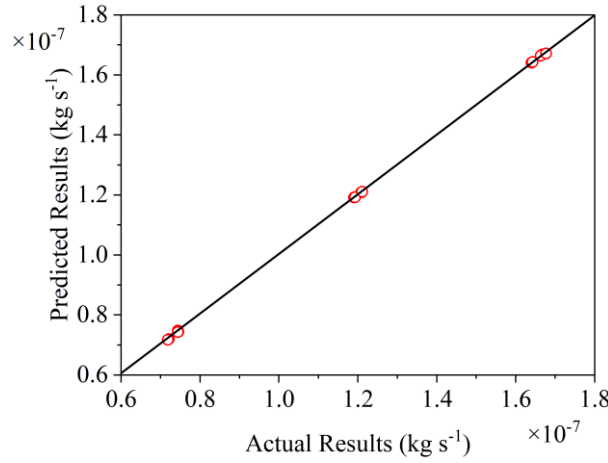
$$\begin{aligned}
 &= -1.2661 \times 10^{-8} - 6.76 \times 10^{-10} * A + 2.98 \times 10^{-8} * B + 2.446 \times 10^{-9} \\
 &* C + 3.33 \times 10^{-10} * A * B - 9.78 \times 10^{-12} * A * C - 1.55 \times 10^{-10} * B * C \\
 &+ 3.49 \times 10^{-10} * A^2 - 1.1038 \times 10^{-8} * B^2 + 2.04 \times 10^{-13} * C^2
 \end{aligned}$$

Maximum Temperature

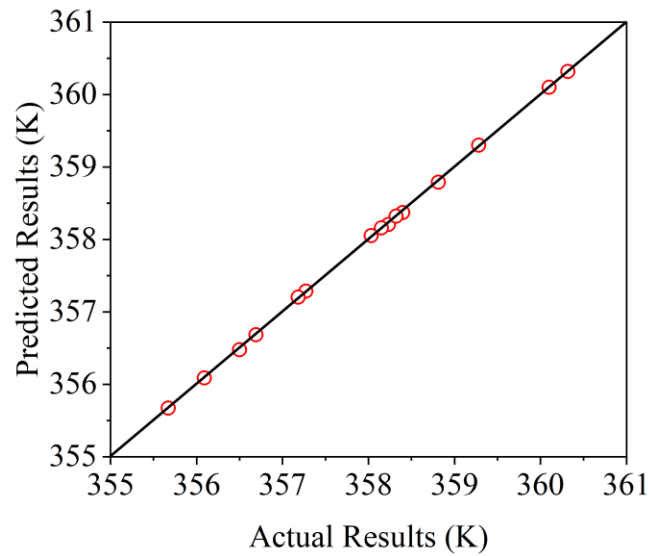
$$\begin{aligned} &= 351.39875 + 0.578333 * A + 5.79736 * B + 0.037947 * C - 0.9375 * A \\ &\quad * B + 0.00625 * A * C + 0.0275 * B * C + 1.4 * A^2 - 1.68056 * B^2 \\ &\quad - 0.000297 * C^2 \end{aligned}$$

Where A, B, C represent for the three input geometrical parameters PTL thickness, channel width and cell length, respectively.

Figure 38 indicates the comparison of simulation results and RSM predicted results of hydrogen production rate and maximum temperature. The points are all near the curve $y=x$, which means the differences between simulation results and predicted results are small. This indicates good fitting towards the selected geometrical parameters and hydrogen production rate/maximum temperature.



(a)



(b)

Figure 38. Comparison of simulation results and predicted results by RSM of (a) hydrogen production rate and (b) maximum temperature

4.2.2 Sensitivity Analysis

Sensitivity analysis is a significant technique in modelling and statistical inference, used to quantify the extent to which variations in model outputs can be attributed to uncertainties or changes in input parameters. [132], [133] Sensitivity analysis always incorporates hypothesis testing to assess the significance of input variables. Generally, sensitivity analysis incorporates following steps:

1. Define the model and inputs
2. Select a sensitivity analysis method
3. Run simulations
4. Analyze the results
5. Interpret and apply the insights

P-value-based sensitivity analysis is an approach which uses p-value to determine the significances of independent input variables on output of regression-based model. Each input has its own constant related to this model. Different hypothesis tests should be done for each input. Aftermath, p-value can be calculated based on the results of hypothesis tests. [132]

- If $p \leq 0.05$, the variable is considered sensitive.
- If $p > 0.05$, the variable is not sensitive.

The inputs are also can be ranked for sensitivity based on the p-value, lower p-value indicates the variable is more significant. Coefficient of Determination R^2 is generally used for evaluate the fitness of the predicted model. [133] Based on the established equations, the sensitivity analysis is completed.

Table 7. Sensitivity Analysis results of Hydrogen Production Rate

Source	F-value	p-value
Model	20595.34	< 0.0001
A-PTL thickness	1.35	0.2976
B-Channel width	0.0777	0.7917
C-Cell length	1.85E+05	< 0.0001
AB	0.0493	0.8331
AC	0.1064	0.7575
BC	106.82	0.0001
A ²	0.0043	0.95
B ²	69.66	0.0004
C ²	0.1482	0.7161

P-values less than 0.0500 indicate model terms are significant. In this case C, BC, B² are significant model terms. The R^2 is approaching to 1 which means the predicted values by the RSM equation are close to the simulation results. That indicates the accuracy of the established model. The Predicted R^2 of 0.9998 is in reasonable agreement with the Adjusted R^2 of 0.9999; i.e. the difference is less than 0.2. The Model F-value of 20595.34 implies the model is significant. There is only a 0.01% chance that an F-value this large could occur due to noise.

Table 8. Sensitivity Analysis results of Maximum Temperature

Source	F-value	p-value
Model	3493.74	< 0.0001
A-PTL thickness	298.75	< 0.0001

B-Channel width	23560.53	< 0.0001
C-Cell length	6682.69	< 0.0001
AB	53.18	0.0008
AC	5.91	0.0593
BC	457.56	< 0.0001
A ²	9.57	0.0271
B ²	219.7	< 0.0001
C ²	42.95	0.0012

P-values less than 0.0500 indicate model terms are significant. In this case A, B, C, AB, BC, A², B², C² are significant model terms. R²=0.9998 also means the predicted values by the RSM equation are close to the simulation results. The Predicted R² of 0.9983 is in reasonable agreement with the Adjusted R² of 0.9996; i.e. the difference is less than 0.2. The Model F-value of 3493.74 implies the model is significant. There is only a 0.01% chance that an F-value this large could occur due to noise.

4.2.3 Influence of Single Parameter

4.2.3.1 PTL Thickness

The effects of PTL thickness on the performance of PEMWE was investigated. 0.1mm, 0.2mm, 0.3mm, 0.4mm, 0.5mm were selected for the thickness of PTL of both anode and cathode. The hydrogen production rate results are shown in Figure 39. The hydrogen production rate decreases proportionally from $1.2109 \times 10^{-7} \text{ kg s}^{-1}$ to $1.2083 \times 10^{-7} \text{ kg s}^{-1}$ with the increasing thickness of PTL from 0.1 mm to 0.5 mm. This is because the increase of PTL thickness decreases the electrochemical reaction rate, which reduces the current density under same electric potential. This indicates that a lower PTL thickness for both anode and cathode will lead to positive effects for hydrogen production.

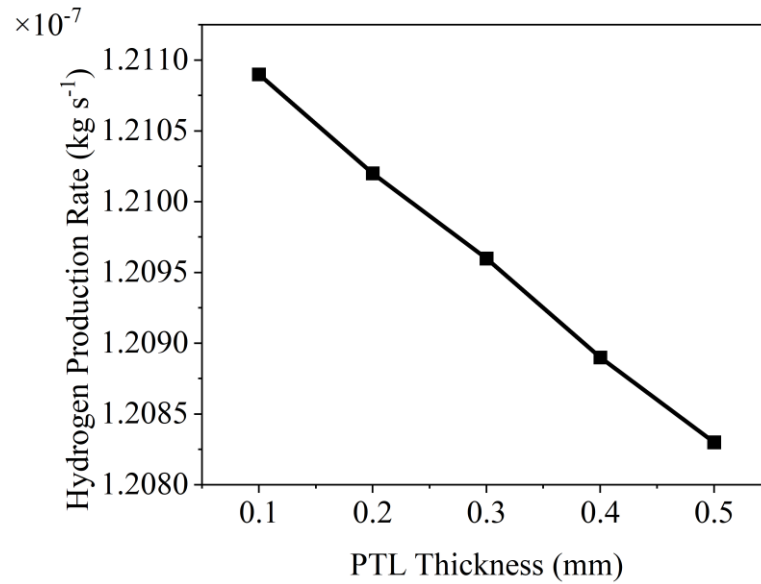


Figure 39. Simulation results of hydrogen production rate with different porous transport layer (PTL) thicknesses from 0.1 mm to 0.5 mm.

Figure 40 presents the effects of PTL thickness on the maximum and minimum temperatures at both the anode and cathode. At the anode side (Figure 40a), the maximum temperatures exhibit an increase with increasing PTL thickness from 358.03 K to 358.4 K, while the minimum temperature at anode side is stable around 353.14 K. In addition, a clear linear increase is observed in both temperature metrics with increasing thickness, indicating a consistent thermal response. The maximum temperature for cathode is also increasing from 354.4 K to 354.91 K due to the PTL thickness variation. This suggests that thicker PTLs hinder effective heat dissipation on both sides, leading to elevated thermal accumulation. Overall, the data implies that PTL thickness plays a significant role in thermal management, with both electrodes experiencing rising temperatures, but the anode exhibiting more variability and sensitivity to thickness changes. Both anode and cathode temperatures have slight increase since the increasing PTL thickness because of higher Joule heating generation since the resistance is increasing with PTL thickness raising, which leads to a higher temperature.

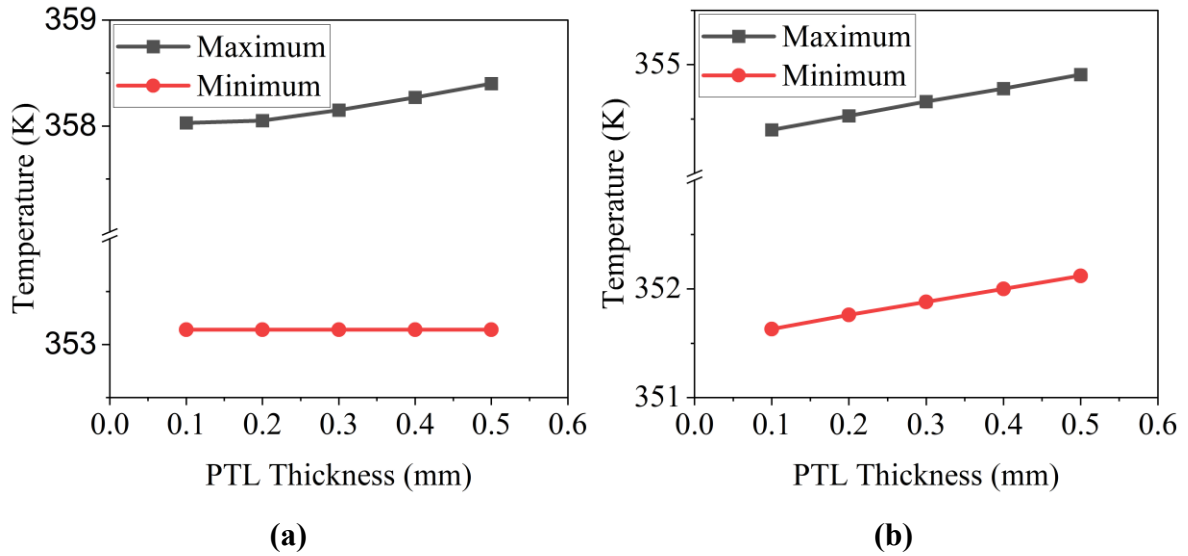


Figure 40. Simulation results of maximum and minimum temperature on (a) anode and (b) cathode with different porous transport layer (PTL) thicknesses from 0.1 mm to 0.5 mm.

Figure 41 indicates the average temperature of anodic and cathodic CL and their variance. The variance represents the uniformity of the temperature distribution at CL, which is the most important part for PEMWE due to the electrochemical reactions happen here. Both the anodic and cathodic CL average temperatures are increasing with the increase of the PTL thickness, from 355.89 K to 356.42 K at anode and 352.97 K to 353.44 K at cathode. The temperature variance is increasing from 1.568 to 1.6817 with higher PTL thickness at the anode side but shows conversed trend (varying within 2%) at cathode side, which means the temperature distribution becomes more uniform with the increasing PTL thickness at cathode side, and cathode is less sensitive to the variation of PTL thickness. The trends showed previous are mainly because of the Joule heating generation, the increasing PTL thickness raise the CL temperature because of the increasing contact resistance based on Ohm's Law.

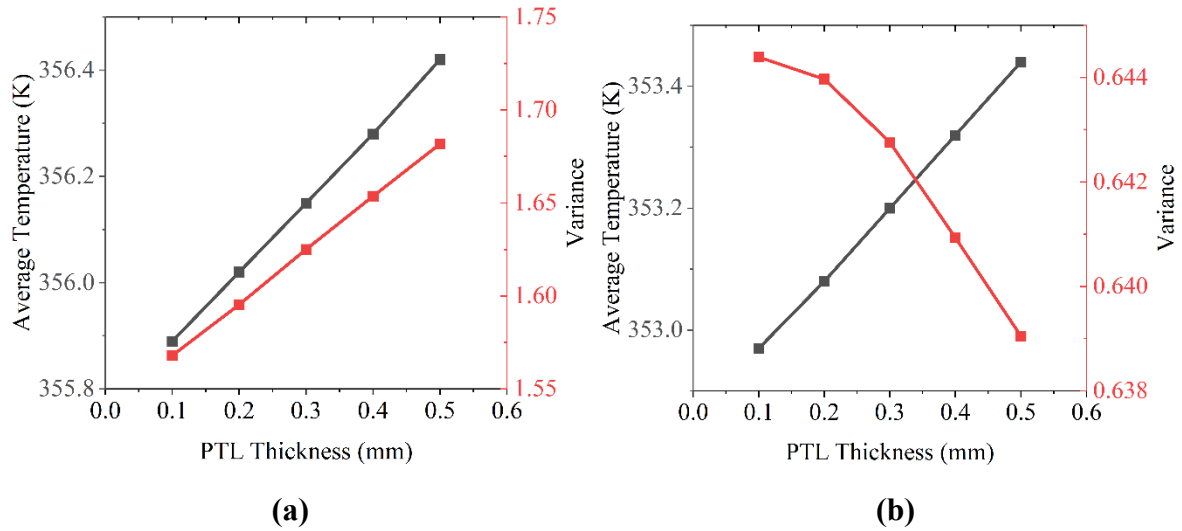
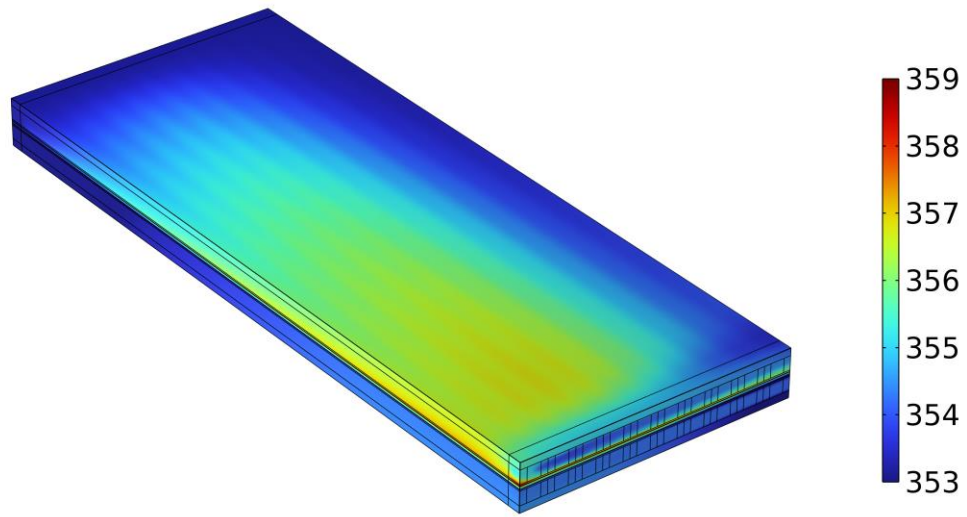
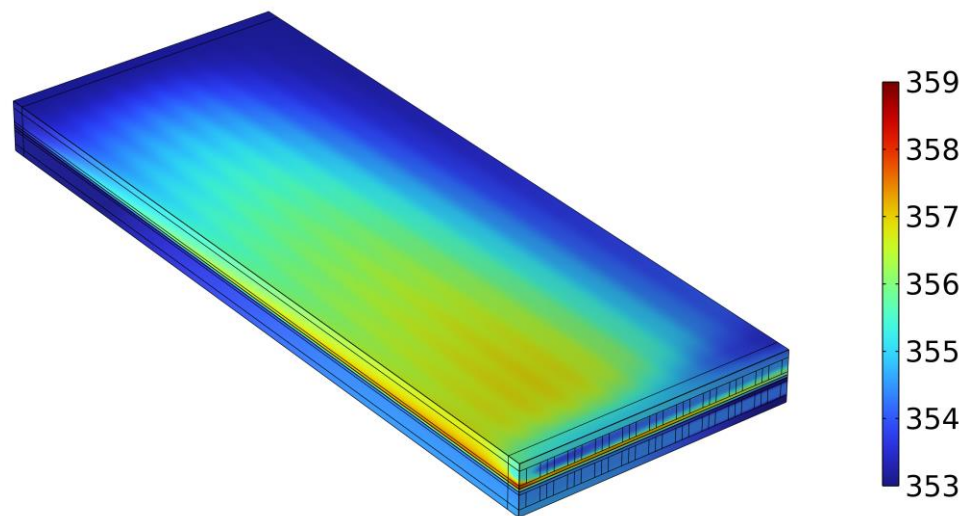


Figure 41. Average temperature and temperature variance of catalyst layer (CL) on (a) anode and (b) cathode with different porous transport layer (PTL) thicknesses from 0.1 mm to 0.5 mm.

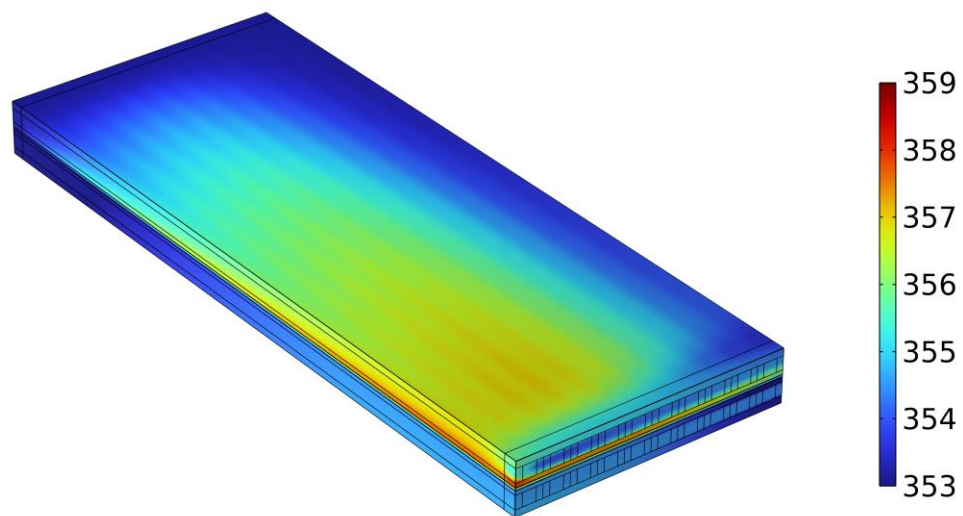
Figure 42 shows the water mole fraction of the surface between anode CL and PTL. This surface is the interface where water first approaches to the catalyst and the electrode reaction starts. For the first figure with 0.1mm PTL thickness, the gaps among different flow channels are obvious, which means the PTL in this thickness can't manage the water distribution well. On the other hand, it's not uniform water distribution for 0.1mm PTL thickness. However, the first case has a lower water mole fraction near the outlet areas. Water reaches the catalyst and starts to react quickly from the anode flow channels because of the low PTL thickness. The gaps among the flow channels become blurred with the increase of PTL thickness. This indicates that the higher PTL thickness leads to better water distribution of the interface between anode CL and PTL.



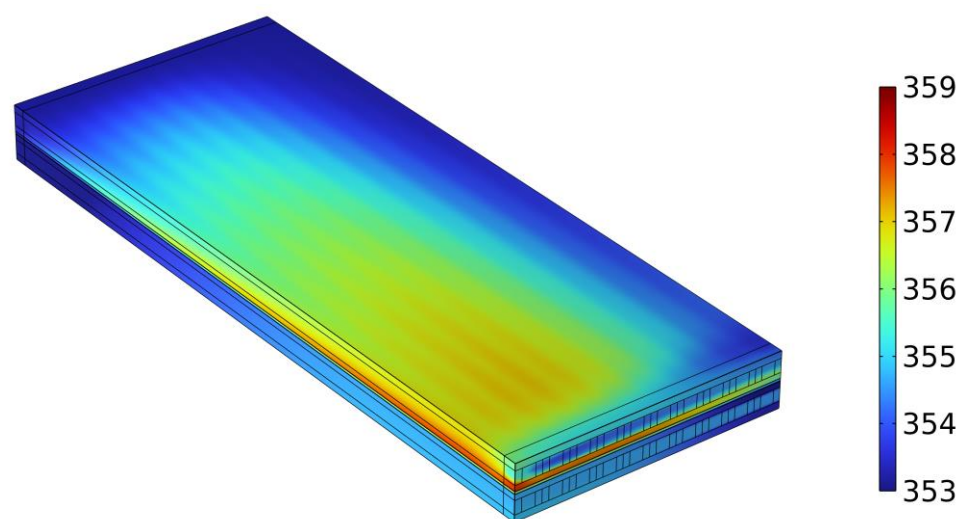
(a)



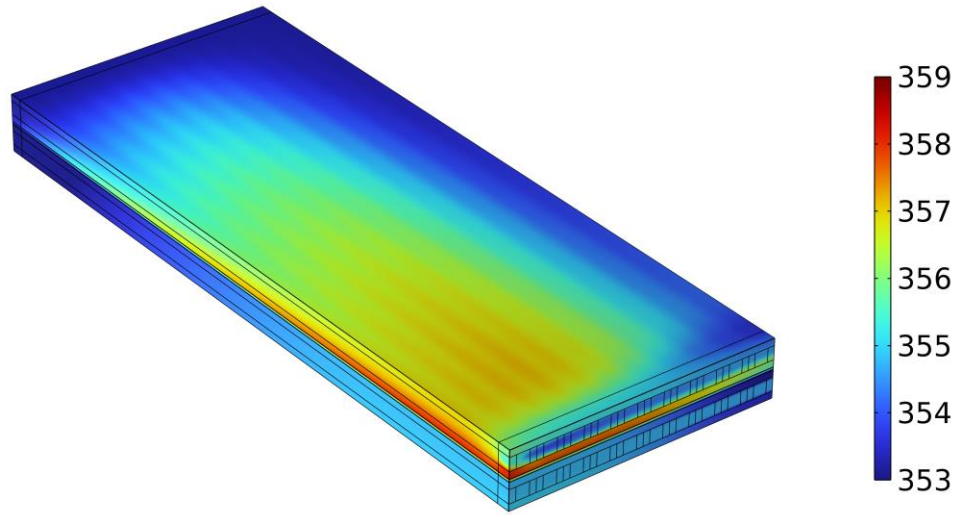
(b)



(c)



(d)



(e)

Figure 42. Temperature distribution with different PTL thicknesses (a) 0.1 mm, (b) 0.2 mm, (c) 0.3 mm, (d) 0.4 mm, and (e) 0.5 mm.

Figure 43 indicates the average outlet temperature of each channel with different PTL thicknesses. The results show that the average temperature of each channel outlet is increasing with the increase of PTL thickness, but there is only a tiny difference among average outlet temperatures on the anode side. The outlet temperatures show a parabolic trend changing with channel numbers on the anode side, while maximum temperature always occurs at Channel #3 and #4. On the other hand, the outlet temperatures are decreasing with the increase of channel numbers. The maximum difference is observed at channel #2, which is 0.22 K, while the minimum difference is 0.06 K at Channel #10. The average temperature of channel outlet is more sensitive on the cathode compared with the anode side, with the maximum difference of 0.57 K at Channel #10.

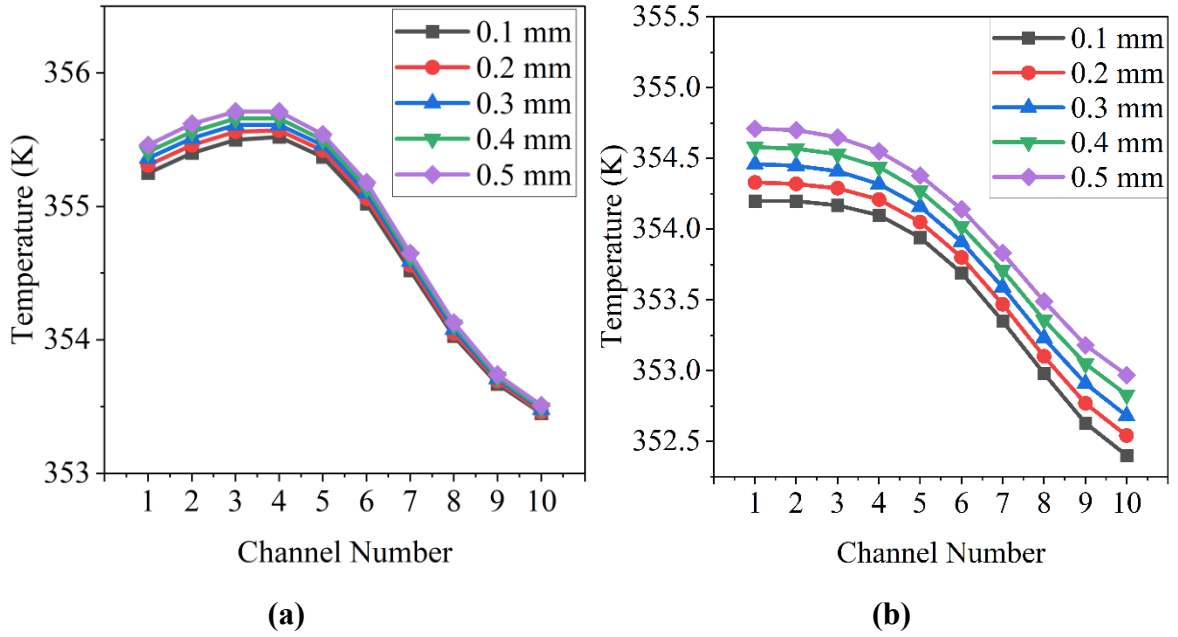
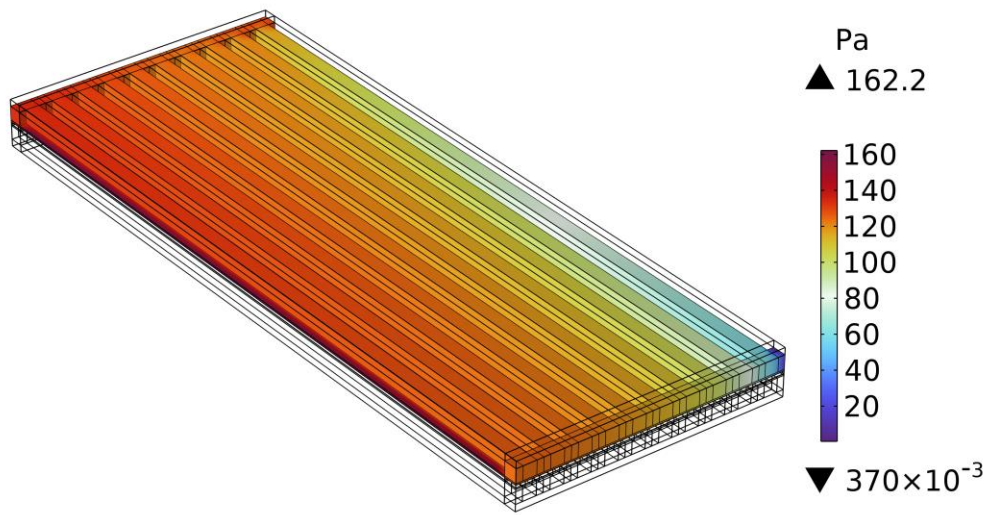
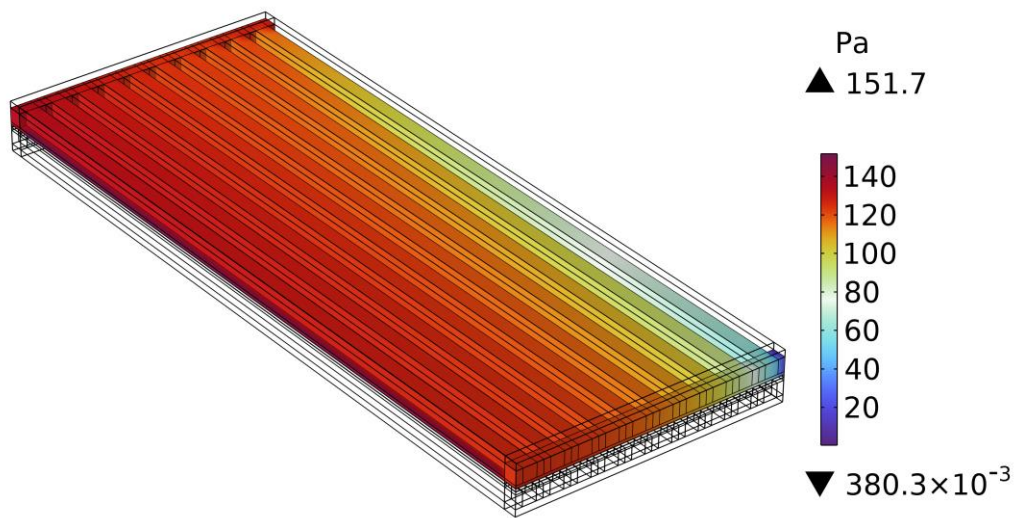


Figure 43. Average temperature of each anode channel outlet of different PTL thickness on the (a) anode and (b) cathode.

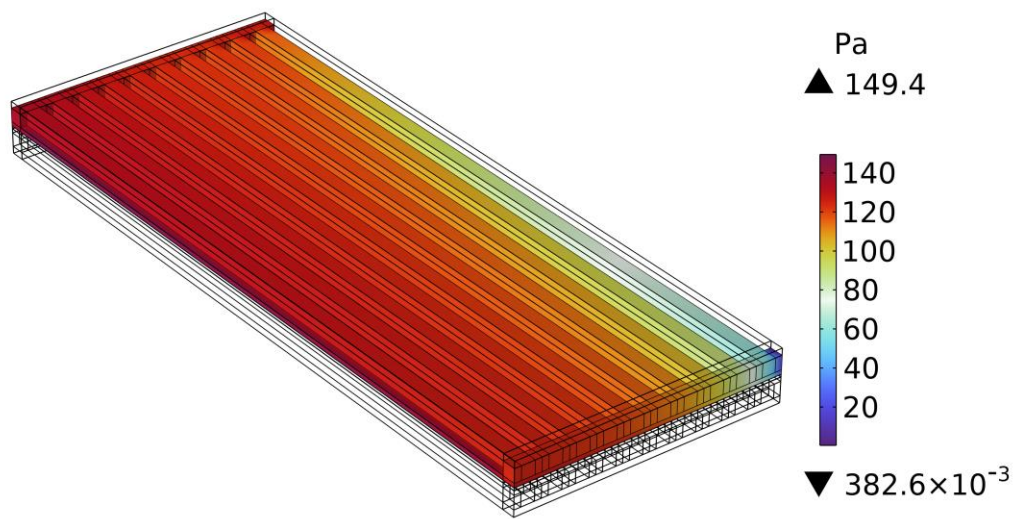
The pressure distributions on the anode side are also shown. The anode pressure distributions of all 5 PTL thicknesses show similar patterns, which is water inlet has higher pressure and outlet has lower pressure. A significant higher pressure is observed in PTL near the interface between ribs and PTLs. This phenomenon can be explained as gas under ribs has a longer distance to diffuse into the channels, the larger volume of gas here increases the pressure. For the highest pressure at anode side for different PTL thicknesses, it is also indicated that a bottom value occurs at 0.4 mm PTL thickness. 0.1 mm case is higher while the highest pressure is decreasing with increased PTL thicknesses from 0.1 mm to 0.4 mm. It is beneficial for a PEM water electrolyzer that was operated under a lower pressure, which will enhance the durability and improve the durability. On the other hand, higher pressure is beneficial for the gas removal on the anode side, but too high pressure proposes challenges for PEM water electrolyzer design, which induces a more complex design and extra cost.



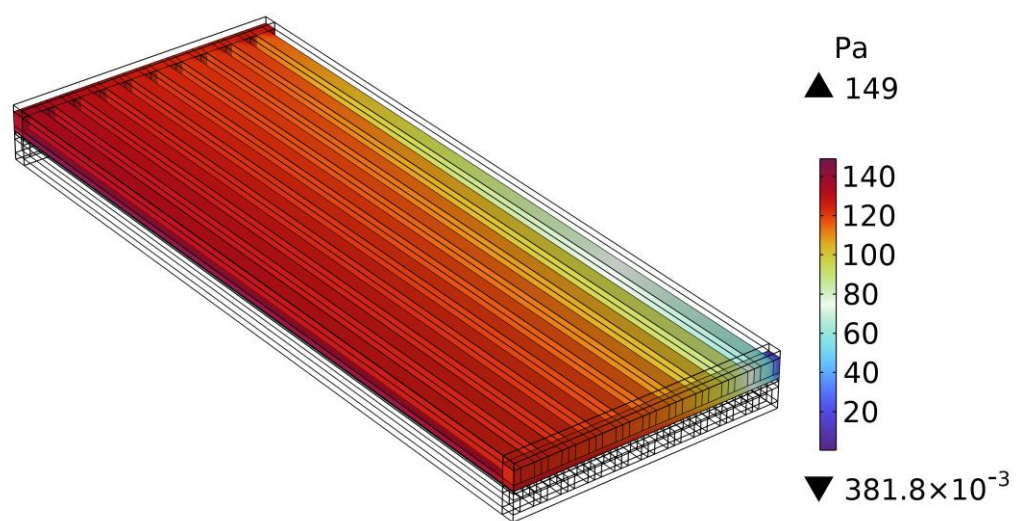
(a)



(b)



(c)



(d)

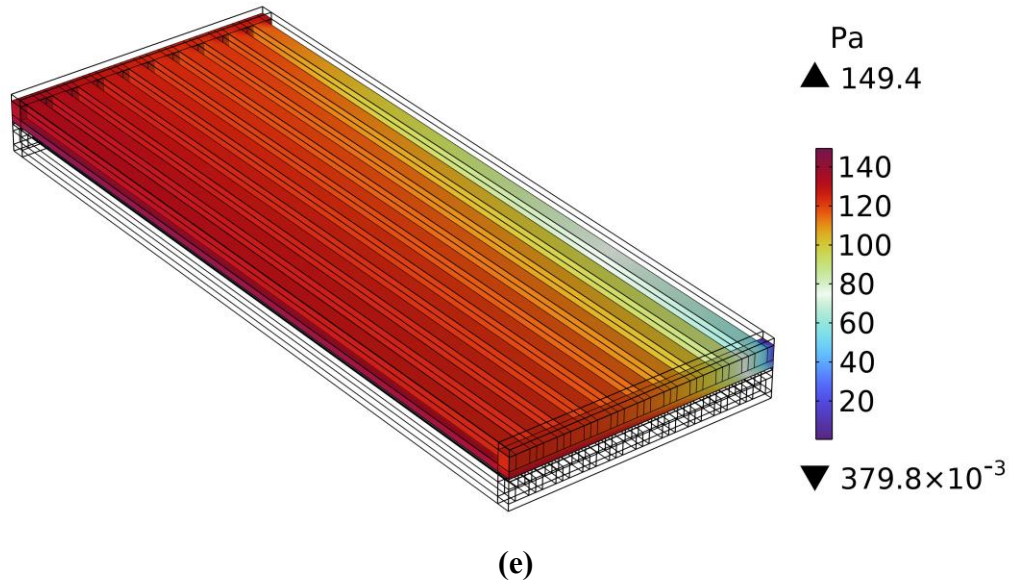


Figure 44. Anode pressure distribution with different PTL thicknesses (a) 0.1 mm, (b) 0.2 mm, (c) 0.3 mm, (d) 0.4 mm, and (e) 0.5 mm.

A decreasing trend is observed for hydrogen production rate through increasing PTL thickness, while higher PTL thickness also results in higher temperature distribution, CL average temperature and temperature variance. A lower CL average temperature and temperature variance represents more uniform temperature distribution and lower temperature, which is positive for long-term operation. A lower PTL thickness is beneficial for both hydrogen production and durability. On the other hand, the PTL thickness is also limited by the mechanical strength where PTL thinner than 0.1 mm is susceptible to fracture under the compressive clamping of PEMWE components [22] [44] [45]. Based on the results of this study, PTL thickness is suggested within the range of 0.2-0.5 mm to balance performance and mechanical strength.

4.2.3.2 Channel Width

Figure 45 shows the PEMWE hydrogen production rate as a function of the channel width. In this study, the channel width is systematically varied while maintaining a constant total width of the channel and rib. Accordingly, increasing the channel width results in a higher channel-to-total width ratio; thus, the channel width serves as the representative geometrical parameter in this analysis. Channel widths of 0.6 mm, 0.8 mm, 1.0 mm, 1.2 mm, and 1.4 mm are selected

for investigation. Hydrogen production shows a parabolic trend with increasing channel width. The hydrogen production rate initially increases from $1.19 \times 10^{-7} \text{ kg s}^{-1}$ to $1.21 \times 10^{-7} \text{ kg s}^{-1}$ with channel width from 0.6 mm to 1.0 mm but then decreases consistently to $1.193 \times 10^{-7} \text{ kg s}^{-1}$. This suggests that there is an optimal channel width that maximizes the hydrogen production rate. And for this case, this optimized value should be between 0.8 mm and 1.2 mm. This is because the increase of channel width results in reduction of rib width, which means increase the charge conducted resistance of ribs part. This impairs the electrons conduction. Furthermore, reduce hydrogen production.

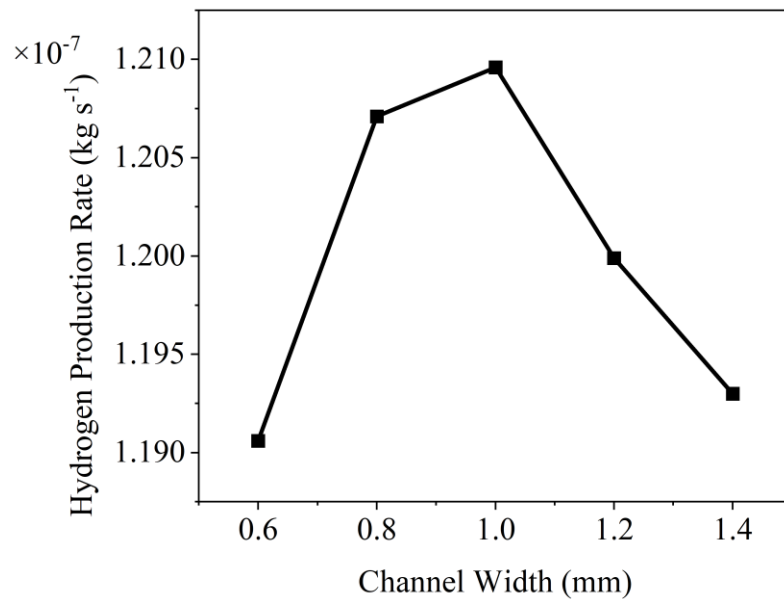


Figure 45. Simulation results of hydrogen production rate with channel widths from 0.6 mm to 1.4 mm.

Figure 46 also shows the sharp increase of the temperature at both anode and cathode. The maximum temperatures of both anode and cathode increase with the increase of flow channel width, which has the ranges of 356.5 K – 359.29 K and 353.1 K – 355.62 K for anode and cathode. The anode minimum temperature remains constant while cathode minimum temperature shows an increasing trend with channel width increases. For the first 3 cases, the temperature increases due to higher production rates, which is the source of electrochemical heating. For the latter cases, a wider channel width weakens the cooling effect of water on the

anode side, which leads to an increase of temperature. The increase of BPP and PTL resistance leads to more Joule heat generation depends on Ohm's law. A higher anodic temperature also results in an increasing temperature at cathode side.

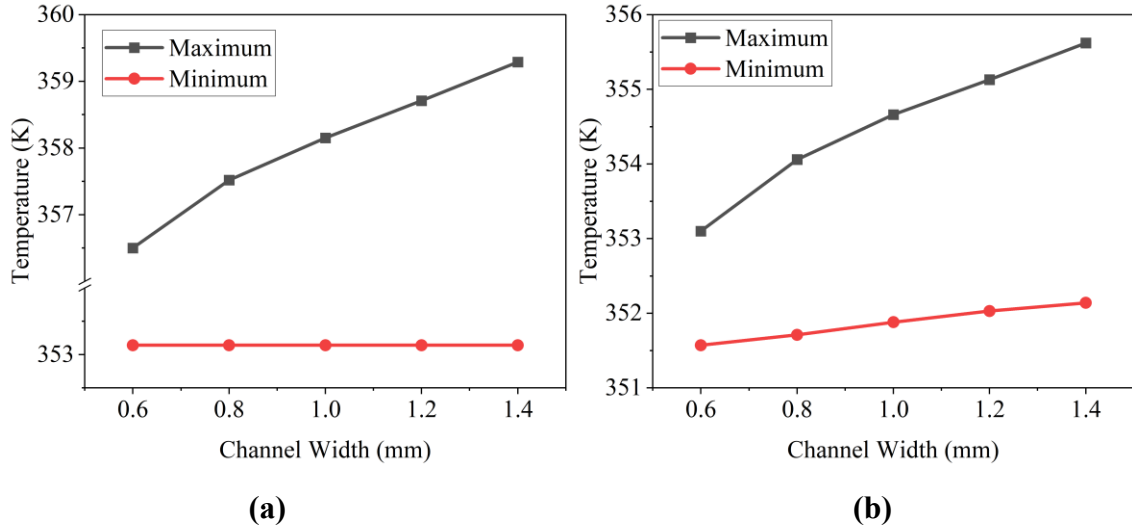


Figure 46. Simulation results of maximum and minimum temperature on (a) anode and (b) cathode with different channel widths from 0.6 mm to 1.4 mm.

Figure 47 represents the average temperature and variance change due to various channel widths. The average temperatures show the same trends as the maximum temperature change that described before. The variance is increasing at both sides, from 0.558 to 2.483 at anode and from 0.184 to 0.995 at cathode. In addition, the increase of electrode maximum temperature results in higher temperature variance. The increasing channel width results in higher resistance for BPP and lower anode velocity, which increases Joule heating generation and impairs the cooling effect of water. These two factors contribute to the increase of average temperature and variance, which results in more potential for durability issues.

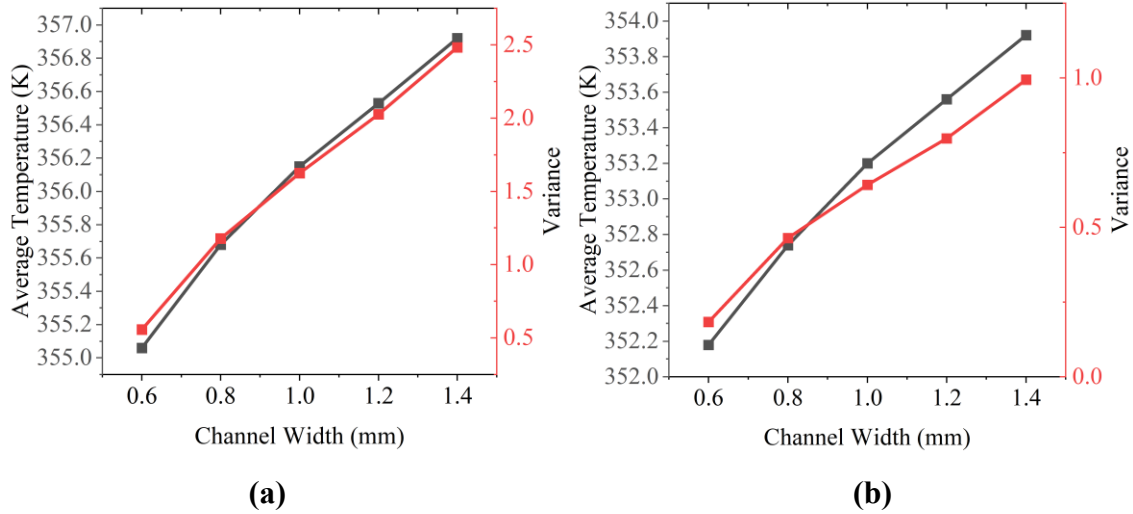
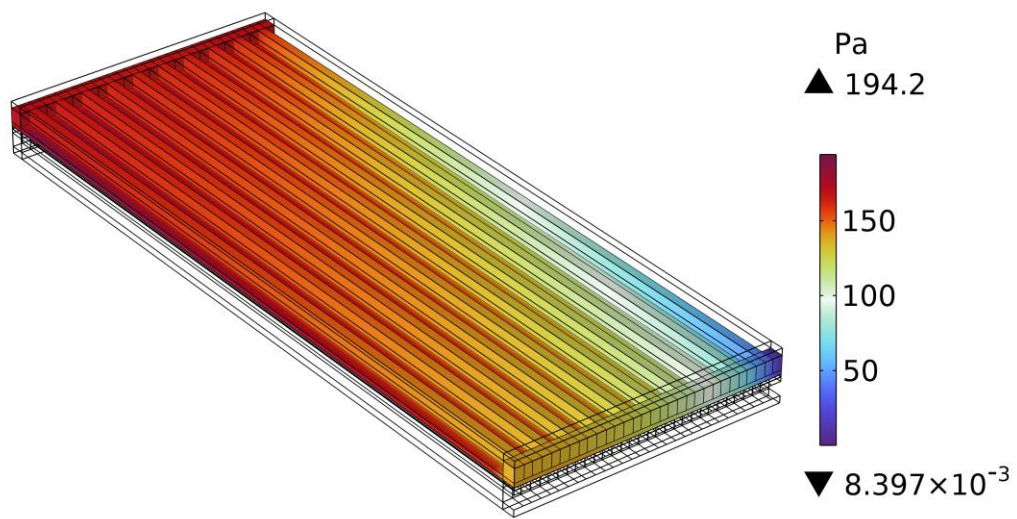
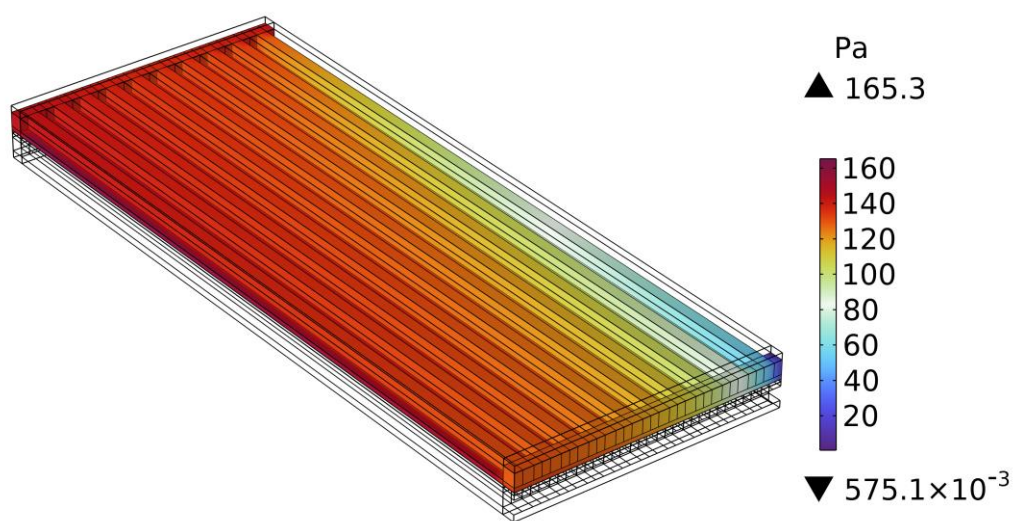


Figure 47. Average temperature and temperature variance of catalyst layer (CL) on (a) anode and (b) cathode with different channel widths from 0.6 mm to 1.4 mm.

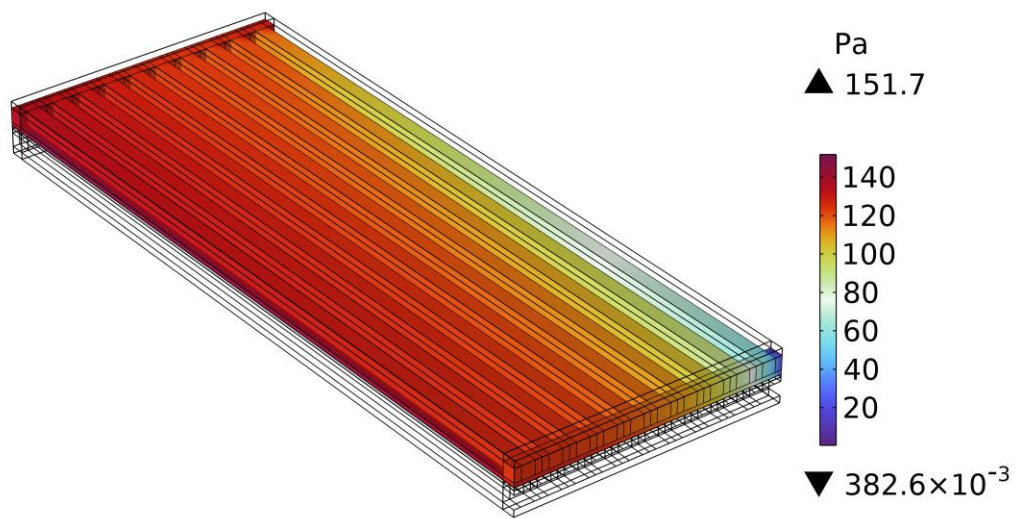
The results of anode pressure distribution with different channel widths are shown in Figure 48. The highest pressure at anode side has a relatively linear relationship with the channel width in selected range. The increasing channel width results in lower pressure drop of flow channels. Higher channel width results in higher cross-sectional area for water, which directly leads to a lower pressure drop at the same water feed rate. Narrower channels increase pressure drop, requiring more energy to pump water, which reduces system efficiency. On the other hand, wider channels and lower pressure drop might cause problems related to water distribution uniformity. Additionally, narrower channel width means wider rib width, the PTL area under ribs might have more gas and it is hard to be moved through the water in flow channels because of the lower contact surface. Therefore, there is an optimal channel width value to enhance the PEM water electrolyzer performance.



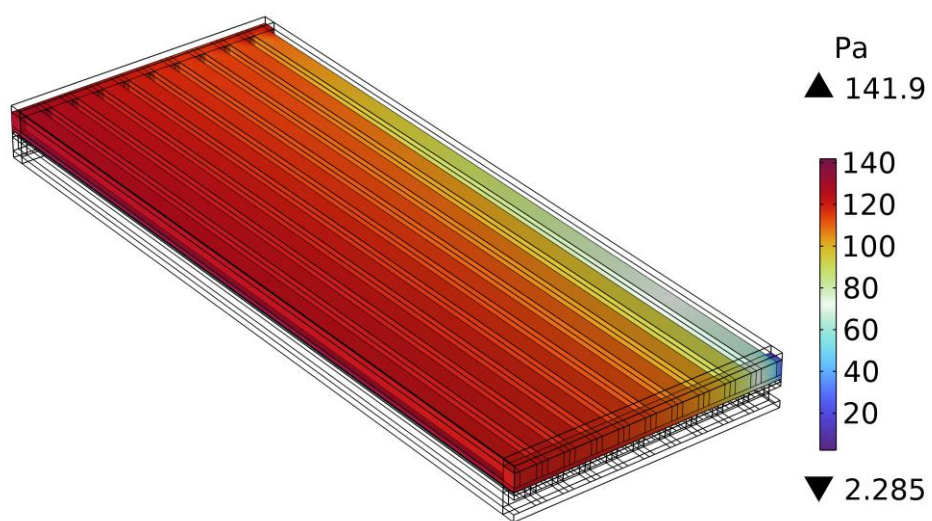
(a)



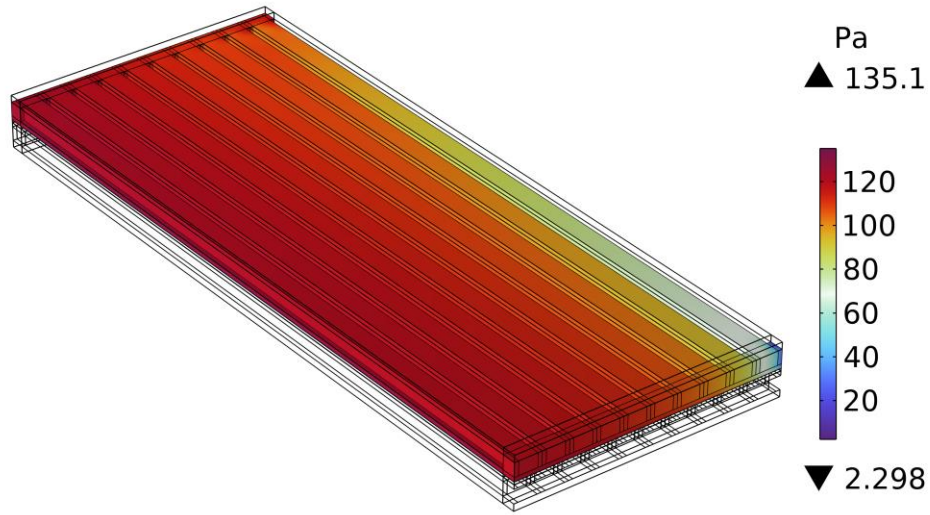
(b)



(c)



(d)



(e)

Figure 48. Anode pressure distribution with different channel widths (a) 0.6 mm, (b) 0.8 mm, (c) 1.0 mm, (d) 1.2 mm, and (e) 1.4 mm.

The velocity distributions of the header are analyzed. The cut plane is xy-plane, $z=2.818$ mm, which shows the velocity distribution of the middle surface at the inlet manifold.

The edge of higher velocity part, which is shown as dark red in Figure 49, approaches to the end of header with increasing channel width. In other words, higher channel width makes more uniform water distribution at the header. The uniform water distribution helps to improve gas removal and enhance long-term stability.

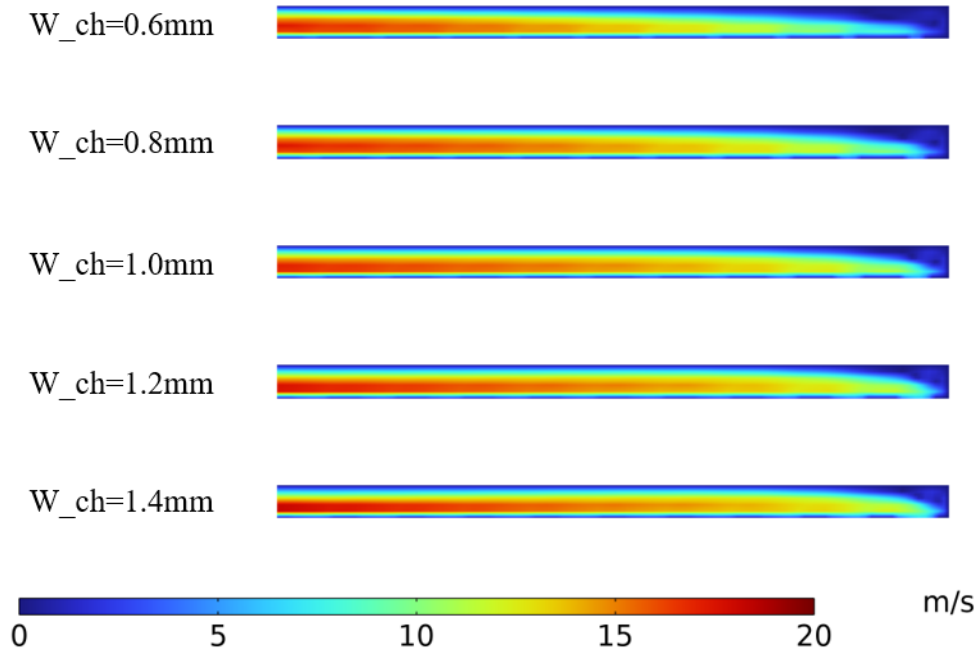


Figure 49. Header velocity distribution with different channel widths

Figure 50 demonstrates the average outlet temperature of each flow channel with different channel widths. The trends are similar to the cases in various PTL thicknesses for both anode and cathode. However, the maximum outlet temperature occurs at Channel #5 on the anode. The channel outlet temperatures are increasing with the increase of channel width. Additionally, the maximum difference between different channel widths is larger than the previous case, which are 2.25 K and 2.59 K for Channel #5 on the anode and cathode, respectively. This temperature difference is much larger than the cases in various PTL thickness, this also verifies the sensitivity analysis results in the previous section.

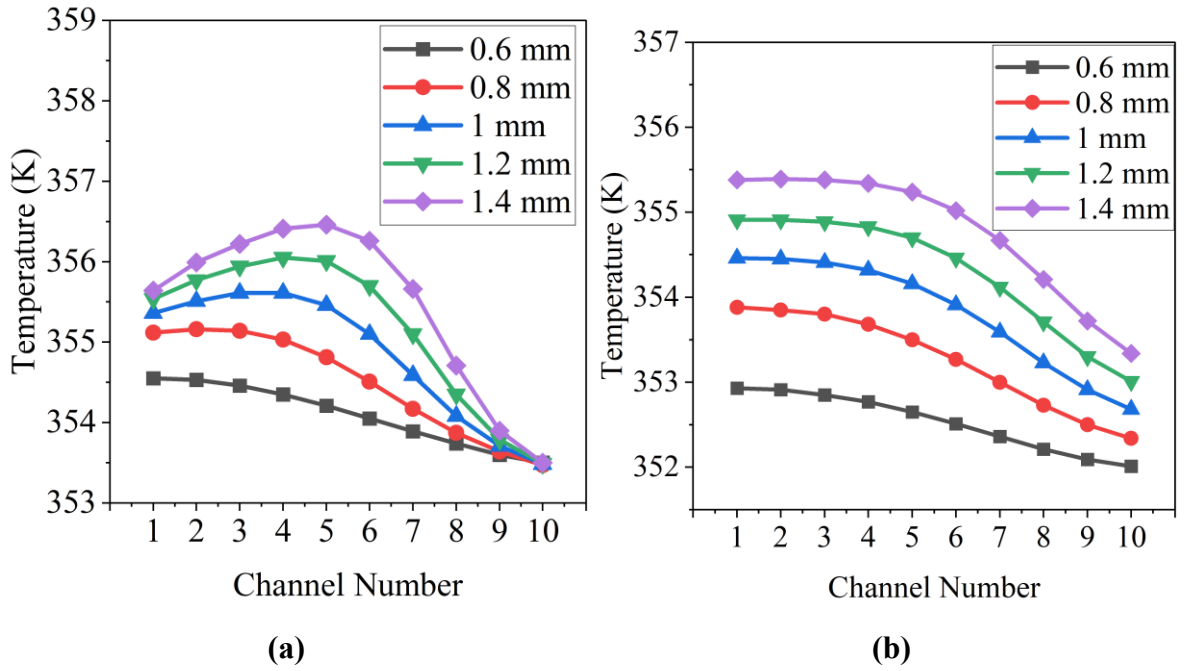


Figure 50. Average temperature of each anode channel outlet of different channel width on the (a) anode and (b) cathode.

The temperature distribution, average CL temperature, and CL temperature variance show increasing trend with increasing channel width, which indicates more potential of durability reduction. However, optimizable results are shown for hydrogen production with channel width variation. Therefore, an optimized channel width can be determined based on hydrogen production, and this value should not affect durability and stability. Therefore, 1:1 is the optimal value of ratio of channel width/rib width for the simulated PEMWE system.

4.2.3.3 Cell Length

The cell length that has been studied here means the length on x direction. The investigated range is 30 mm – 70 mm with an interval of 10 mm. The hydrogen production rate results are shown in Figure 51. It is increasing from $0.74 \times 10^{-7} \text{ kg s}^{-1}$ to $1.68 \times 10^{-7} \text{ kg s}^{-1}$ with a longer cell length, which indicates a higher performance. The hydrogen production rate increases by 125% compared with the lowest tested cell length (30 mm). The increase of cell length leads to higher contact area and active surface area. Furthermore, it has a higher hydrogen production rate. However, the cell length cannot be too long since increasing the cell length results in more

water consumption, nonuniform water distribution and higher pressure drop, which increases the required energy input and decreases the efficiency. [22]

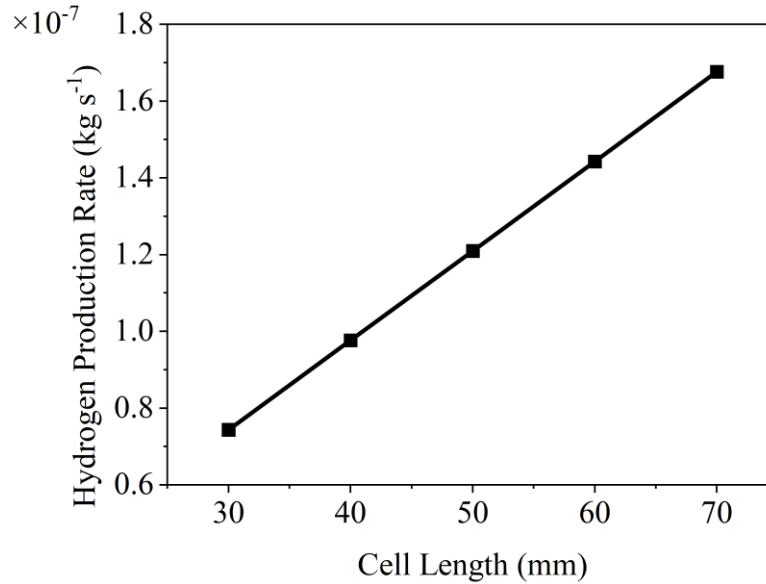


Figure 51. Simulation results of hydrogen production rate with different cell lengths from 30 mm to 70 mm.

The temperature distributions are shown in Figure 52. A higher cell length is also leading to a higher temperature at both sides, from 357.27 K to 358.81 K at anode and from 353.87 K to 355.22 K at cathode. The maximum temperature increases to 358.81 K for anode when the cell length is 70 mm. The increasing temperature distribution is caused by more heat generation from the reactions due to more contact area. Longer cell length results in the increase of contact surface area, which significantly influences the reaction rate. The increase of cell length also leads to higher resistance based on Ohm's Law. These result in more Joule heating and electrochemical heat released at both anode and cathode. Higher reaction rate also increases the consumption of water on the anode side, reducing the cooling effects of water.

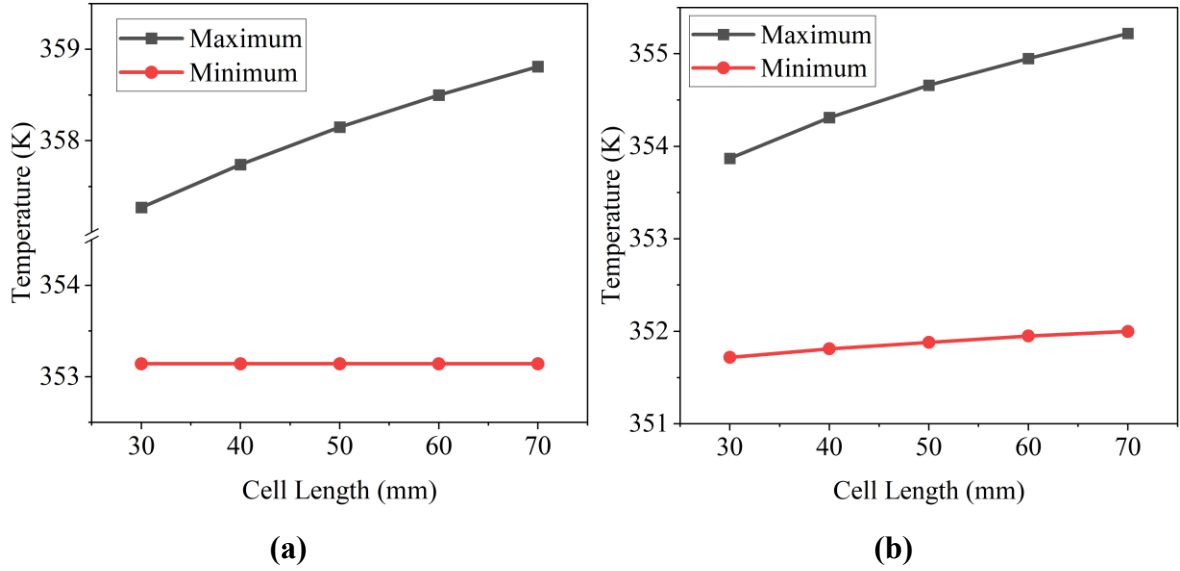


Figure 52. Simulation results of maximum and minimum temperature on (a) anode and (b) cathode with different cell lengths from 30 mm to 70 mm.

Figure 53 shows the increasing trends of both average temperature and variance of CL. The average temperature of the anode CL increases rapidly from 355.58 K to 356.57 K, while it rises from 352.72 K to 353.55 K for cathode. Additionally, higher temperature variance is reported with higher cell length, which is increased from 1.146 to 2.0038 at the anode side. The variance is lower for cathode but also shows an increasing trend from 0.385 to 0.8599. This is because the increase of cell length leads to higher contact area, which means more water can be consumed, generates oxygen and hydrogen. The increase in contact area also results in higher temperature spots since the increase of reaction rate. High variance should be avoided since the non-uniform temperature distribution will lead to the reduction of PEMWE durability.

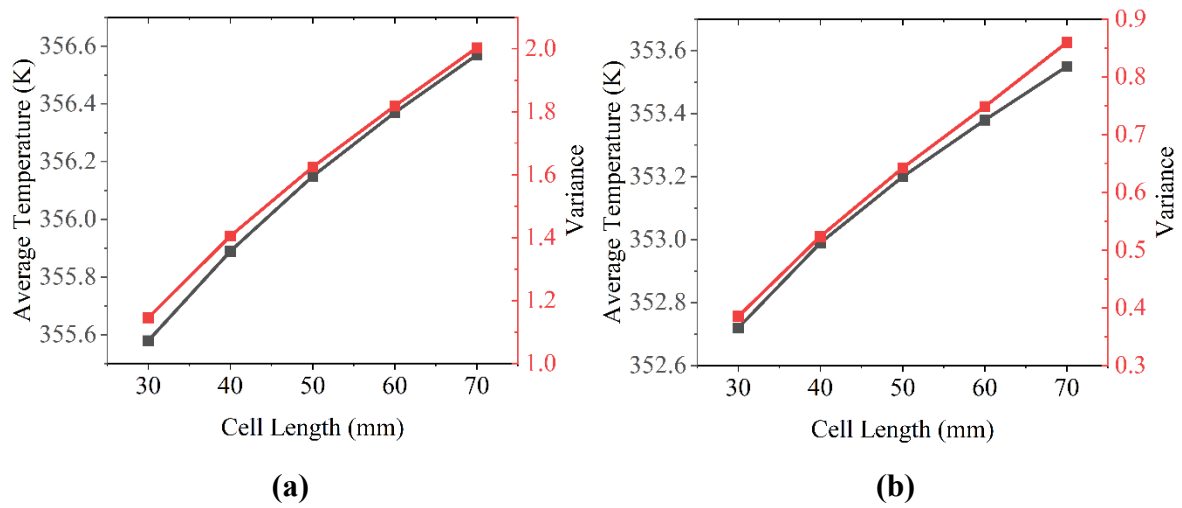


Figure 53. Average temperature and temperature variance of catalyst layer (CL) on (a) anode and (b) cathode with different cell lengths from 30 mm to 70 mm.

Figure 54 shows the outlet temperatures with different cell lengths. Similar trends are observed as in the previous two cases. The maximum temperature difference among different cell lengths is 1.58 K and 1.34 at Channel #1 on the anode and cathode, respectively, which is slightly lower than the various channel width cases but still higher than the different PTL thickness cases. This indicates that channel outlet temperature is more sensitive for various cell lengths and channel widths.

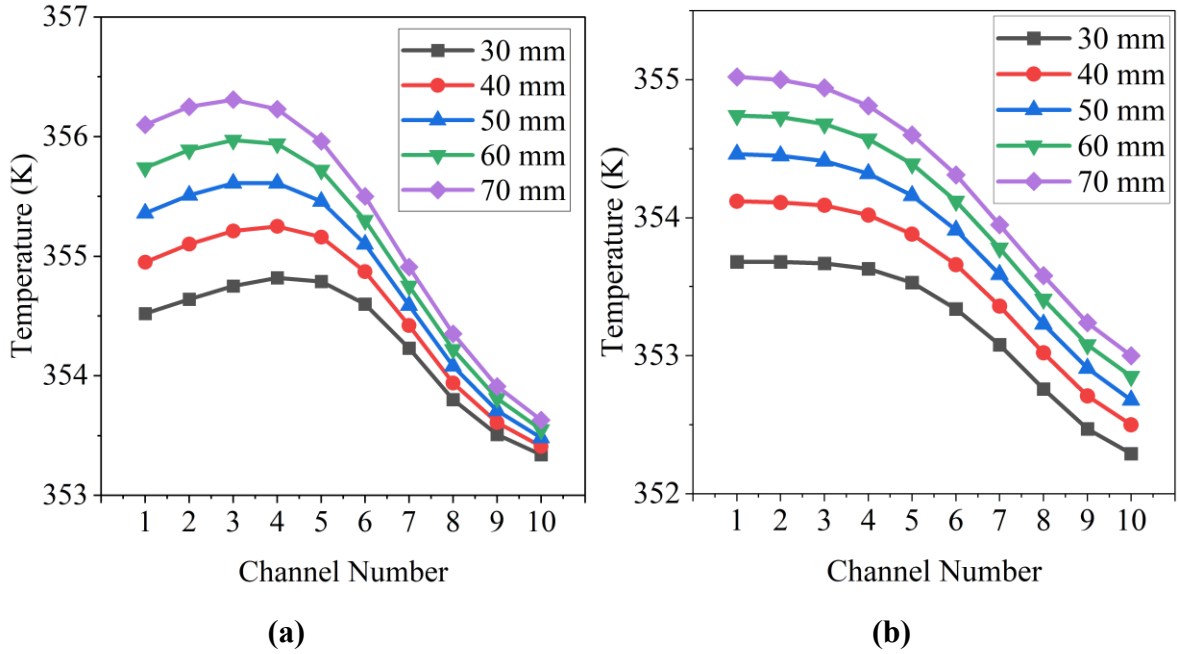
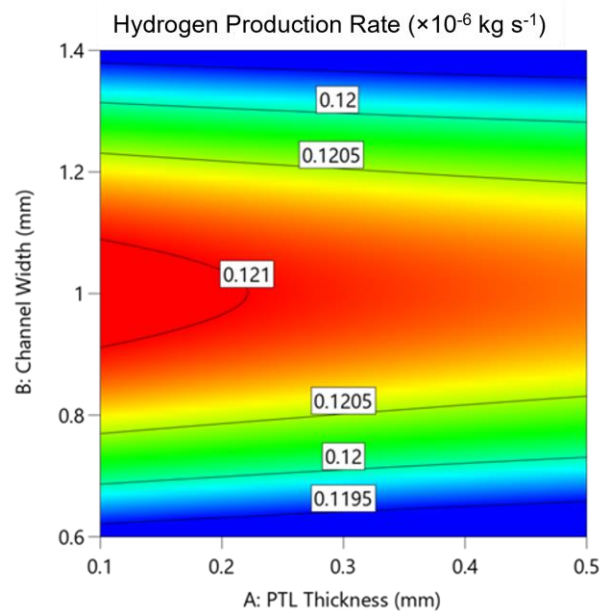


Figure 54. Average temperature of each anode channel outlet of different cell length on the (a) anode and (b) cathode.

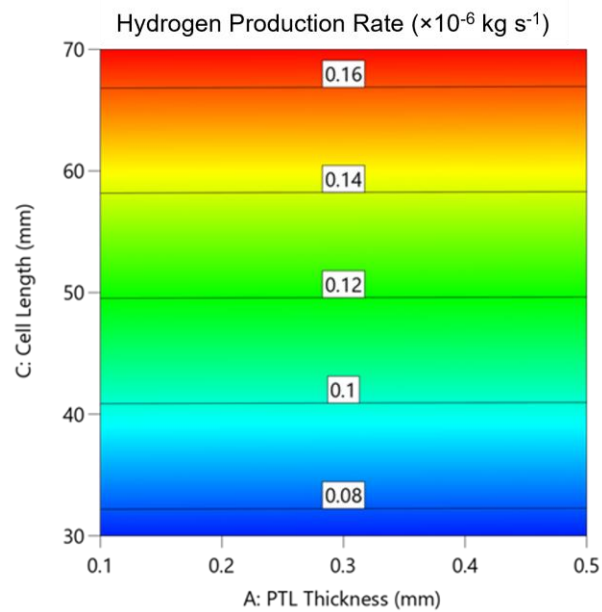
Increasing the cell length enhances the hydrogen production rate; however, it also leads to greater temperature gradients and higher CL temperature variance, which can negatively impact the durability of PEMWE. Therefore, selecting an appropriate cell length requires balancing performance gains against thermal management challenges. For cells with greater length, increased water flow is necessary to maintain lower operational temperatures and mitigate adverse effects on long-term system stability. Nevertheless, long cells incur high energy consumption due to increased pressure drops, and they introduce additional challenges related to structural integrity, manufacturing, and assembly. Furthermore, PEMWE cell operation is subject to critical constraints: the cell pressure must remain below 30 bar [22], and the operating temperature is recommended to stay below 363.15 K to preserve membrane performance. Consequently, cell length optimization must consider these limitations on pressure and temperature to ensure both efficiency and durability.

4.2.4 Influence of Parameter Interaction

After analyzing the effects of single parameters on Hydrogen production rate and Maximum Temperature, the influences of parameter interactions are also analyzed because of the existence of variance of the prediction model.



(a)



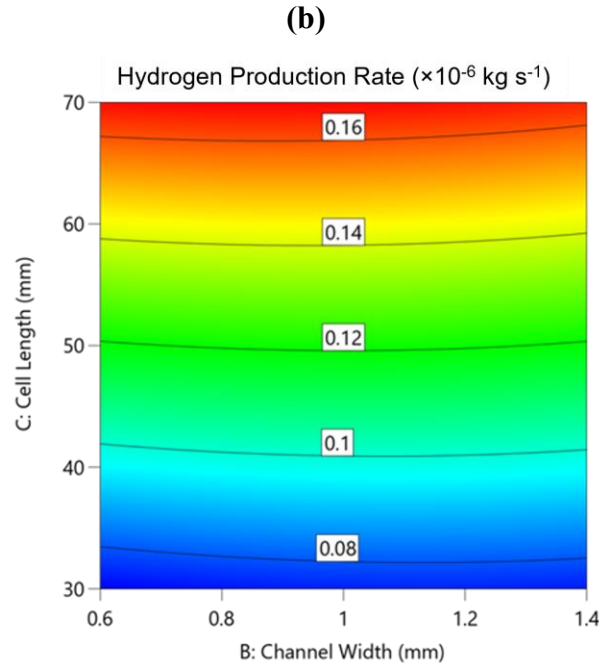
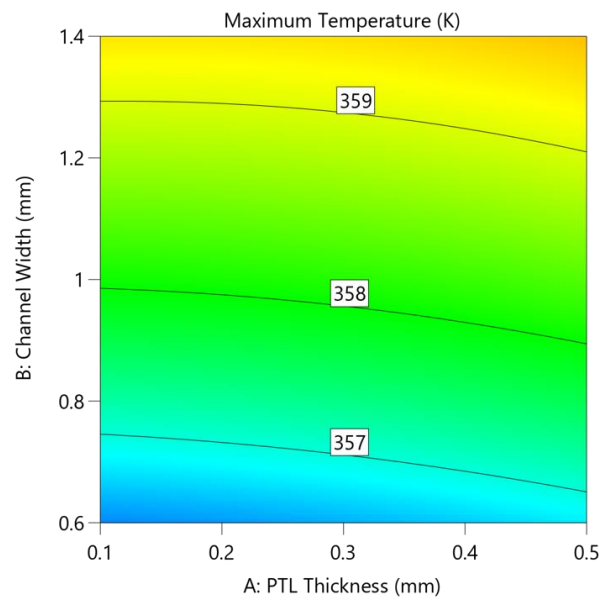
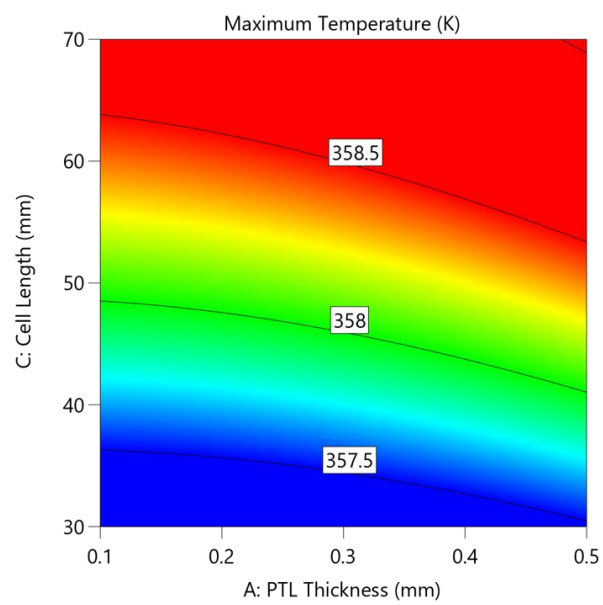


Figure 55. Effects of interaction parameters of (a) PTL thickness and channel width, (b) PTL thickness and cell length and (c) channel width and cell length on Hydrogen production rate.

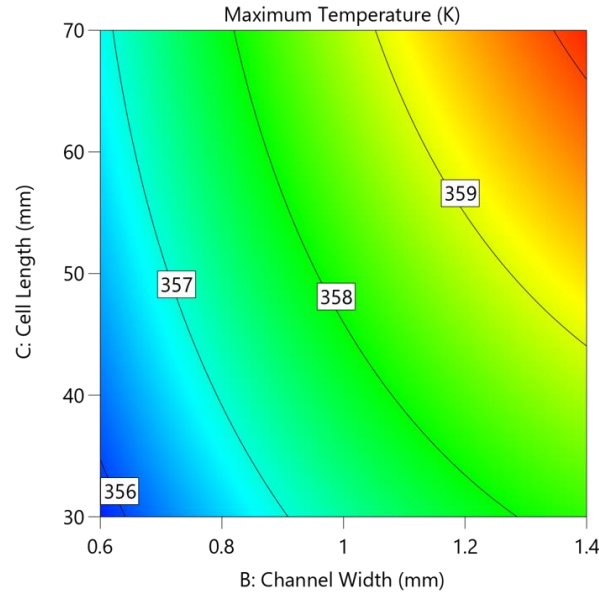
Figure 55a indicates that when PTL thickness is fixed, a maximal hydrogen production rate occurs around channel width equals 1 mm and becomes lower if the channel width is increased or decreased. If the channel width is fixed, the hydrogen production rate decreases when increasing the PTL thickness. In addition, PTL thickness has a more significant effect in BC term than AC term, since the hydrogen production rate is nearly stable when cell length is fixed in AC term. In addition, the maximum hydrogen production rate occurs around 0.1 mm PTL thickness and 1 mm channel width under the effects of these two parameters. While the maximum values occur at high cell length under interactive effect of PTL thickness and cell length, and effect of channel width and cell length. PTL thickness has nearly zero effect on hydrogen production rate in Figure 55(b), but the single parameters sensitivity analysis results show it's more sensitive than channel width, which emphasizes the importance of interactive parameters analysis.



(a)



(b)



(c)

Figure 56. Effects of interaction parameters of (a) PTL thickness and channel width, (b) PTL thickness and cell length and (c) channel width and cell length on Maximum temperature.

Figure 56 demonstrates the effects of interaction parameters on the maximum temperature of PEMWE unit. The lower variations range of AC term also verifies the insignificance of AC term. Furthermore, all the three interaction terms indicate higher input variables will lead to higher temperature, which shows the same analysis results of single parameters. BC term is the most significant term for maximum temperature in PEMWE, followed by AB term and AC term. This can be verified by the isothermals in the figures, BC term incorporates 4 isothermals from 356 K to 359 K, which has a wider variable range compared with the other two.

The effects of parameters interaction indicate that the effect of single parameters is not comprehensive, also provides the methods to predict the variations of hydrogen production rate and maximum temperature variations under random geometrical parameters.

4.3 Optimization

The relationship between three input parameters and two outputs (Hydrogen production rate and Maximum Temperature) are established in the previous chapter. For practical use, the PEMWE unit can be optimized to have a higher hydrogen production rate and lower maximum temperature. The optimization is conducted by MATLAB R2024b. The *gamultiobj* function is used for optimization in this study, which is part of the Global Optimization Toolbox to solve multiobjective optimization problems using genetic algorithm. [136] This function can optimize multiple objectives by finding several solutions on the Pareto Front. The optimized equations are normalized based on the two RSM models that have been built before. The variables are normalized by their ranges:

$$A' = \frac{A - 0.1}{0.4}$$

$$B' = \frac{B - 0.6}{0.8}$$

$$C' = \frac{C - 30}{40}$$

Therefore, the equations of the two objectives with dimensionless input variables can be written as:

$$X_1(A', B', C') = 5.584 \times 10^{-11} \times A'^2 + 1.0656 \times 10^{-10} \times A'B' - 1.5648 \times 10^{-10} \times A'C' \\ - 2.7992 \times 10^{-10} \times A' - 7.06432 \times 10^{-9} \times B'^2 - 4.96 \times 10^{-9} \times B'C' \\ + 9.55016 \times 10^{-9} \times B' + 3.264 \times 10^{-10} \times C'^2 + 9.457048 \times 10^{-8} \times C' \\ + 7.194545 \times 10^{-8}$$

$$X_2(A', B', C') = 0.224 \times A'^2 - 0.3 \times A'B' + 0.1 \times A'C' + 0.1933332 \times A' \\ - 1.0755584 \times B'^2 + 0.88 \times B'C' + 3.6095504 \times B' - 0.4752 \times C'^2 \\ + 1.49008 \times C' + 355.6726077$$

The ranges of objectives X_1 and X_2 are calculated by Monte Carlo sampling.

$$X_1 \in [7.172 \times 10^{-8}, 1.676 \times 10^{-7}]$$

$$X_2 \in [355.673, 360.319]$$

So the Objectives are further optimized by the ranges of objectives

$$X'_1 = \frac{X_1 - 7.172 \times 10^{-8}}{1.676 \times 10^{-7} - 7.172 \times 10^{-8}}$$

$$X'_2 = \frac{X_2 - 355.673}{360.319 - 355.673}$$

The final normalized optimization equations are:

$$X'_1(A', B', C') = 5.8248 \times 10^{-4} \times A'^2 + 1.1116 \times 10^{-3} \times A'B' - 1.6323 \times 10^{-3} \times A'C'$$

$$- 2.9199 \times 10^{-3} \times A' - 7.369 \times 10^{-2} \times B'^2 - 5.174 \times 10^{-2} \times B'C'$$

$$+ 9.962 \times 10^{-2} \times B' + 3.405 \times 10^{-3} \times C'^2 + 0.9865 \times C' + 0.00234$$

$$X'_2(A', B', C') = 4.821 \times 10^{-2} \times A'^2 - 6.457 \times 10^{-2} \times A'B' + 2.152 \times 10^{-2} \times A'C'$$

$$+ 4.161 \times 10^{-2} \times A' - 0.2315 \times B'^2 + 0.1894 \times B'C' + 0.7769 \times B'$$

$$- 0.1023 \times C'^2 + 0.3207 \times C' - 8.44 \times 10^{-5}$$

X'_1 and X'_2 are the dimensionless objectives within range [0,1], which denote hydrogen production rate and maximum temperature in this case.

Genetic algorithm (GA) is a method for solving both constrained and unconstrained optimization problems on a natural selection process that mimics biological evolution. [137] Comparing with Classical Algorithm, GA can generate a population of points at each generation, while only one single point is generated at each iteration for Classical Algorithm. The flow chart of GA is shown in Figure 57. A random initial population is generated when the algorithm starts, then each individual is evaluated using a fitness function that quantifies how good the solution is. After the evaluation, it will select the individuals from the current population to become parents depending on the fitness. Different parents will be combined to create new offspring. Mutation, randomly altering one or more genes in the offspring, will also happen in this step. Finally, the individuals are evaluated by the termination criterion, if the generation met the criterion, the program would terminate and output the results. If not, it will repeat the previous steps until an optimal generation has occurred.

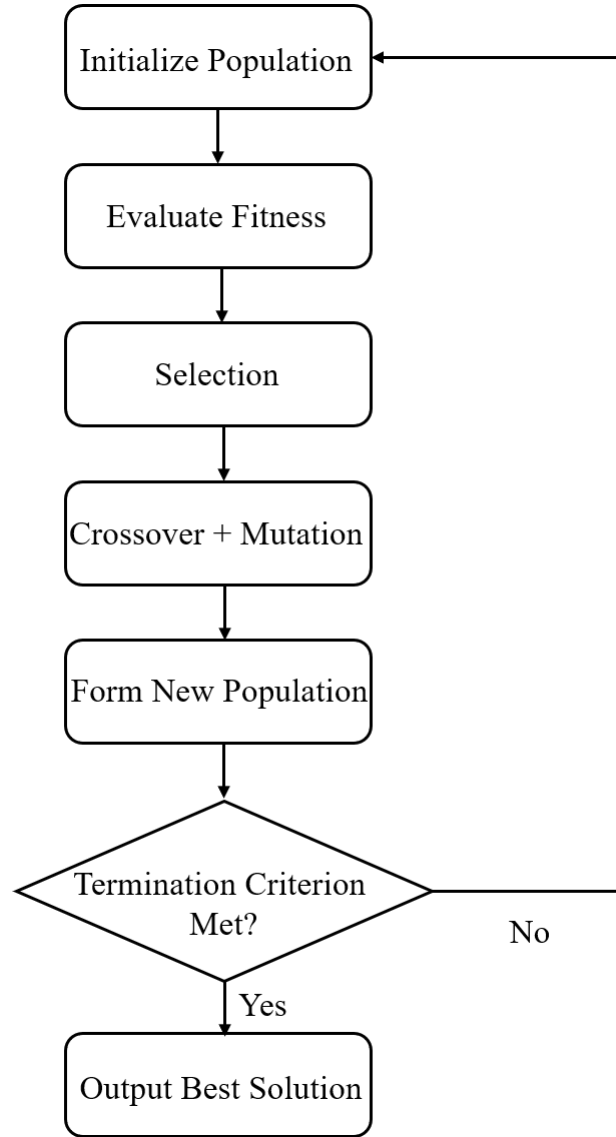


Figure 57. Flow chart of Genetic algorithm

Based on the simulations results and sensitivity analysis, the targets of the optimization in this study are

- Maximize the Hydrogen production rate
- Minimize the Maximum Temperature

The weights of the two objectives are 50% and 50%, respectively. Therefore, the objective function f can be written as:

$$f = -0.5X'_1 + 0.5X'_2$$

The negative sign of X'_1 denotes maximization of this objective, since the function is automatically optimized to search for the minimal value of the objective. The maximum generation is set to 3,000 to make sure it is not a factor that influences the results. Function tolerance is set to $1e-10$ to engage the accuracy of the optimization. The optimized results are shown in Figure 58.

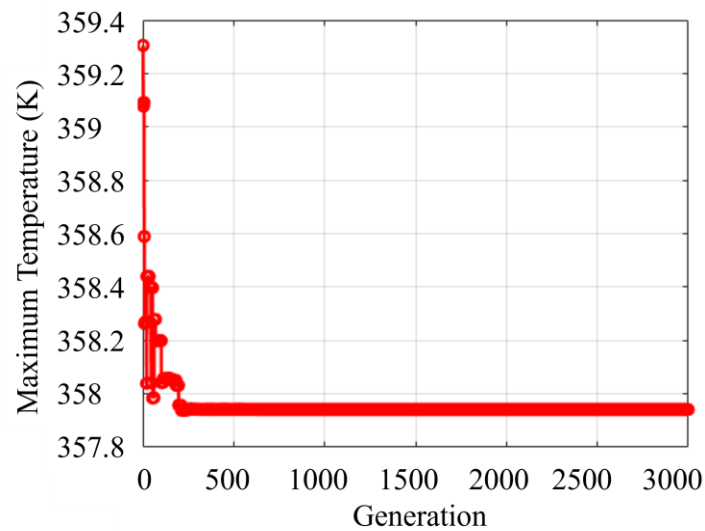
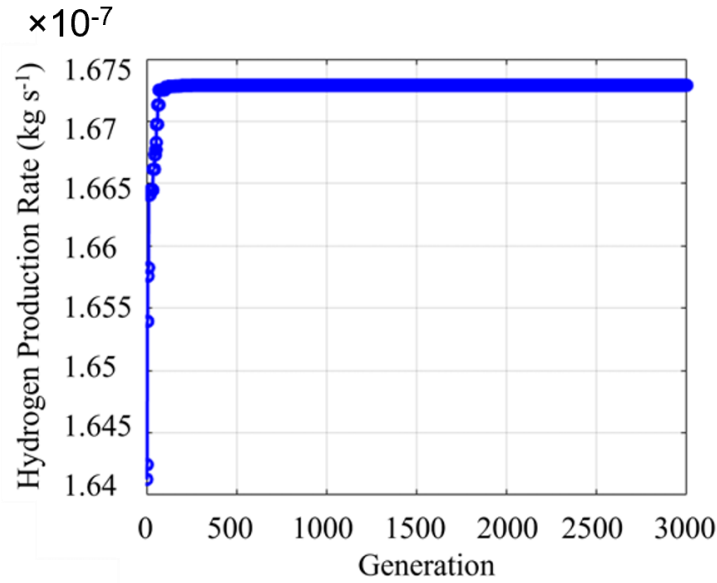


Figure 58. Variations of Hydrogen production rate (top) and Maximum Temperature (bottom) with generations

The results indicate that at the beginning part of the optimization, the values of both outputs are unstable, varying with the increase of the generations. This indicates that these values are not optimized values. With the increase of generation, two outputs become stable and do not change with generations, which demonstrates these are the best outputs that we can get in these ranges. The details of the optimization are shown in Table 9, while the comparison between baseline design and the optimized case is shown in Table 10.

Table 9. Geometrical parameters after GA optimization

Parameters	Unit	Original Values	Optimized Values
Total length	mm	50	70
Channel width	mm	1	0.8439
Ribs width	mm	1	1.1561
PTL thickness	mm	0.3	0.1

Table 10. Comparison of outputs between original design and optimized case

Output	Unit	Original Values	Optimized Values
Hydrogen production rate	kg s ⁻¹	1.2096×10^{-7}	1.673×10^{-7}
Maximum temperature	K	358.15	357.9416

From the optimized results, the PTL thickness is reduced to 0.1 mm, cell length is extended to 70 mm, and channel width is optimized to 0.8439 mm. The results indicate that the Hydrogen production rate can be enhanced to 1.673×10^{-7} kg s⁻¹ and the Maximum Temperature can be improved to 357.9416 K. The optimized hydrogen production rate achieves a 38.31% increase, while the maximum temperature is reduced simultaneously. The optimized geometrical parameters can increase hydrogen production and reduce the temperature simultaneously. The polarization curves of original model and optimized model are compared in Figure 59. The current density has a relative improvement at the same electric potential, which also indicates the enhancement of the PEMWE performance.

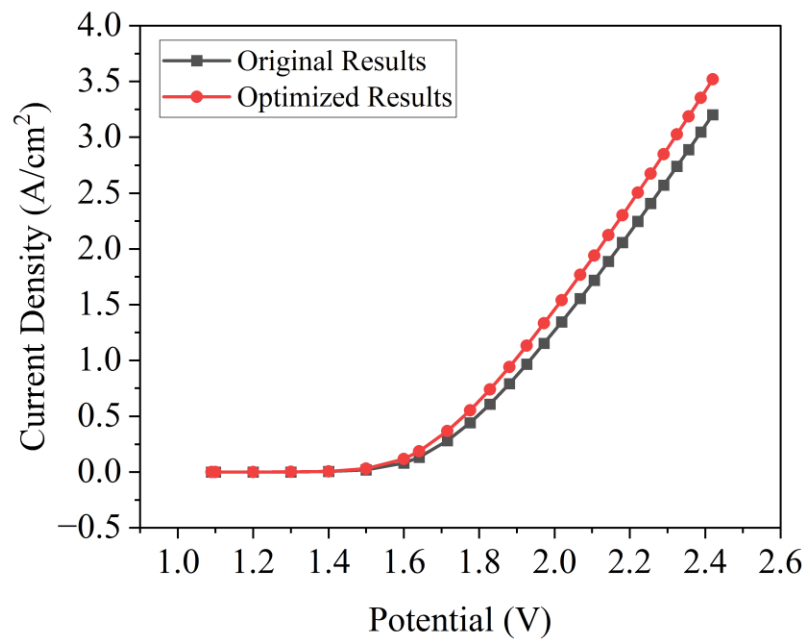


Figure 59. Comparison of original and optimized model

5. Conclusions and Future Work

5.1 Conclusions

This study explored the integration of green hydrogen production via Proton Exchange Membrane Water Electrolyzers (PEMWEs), by employing a comprehensive numerical simulation, the influence of key geometrical parameters-porous transport layer (PTL) thickness, channel width, and cell length-on PEMWE performance was systematically assessed.

Cell length is a dominant factor affecting hydrogen production, while all three parameters significantly influenced the internal temperature distribution. The simulation results indicated that increasing the cell length from 50 to 70 mm led to a 38.62% increase in hydrogen output, and that a thinner PTL enhanced hydrogen generation efficiency. Furthermore, channel width exhibited a non-linear (parabolic) relationship with both temperature and hydrogen production, suggesting the existence of an optimal width for thermal and performance efficiency. However, higher temperature variances are observed at catalyst layer (CL) with higher channel width. These results indicate the possibility of optimizing the geometrical design of PEMWE. A suitable optimization can maximize the performance of PEMWE, which increases the hydrogen production rate and keeps the temperature distribution as low as possible.

To enhance operational efficiency, a multi-parameter optimization with Genetic Algorithm (GA) was conducted, targeting maximization of hydrogen output and minimization of temperature rise. The optimized configuration achieved a 38.31% increase in hydrogen production and 0.21 K reduction in peak temperature compared to the baseline design.

This study provides the effects of geometrical parameters variations on the PEMWE performance, especially hydrogen production rate and temperature distribution. It provides valuable and comprehensive evaluation methods for a PEMWE unit in green hydrogen production.

5.2 Future Work

It is obvious that geometrical parameters have significant effects on the performance of PEMWE. The change of geometrical parameters can increase the hydrogen production rate and reduce the temperature simultaneously with appropriate optimization. In this study, the influences of PTL thickness, channel width and cell length are investigated, and the design was optimized for proposed hydrogen production and storage pathway.

Further, other parameters can also affect the performance of PEMWE, such as operational parameters and flow pattern design. For example, different operation temperatures and water feed rates can affect the polarization curve and cooling efficiency. Different flow patterns, like serpentine, parallel, pin will lead to different PEMWE design due to various pressure and velocity distribution. Therefore, the sensitivity analysis and optimization of operational parameters and flow pattern are also an essential part for PEMWE performance investigation.

In addition, with optimized PEMWE by considering geometrical parameters, operational parameters and flow pattern design, the stability of PEMWE is another important topic. Stability is strongly related to the lifespan of the PEMWE, further, the economics of the hydrogen system. Therefore, the stability related to PEMWE should be investigated in the future. .

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