UNIVERSITÉ DU QUÉBEC À TROIS-RIVIÈRES

Gestion d'énergie d'un électrolyseur PEM modulaire

THÈSE PRÉSENTÉE
COMME EXIGENCE PARTIELLE DU

DOCTORAT EN GÉNIE ÉLECTRIQUE

PAR
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Avril 2025

UNIVERSITÉ DU QUÉBEC À TROIS-RIVIÈRES
GÉNIE ÉLECTRIQUE (DOCTORAT)

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Thèse soutenue le 7 avril 2025

REMERCIEMENTS

Au terme de cette thèse, il m'est particulièrement cher d'exprimer ma profonde gratitude envers ceux qui ont rendu ce voyage possible et enrichissant.

Je tiens à remercier chaleureusement le Professeur Loïc Boulon, mon directeur de thèse, qui a toujours cru en moi. Sa confiance indéfectible, sa disponibilité constante et ses précieux enseignements ont été une source inestimable d'inspiration et de motivation tout au long de ce parcours.

Je suis également profondément reconnaissant envers le Professeur Bruno Pollet, dont l'énergie débordante et l'enthousiasme sans limites m'ont constamment émerveillé. Son dynamisme exemplaire est une véritable source d'inspiration, et j'espère un jour atteindre son niveau d'activité et de passion.

Mes sincères remerciements vont à cher Mohsen Kandidayeni, mon premier guide scientifique, qui est pour moi bien plus qu'un mentor. Tel un grand frère, il a toujours été là pour me soutenir, partageant généreusement ses idées novatrices et son aide précieuse. Sa présence a été essentielle dans les moments clés de cette recherche.

Je souhaite également exprimer ma gratitude envers cher Meziane Ait-Ziane, mon conseiller scientifique. Sa positivité contagieuse et ses paroles encourageantes ont été une véritable bouffée d'air frais, me motivant à persévérer et à donner le meilleur de moi-même.

Mes remerciements s'étendent à mes amis et collègues, sans qui cette aventure académique n'aurait pas eu la même saveur. Et tous ceux qui m'ont soutenu et accompagné, merci de ne jamais m'avoir laissé seul. Votre camaraderie et votre soutien ont rendu ce voyage non seulement enrichissant, mais également mémorable.

Enfin, mes mots les plus tendres sont pour mon épouse, qui a été ma seule famille durant cette période. Elle a accepté avec courage toutes les pressions et les moments difficiles que cette thèse a impliqués. Son amour et son soutien inconditionnels ont été ma plus grande force. Je tiens également à remercier nos parents, qui nous ont toujours soutenus. Leur affection et leurs encouragements ont été le socle sur lequel j'ai pu construire et avancer.

À tous, je vous exprime ma profonde reconnaissance. Votre présence à mes côtés a fait de cette étape une expérience inoubliable et précieuse.

RÉSUMÉ

Cette thèse présente une étude complète sur l'amélioration de la gestion de l'énergie des électrolyseurs à membrane échangeuse de protons (PEMWE) modulaires, une technologie clé pour la production d'hydrogène vert. En réponse au besoin crucial de systèmes de production d'hydrogène efficaces et évolutifs, cette recherche examine l'intégration des PEMWE avec des sources d'énergies renouvelables (RES), en se concentrant sur l'optimisation de l'efficacité opérationnelle et de la longévité des systèmes à travers des stratégies avancées de gestion de l'énergie.

La recherche commence par une revue exhaustive de la littérature, établissant une compréhension fondamentale des opérations des PEMWE, de l'importance des configurations modulaires, et des pratiques existantes de gestion de l'énergie. Les chapitres suivants présentent des méthodologies innovantes pour le benchmarking des modèles électrochimiques adaptés aux systèmes PEMWE modulaires, en mettant l'accent sur la sélection de modèles qui équilibrent efficacement l'efficacité énergétique et le contrôle de la dégradation.

Au cœur de cette thèse se trouve le développement d'un Système de Gestion de l'Énergie (EMS) sophistiqué, conçu pour optimiser la distribution de l'énergie à travers les unités modulaires, s'adaptant dynamiquement à la nature variable des entrées RES. Ce système utilise une combinaison d'analyses de données en temps réel, de modélisation prédictive, et d'algorithmes de contrôle avancés pour améliorer la stabilité opérationnelle et l'efficacité des systèmes PEMWE.

La validation empirique, réalisée à travers des simulations et des configurations expérimentales, démontre l'efficacité du EMS proposé, révélant des améliorations significatives dans l'efficacité de la production d'hydrogène et la durabilité du système. La recherche se conclut par une discussion sur les orientations futures, incluant l'intégration d'algorithmes d'apprentissage automatique pour une optimisation supplémentaire et le potentiel d'extension des systèmes PEMWE modulaires pour des applications industrielles.

En comblant le fossé entre les modèles théoriques et la gestion de l'énergie pratique, cette thèse apporte des insights précieux dans l'optimisation de la production d'hydrogène vert, soutenant l'avancement des solutions énergétiques durables.

Abstract

A thorough investigation into improving the energy management of modular proton exchange membrane water electrolyzers (PEMWE), a crucial technology for the generation of green hydrogen, is presented in this thesis. This study explores the integration of PEMWEs with renewable energy sources (RES) to meet the urgent demand for scalable, efficient hydrogen-generating systems. It focuses on employing advanced energy management strategies to decrease degradation and increase operational efficiency.

The research begins with a thorough literature review, establishing a foundational understanding of PEMWE operations, the significance of modular configurations, and existing energy management practices. Subsequent chapters present novel methodologies for benchmarking electrochemical models tailored to modular PEMWE systems, emphasizing the selection of models that effectively balance energy efficiency and degradation control.

A key component of this thesis is the creation of an advanced Energy Management System (EMS) that dynamically adjusts to the changeable nature of RES inputs to improve power distribution across modular units. A sophisticated control algorithm, a real-time data analytics platform, and rotary modelling are incorporated into the PEMWE system to enhance its operational stability and effectiveness.

Numerous empirical validations based on simulations and tests have proved the practical use of the proposed EMS, demonstrating significant improvements in the lifetime and efficiency of hydrogen production. Potential future trends are covered in the study's conclusion, including the potential for expanding modular PEMWE systems for industrial applications and the adoption of machine learning techniques for more optimization.

This thesis supports the development of sustainable energy solutions by providing important insights into the optimization of green hydrogen generation by bridging the gap between theoretical models and real-world energy management.

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A_L	**Active large surface area (mm)**
A_S	Active small surface area (mm)
B_r	temperature coefficient
CP_{PV}	Coefficient of Performance
G_{nr}	Solar irradiance (W/m^2)
I_C	cell current (A)
I_S	stack current (A)
I_{cn}	each cell current (A)
P_C	cell power (W)
P_{el}	electrolyzer required power
P_{pv}	PV Power (W)
T_{pv}	PV temperature(°C)
T_r	operating reference temperature (°C)
U_a	Activation overvoltage (v)
U_c	Concentration overvoltage (v)
U_o	Ohmic overvoltage (v)
U_b	Bubble overpotential
V_C	cell voltage (v)
V_{OC}	Open circuit voltage (v)
V_S	stack voltage (v)
V_{cell}	cell voltage (v)
V_{cn}	each cell voltage (v)
V_{rev}	Reversible cell voltage (v)
$V_{rev,s}$	Standard reversible cell voltage (v)
V_{th}	Thermoneutral voltage (v)
n_{el}	number of electrolyzers
n_p	number of PV panels
t_r	reference time
$\alpha HyPro_S$	HyPro system (in a stack) efficiency
η_v	voltage efficiency (%)
η_c	cell efficiency (%)

η_e	Electrolyzer efficiency (%)
η_s	Electrolyzer system energy efficiency (%)
η_{BP}	Balance of plant efficiency (%)
A	Area (square meter, m^2)
E	Energy ($Wh \approx 3600\ joules$)
F	gas flow rate (Normal Meter Cubed per Hour Nm3/hr)
F	Faraday constant (C/mol)
G	gradient
$HHVH$	Higher Heating Value of Hydrogen (kWh/Nm^3)
P	Power (W)
Rct	charge transfer impedance (Ω)
R	The universal gas constant 8.314 (J/mol·K)
t	Time (h and H/2)
W	electrical work of electrolysis (J/mol)
W_{irrev}	Irreversible energy (J/mol)
W_{rev}	Reversible energy (J/mol)
Υ	surface coverage ratio (/)
ΔH_R^0	Electrolysis required energy (J/mol)
Ω_E	Electric resistance in electrodes (Ω)
Ω_{eq}	Equivalent electric resistance in PEMWE (Ω)
Ω_M	Electric resistance in membrane (Ω)
θ	Thickness of the membrane (cm)
℧	Conductivity of the membrane (umho/cm)
λ	Humidification of the membrane

List of abbreviations

AC	Alternating Current
ANN	Artificial Neural Network
CNC	Computer Numerical Control
CO_2	Carbon Dioxide
DC	Direct Current
e_-	electron
ERC	Ejector Refrigeration Cycle
FC	Fuel Cell
H_2	Hydrogen
HyPro	Hydrogen Production
kW	Kilo Watt
L	Liter
MES	Modular energy system
ML	Machine Learning
MW	MegaWatt
NPV	Net present value
O_2	Oxygen
ORC	Organic Rankine Cycle
PEMFC	Proton Exchange Membrane Fuel Cell

PEMWE	Proton Exchange Membrane Water Electrolyzer
AWE	Alkaline Water Electrolysis
AEM	Anion Exchange Membrane
SOE	Solid Oxide Electrolysis
PTC	Parabolic Trough (solar) Collector
PtG	Power-to-Gas
PV	Photovoltaic
RES	Renewable Energy Source
RO	reverse osmosis
WECS	wind Energy Conversion System
SIBC	stacked interleaved buck converter
MEA	Membrane Electrode Assembly
PTL	porous transport layer
OER	Oxygen Evolution Reaction
MSE	Mean Squared Error
RMSE	Root Mean Squared Error
GA	Genetic Algorithm

1 Introduction

1.1 Background and Motivation

1.1.1 The increasing demand for green hydrogen

In the pursuit of sustainable energy solutions, the importance of green hydrogen is paramount. As worldwide energy needs rise [1-3], we face the urgent task of identifying clean, efficient energy sources [4]. Green hydrogen, a key player in this field, is gaining momentum due to its potential to reduce carbon emissions and contribute to a sustainable energy future. Green hydrogen is produced by splitting water into hydrogen and oxygen using renewable energy. This process is carbon-free, making green hydrogen a clean energy source. It aligns with global sustainability goals, including the United Nations Sustainable Development Goals and the Paris Agreement, underscoring its role in combating climate change [5, 6]. The demand for green hydrogen is driven by global policies, strategic initiatives, and the push for renewable energy across various sectors. Governments, industries, and organizations are incorporating green hydrogen into their energy strategies, recognizing its transformative potential in transportation, industry, and grid management [7, 8].

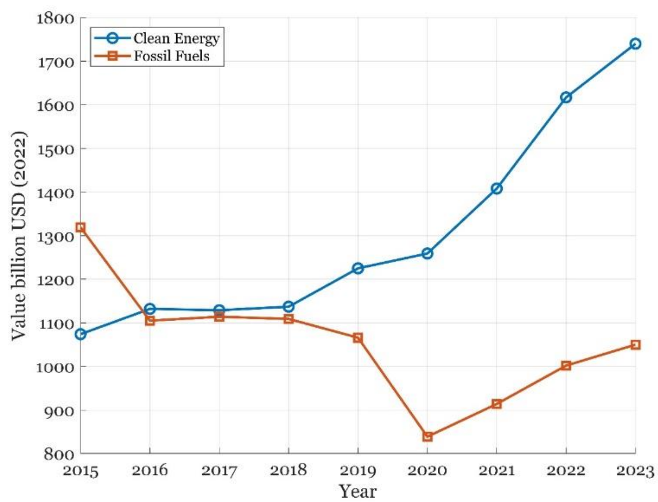


Figure 1-1 Global energy investment in clean energy and in fossil fuels [9]

Investment trends show a steady increase in clean energy, with green hydrogen playing a crucial role (Figure 1-1). Technological innovation and research are vital in enhancing the efficiency, scalability, and economic viability of green hydrogen. These advancements support its integration into diverse energy systems and applications [10, 11]. The economic landscape is increasingly attuned to the potential of green hydrogen. Market trends and investment flows, as highlighted in the accompanying graph, indicate a robust commitment to this clean energy source. Figure 1-2 from the International Renewable Energy Agency (IRENA) and the International Energy Agency (IEA) projects a significant increase in installed electrolyzer capacity over the coming decades, which is crucial to produce green hydrogen. The steep upward trajectory showcases the expected growth in this sector, reflecting investor confidence and the prioritization of green hydrogen in energy strategies [12, 13].

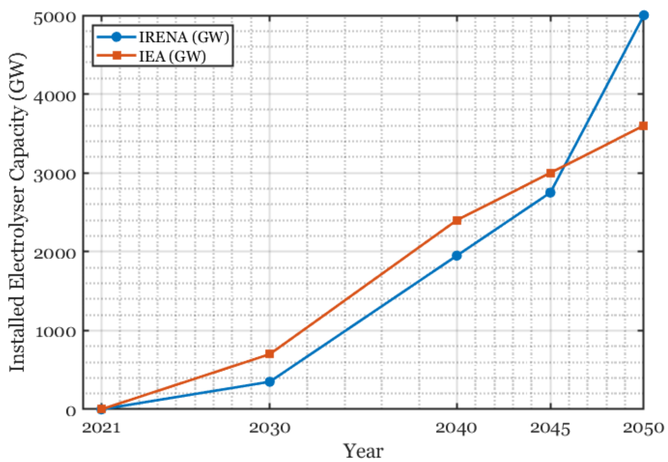


Figure 1-2 Installed Electrolyser Capacity Estimates [ref]

This surge in electrolyzer capacity is a clear indicator of the green hydrogen sector's expansion. As we transition to the next chapter, we will delve deeper into the technology behind this rise—the electrolyzers themselves. These devices are central to the production of green hydrogen, splitting water into hydrogen and oxygen using electricity from renewable sources. We will explore how advancements in electrolyzer technology contribute to the scalability and efficiency of green HyPro, and how they may shape the future of sustainable energy.

1.1.2 Role of Electrolyzers in Green HyPro

Water electrolysis is pivotal for HyPro, offering a sustainable energy path. Various electrolyzers, such as PEMWE (Proton Exchange Membrane Water Electrolyzer), AWE (Alkaline Water Electrolysis), AEM (Anion Exchange Membrane), and SOE (Solid Oxide Electrolysis), have their specific strengths for different scenarios.

PEMWE respond quickly to power changes and are highly efficient, ideal for energy storage and vehicular use. They work at low temperatures, aiding rapid operation, but require pricey catalysts like platinum and rigorous water purification due to their sensitivity to impurities [14, 15]. AWE electrolyzers are cost-effective and robust, able to handle impure water, making them great for large-scale HyPro. They are stable and durable but slower to respond to energy changes and need higher temperatures and regular maintenance due to possible scaling [16]. AEM electrolyzers, still in development, use cheaper catalysts and are more durable than PEM types, functioning across a broad range of conditions. However, they face challenges like membrane stability and aren't widely available yet [17]. SOE electrolyzers operate at high temperatures, which allows them to use waste heat effectively, making them efficient. They're suited for high-temperature industrial processes but require time to warm up and face material durability challenges [18].

In essence, each electrolyser type presents unique attributes for HyPro. PEM electrolysers are renowned for their quick operational pace and compact nature, fitting for on-demand energy applications and mobile integration. Their downside includes their cost and a need for pure input water. AWE units, conversely, are cost-efficient and robust, capable of processing less pure water, aligning with large-scale production needs. Their limitations lie in their slower responsiveness and maintenance needs. AEM technology, still under refinement, promises cost and durability improvements, while SOE systems offer high efficiency at elevated temperatures but face slower start-ups and materials-related challenges. Table 1-1 compares various electrolyzers. PEM is preferable for rapid, space-efficient scenarios, AWE for cost-sensitive, large-scale operations, AEM for cost and durability in developing contexts, and SOE for high-temperature, efficiency-focused uses.

Recognizing each technology's pros and cons aids stakeholders in making informed choices for water electrolysis systems, aligning them with specific application needs, and optimizing for performance and cost-efficiency.

Table 1-1 Comparision of various electrolyzers

Type	Advantages	Disadvantages
PEM	High current density	Expensive due to the use of noble metals like platinum
	Low operating temperature (around 80°C)	Sensitive to impurities
	Fast response to variable power inputs	Requires high purity water
	Compact design	Limited lifetime due to membrane degradation
	Suitable for large-scale operations	
AWE	Well-established technology	Lower current densities compared to PEM
	Tolerant to impurities in the feed water	Higher operating temperatures (60-80°C)
	Lower cost due to the absence of noble metals	Slower response to variable power inputs
	Suitable for large-scale operations	Bulkier design
AEM	Operates at intermediate temperatures	Less established technology, still under research
	Potential for lower costs without noble metals	Membrane stability and lifetime are still under evaluation
	Can handle some impurities	Limited commercial availability
	Flexible response to power input variations	
SO	High efficiency, especially at high temperatures	High operating temperatures (700-1000°C)

Can utilize heat from other processes (waste heat)	Expensive due to the use of ceramic materials
Suitable for integration with other industrial processes	Slower start-up times
Capable of both electrolysis and fuel cell operation	Materials subject to degradation at high temperatures

As hydrogen's role as a sustainable energy carrier becomes more prominent, electrolysers are crucial for large-scale, renewable-based HyPro. Ongoing research and development are key to enhancing these technologies' efficiency, longevity, and affordability.

This research emphasizes PEMWEs, with its rapid response and compatibility with renewable energy, making it well-suited for fluctuating power sources like wind and solar. This aligns with sustainability objectives and greenhouse gas reduction. PEM's modularity and scalability are also advantageous, fitting various industrial applications and mass HyPro.

1.1.3 Advancements in PEM Water Electrolysis

The integration of PEMWEs into the renewable energy sector marks a technological leap forward in sustainable HyPro. PEMWEs are adept at matching the intermittent nature of wind and solar power, and their growing capacity, as shown in recent trends (Figure 1-3), underscores their expanding role [19, 20].

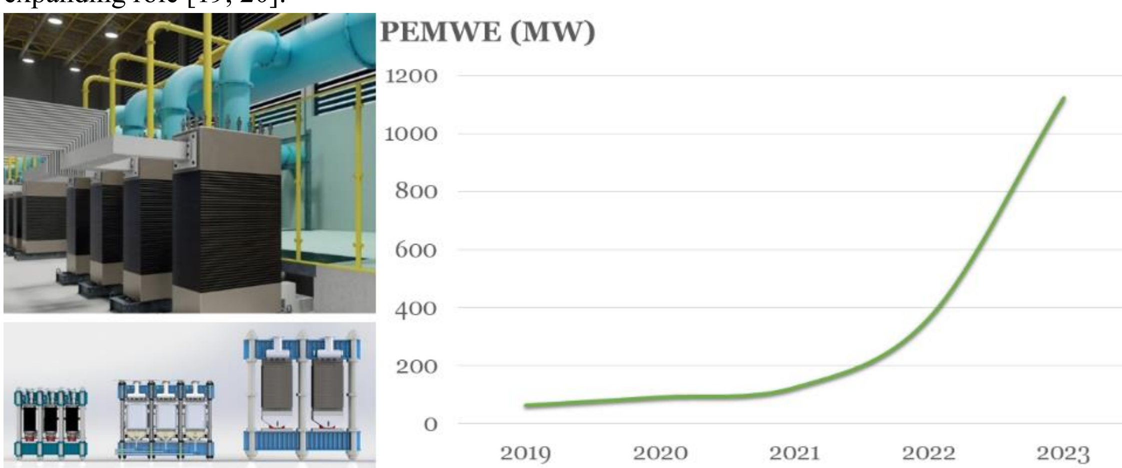


Figure 1-3- The increasing installation of PEMWEs [21]

Renewable energy's variability calls for adaptable conversion systems like PEMWEs, which can harness excess energy during peak periods for HyPro, a storable energy form. This conversion not only maximizes renewable energy use but also strengthens the energy system's resilience.

PEMWEs' operational dynamics mirror society's adjustment to fossil fuels, necessitating a similar evolution to harmonize with renewable energies [22, 23]. Efficiency is the cornerstone of PEMWEs in HyPro, with continuous improvements enhancing their performance. Still, challenges like optimizing operational parameters and reducing costs remain focal points for research [24-26].

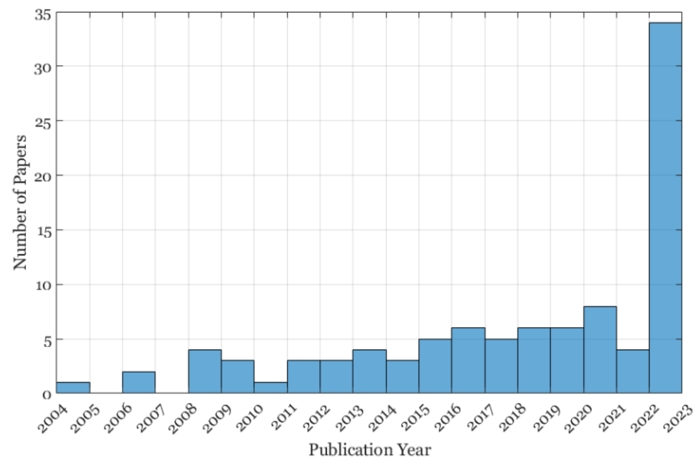


Figure 1-4 Distribution of Published Papers on Electrochemical Models of PEMWE Over the Years

PEMWEs are lauded for their quick response and high current density, crucial for adapting to renewable energy fluctuations. However, their sensitivity to impurities and material costs present hurdles that call for innovative solutions.

In the broader context of HyPro, PEMWEs are significant players, whose roles involve adaptability, efficiency, and ongoing optimization. Dedicated enhancements in PEMWE compatibility and operational strategies will ensure their significant impact on sustainable HyPro.

As we move forward, the research will explore optimizing a modular PEMWE system for energy efficiency, setting the stage for further advancements in energy management. This will involve a deep dive into the electrochemical modeling of PEMWEs, a field that has seen exponential growth in scholarly interest, reflecting the technology's potential and the energy sector's prioritization of sustainable solutions.

1.1.4 Modular PEMWE for scalable and efficient operations

Modularization of PEMWEs has risen as a key strategy to integrate HyPro with renewable energy, addressing its variability. Modular PEMWEs, using several smaller units instead of a large one, enhance control, adaptability, and reliability, as depicted in Figure 1-5. However, challenges include higher initial costs, complex control needs, and more space required. Yet, the flexibility of modular PEMWEs makes them well-suited for renewables like wind and solar, which don't always provide steady power. Modules can be adjusted to work with the energy available, ensuring a steady hydrogen output [27, 28].

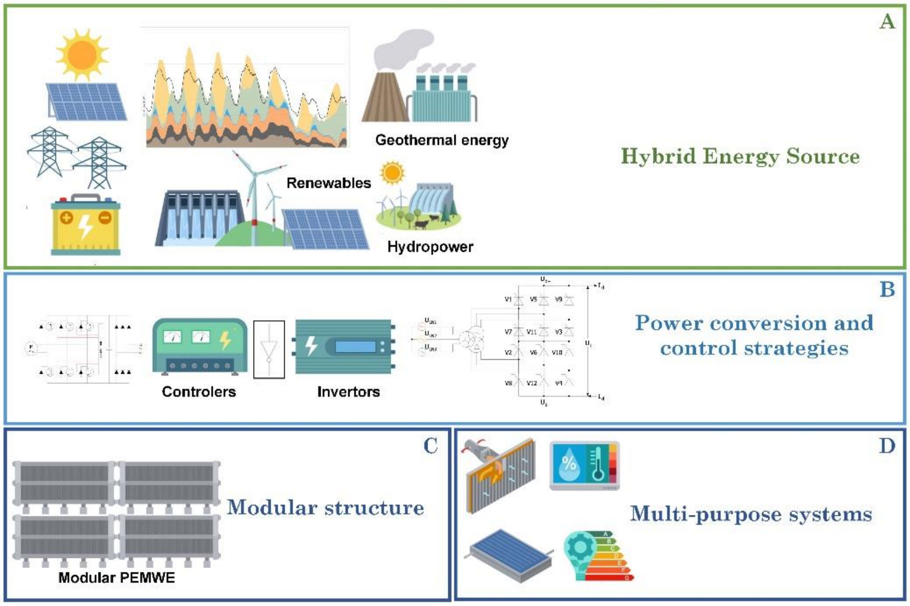


Figure 1-5- Modular system as possible solutions to RES utilization challenges in PEMWE

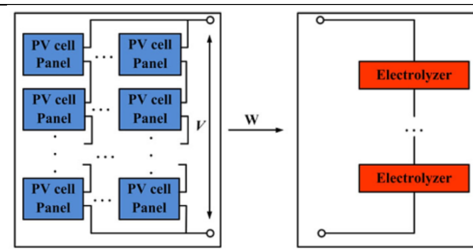
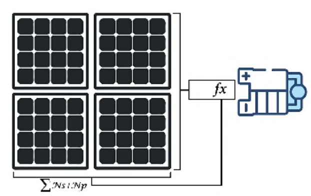
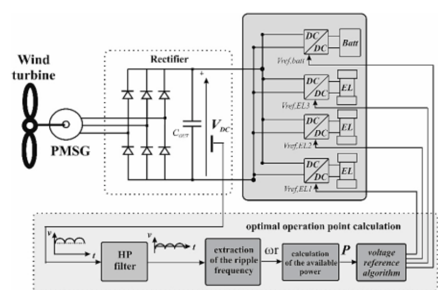
In essence, modular PEMWEs offer a promising path forward for efficient, scalable HyPro in line with renewable energy use, despite some drawbacks. Ongoing research aims to refine these systems for better renewable integration, marking a significant step in sustainable energy development.

This adaptability highlights the unique advantage of modular PEMWE systems. Nevertheless, the research landscape reflects notable gaps in understanding the specific operational characteristics and optimization needs of these systems. Although modular PEMWEs are scalable and flexible, existing studies on their performance optimization and degradation mitigation strategies are sparse. Addressing these gaps is essential for realizing the full potential of modular designs in renewable energy integration and for advancing PEMWE technology overall.

There is a notable gap in research regarding modular PEMWE systems. These systems differ from traditional ones in their adaptability and scalability, suited to varying energy scenarios. However, studies on their specific operational characteristics and optimization are limited, leaving aspects like control strategies and degradation mitigation underexplored.

Key contributions in this area include Guilbert and Vitale's (2020) [43] development of a power management control system for wind turbine-PEM electrolyzer integration, focusing on efficiency and reliability through a specialized converter design. Wirkert et al. (2020) [44] Improved PEMWE design for uniform cell compression and temperature control, enhancing efficiency and scalability. Lux et al. (2022) [45] created a modelling framework for multi-stack PEM electrolyzers, incorporating degradation effects, enabling effective simulation and control strategy evaluation. Lu et al. (2023) [46] proposed a power allocation strategy for wind-hydrogen systems, addressing electrolyzer efficiency and degradation, demonstrating significant improvements in system viability. Tully et al. (2023) [47] explored heuristic control strategies for wind-hydrogen systems, focusing on electrolyzer degradation, showing that intelligent control can significantly extend plant lifetime and efficiency.

These studies highlight the importance of advanced control systems and operational strategies in optimizing PEMWE systems, especially in modular configurations, for sustainable, large-scale HyPro.

Ref	Modularity (Strategy)	Superiority and creativity	Schematic
[48]	Modular direct coupling with PV (With optimization	• higher HyPro efficiency • more leakage resistance • No converter • Compact	
[49]	Single-stack direct coupling with PV (With optimization	• No need for electrical converters • More compact • Less connections	
[43]	Modular (Control and conversion)	• Eliminating the intermittency of input energy • Faster dynamic behavior than the wind turbine • Avoiding overvoltage during transients • The operation of each converter in the mode of maximum efficiency	

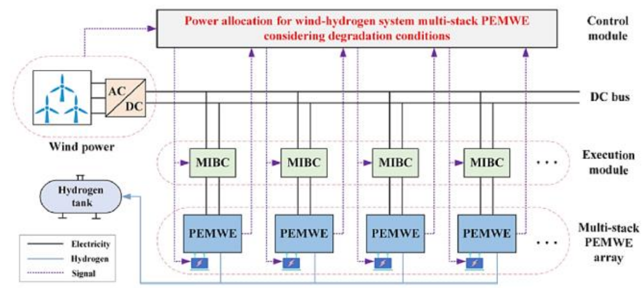
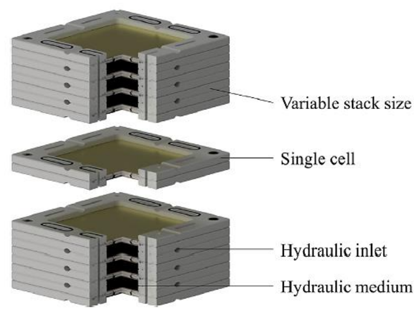
[50]	Modular (Power allocation Optimization)	• PEMWE Maximum efficiency • Lower degradation • Shortened control transient time	
[44]	Multistack (flexible pocket)	• Dynamic high-pressure HyPro • Compact structure and easy stack adjustment and size upgrade • Improved heat management • Direct current and media conduction • Full flexibility	

Figure 1-6 Modular PEMWE configurations in letriture

Despite advancements in modular PEMWE technologies, there remains a significant gap in understanding the full range of configurations and the efficiency of different system structures. Studies are particularly lacking in identifying the most effective parameters influencing these systems. This gap signifies the need for comprehensive research to optimize modular PEMWE configurations and fully explore the impact of various operational parameters on their efficiency and effectiveness in renewable energy applications. Additionally, economic aspects specific to modular PEMWE technologies, such as cost-efficiency and strategies to reduce expenses while enhancing performance, are not extensively covered in the existing literature. In summary, the current body of research on modular PEMWE technology is somewhat disjointed, highlighting the need for comprehensive studies to fill these knowledge gaps. Such research is essential to fully exploit the benefits of modularity in PEMWE systems, leading to more advanced, scalable, and efficient HyPro methods.

This thesis seeks to address the critical knowledge gaps in modular PEMWE systems by advancing our understanding of energy management and operational efficiency. By investigating the literature, characteristics, structures, control strategies, degradation mechanisms, and configuration optimization, the study aims to enhance the scalability and sustainability of modular PEMWE technology. A key objective of the project is to develop energy management system that are aligned with the fluctuating nature of RESs, as well as to improve the efficiency and longevity of PEMWE systems. Detailed analysis and reviews of existing literature are provided in Chapter 2, Section 2.3, where a thorough examination of PEMWE modular systems is conducted, assessing current methodologies and potential advancements. This approach ensures a comprehensive basis for exploring modular PEMWE's potential to contribute to green hydrogen production.

1.1.5 Importance of a comprehensive energy management strategy

Effective energy management is vital for hydrogen production through PEMWE, especially when scaled to the gigawatt level. At this scale, the complexities of energy procurement, conversion, distribution, and utilization require a coordinated strategy that balances environmental sustainability with economic efficiency. Optimizing energy inputs in PEMWE systems is key to achieving sustainable, cost-effective hydrogen production. The modular design of PEMWE systems further amplifies the need for energy management, as modularity introduces flexibility and scalability that are essential for efficient operation at high capacities, particularly when integrated with RESs [29, 30].

The adoption of a modular approach enhances this need due to the operational flexibility and scalability it provides [31, 32]. In PEMWE systems, energy management is crucial for several reasons. Firstly, it optimizes resource use. PEMWEs often rely on RESs, which are inherently variable. Effective energy management ensures this energy is used efficiently, enhancing HyPro and extending the PEMWE's lifespan [33]. Secondly, it contributes to economic viability. Efficient energy management can lead to significant cost savings over time, making the production of green hydrogen more competitive with traditional hydrogen sources [34, 35]. Thirdly, it addresses environmental considerations. Proper energy management minimizes the environmental impact of HyPro, fulfilling the promise of 'green' hydrogen [36]. Lastly, it ensures operational stability. This is particularly important in complex modular PEMWE systems, where energy management provides the necessary oversight and control for stable and consistent operations [37].

Comprehensive energy management, learned from sectors like data centers, manufacturing, and electric vehicle industries, notably fuel cell applications, is crucial in reducing operational costs and enhancing efficiency [38-40]. In fuel cell vehicles, for example, energy management optimizes fuel cell performance, extending vehicle range and lifespan [41, 42]. For PEMWE systems, this approach is essential, especially in modular designs. It involves dynamic decisions on module operations based on real-time energy availability and demand, ensuring peak efficiency despite the variability in RESs.

The selection of appropriate models is central to efficient energy management and operational resilience in modular PEMWE configurations, as detailed in Chapter 2. Model selection influences both the precision of performance predictions and the effectiveness of control strategies. In modular PEMWE configurations, each module or stack must work harmoniously within the larger system, which demands models that can handle segmented control, variable operational conditions, and seamless integration with RES. A well-suited model is critical for optimizing energy distribution, maintaining efficiency, and minimizing degradation across all modules.

Modular PEMWE systems present unique modelling challenges, requiring models that account for factors such as power allocation across modules, variable load conditions, and degradation management. Traditional single-stack models lack the necessary flexibility to manage these aspects effectively. Consequently, advancing modular PEMWE technology depends on developing and implementing models that provide granular control and adapt to variable energy inputs. This thesis adopts a structured approach to model selection, focusing on models that meet the specific demands of modular PEMWE technology. By analyzing various electrochemical models and evaluating their suitability for modular operations, this study aims to establish a foundation for choosing models that optimize efficiency and extend the lifespan of PEMWE systems. This model selection framework sets the stage for the following chapters, where specific methodologies for energy management and degradation mitigation in modular PEMWE systems are explored.

1.2 Integrating Energy Management with Operational modes for Enhanced Industrial Solutions

Considering the operational modes of the modular PEMWE system is essential when developing an energy management strategy. This integrated approach not only tackles technological challenges but also adapts to the variable nature of RESs. Operational modes like temperature, pressure, humidity, and feedstock purity significantly influence the efficiency and longevity of PEMWE systems. Merging these factors with an energy management strategy leads to more effective HyPro solutions.

Key advantages of this integrated method include adaptive operations, which allow PEMWE systems to adjust to varying energy inputs for optimal performance [27, 51], and improved system longevity by maintaining operations within optimal ranges, thereby extending the system's lifespan [52]. Economic efficiency is enhanced as the strategy reduces operational costs, making green HyPro more cost-effective [23, 53]. Scalability is also improved, allowing modular PEMWE designs to adjust according to energy availability and demand, ensuring efficient operation regardless of input variability [54, 55]. Additionally, this approach reduces the environmental impact of HyPro, supporting the concept of 'green' hydrogen [56, 57].

PEMWE systems are key in HyPro, particularly when linked with RESs. The success of these systems heavily relies on energy management strategies, which impact their efficiency, durability, and overall HyPro performance. These strategies typically involve real-time monitoring and adjustments to the electrolyzer's power input, responding to changes in energy supply, especially from variable sources like wind and solar. Figure 1-6 illustrates this process, showing the power distribution between the electrolyzer and the battery storage system over time, highlighting the adaptability of the system to the fluctuating energy input.

There are various methods for managing energy in PEMWE systems. A common approach is directly connecting RESs, such as wind turbines or solar panels, to electrolyzers [48, 49, 58-60]. This direct coupling can be effective but often requires advanced control systems to manage the unpredictability of renewable energy [61-64]. Another strategy involves using intermediate energy storage, like batteries or supercapacitors, to stabilize the energy supply, protecting the electrolyzer from sudden power fluctuations , as demonstrated in Figure 1-6.

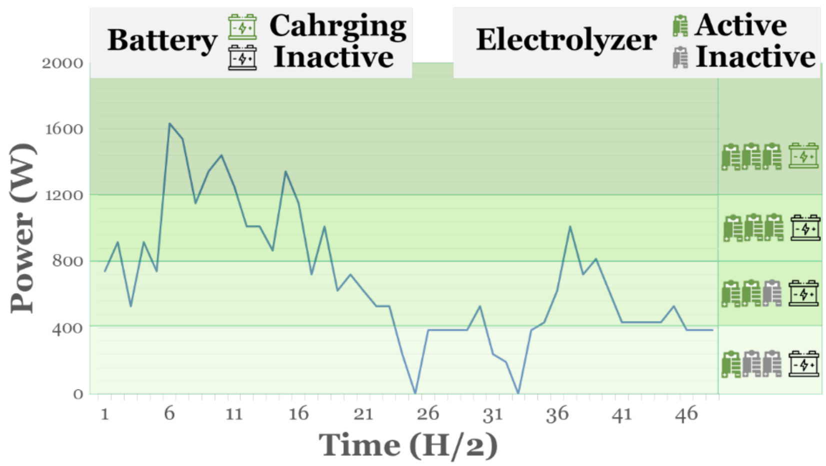


Figure 1-7 How a simple energy management can increase efficiency and decrease degradation

Research has also focused on advanced control algorithms, including heuristic controllers, model predictive control, and fuzzy logic controllers, to enhance PEMWE system performance. These controls aim to optimize HyPro, reduce energy waste, and manage the electrolyser's operational load, thus extending its lifespan [64, 65]. However, there are gaps in research, as some energy management studies lack comprehensive testing, and the models used aren't standardized or widely benchmarked. Additionally, these models often use constant degradation rates, not accounting for the variable conditions that a real-world electrolyzers would face.

1.3 Knowledge Gap

Despite substantial progress in understanding the fundamental principles and operational efficiencies of PEMWEs, significant gaps persist, particularly concerning modular designs and their integration into modern energy systems. While the electrochemical foundations of PEMWEs are well-established, their application to modular configurations and energy management strategies remains underexplored. Addressing these gaps is crucial for advancing PEMWE technology.

Firstly, there is a notable absence of comprehensive studies identifying and analyzing the factors and parameters that increase or maintain efficiency in modular PEMWE systems. Existing research provides limited insight into how different operating conditions—such as temperature, pressure, and current density—affect performance and efficiency at the electrochemical level, especially in modular configurations. Furthermore, the lack of detailed design guidelines impedes the development of optimized modular systems tailored to specific needs and applications. Understanding how different design choices impact system efficiency, stability, and scalability is essential for optimizing the design and operation of modular PEMWEs.

Secondly, there is a scarcity of comparative analyses and benchmarking of electrochemical models specifically for power allocation and energy management in modular PEMWE systems. The absence of specific models integrating power distribution among individual modules affects overall system performance and limits the potential for scalability and efficiency improvements. Additionally, existing research lacks a unified classification or comprehensive review of degradation mechanisms and efficiency models. This gap complicates the selection of suitable models for accurate simulation and optimization of system behaviour.

Thirdly, the energy management of modular PEMWE systems has not been thoroughly investigated, particularly regarding its effects on performance, efficiency, and degradation. Without analyzing how energy management strategies influence these factors, it is challenging to implement practices that enhance system effectiveness. Moreover, there is a need for advanced energy management strategies that optimize the balance between energy efficiency and system degradation under fluctuating renewable energy conditions. Developing robust control systems capable of adapting to changes in energy availability is essential for improving operational efficiency and extending the system lifespan.

In addition to these gaps, other challenges also hinder the widespread adoption and optimal performance of PEMWE systems. Issues such as integrating PEMWEs into existing power grids [66], handling grid variability [67], and ensuring economic viability for large-scale hydrogen production require further exploration [68]. Long-term durability of components under fluctuating operational conditions [69], effective thermal management in integrated systems, and the development of regulatory frameworks and industry standards are additional areas needing attention [70]. Furthermore, comprehensive environmental impact assessments and adaptive economic models are crucial for understanding the true sustainability of PEMWE systems.

The literature addressing these topics is reviewed partly in the Introduction chapter and further explored in Chapter 2: Literature Review. By addressing these knowledge gaps, this research aims to contribute to the advancement of PEMWE technology, focusing on optimizing efficiency, improving energy management strategies, and enhancing the design and operation of modular PEMWE systems.

1.4 Research objectives

This thesis aims to advance the understanding and application of energy management strategies in modular PEMWEs. By addressing identified knowledge gaps related to integration, efficiency, and sustainability—especially in modular designs—the research seeks to enhance the operational efficiency and lifespan of PEMWE systems. This is crucial for aligning these systems with the dynamic demands of renewable energy applications and improving their overall effectiveness in practical use.

Objective 1 To conduct an in-depth literature review to identify and analyze the factors and parameters that increase or maintain efficiency in modular PEMWE. This involves exploring possible solutions to enhance efficiency in PEMWE. By evaluating various PEMWE models—including detailed electrochemical models that account for overpotentials and other losses—the objective aims to understand the fundamental mechanisms affecting efficiency at the electrochemical level. This includes studying how different operating conditions, such as temperature, pressure, and current density, influence the performance and efficiency of PEMWEs.

Furthermore, the objective examines the modular structure of PEMWEs by conducting a comparative analysis of single-cell configurations and modular designs. By comparing different configurations, the objective seeks to identify key parameters that influence efficiency, stability, and scalability in modular PEMWE systems. The investigation will highlight important factors. This comprehensive analysis aims to provide insights into optimizing the design and operation of modular PEMWEs to achieve higher efficiency and better performance.

Objective 2 aims to benchmark and select electrochemical models specifically for power allocation and energy management in modular PEMWE systems. This involves two key components:

First, to conduct a thorough analysis of the existing literature to compare various electrochemical models. Through this comparison, a systematic selection process will be introduced to identify the most suitable model for power allocation and energy management in modular PEMWEs. This selection process addresses a gap in the literature by providing a clear methodology for model choice, ensuring that the selected model aligns with the specific needs of modular systems.

Second, identifying important parameters and operational modes in PEMWE operation. This includes reviewing and classifying efficiency and degradation models to understand their effects on the performance of modular PEMWEs—an area previously underexplored in research. Recognizing these effects is crucial for accurately simulating system behaviour and for improving operational strategies.

Objective 3 is dedicated to developing and implementing an advanced energy management strategy for modular PEMWEs. Using the insights and models from the previous objectives, this strategy will focus on optimizing the balance between energy efficiency and system degradation, considering the fluctuating conditions of renewable energy supply. Comparative analyses of existing strategies will be conducted to assess effectiveness, and simulations of various operational modes will help understand their effects on system degradation. The outcome will be a robust energy management system that enhances operational efficiency and extends the system's lifespan while adapting to changes in energy availability.

1.5 Methodology overview

The methodology of this thesis will address the critical knowledge gaps identified in previous sections, focusing on advancing the energy management and operational efficiency of PEMWE systems, particularly in modular configurations. This section will provide an integrated overview of the methodological approaches employed throughout the study, connecting prior research objectives, and identified gaps to the techniques used in the investigation. The overarching aim will be to establish a systematic, data-driven approach for optimizing the performance, scalability, and longevity of modular PEMWE systems.

The methodology will be structured around three primary research objectives, each aligned with specific gaps in the literature:

Objective 1: Identification of factors to increase efficiency in Modular PEMWE
Objective 2: Benchmarking and Selection of Electrochemical Models
Objective 3: Advanced Energy Management System (EMS)

The methodology will integrate increasing efficiency factors with electrochemical models, structural design processes, and advanced energy management techniques to provide a robust framework for improving system efficiency and degradation management.

1. Identification of factors to increase efficiency in Modular PEMWE

An extensive literature review will be conducted to identify and analyze the key factors influencing the electrochemical performance of modular PEMWE systems. This review will deeply explore current PEMWE models, particularly those addressing overpotentials and operational losses, to grasp the underlying mechanisms impacting efficiency. Key variables such as temperature, pressure, and current density will be systematically examined to determine their impact on system performance and efficiency.
Additionally, a comparative analysis of single-cell versus modular PEMWE configurations will be performed to identify parameters influencing efficiency, stability, and scalability. This analysis is intended to guide optimized design choices tailored to specific operational needs by elucidating the differences and interactions between various configurations. Empirical validation will involve

experimental studies on a modular PEMWE test bench, collecting data on hydrogen output and efficiency rates to provide practical insights under actual operational conditions.

Our research will also encompass a review of existing methodologies and technological advancements that could enhance PEMWE efficiency. This includes evaluating innovative materials, design modifications, and operational techniques previously proposed or implemented. Moreover, various PEMWE models that incorporate detailed electrochemical considerations of overpotentials and other losses will be analyzed. Identifying areas for improvement within the design and operation of these systems is vital for a more profound understanding of efficiency determinants at the electrochemical level.

By studying how operating conditions—such as temperature, pressure, and current density—affect electrochemical reactions and overall system behaviour, we can pinpoint optimal operational parameters.

This comprehensive study will ultimately furnish a detailed understanding of the factors affecting the efficiency of modular PEMWE systems. The insights gained will inform future research directions and help optimize design and operational strategies, thereby enhancing the performance and scalability of PEMWE systems. Empirical data from the test bench experiments will validate theoretical models and establish a strong basis for practical applications in hydrogen production technology.

2. Benchmarking and Selection of Electrochemical Models

Understanding and modeling complex systems like PEMWE is crucial. We use models as simplified representations, applying mathematical or computational methods for analysis and simulation. These models are categorized into white box, grey box, and black box, each with different levels of system understanding and application, as shown in Figure 1-8.

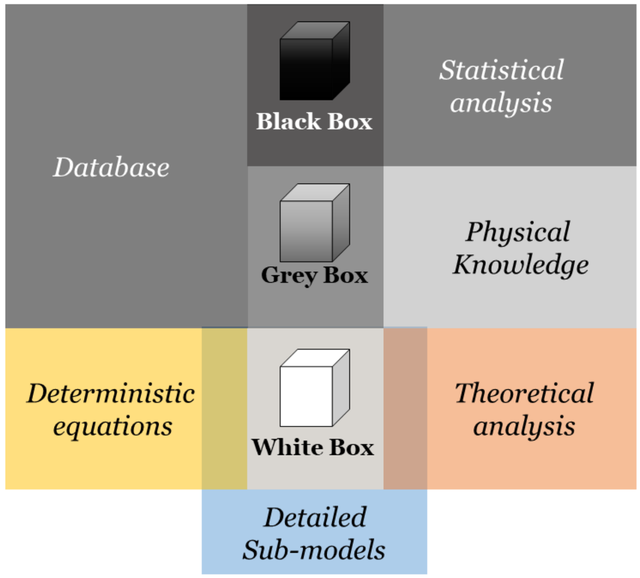


Figure 1-8 Different types of models

In the development of PEMWE energy management systems, the focus is on implementing grey box modeling. This method strikes a balance between comprehensive understanding and adaptive flexibility. It's ideal when we have partial system knowledge, capturing essential dynamics without overfitting. Unlike the detailed white box or the opaque black box models, grey box models offer a practical middle ground. They integrate known relationships and physical principles, allowing for better generalization and adaptability to modular systems. This makes them suitable for managing the energy dynamics of multiple stacks in PEMWE systems.

The first methodological step will involve a detailed review and benchmarking of existing electrochemical models for PEMWE systems. This will be crucial for establishing a foundation of models that can be used for energy management in modular configurations. The primary focus of this process will be to identify and compare models based on their accuracy, complexity, and computational efficiency. Key parameters such as overpotential, cell voltage, current density, and temperature will be analyzed to assess how well each model predicts system performance under varying operational conditions.

The benchmarking process will employ both theoretical and empirical methods. Theoretical models will be evaluated based on their ability to predict voltage losses and efficiency, while empirical models will be tested using experimental data from existing PEMWE systems. This dual approach will ensure that selected models are both scientifically sound and practically applicable to real-world PEMWE operations.

Additionally, a test bench will be designed to validate model accuracy, using statistical metrics like MSE, RMSE, and R^2 values to quantify performance. The inclusion of optimization algorithms, particularly Genetic Algorithms (GA), will allow for the fine-tuning of model parameters, ensuring that they can adapt to different operating scenarios. The results will guide the selection of models most suitable for integration into energy management systems of modular PEMWE setups.

3. Advanced Energy Management System (EMS)

The final methodological focus will be on the development and implementation of an advanced EMS tailored to modular PEMWE configurations. This system will aim to balance energy efficiency and degradation by dynamically allocating power across multiple stacks, considering the fluctuating conditions of renewable energy supply.

The system will use a nonlinear optimization function to maximize efficiency while minimizing degradation. This optimization problem is solved using advanced nonlinear programming techniques, with constraints to ensure that no stack is over-utilized. The solution dynamically adjusts power allocation in real-time, optimizing the system for both efficiency and longevity. The EMS will use the Rotary Power Allocation Strategy (RPAS), which will systematically distribute power among stacks to prevent overloading and ensure that each stack operates within its optimal efficiency range. The system will adjust power allocation dynamically to ensure long-term operational stability and efficiency. The EMS will also include degradation models to monitor and respond to real-time system health, improving both system longevity and performance.

To validate the EMS, simulations will be conducted to compare the RPAS with simpler rule-based systems. These simulations will demonstrate how the RPAS improves system efficiency and distributes the operational load evenly across stacks, thus reducing degradation rates and extending the operational lifespan of the PEMWE system. Empirical data will further validate the performance of the EMS under fluctuating renewable energy conditions.

Connection to Research Objectives and Gaps

This integrated methodology will directly address the key gaps identified in the knowledge gaps section. The benchmarking of electrochemical models will respond to the lack of comparative analyses in existing research, providing clarity on model selection for PEMWE systems. The modular design process will fill the gap in detailed structural guidelines for PEMWE systems, allowing for optimized designs tailored to specific operational requirements.

Lastly, the development of the EMS will address the significant gap in energy management in modular configurations. By offering a dynamic and adaptable solution, the EMS will enhance both system performance and longevity, ensuring that PEMWE systems can meet the growing demand for green HyPro while maintaining high levels of efficiency.

As the thesis progresses, the methodological insights gained from these three objectives will inform the development of practical solutions for scaling PEMWE systems to industrial levels. An emphasis will be placed on integrating RESs and addressing the challenges associated with real-time energy management. The final chapters will explore the broader implications of these methodologies, contributing to innovations in HyPro and PEMWE technology.

1.6 Dissertation organization

This dissertation is organized into five chapters, each contributing to a comprehensive understanding of PEMWE and its EMS. The structure is designed to systematically address the research objectives and fill the identified knowledge gaps.

This thesis is structured into five chapters:

1. ***Chapter 1: Introduction***
   - ❖ Introduce the growing significance of green hydrogen as a sustainable energy source.
   - ❖ Discusses the role of PEMWEs in hydrogen production and the potential for modular designs.
   - ❖ Identifies critical gaps in energy management and degradation analysis within modular PEMWEs, setting the foundation for the research objectives and methodology.
2. ***Chapter 2: Literature Review***
   - ❖ Provides an in-depth analysis of existing PEMWE models, particularly electrochemical models essential for optimizing efficiency and managing degradation.
   - ❖ Reviews advancements in modular electrolyzer designs, exploring factors that affect performance, scalability, and control strategies.
3. ***Chapter 3: Model Benchmarking and Selection***
   - ❖ Benchmarking various electrochemical models applicable to PEMWE systems, particularly in modular configurations.
   - ❖ Identifies optimal models for balancing power allocation, efficiency, and durability within the unique operational needs of modular systems.
4. ***Chapter 4: Energy Management Strategy***
   - ❖ Develops an advanced energy management strategy tailored to modular PEMWE systems.

- ❖ Implements dynamic power distribution techniques to enhance system efficiency, minimize degradation, and adapt to fluctuating renewable energy inputs.

5. ***Chapter 5: Conclusion and Future Directions***

- ❖ Summarizes the findings and contributions of the research to the field of PEMWE technology.
- ❖ Proposes future research avenues, including machine learning integration, temperature regulation, and cold weather adaptations, to further optimize modular PEMWE performance.

2 Literature review

2.1 Possible solutions to increase efficiency in PEMWE

Efficiency enhancement directly impacts the operational sustainability and economic viability of PEMWE systems. The purpose of this thesis is to investigate advanced energy management strategies to optimize PEMWE performance. It is important to examine existing methodologies that address efficiency improvements in comprehensive detail. The review paper that follows carefully summarises the most recent cutting-edge research, offering a fundamental comprehension that is essential for creating creative energy management solutions.

In its thorough analysis of multidisciplinary techniques, the review paper "A perspective on increasing the efficiency of proton exchange membrane water electrolysers – a review" highlights:

Material Innovations and Component Optimization: Key advances in stack components, including membranes, catalysts, and gas diffusion layers, demonstrate the substantial potential of material science in enhancing PEMWE efficiency.

Operational Conditions Optimization: Strategic adjustments in operational parameters such as temperature, pressure, and flow rates are critically evaluated for their role in significantly influencing overall efficiency.

The review demonstrates how merging PEMWEs with renewable energy sources can efficiently address intermittent energy supply concerns, with a focus on hybrid systems and power-to-gas solutions.

Research and Development Pathways: The study ends with well-defined suggestions for additional study, highlighting ongoing advancements in improved operating techniques, hybrid system designs, and materials innovation.

Positioned strategically in the thesis, this detailed review effectively bridges theoretical discussions from prior sections on PEMWE efficiency with empirical, research-driven insights. By providing a comprehensive introduction to PEMWE performance improvements, it establishes a basis for understanding how technology can enhance performance.

2.1.1 A perspective on increasing the efficiency of proton exchange membrane water electrolyzers–a review.

Journal: International Journal of Hydrogen Energy (Elsevier)

Publication date: 12 May 2023

Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/he

Review Article

A perspective on increasing the efficiency of proton exchange membrane water electrolyzers– a review

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ARTICLE INFO

Article history:
Received 22 November 2022
Received in revised form
3 January 2023
Accepted 4 January 2023
Available online 27 January 2023

Keywords:
PEMWE
HyPro
Electrolyzer efficiency
Membrane electrolyzer
Hydrogen

ABSTRACT

Decarbonized hydrogen production using renewable energy sources and water electrolysis is perceived as a promising solution for a sustainable future. The efficiency of PEMWEs relies on several multiphysical aspects and even a slight increase in their efficiency may change the future of sustainable energy routes. Hence, this paper reviews the most compelling research on increasing PEMWE efficiency, which is one of the main pillars for the advancement of this technology. Various publications, including chemical engineering, materials, mass transfer, energy transfer, electrical control, power generation, and hybrid systems, are considered. From the electrolyzer power sources (renewable energy, hybrid, power to gas), inputs (power regulation, water temperature, pressure, ambient temperature), and stack, to components design, control strategy, and new hybrid designs have come under scrutiny in this manuscript. Finally, five essential recommendations are given as the pathways for future studies on PEMWE efficiency.

Contents

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https://doi.org/10.1016/j.ijhydene.2023.01.048

Nomenclature

Renewable Energy Source RES
Hydrogen Production HyPro
Proton Exchange Membrane PEM
Water Electrolyzer WE
Fuel Cell FC
Photovoltaic PV
Power-to-Gas PtG
Catalyst Layer CL
Computational fluid dynamics CFD
Fuzzy Logic Control FLC
Oxygen Evolution Reaction OER
Platinum Group Metal PGM
Stainless Steel SS
Transport Layer TL
Gas Diffusion Layer GDL
Membrane Electrode Assembly MEA
Temperature Swing Adsorption TSA
Porous Transport Layer PTL
Catalyst Coated Membrane CCM
Mass Transport Limitation MTL
Charge Transfer Coefficient CTC
Maximum Power Point Tracking MPPT
Dual Organic Rankine Cycle DORC
Ground Source Heat Pump GSHP
Balance of Plant BOP

Introduction

One of the most practical alternatives to traditional energy, which mainly depends on fossil fuel, is renewable energy sources (RESs) [1]. They are much less detrimental to the environment. The key downsides of renewable energy are its reliance on the weather [2], its incapacity to store, and its availability when needed. In this regard, power-to-gas (PtG) is undoubtedly one of the best environmentally friendly solutions for storing renewable energy [3,4], which is dominating the market [5]. In the literature, PtG is reviewed from various points of view, such as technology [6], economics [7], market and portfolio effects [8], electrolysis and methanation status [9], thermochemical water splitting cycles [10], and solar energy [11]. In recent years, hydrogen production (HyPro) has drawn the attention of policymakers, industries, and individuals. The production and use of hydrogen are also on the rise worldwide [12,13], with technologies such as hydrogen vehicles, hybrid cars, and other green systems [14,15]. Researchers predict that HyPro from RESs will be critical in transforming the global energy system into a sustainable energy system by 2050 [16–20].

Electrolysis is now a crucial technology for HyPro, forming the basis of future energy systems as an energy carrier. Most PtG systems use the electrolysis process to produce hydrogen [21]. Electrolyzers are rapidly expanding in the market to meet the world's clean energy demand, although they need additional durability, efficiency, and performance improvement [22]. Brynolf et al. studied the production costs of modern fuel (electrofuels or PtG) for transportation systems. Based on a review of more than 130 articles, they concluded that HyPro with electrolysis could be reliable in both small and large-scale applications if capital costs and stack life are considered [23].

This study reviews all of the struggles in increasing the PEMWE's efficiency. After this short introduction, in the second section, the PEMWE's importance, advantages, industrial status, literature review, drawbacks, and possible solutions are reviewed. Section 3 discusses; operational conditions and the stack component's role in increasing efficiency, system configuration, models, and energy control. There is a discussion of future perspectives in section four, and a conclusion and some recommendations for future research are provided in section five.

Polymer electrolyte membrane water electrolyzer (PEMWE)

PEMWE is an efficient and clean method for generating H_2 from water by electrolysis. Proton conduction, separation of the produced gases, and electrical insulation of the electrodes occur in a zero-gap cell equipped with a solid polymer electrolyte in a stack section. From this reaction among cathode and anode sides and catalyst layers, H_2 and O_2 are generated [24]. PEMWE has a considerable potential of HyPro from RES by its privileges to play an essential role in reducing greenhouse gas emissions in the hydrogen sector. Studies show that PEMWE may eliminate conventional steam methane reforming from the field of HyPro by 2050 [25].

Popularity of PEMWE

PEMWE has been attracting significant attention in recent years due to its superiority over other green HyPro methods, and its excellent potential to connect to RESs. These clean and free sources, such as solar and wind, are tremendously dynamic. This challenging operational condition makes the HyPro complicated and inefficient because the energy intensity is intermittent. However, unlike alkaline water electrolyzers, PEMWE quickly reacts to the fluctuations of RESs, withstand high-temperature ranges, performs well in variable power input modes, operates at higher current densities, and has high energy conversion efficiencies [26,27]. PEMWE can either be directly coupled with other sources in proper circumstances or use maximum power point tracking (MPPT) tools by a regulator (DC/DC).

Moreover, PEMWE is more straightforward than the alkaline type since it delivers high-quality gas and has lower maintenance requirements. Therefore, the operational, maintenance, and repair costs of HyPro are reduced, and energy efficiency is increased using PEMWE [28]. Mohammadi and Mehrpooya reviewed several studies on the performance of various electrolyzers linked with a variety of RESs. The positive aspect of such research is to optimize the electrolyzer's connection with RESs [29].

It is also shown in [30] that PEM electrolyzers can generate hydrogen and oxygen as a byproduct at up to 350 bar pressures with small additional power consumption, which is attractive for hydrogen storage usage or applications that use pressurized hydrogen. In addition, depending on the material used, PEMWE can maintain high efficiency while operating at high pressures [31]. A PEMWE can produce ultrapure hydrogen with higher than 99.999% purity, and even a fuel cell can be fed by it [32].

The benefits of the PEMWEs, such as less corrosivity [33], flexibility, high proton conductivity [34], thin proton exchange membranes [35], relatively low operating temperature [36], and low computational complexity [37], are explained in numerous articles. In this regard, decarbonization [38], fast response [39], and fast cold start [40] are also noticeable.

PEMWE modules require less space than alkaline ones (about 20%) [31]. Hence, they have a higher density (smaller footprint) than their rivals. On a small scale, it is efficient, clean, and has good compactness. Increasing the electrolyzer's scale to enormous sizes [32]. The produced hydrogen in the output can also be compressed to reduce transport storage costs [41].

In a nutshell, fast response to the power source, high differential operating pressure, high current densities, high power densities, hydrogen purity, high production rates, compact design, and the capability of working in variable operating conditions are the upper hands of PEMWE in its industrial success [59]. Currently, PEMWEs are in a state of development with various limitations. A complete list of these limitations and disadvantages is discussed in section 1.4.

The embracement of PEMWE by industry

As mentioned in the previous section, due to the ability to connect to new energy sources, PEMWEs are becoming more popular year by year. The first commercial version was sold in 1978 [42]. However, the competition among companies and even countries is in progress to set a new record for HyPro nowadays [43]. Mittelsteadt expressed, "today at least five companies are at or near the launch of MW electrolyzers systems" in 2015 [44], and now, every forward-looking company knows the only path for the future is RES." The capability of PEM electrolyzers to rapidly change the power consumption has a desirable feature for frequency stability," said Alshehri et al. [44]. Fig. 1 illustrates these concepts and the industrialization process of PEMWEs. Several key events have occurred along the path to PEMWE improvements, including obstacles, critical successes, and significant advances. According to this Figure, the modern design of PEMWE has caused models and control strategies to become more sophisticated after the 19th century. The flowchart shows that efficiency is among the highest importance for future scenarios, same as durability and cost.

Table 1 illustrates the size, output pressure, energy demand, and model of nearly all PEMWE providers. From this table, the United States of America, France, Germany and China are the greatest PEMWE providers. It is also noticeable that there are of course other laboratory and industrial manufacturers, however only the census of prominent companies has been conducted. Furthermore, The largest operating unit of PEMWE using 20 MW RES is implemented in Bécancour, Canada (Quebec) by the Air Liquide company and Cummins technology. This unit ensures the low-carbon hydrogen supply for industrial use and mobility in North America by up to 8.2 tons of HyPro per day [45,46]. Cummins Inc. also claims that they have constructed the largest PEMWE in the USA at the Douglas County Public Utility District in Washington [47]. Thus, it is the beginning of the competition for manufacturing more outstanding PEMWEs. Shortly after, Linde announced that the worlds largest PEMWE (24-MW) will be established at the Leuna chemical complex in Germany and then some months later a 35-MW in Niagara Falls, New York [48,49], and Air liquid unveiled a 30-MW project by 2023 [50].

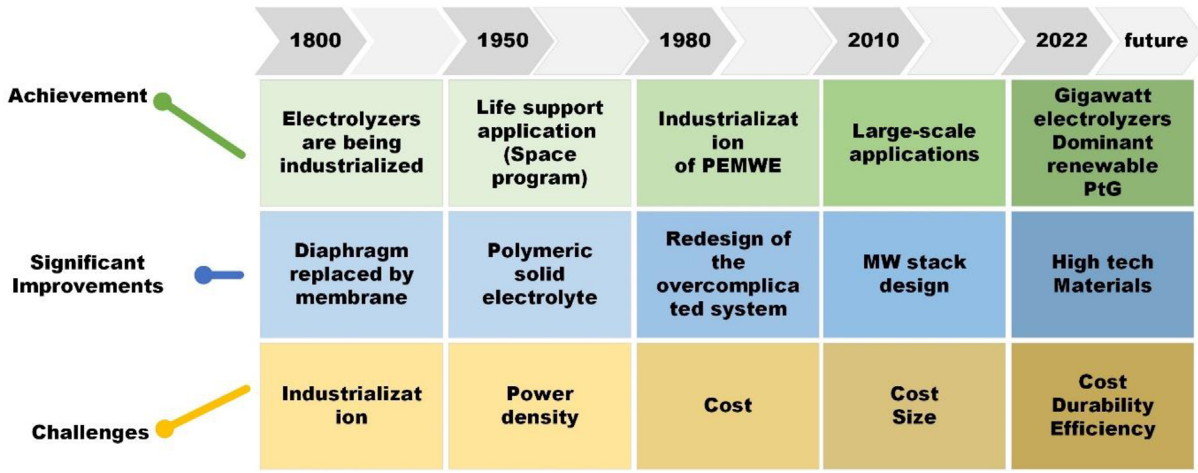


Fig. 1 – Improvements, turning points, and challenges of PEMWEs.

State of the art, obstacles and possible solutions regarding PEMWEs

Carmo et al. examine the new and old challenges relating to electrocatalysts, solid electrolytes, current collectors, separator plates, and modeling efforts. The structure of PEMWE is analyzed, materials are discussed, and the challenges are noted [28]. Shiva Kumar and Himabindu's paper contains new studies, graphical comparisons, and PEMWE models [23]. Ayers's publication in "Current opinion in electrochemistry" is about the potential of PEMWEs and their associated components. A description of the performance of a typical electrolyzer can also be found in this paper [51].

HyPro using PEMWE can be tracked in review papers from 2004 when Zoulias et al. published a review article on WE with a deep insight into various techniques of that time and its history from 1789 [52]. Almost all review articles on electrolyzers are included in this section; most of these publications discuss PtG [53,54], different methods of HyPro [55–61], and HyPro by RES [62–64]. For instance, Berstad et al. [65] review liquid hydrogen as a prospective energy carrier. They studied the impact of battery limits on hydrogen value chain studies and identified the knowledge gaps that need to be addressed. They also mentioned that it needs a comprehensively bottom-up approach to understand better the pros and cons of different hydrogen energy carriers. Shan et al. [66] have reviewed long-duration energy storage technologies. They mainly focused on projects that were commercially mature or industrialized. This work also compares modularity, long-term energy storage capability, and average capital cost with varying durations. Insights gained from this study can assist the development of long-duration energy storage projects, inspire use cases for different long-duration energy storage technologies, and be used to create a foundation for future relevant modeling and decision-making studies. Some highlight chemical and fundamental topics, which are the basis of PEMWE [67,68]. HyPro in a particular country is also the subject of two publications [69,70]. Some authors propose increasing the efficiency approach in a particular component or process, intensification [71], the definition of energy efficiency coefficient [72], verification of existing HyPro systems, and PEMWE models [73–75]. Other articles consider varying points of view, such as exergy attention [55], techno-economics [76,77], economics [78], transportation [79], special applications in space [80,81], and specific supplements (geothermal [82], wastewater [83]). The number of all review papers that PEMWE is the main or part of their concerns is presented in Fig. 2. From 2014 to 2018 and 2010–2014, the number of reviews has increased by over twofold and fivefold compared to 2018–2022, respectively, which illustrates that PEMWEs are becoming more popular. The main concern of all these publications is demonstrated in Fig. 3, as no publication has not directly reviewed all possible ways of enhancing PEMWE efficiency.

Based on the studies conducted on PEMWEs, their development challenges are mainly attributed to production costs, component durability, and high efficiency. Decreasing electrolysis costs is expected to make PEMWE technology more welcome [84]. Most publications point out the cost of platinum group metal (PGM) materials, such as iridium (Ir) and platinum (Pt), as the major disadvantage, and researchers explore solutions [85,86]. The PEMWE cost has experienced a dramatic reduction in recent years due to mass production and scaling up. Additional savings will be feasible based on technology advancements and manufacturing developments, similar to the PEM fuel cells pathway [87]. In addition, Young et al. prove that existing fuel cell materials and hardware can also be applied to PEMWEs, in particular cases adhering to the associated limitations [88]. Therefore, the existing fuel cell pathway can be tracked and transferred to the younger and rapidly growing PEMWEs. The evolution of PEMWE technology involves both process and material advancement, which are currently under investigation by scientists and engineers worldwide. Two significant system costs are manufacturing the PEMWE stack and the balance of plant (BOP). BOP expenses would account for about two-thirds of the total system cost. The share of these costs can be different for various electrolysis scales [89–91]. The final price of the stack mainly depends on cell power density, manufacturing process, membrane and its catalyst, the thickness of the transport layers. Fig. 4 shows the general range of prices mentioned in the explored

Table 1 – Origin, model, sze and energy requirement of PEMWE providers.

Brand (Company)	Model	HyPro	Required power	Average power consumption	Maximum Output pressure	Country
Cummins	HyLYZER	200-250 (Nm^3/h)	1.4–1.7 (MVA)	55 (kWh/kg)	435 (PSIG)	USA
		400-500 (Nm^3/h)	3.2 (MVA)	54 (kWh/kg)		
		1000 (Nm^3/h)	7 (MVA)	51 (kWh/kg)		
		4000 (Nm^3/h)	23 (MVA)	51 (kWh/kg)		
Proton on site	M	104-417 (Nm^3/h)	0.53–2.2 (MVA)	59 (kWh/kg)		
	G	200-600 (cc/min)	120-230 (VAC)	(9.17–6.94) (Wh/L)	116 (PSIG)	
	G4800	4.7 (L/min)	205–240 (VAC)	6.17 (Wh/L)	200 (PSIG)	
	S	9.4–18.8 (L/min)	205-240 (VAC)	6.7 (kWh/Nm^3)		
Plug Power	EX-425D	200 (Nm^3/h)	1 MVA	49.9 (kWh/kg)	580 (PSIG)	
	EX-2125D	1000 (Nm^3/h)	5 MVA	49.9 (kWh/kg)		
Nel	S	027–1.05 (Nm^3/h)	NA	6.1 (kWh/Nm^3)	200 (PSIG)	Norway/
	C	10-30 (Nm^3/h)	85-236 (kVA)	68.9–64.5 (kWh/Nm^3)	435 (PSIG)	Denmark/US
	M	1,698–4,920 (Nm^3/h)	NA	4.5 kWh/Nm^3		
	MC	264-492 (Nm^3/h)	NA	4.5 (kWh/Nm^3)		
	H	2-6 (Nm^3/h)	22-55 (kVA)	7.3–6.8 (kWh/Nm^3)		
Elogen	ELYTE	10-260 (Nm^3/h)	100-1680 kVA (AC)	4.9 (kWh/Nm^3)		France
	Open Power	Min. 500 (Nm^3/h)	Min. 3.2 MVA (AC)	5 (kWh/Nm^3)		
	Multi MW Systems	Min. 2000 (Nm^3/h)	Min. 13 (MVA) (AC)	4.8 (kWh/Nm^3)		
AREVA H2Gen	E	5-120 (Nm^3/h)	40-960 (kVA) (AC)	5.7–4.8 (kWh/Nm^3)	507.6 (PSIG)	
HIAT	PURIFIER	1.2 (Nm^3/h)	7.3 (kVA) (DC)	NA	580 (PSIG)	Germany
	CUSTOMIZER	2.8 (Nm^3/h)	17.5 kVA (DC)			
	SUPPLIER	7.6 (Nm^3/h)	47.3 (kVA) (DC)			
	STORAGER	19.4 (Nm^3/h)	120.6 (kVA) (DC)			
	PURIFIER 100	0.8 (Nm^3/h)	4.6 (kVA) (DC)			
	CUSTOMIZER 100	1.9 (Nm^3/h)	11.1 (kVA) (DC)			
	SUPPLIER 100	4.8 (Nm^3/h)	30.1 (kVA) (DC)			
	HYP	5-20 (Nm^3/h)	35-102 (kVA) (DC)		1450 - 580 (PSIG)	
H-TEC SYSTEMS	HCS	420-2100 (Nm^3/h)	2-10 (MVA)	4.8 (kWh/Nm^3)	435 (PSIG)	
	ME450	210 (Nm^3/h)	1 (MVA)	4.8 (kWh/Nm^3)		
	S	0.22–1.1 (Nm^3/h)	1-5 (kVA) (AC)	NA	NA	
	ME	46.3–210 (Nm^3/h)	500–1.707 (kVA) (AC)			
Igas	gEl PEM MD	10 (Nm^3/h)	75 (kVA) (DC)	5.4 (kWh/Nm^3)	580 (PSIG)	
		30 (Nm^3/h)	205 (kVA) (DC)	5.2 (kWh/Nm^3)		
		60 (Nm^3/h)	400 (kVA) (DC)	5.2 (kWh/Nm^3)		
		100 (Nm^3/h)	660 (kVA) (DC)	5.4 (kWh/Nm^3)		
		160 (Nm^3/h)	1050 (kVA) (DC)	5.4 (kWh/Nm^3)		
		320 (Nm^3/h)	2070 (kVA) (DC)	5.3 (kWh/Nm^3)		
Siemens	Silyzer	100 up to 2000 (kg/h)	70 (MVA)	NA	NA	
		21 (kg/h)	1.25 (MVA)		507.6 (PSIG)	
AUKEWEL/ANBOS	ABS-XQ-06	300 (ml/min)	180 (VA) (AC)		NA	China
BEIJING CEI TECHNOLOGY	HGPM	300-1500 (ml/min)	NA			
Zhongrui	ZRA3	50 (ml/min)	30 (VA) (DC)			
Saikesaisi	QLSC-H4	4 (Nm^3/h)	22 (kVA) (DC)			
	QLC	60-1000 (ml/min)	(45–540) (VA) (DC)			
Cawolo	150–600	150-600 (ml/min)	70 -300 (VA) (DC)			
Eason Industrial Engineering Co., Ltd	GH	2-100 (Nm^3/h)	(12.88–469.2) (kVA) (DC)			
PERIC	ZDQ-12	12 (Nm^3/h)	90 (kVA) (DC)			
	CNDQ-(5–12)	5-12 (Nm^3/h)	40-120 (kVA) (DC)			
SENZA	SZPE	300-1200 (ml/min)	80-260 (kVA) (DC)			
ITM Linde Electrolysis	N/A	N/A	N/A			Germany
Swiss hydrogen	PEM electrolyser	1 (Nm^3/h)	6 (kVA) (AC)		435 PSIG	Switzerland
Hydrogenics Corp	HyLYZER	1-5000 (Nm^3/h)	6.7–25000 (kVA) (AC)		NA	Canada
ITM Power	Hgas	0-2000 (Nm^3/h)	0-10 (MVA)			UK
GreenHydrogen.dk ApS	A	30-90 (Nm^3/h)	135–418.5 (kVA) (AC)			Denmark
McPhy Energy S.A.	NA	NA	NA			France
Giner, Inc	NA	NA	NA			USA

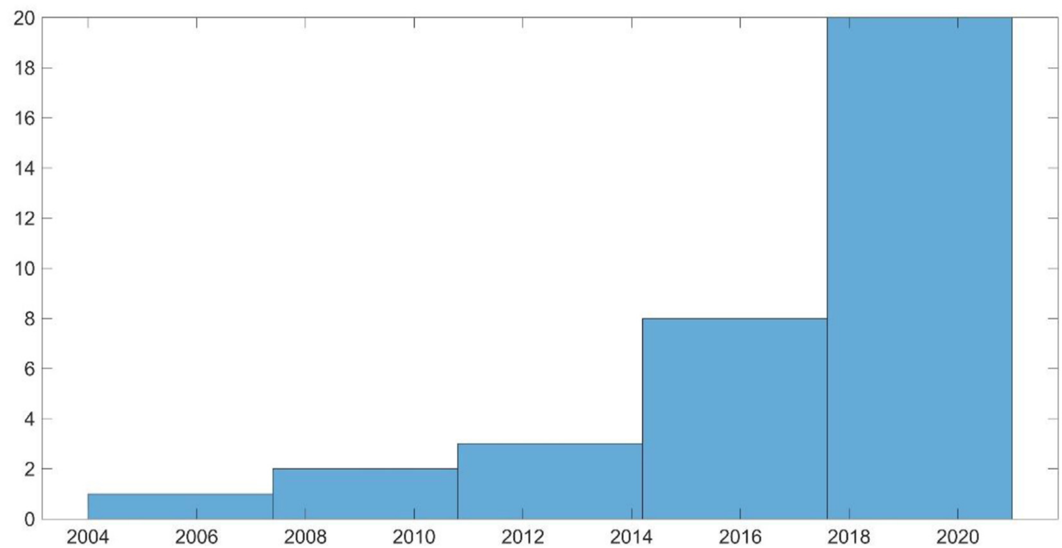


Fig. 2 – Number of review papers on PEMWE and its associated components.

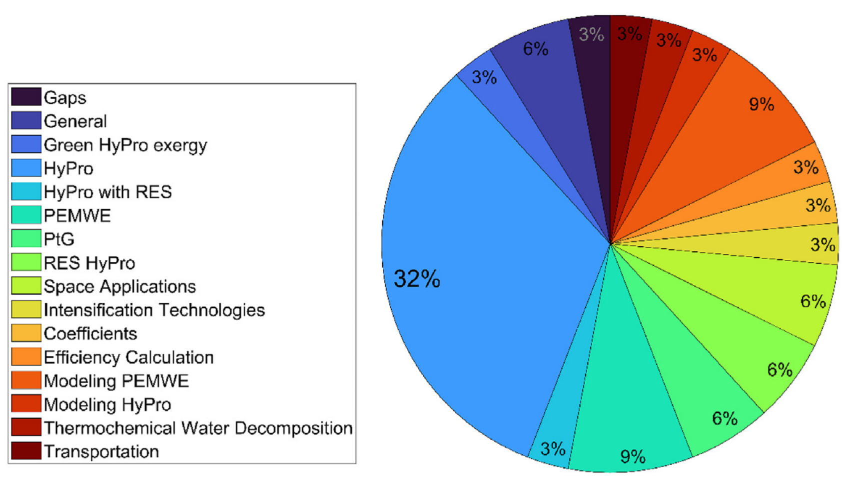


Fig. 3 – The main concern of review papers.

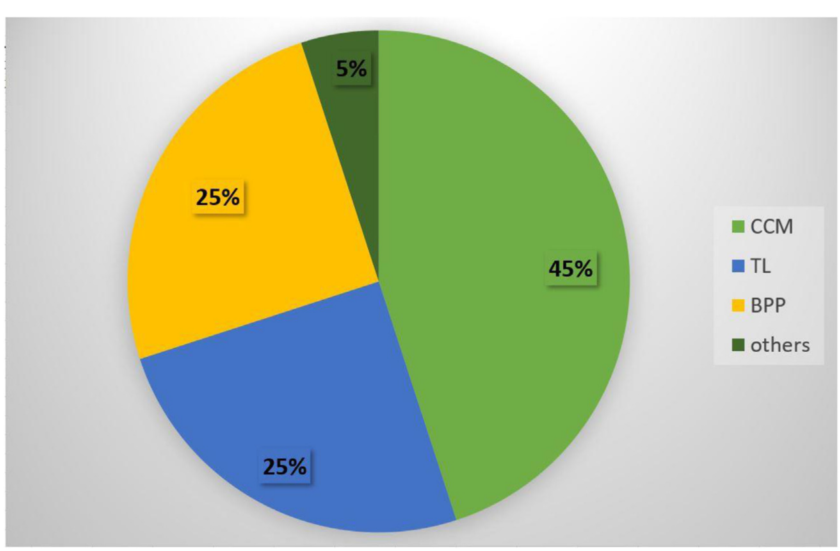


Fig. 4 – Approximate shares of Influential components on a stack price.

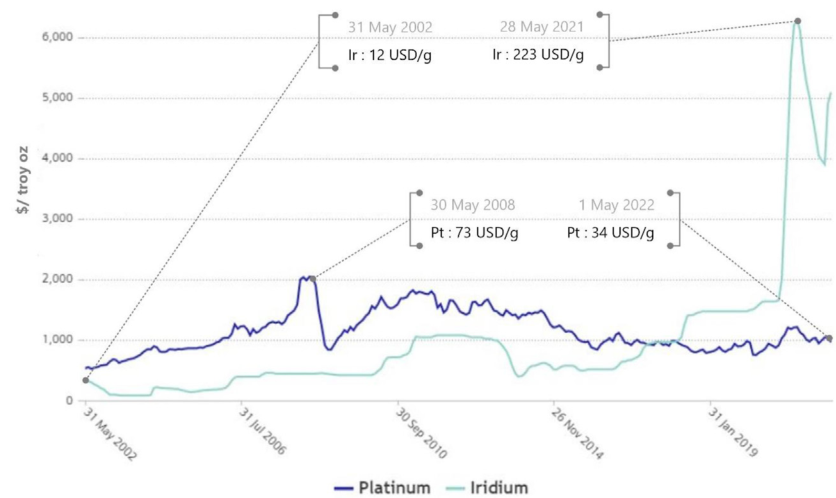


Fig. 5 – PEMWE catalysts (PGM)prices [97].

references. From this figure, the costliest part is the heart of the electrolyzer. Catalysts and membranes have an integrated design in new generations of PEMWE (Catalyst Coated Membrane (CCM)). However, if they were designed separately, they would be even more expensive. Secondly, various layers designed for mass and gas transfer are called Porous Transport layers (PTL). Finally, BPs are other costly parts of a stack.

PEMWE materials and constructions are expensive, and their prices also fluctuate drastically. As illustrated in Fig. 5, the PGM cost, a primary catalyst in PEMWE, fluctuates wildly. HyPro's large-scale by PEMWE faces severe obstacles because of the iridium demand and potential bottlenecks [92].

Alternatively, researchers have found a number of general solutions for reducing hydrogen production costs, including the use of small independent hydrogen production stations that not only eliminate transmission and loss costs but are also economically viable [93,94]. Examples are wind [95] and photovoltaic [96] systems which can cooperate with electrolyzers in one area and provide hydrogen as required.

In addition to the cost, another criticism of the PEMWE is its acidic environment, which is responsible for corrosion, degradation, and reduced lifespan [77]. The mechanisms of the individual component degradation are investigated by Feng et al. They showed significant failure in the PEMWE components (the catalyst/catalyst layer, membrane, current collector, and bipolar plate) [98]. The strategies to mitigate the degradation are also presented. Some methods to increase electrocatalyst stability are as follows: adding inert oxides, forming or single-phase alloy of binary or ternary catalysts, catalyst morphology tailored to the application, and increasing the adhesion between the catalyst layer and membrane via unique methods. They divided the membrane degradation into mechanical, chemical, and thermal degradation. Some solutions, such as reducing the creep characteristics of PFSA membranes, membrane reinforcement, or modification by incorporating reinforcement materials in polymer chemistry, are advised to be adopted. Current collectors and bipolar plates are susceptible to degradation mechanisms, such as corrosion, embrittlement, and passivation. Furthermore, current collectors may be damaged by improper clamping force. BPs are coated by stainless steel (ss), advanced materials and compounds (e.g., metal nitride), and a new deposition to minimize the coating defects and decrease the component's expenses significantly. Furthermore, Stiber et al. [99] index that BPs and ss meshes can be used instead of the expensive porous structure of PTLs. Tajuddin et al. have shown how recycling can tackle specific acidic electrolyte problems with remarkable stability and relatively cheap prices [100]. In addition, Khatib et al. completely covered the material degradation of PEMWE components in a review paper and strategies for improving cells' durability and efficiency [101].

Shirvanian & van Berkel have published an exciting minireview on the PEMWE limitations. The study is mainly about the performance and durability of different components. They considered long-term implementation and short-term strategies for decreasing costs and significantly improving lifetime [102]. Another problem listed for PEMWE is the water inlet. It must be purified for the current membranes, which can be detrimental to its reputation. Since desalination and water treatment are necessary before the initial process, more cost, technology, and time will apply consequently [57]. However, ongoing studies show efforts to make electrolyzers available to consume a more comprehensive range of H_2O [103]. The main concern of papers that studied PEMWE problems are listed in Table 2, and the possible solutions suggested by the authors are also mentioned.

All in all, any efficiency increase in the electrolyzer will help raise the HyPro and reduce the cost of the process. Consequently, a lower cost, higher capacity, and more durable PEMWE system would be a technological leap that can lead to the higher application of the zero-carbon hydrogen for various applications. In this regard, no review article has explicitly looked at increasing PEMWE efficiency.

In this paper, several articles are reviewed to comprehensively define methods for improving the electrolyzer's efficiency. Numerous efforts have been made to enhance the PEMWE efficiency, durability, and affordability. The roots of

Table 2 – Summarizes the main indicated obstacles and their solutions in the discussed papers.

Perspective	Obstacle				Solutions and suggestions	Ref.
	Cost	Durability	Operating	manufacturing		
PGM materials	✓				Catalyst separation, recovery, and recycling	[85]
	✓		✓		replacement of conventional PGM metal catalysts with non-noble metal catalysts	[100]
Techno-economic analysis (TEA)	✓	✓	✓		material reduction, substitution, scale-up, and learning by doing	[86]
	✓				large-scale, high-temperature technologies source availability and uninterrupted energy supply	[77]
Technology and performance	✓			✓	material and process development	[87]
	✓		✓		Carbon paper as anode PTLs Avoid Contact between membrane and graphite	[88]
		✓		✓	Mitigation and alleviating strategies catalyst, membrane, current collector, bipolar plate	[98]
	✓	✓	✓		Adding inert oxides and forming a solid solution reinforcing materials such as polymer fibers Coating the bipolar plate, improving materials	[101]
	✓	✓	✓		reinforced membranes, overpotential operation, stable support and coating materials	[102]
Input water	✓		✓		chlorine evolving reaction, utilization of ion-selective membrane	[57]
	✓	✓	✓		ion crossover in direct saltwater electrolysis, preventing cathode fouling and considering HER-catalyst crystal structure, morphology, and loading effects	[103]

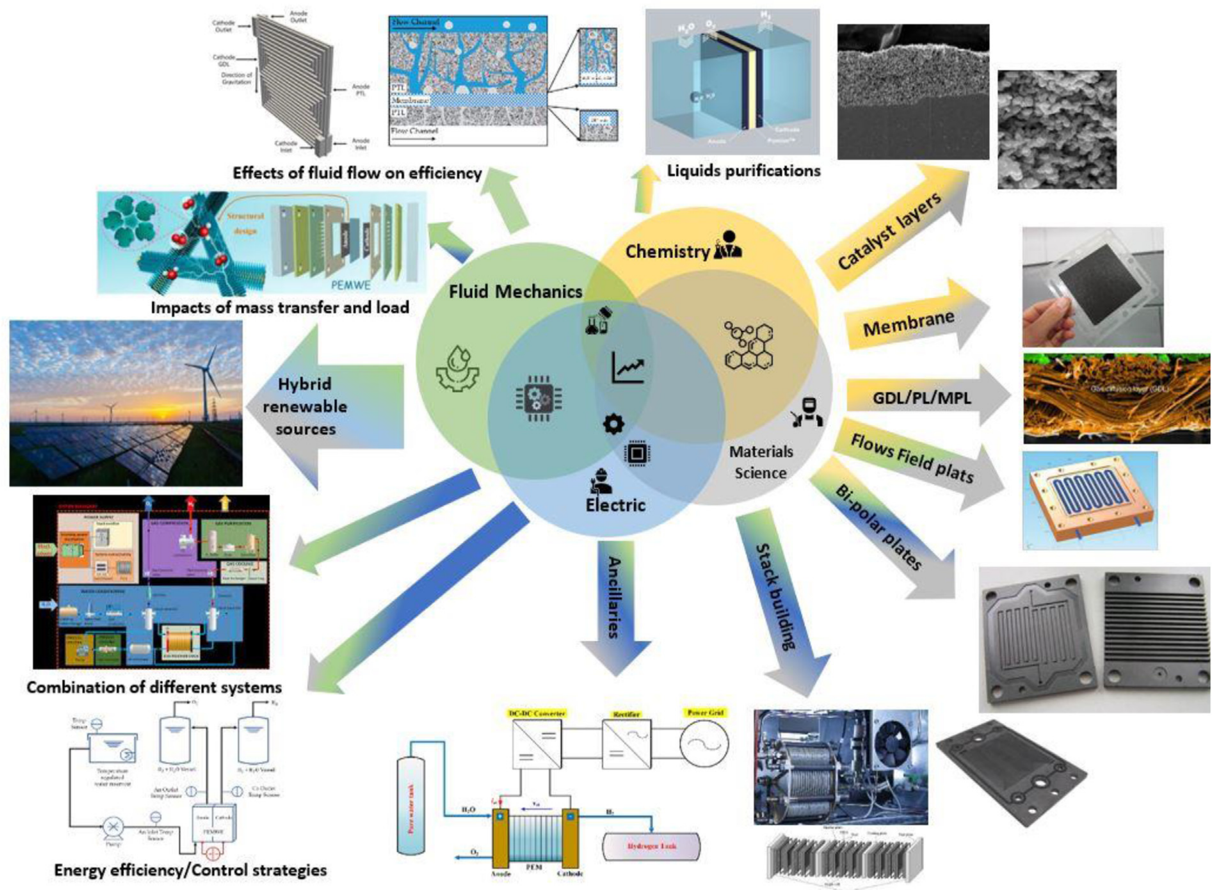


Fig. 6 – Various science branches that can increase different parts of PEMWE efficiency.

most of these methods offer material science or chemistry solutions to study and improve electrolyzer fundamentals. However, some suggest energy management or integration with other systems. Furthermore, some studies work on the flow system with a fluid mechanic approach (Fig. 6).

Increasing PEMWE energy efficiency

Considerable efforts have been made to enhance the efficiency of PEMWEs. The roots of these studies for increasing PEMWE efficiency are represented in Fig. 6. From this figure, It is evident that the four main science branches that can increase PEMWE efficiency are; Chemistry, Material science, Electrical engineering, and Fluid mechanics. It also illustrates that the studies on PEMWE are in three main areas: in-situ, ex-situ, and as a black box. First, in the in-situ research, a part of PEMWE or an action is studied in its original place. Second, ex-situ is the investigation of a section, component, or phenomenon out of the PEMWE and separately from the other parts. Finally, from the black box point of view, the researcher studies the PEMWE as a whole system and analyzes it with inputs and outputs. Lamy and Millet have studied the rate of energy efficiency by collecting various coefficients. Their work focuses on the most common electrolyzers near ambient temperature [72]. Other authors also employ process investigation, exergy calculation, and alternative methods to increase efficiency. Burton et al. have reviewed various methods, including hybrid coupling technology, magnetic fields, light energy, ultrasonic fields, and pulsating electric fields, to realize their effect on the efficiency of HyPro using RESs [104].

Operation conditions

The main electrolysis process in a PEMWE takes place in its stack, where operation occurs by gas interaction and mass transfer [105,106]. The influence of different operating conditions on the performance of PEMWEs has been investigated in different papers and is shown in Table 3. According to this table, several studies have focused on the effect of operational conditions and input currents on the PEMWE efficiency. Moreover, other factors have been influential, including temperature, pressure, flow rate, and current density. In this regard, Fritz et al. [107] focused on the simulation of capturing the performance of a PEMWE model operating at high current densities. Their study entailed predicting membrane proton transport and accurately studying the mass transport and ohmic losses under electrolyzing conditions. Marangio et al. analyzed different new objectives for PEMWE performance. First, a break-even value of the operating pressure in the range of 30–45 bar was considered. Second, a new design with a

Table 3 – Operating conditions and their influence over the performance of the PEMEW.

Main study	Operating conditions				Result/Suggestion	Ref.
	Pressure	Temperature	Current	Transport		
Water transport		✓	✓		Calculation of electro-osmotic drag coefficient, mass flow rate equation of discharged water with hydrogen in a cathode	[105]
Bubble formation and porous structures				✓	Observation with Synchrotron radiography new transport pathways	[106]
Zero dimensional simulation	✓	✓		✓	prediction of the ohmic losses, maximizing the conductive contact areas	[107]
Manufacturing	✓	✓			new activity should aim at a pressure of about 30–45 bar and higher temperatures	[108]
Thermal and electrochemical performance	✓	✓	✓		Best size of membrane, GDL, catalyst for highest performance in the sample	[109]
Anodic PTL			✓	✓	the in-plane and through-plane permeabilities should be measured in order to properly characterize PTL structures	[110]
Heat and charge transport in the anode and membrane	✓	✓	✓	✓	electrochemical performance parameters for obtaining the highest accuracy	[111]
The pattern of anode channel and effect of gravity		✓	✓		high operating temperature and low flow rate reduce the activation and ohmic losses, and bubble coverage on the catalyst should be reduced	[112]

metal foam layer as the support at the anode side of MEA was successfully tested and validated [108]. Toghyani et al. studied different design parameters and operating conditions to analyze the performance of PEMWE at the steady-state condition with a three-dimensional numerical model. They have done one of the most comprehensive research by surveying temperature, pressure, gas diffusion layer (GDL) thickness, and membrane thickness. At a voltage of 1.65 V, temperature varies from 373 K to 403 K, the maximum HyPro from 1.9×10^{-4} to 2.2×10^{-4} mol/m^3. GDL change from 0.2 mm to 0.5 mm decreased current density from 0.426 A/cm^2 to 0.40 A/cm^2. Thickening membrane from 50 to 200 μm caused a drop of current density from 0.32 to 0.16 A/cm^2. Operating pressure variation from 5 bar to 20 bar led to higher open-circuit voltage and the partial pressure of different species responsible for reducing the charge transfer rate and, consequently, the inferior performance of the PEMWE [109].

In [110], the influence of temperature, pressure, and flow rate in two different cell designs (with and without flow channels on the anodic side) was presented. Five different PTL structures were also investigated by analyzing the polarization curves. Lickert et al. observed significant differences in the performance between the two cell configurations. The electrolyzer performance without a flow field was with lower pressure and temperature, and consequently, the flow rate increased. However, they observed significant losses for incomplete removal of oxygen gas induced by anodic PTL. Finally, they announced that the transport properties related to porosities and particle/fiber diameters as PTL characterization and the in-plane and through-plane permeabilities should be measured to characterize PTL structures for PEMWE properly. A uniformly distributed heat, mass, and charge system is explained by Olesen et al. [111]. They studied a high pressure and high current density operation of PEM electrolysis cells using a dynamic flow approach. The effect of gravity has been examined by Choi et al. [112]. They studied different parameters by the orientation of the cell, and the gravity impact on the electrolyzer performance was explored. It was concluded that the single serpentine channel affected the performance at high current density (about 8.3% more than the quintuple serpentine channel). Moreover, the two-phase flow regime of water and oxygen in this channel and the PTL varied with the cell orientation. It was also noticed that it did not affect the performance of the PEMWE cell with the quintuple serpentine channel because its active areas did not vary with the cell orientation.

Two influential operating parameters of PEMWEs are pressure and temperature because they affect various components [113,114]. It has always been a question for designers and researchers about the relationship between temperature, pressure, and maximum efficiency in different systems. Should the operating pressure or temperature be higher, or an external process is necessary for compaction? Tjarks et al. tried to find the answer about PtG systems with electrolyzer pressure levels up to 20 bar. They studied the overall PtG plant's energy demand optimization, considering compression and temperature swing adsorption (TSA). They concluded that a particular optimum pressure exists for various operating conditions in the electrolyzer, which depends on the stack's current density and the hydrogen storage pressure [115]. Some authors expressed how the high-pressure PEMWE operation eliminates the need for external compression in the HyPro process. Saebea et al. showed the advantage of delivering hydrogen at high pressure with a more negligible effect on performance and low power requirement by simulating the PEMWE based on an electrochemical model [116]. Scheepers et al. investigate the capability of PEMWE membrane for efficiency improvement [117].

A mini-review of the high-pressure PEMWE system until 2014 can be found in the introduction of Bensmann et al.'s paper [118]. Then, three possible thermodynamic models are energetically evaluated in this work. The models are named pathways and are compared by balances for energy, entropy, and mass. Finally, they mentioned the importance of this evaluation in decreasing the costs and lessening the process, especially compacting the gas, as they studied PEMWEs up to 40 bar. Kim et al. predicted high-pressure PEMWE behavior for gaining the advantage of a new generation of large-scale electrolyzers by developing a one-dimensional dynamic model. They studied voltage-current relations, overvoltages, water and gas permeation through the membrane, 1-*D* profiles of two-phase flow, temperature, concentration in the anode and cathode channels, and profile over the MEA [119]. In 2021, Afshari et al. worked on a mathematical model of PEMWE (a combination of electrochemical, and fundamental thermodynamic relations) [120]. They studied the crossover phenomenon, water transferring mechanisms, and diffusion concentration. Their final goal was to improve electrolyzer efficiency by controlling voltage loss, so the contribution of electrodes, BP, and membrane resistance to electrolyzer performance was examined. They have also investigated the influence of membrane thickness, cathode pressure, and temperature on the anodic hydrogen content. So, they showed a significant reduction in hydrogen crossover from cathode to anode due to a thicker membrane, whereas a larger cathode pressure will result in an increased rate of crossover as the pressure difference between anode and cathode channels increases, at a current density of 10,000 A/m2 results in 85% and 3% contribution of concentration and activation over potentials, respectively.

Stack components

A stack primarily consists of the membrane, electrodes, catalyst, TLs, and BPs. A general view of a cell from a PEMWE stack is shown in Fig. 7. However, thanks to new research and cutting-edge technology in unique modern designs, some components can be added, and some can be changed or removed.

Membrane

The membrane is one of the stack components in the heart of the PEMWE cell. Its superior performance will increase system efficiency. This part can be developed by replacing more appropriate materials [121,122] or using new electrochemical and physicochemical techniques [123]. The coated membrane with catalysts, such as Iron (Fe) and Nickel (Ni) [124] porous titanium [125], decreases the level of corrosion and increases the efficiency and durability [126].

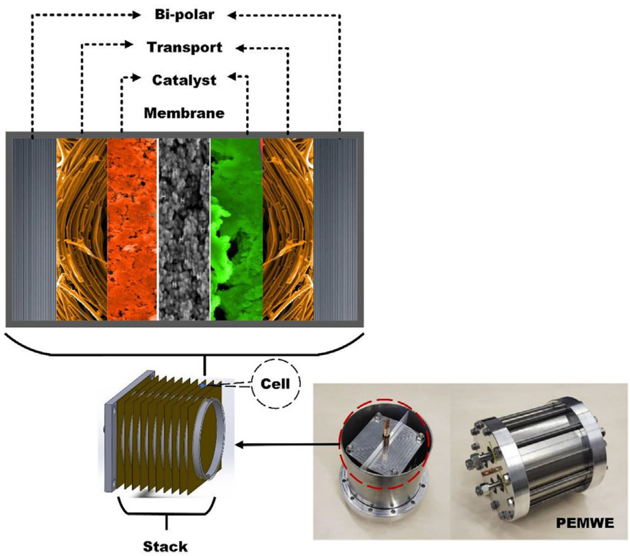


Fig. 7 – PEMWE stack components.

Catalyst

The Catalyst Layer (CL) in CCMs is another important PEMWE cell component. Currently, almost all PEM electrolyzers use expensive PGM catalysts. They are expensive, and their degradations are costly [127]. So, replacing them with low-cost [128], earth-abundant [129] non-precious catalysts, such as molecular catalysts [130], metal cobalt phosphide (CoP) [131], MoS_2 based materials [132] and [Mo_3S_{13}] clusters anchored to N-doped carbon nanotubes [133], seems reasonable. Iridium, Titanium, and Platinum compounds, as well as new versions of these compounds, offer substantial improvements through the use of cutting-edge technology. For example, iridium core/shell catalysts via galvanic exchange [134], nano-size IrOx catalyst with high activity and stability [135], N–TiO_2 nanofibres [136], or simply applying aerogel supports to them [137].

Performance and durability at the cell level are not only affected by individual components but also by fabrication methods. In addition, the parameters during fabrication also matter, impacting the CL morphology [138,139]. Alia et al. examined the effects of ink and ultrasonic spray variables on CL properties, PEMWE performance, and durability. These parameters include the ionomer content, solid concentration, solvent ratio, pump rate, and drying temperature. It was found that kinetic performance was greatly affected by changes in ionomer quantity or dispersion. As a result of increased ionomer concentrations and poor ionomer incorporation (catalyst-ionomer segregation), the kinetics have been slowed, likely because the ionomer limits access to the Ir sites. Besides, inconsistencies in catalyst layer thickness adversely affected ohmic loss, possibly by reducing catalyst layer-PTL contact and increasing contact resistance [140]. For enhancing the CL engaging and optimizing catalyst service even at high current density, transport resistance should fall, and as a result, protonic and electronic conductivities rise [141]. It applies to electrolytes, and their concentration will help their conductivity and increase their performance [142].

Gas diffusion layers

The next layer in PEMWE is the GDL. There is a lengthy research background [143] about it, a vast improvement potential [144,145], and studies on reducing its costs [146]. Accumulating oxygen gas in PEMWE transition layers is a severe obstacle to achieving higher efficiencies. For facilitating mass transport and increasing electrical conductance, a porous layer is ingrained in the design of PEMWE, which is named PTL [147]. Research is still ongoing in this area to raise the benefits of PTL [148]. Lee et al. have collected these studies and focused on PTL mass transport losses in PEMWE to improve efficiency [149]. PTL development can diminish mass transport losses, increase catalyst utilization and minimize the ohmic and kinetics losses of the PEMWE [150].

A common problem in the flow of the PEMWE cell potential in high current density is called the mass transport limitation (MTL). It decreases PEMWE efficiency by crippling transport in the PTL. Panchenko et al. studied this effect on mass transfer processes comprehensively with neutron-based imaging (neutron visualization techniques). They observed different in-situ stoichiometries during the absorption of polarization curves. The importance of their study lies in the optimized and efficient cell design [151]. In their publication introduction, Kim et al. have brought a valuable review of PTL and CL techniques and materials until 2022. They presented a new method of PTL and CL combination. They described it as tailoring the CL interfacial contact in a PEMWE with bilayer titanium mesh PTL [152]. Ojong et al. have a compelling discussion about predicting the PEMWE cell operation without a flow channel in PTL. They developed this subject by studying coupled momentum, heat, and mass transport phenomena on a semiempirical non-isothermal model [153]. Parra-Restrepo et al. studied the effect of the PTL and CL properties on the mass and charge transfer in a PEMWE. They demonstrated that the PTL optimal outlet depends not only on the operational condition of the PEMWE but also on the thickness and the electrical conductivity of the CL. Based on this fact, they proposed a new model for the constriction resistance between the CL and the PTL [154].

Bipolar plate

The last key element of the PEMWE is the BP (Bipolar Plate). This multi-functional component uniformly distributes air and liquid, manages electrical current from cell to cell, controls heat, and prevents gases and coolant leakage [155,156]. They must have the least interfacial contact resistance and high resistance counter corrosion to withstand the operational conditions within the stack. Furthermore, a coating layer may also be necessary for BPs [157]. These detailed considerations have made a relatively expensive part out of BP [158].

On the other hand, cost reduction of stack components in PEMWEs is a priority nowadays. So, inexpensive materials coated with anti-corrosive layers can be desired to replace conventional BPs, reduce cost, and hopefully increase performance [159–162]. Taner et al. (2019) performed a prototype HyPro study using PEMWE, and the result shows that this system can produce H_2 about 4.5 times more efficiently than the other systems. PEMWE with a magnet (Cr–C Coated SS304 BP) shows higher efficiency than the bare one [163]. As a result of advances in manufacturing technology and 3D printing, electrolyzers, BP, and some integrated components are now being produced [164].

Charge transfer in cell components

Investigating the Charge Transfer Coefficient (CTC) is essential in anticipating electrolyzers' current-voltage characteristics. Furthermore, this estimation provides insight into the electrode properties. Biaku et al. studied the temperature dependency of the oxygen electrode CTC of a commercial PEMWE stack [165]. Tijani et al. evaluated the operating temperature effects on the CTC and its consequences on the operating voltage of PEMWE. Their study is essential in PtG systems where activation overpotential plays a crucial role in the operating voltage. Their study results show that CTC's value increases at higher operating temperatures. However, it enhances the anode more significantly than cathode electrodes. In addition, it was observed that pressure does not significantly affect CTC at each electrode [166]. In the next step, they investigated the effect of exchange current density and CTC on PEMWE performance and its polarization. They demonstrated that CTC needs are lower in higher exchange current density, so less activation overvoltage and, subsequently, lesser operating voltage systems are required. In simpler terms, using overvoltage in PEMWE will be more efficient, and all the excess energy capacity can be used in this design. They also completed studies on the relation between temperature and CTC, primarily effective on the oxygen electrode [167]. Table 4 demonstrates different solutions for improving PEMWE performance, and the viewpoints of different studies are also explained.

System function, configuration, control, and energy management

PEMWE has also been studied from other perspectives, considering system control, energy, and configuration efficiency analyses. Preliminary studies on PEMWE efficiency have encountered severe obstacles such as electrode pressure increase, electrode destruction, membrane melting, membrane drying, overheating, or membrane rupture [168]. Zhang et al.'s design with a thermodynamic and electrochemical outlook improves the system's overall performance, avoiding irreversible losses. Interestingly, they expressed how the efficiency of their developed configuration was higher than the conventional system, which directly released redundant heat into the environment. PEMWE efficiency increases by surging the impact of the heat exchanger and working temperature. In contrast, the efficiency is reduced by the increase in the electrolyte membrane's thickness and the inlet water flow rate [169].

Koponen et al. studied control and energy efficiency in a commercial PEMWE system powered by PV. They proved that wise pressure selection and control of PEMWE operation could minimize consumption and maximize the real HyPro. They doubled the hydrogen outlet pressure and observed that the electrical energy consumption did not significantly increase. However, the specific energy consumption of the stack has increased significantly. In addition, they concluded that attention to the PEMWE system's dynamic control would prevent accelerated cell degradation [170]. A standard evaluation method for the performance of electrolyzers is to focus on fluid flow. The fluidic phenomena that occur continuously in an electrolyzer can be modeled with Energetic Macroscopic Representation (EMR) viewpoint [171]. Computational Fluid Dynamics (CFD) is a known branch of fluid mechanics that equips researchers with numerical analysis and algorithms to simulate the whole or part of PEMWE. For instance, using CFD, Upadhyay et al. provided a deep insight into the flow pattern factors by assessing the anode flow field hydrodynamic behavior. They considered the velocity value of the inlet and outlet port configuration in a new circular PEMWE design. Furthermore, their findings helped the understanding of a uniform velocity outline, maintenance of the desired temperature, reduced pressure drop, and active removal of oxygen bubbles effectively [172].

Olivier et al. developed a new model using the bond graph tool for improving PEMWE entire system design for green HyPro, considering its exposure to intermittent electrical sources [173]. Martinson et al. also focused on RES nature and the current interrupt method on the electrochemical characterization of PEMWE. They announced that increasing the working current density and temperature decreases concentration losses [174].

Another solution proposed to increase system efficiency is using control strategies to protect the electrolyzer against overvoltage, ensure input capacitors in dynamic operations, manage ripples current and voltages, and increase reliability, durability, and efficiency [175,176]. For instance, Parache et al. observed a rise in ohmic resistance, titanium mesh corrosion and passivation, and mass transport limitations. These effects seem to increase by triangular current ripples [177]. Various parameters can be determined by accurately modeling the PEMWE [178–187]. Dang et al. [188] have represented a high-differential pressure PEMWE zero-dimensional steady and dynamic model with high accuracy by calibrating a 0–700 bar pressure electrolyzer at different cathode pressures and temperatures. Some unclear parts of previous models, such as the concentration overpotential in the voltage composition, the cathode water flow problem, the double-layer, and mass transfer lag effects, are also considered in their study.

Load modeling is essential for control goals, increasing system efficiency, and improving performance [189–192]. Yodwon et al. reviewed PEMWE various load modeling with a control approach and their comparison [193]. Keow and Chen used an automated adjustment approach to establish an online proportional-integral control. In simple terms, they achieved the desired current output by automatically adjusting the voltage applied to the PEMWE. The PEMWE inlet is a nonlinear voltage and current, so its properties need to be investigated and controlled. They evaluated and compared two tuning methods, Ziegler–Nichols and phase margin [194]. Other authors, such as Fuzzy Logic Control (FLC), relied on water temperature to control and optimize the PEMWE system, such as Fuzzy Logic Control (FLC) [195]. Wirkert et al. mainly focused on heat management and how it affects PEMWE efficiency. They developed a high-performance modular PEMWE system operation, dynamic high-pressure HyPro.

Moreover, the process water was experimentally validated regardless of heat management. They claimed that future

Table 4 – Different ways for efficiency enhancement by each of the stack components.

Component: membrane	CL	TL	BP	Focus	Results or Effects	Ref.
✓				Solid acid	high proton conductivity at temperatures above 130 °C	[121]
✓				Nafion properties (Review)	high-pressure operating	[122]
✓				Degradation issues Hot pressing treatment	Mitigation/Better performance and stability	[123]
✓	✓			catalyst-coated membranes	increaseperformance and durability	[124–126]
	✓			ultra-low catalyst loading	Insights on the degradation mechanism	[127]
	✓			IrO_2/TNO anode catalyst	low cost and efficient	[128]
	✓			Earth-Abundant Electrocatalysts	efficient and stable	[129]
	✓			Molecular catalysts	tolerate high acidity	[130]
	✓			Cobalt phosphide (CoP) low-cost, non-precious	potential pathway for commercial applications	[131]
	✓			MoS_2 -based catalyst	reasonable and promising	[132]
	✓			$[Mo_3S_{13}]_2$ clusters anchored to N-doped carbon nanotubes	Cost reduction high-performing and stable	[133]
	✓			Iridium Core/Shell	emphasize the manufacturing feasibility	[134]

	✓		Nano-size IrOx	cost-effective, outstanding activity for oxygen evolution reaction (OER) and stability	[135]
	✓		N–TiO_2 Nanofibres	High Efficient HyPro	[136]
	✓		SnO_2:Sb aerogel OER	Better activity and stability	[137]
✓	✓		Reducing anode catalyst layer proton- and electron-transport resistances	maximizing catalyst utilization at the high current density	[141]
✓	✓		Electrolyte Concentration	increasing electrolyzer efficiency	[142]
		✓	GDL review	improving process efficiency	[143,144,147]
		✓	modified titanium porous matrix	calculate the porosity	[145]
	✓	✓	Transport perspective Radiography, CT	visualize the morphology and oxygen transport	[148]
		✓	Mass Transport Losses	minimize small capillary effects and reduce large slug formation	[149]
		✓	Neutron spectroscopy	cell visualized in-situ	[151]
	✓	✓	Tailoring catalyst with titanium mesh	Maximize interfacial contact area	[152]
✓	✓	✓	Channel-less PEMWE cell	costs advantage, mass transport constitutes	[153]

(*continued on next page*)

Table 4 – (*continued*)

Component				Focus	Results or Effects	Ref.
membrane	CL	TL	BP			
		✓		Mass and charge transfer	Optimal performance	[154]
			✓	Pressure and velocity distributions	pressure drops diagonally,	[155]
			✓	Design, material, cost	the coating layer is necessary to protect the substrate	[156]
			✓	pH value, titanium coatings, plasma processing	Improve the adhesion of the coating, Stable	[157,158]
			✓	Electrochemical Evaluation, Niobium Corrosion Resistance	the formation of a very stable, low porosity, the protective oxide layer	[159]
			✓	Additive manufacturing	possibility to design new and more complex flow distribution channels	[160]
			✓	Coated stainless steels	Corrosion resistance	[161]
			✓	Carbon-coated stainless steel	solution for the large-scale application	[162]
			✓	Cr–C Coated SS304	more efficiently and economically	[163]
	✓	✓	✓	all-in-one bipolar electrode	compact and efficient	[164]

industrial-scale PEMWE stacks with optimized media flow homogeneous operation conditions over a wide dynamic pressure range can be constructed using their presented design approach. At the same time, a high degree of modularity provided complete flexibility for individual system design [196].

Caparros Mancera et al. proposed a logic control design to maximize efficiency by evaluating operational factors, observing the environment, and quality testing. The BoP is also considered in power engineering. They tried to find a meaningful relation between performance and minimal BoP in PEMWE [197].

Different sources and hybrid systems

The efficiency of systems can sometimes be increased by integrating multiple electrical sources to ensure a non-stop operation or by combining two or more configurations for maximum effect. This section presents publications that meet these criteria. One of the advantages of PEMWE is production despite intermittent electrical sources and accepting RES as the power source. However, increasing the system's capability to connect this type of electrical current can significantly raise its efficiency [198,199]. Since most designs of PEMWEs operate with low voltage and high current, converters using strategies such as LLC resonant can play a vital role in integrating electrolyzer with a power source [200].

PEMWEs are the most well-known sources of HyPro power supply from RES. If they are assumed as the primary power source, as shown in Fig. 8, power network and individual batteries are overcharged in some terms. Hence, the over-power of powerline, standalone batteries, and even active consumers can turn into green hydrogen. PVs most often supply PEMWEs and therefore electrolyzers' performance in this arrangement is consistently attractive [201]. Optimal coupling approaches have been proposed by Yang et al. to improve the HyPro efficiency using a strategy called direct coupling and increasing leakage resistance [202]. According to their analysis, hydrogen production from solar irradiation of 1,000 W m2 is less than 1% efficient without optimization. Nevertheless, under the same conditions, the efficiency of hydrogen production can be as high as 7.9% when series-parallel PV cells are configured optimally. Some authors researched particular combinations with PEMWE, such as concentrating solar plants [203], Photovoltaic Thermal (PVT) [204], and PV directly coupled with PEMWE [205].

In recent years, hybrid RESs are becoming prominent in the energy sector for achieving more sustainability, especially in standalone systems. So their integration with PEMWE is the subject of new research [206]. As RES's capacity factor is usually low, combining different sources will be helpful. One of the successful scenarios of hybrid sources for PEMWEs is the combination of wind turbines and PV arrays [207]. Zaik & Werle [208] have published an experimental methodology review about PEMWE HyPro with RES. However, the main body of their paper is about a PEMWE running with wind and solar in Poland. Their system produces 158.1 (cc/min) hydrogen with an average efficiency of 69.87%. So, wind energy is another renewable source of power for PEMWE [209]. This continuous energy source will increase the efficiency of HyPro. Seyam et al. worked on optimizing a multi-objective hybrid RES supplied by solar panels, wind turbines, and an absorption cooling system. They expressed that they achieved more than 65% of energy and exergy efficiency [210]. Geothermal is another renewable source that can be combined with PEMWE [211]. This technology brings both fresh

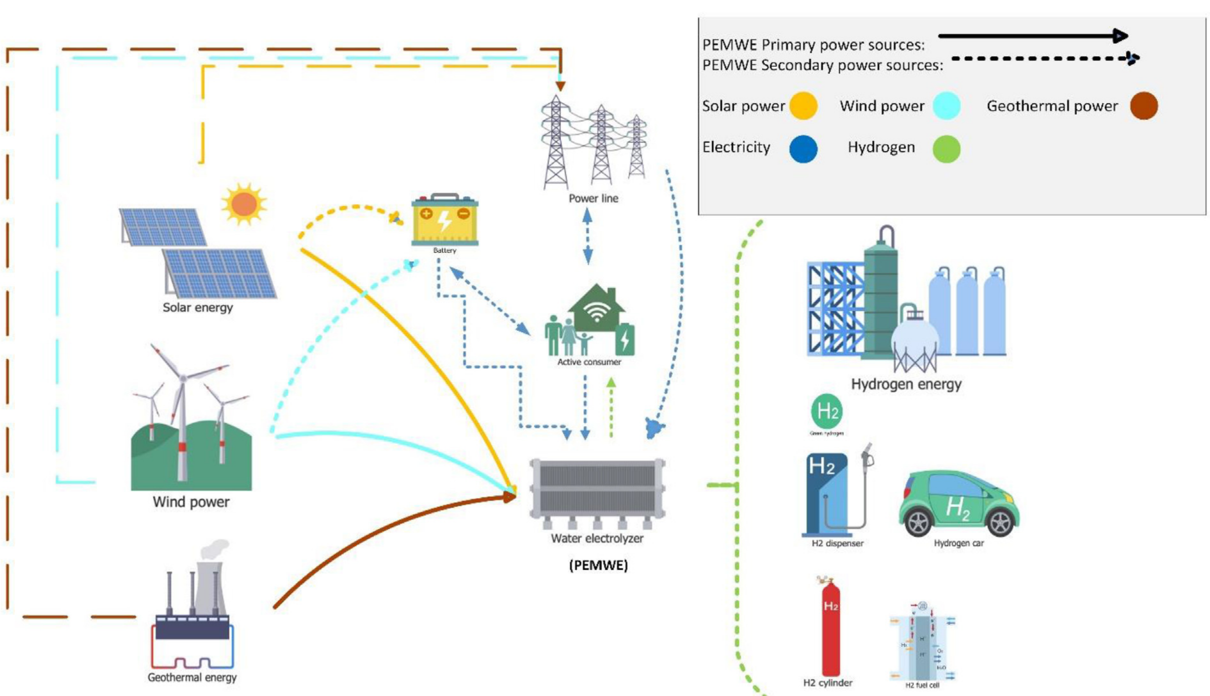
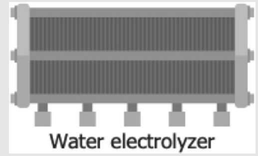
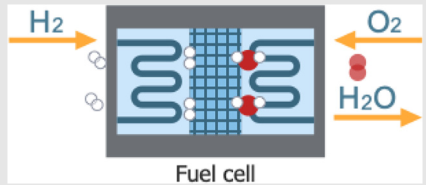
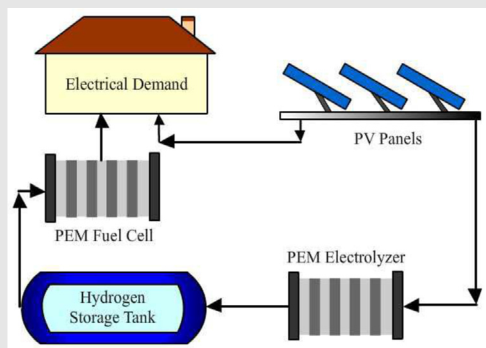
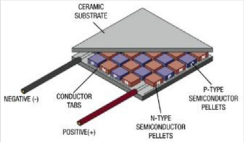
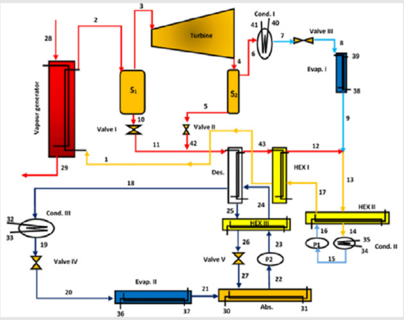
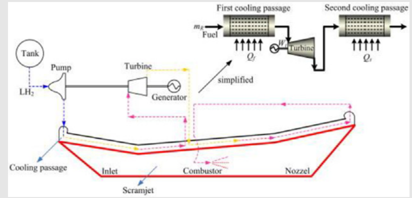
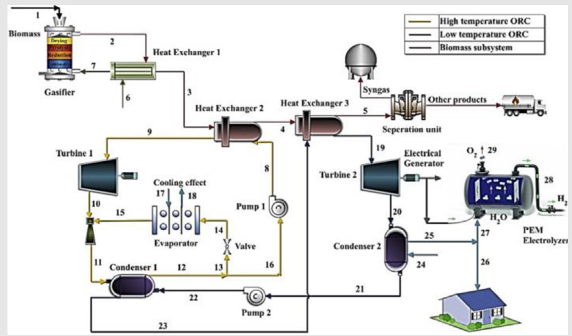
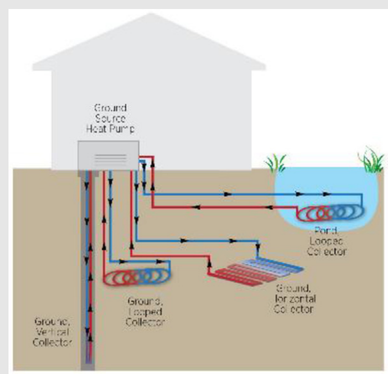


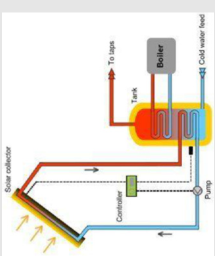
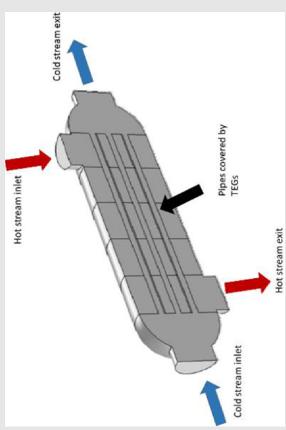
Fig. 8 – Different sources and systems that can be combined with PEMWE.

Table 5 – Hybrid PEMWE systems with their properties.

System integrated with PEMWE		Achievement	Ref.
PEMFC		Energy and temperature sustainability, energy and exergy efficiency improvements, and cost reductions	[219,220,230]
PEMFC + Solar PV		High efficiency, Net-zero emission residental, Freshwater by-product	[221]

Dual-fuel engine		High exergy efficiency	[231]
Thermoelectric generator		Compared to other system, exergy, energy, exergoeconomic, and environmental approaches sound better	[236]
modified Kalina-LNG			

<table>
<tr><td>cooling cycle of scramjet</td><td>
</td><td>Enhance the exergy and efficiency, fuel consumption</td><td>[232]</td></tr>
<tr><td>Dual organic Rankine cycle equipped with an ejector refrigeration loop, a biomass gasification process</td><td>
</td><td>Hydrogen cost and environmental impact per unit exergy are improved within 49.18% and 34.58%. Total cost decreased.</td><td>[233]</td></tr>
<tr><td>ground source heat pump GSHP</td><td>
</td><td>Energy and exergy efficiency is acceptable also improve the flexibility of the energy system</td><td>[234]</td></tr>
</table>

Solar thermal		19.1% increase in H2 production, overall electricity production by recovering the waste heat	[235]
Thermoelectric generator			

water and hydrogen simultaneously. These systems usually use a flash-binary geothermal and Organic Rankine Cycle (ORC) [212]. Alirahmi et al. [213] have equipped ORC-PEMWE system with a lithium/bromide absorption refrigeration cycle. The most influential parameters in their multi-generation system outputs are: geothermal fluid mass flow rate, geothermal fluid temperature, ORC turbines inlet temperature, and evaporator pinch-point. In some studies on power optimization of the geothermal flash systems with Dual-pressure Organic Rankine Cycle (DORC), hydrogen generation performance in the PEMWE is also investigated [214,215]. Mehrenjani et al. [216] used liquefied nature gas (LNG) for the stream as a heat sink. Using this method configuration combined with a PEMWE leads to HyPro and liquefied it through a Claude cycle. Their introduced system produces up to 106.8 kg/h of hydrogen, which can be raised to 154.95 (kg/h) due to optimizations.

According to some research, the overall efficiency of systems can be increased by merging them. Furthermore, hydrogen is often generated along with other products in these systems [217]. For instance, Marefati & Mehrpooya polygeneration system based on PV, PEMWE, PEMFC, and thermoelectric device electrical efficiency is 53.3%, it provides the electrical, thermal and cooling demand [218]. A combination of PEMWE and PEM Fuel Cell (PEMFC) seems to provide sustainability of energy and temperature [219,220]. Pirom & Srisiriwat [221] used this combination and Photovoltaic for a residential house with a compelling overall system efficiency between 1.75% and 7.66%. Freshwater as a byproduct of PEMFC was also available for the net-zero emission residential house. Several proposed system produce fresh water, cooling or heating along side with hydrogen using solar heliostat [222], parabolic solar collectors [223,224], geothermal power [225,226], solar plus geothermal [227], solar plus wind plus geothermal [228], biomass [229] for renewable electricity generation. Moltames et al. expressed that the results of this system optimization were a 22.32% and 8.61% increase in energy and exergy efficiency, respectively. Moreover, the cost rate of the entire system was decreased by 6.65% [230]. Armas-Calderón et al. introduced a hybrid system consisting of a PEMWE, a thermoelectric generator, and a dual-fuel engine. They showed that the overall system would have better exergetic efficiency by integrating this hybrid system. After obtaining positive results, the optimal operating conditions of each subsystem and their behavior were analyzed by varying the effective parameters on their performance [231]. Some systems are more complex and need multi-criteria analysis [232–235]. Zoghi et al. designed a novel biomass-driven multi-generation system to simultaneously produce power, heating, cooling, and hydrogen. They employed a thermoelectric generator, PEMWE, a modified Kalina cycle for power and cooling production. Then they investigated their system from energy, exergy, exergoeconomic, and environmental approaches, which sounds better than other systems. However, there was no clear result to compare original subsystems without this combination, which is necessary for professional conclusions [236]. Table 5 shows various systems integrated with PEMWE, and the total performance, efficiency, cost, or function has been changed. These inventions will give

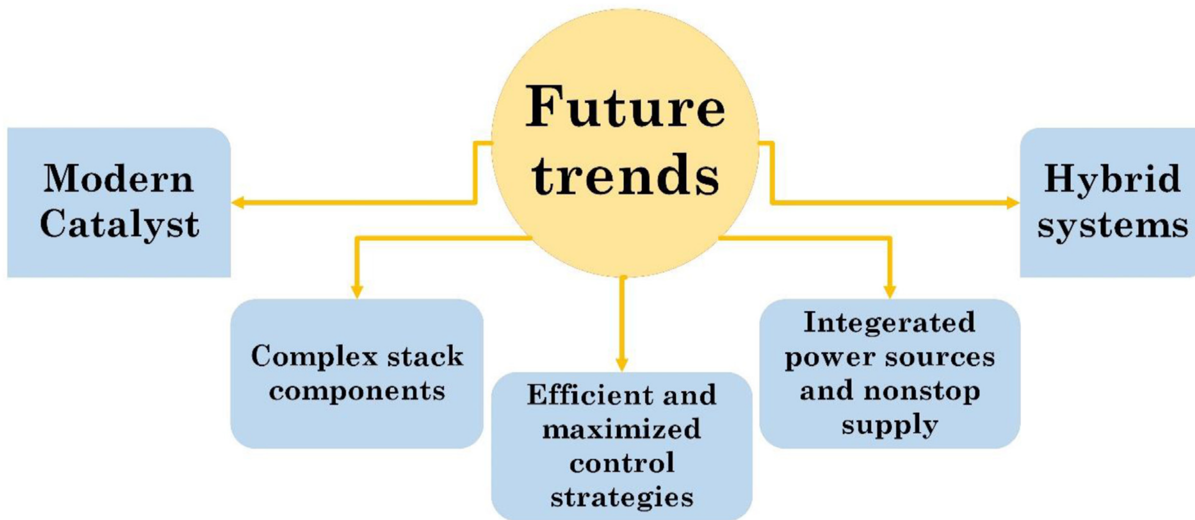


Fig. 9 – Future trends of PEMWE for increasing the efficiency.

modern energy systems a higher level of flexibility, especially in zero-carbon or low-carbon systems.

Future perspectives

The previous chapter mentioned that increasing PEMWE energy efficiency depends upon different scientific disciplines, so improvements in any of these areas will improve PEMWE efficiency. However, multidisciplinary studies also made significant impacts. According to Fig. 9 and the PEMWE trajectory, efficiency, durability, and cost are three main domains that should be considered in future studies.

- Although there has been some progress, further study of the new chemical compounds for catalysts remains essential.
- Material science is expected to make the most remarkable contributions to increasing the efficiency of electrolyzers, meaning new designs of the electrolyzer and its components interfaces can be made with modern materials, such as nanomaterials. The studies of membranes, electrodes, TLs, PTLs, and BPs, are highly recommended.
- The study of independent cases with unique circumstances, as demonstrated in several articles, is strongly suggested in control and the studies on PEMWE operational conditions, since each situation has its formula to thrive and be most effective.
- PEMWE technology in renewable energy storage is in its infancy and has much potential. So it is a valuable recommendation for future scientific investigations and environmentally sustainable energy systems. Another practical recommendation is to study hybrid renewable sources for continuous HyPro in further details.
- Some systems can be integrated to boost efficiency and reduce waste, as was discussed in the last chapter. Therefore, future studies should utilize all available capacities to maximize the entire system's efficiency.

Conclusions

Hydrogen will undoubtedly play an essential role in the zero-emission energy system of the future. Electrolysis is a valuable technology used as an energy carrier generator, forming future energy systems to cross the age of fossil fuels and take advantage of the zero-carbon energy system. The PEMWE is considered one of the best instruments for HyPro from RESs due to its reliability. Although the technology is still in its infancy, many improvements are needed to increase durability, performance, and efficiency. Therefore, this study strives to present a general and realistic picture of improving the efficiency of PEMWE by combining various platforms and research. A review is provided here of the various methods and applications that can be applied to increase the efficiency of PEMWE from a variety of perspectives. These include chemistry, materials, mass and energy transfer, electrical control, power sources, and hybrid systems. Each mentioned concept is explained by summarizing the performed studies in this line of research and development and interpreting their results and discussion. Lastly, five research axes are introduced as the guidelines for future endeavors to enhance the efficiency of PEMWEs.

In this article, various methods of increasing efficiency have been explored, specifically the PEMWE framework. Still, the process of producing green hydrogen from renewable energies involves multiple systems in addition to the electrolyzer. It includes the power and hydrogen systems prior to entering PEMWE and afterwards. The chain before the electrolyzer ring includes power generation, conversion, control, and transmission, which should be discussed in detail in future studies. Also, the chain after the electrolyzer ring consists of hydrogen compression, storage and transfer, each of which involves different fields of science and experts, each of which has its own challenges that should be investigated further and researched in order to increase the efficiency of the entire green hydrogen production system. In light of this, increasing the overall efficiency of green hydrogen production requires both effort and understanding across several fields and the cooperation of researchers in the optimal production and transfer of energy, electrolysis performed with high efficiency, as well as the compression, storage and transfer of hydrogen in the most efficient manner.

Declaration of competing interest

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

Acknowledgements

This work was supported in part by Natural Sciences and Engineering Research Council of Canada (NSERC) [RGPIN-2018-06527].

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Following the insights gleaned from this extensive review, the next section synthesizes these findings within the overarching objectives of this thesis. The review highlights the critical roles of system design, material selection, and optimised control systems while illuminating the complex nature of efficiency increases in PEMWEs. These insights are fundamental for identifying specific challenges and opportunities, particularly in modular PEMWE systems, where flexible scaling and localized control become critical.

This thesis's modular approach implies that specific energy management techniques can maximise operational efficacy, prolong system longevity, and considerably reduce performance losses. Modular PEMWEs are particularly adept at adapting to fluctuating inputs from renewable sources, which necessitates sophisticated, tailored energy management solutions.

This thesis continues with sections that focus exclusively on developing and implementing sophisticated, model-based energy management frameworks that can be applied to modular PEMWE designs and built on the insights gleaned from reading the relevant literature. This methodical process combines theoretical and practical viewpoints, offering a clear route to increased system flexibility, increased productivity, and efficient use of resources. This transition effectively sets the stage for in-depth exploration and practical application of advanced energy management strategies.

2.2 PEMWE Models

The literature review in this section aims to provide a concise overview of the existing research on PEMWE systems. It delves into the modeling approaches used in the field, highlighting their significance and areas of application. Additionally, it reviews key papers that have contributed to the understanding of PEMWE systems.

Modeling plays a crucial role in optimizing PEMWE systems, which involve complex physical and energy coupling phenomena. Various modeling approaches have been employed, ranging from simple analytical models to more complex computational ones. The choice of modeling technique depends on the specific application and requires a deep understanding of the underlying physics and chemistry, as well as expertise in numerical methods and simulation techniques. Accurate and reliable models are essential for advancing PEMWE design and performance. Review papers analyzing existing modeling works offer a comprehensive overview of the field. They highlight the strengths, weaknesses, and research gaps in PEMWE modeling. These reviews help researchers identify areas for future exploration and provide valuable insights.

Lamy and Millet's review [71] focuses on energy efficiency coefficients in water electrolysis cells, emphasizing their importance in comparing performance and cost calculations. The authors provide a method for calculating these coefficients, contributing significantly to the field. Olivier et al. [72] examine low-temperature electrolysis system models, including PEM and alkaline systems. Their work classifies modeling areas and provides a comparative analysis, identifying strengths and weaknesses in existing models.

Falcao and Pinto's article [73] reviews PEM electrolyzer modeling, particularly the main equations predicting cell voltage. They emphasize the empirical and analytical nature of current models and predict increased interest in PEM electrolysis in the future. Hernandez-Gomez et al. [74] review models related to the electrical domain of PEMWEs, highlighting the importance of understanding the interaction with RESs and power electronics. They also address Faraday's efficiency and suggest the development of empirical models for varying operating conditions.

Yodwong et al.'s article [75] focuses on PEMWE modeling for power electronics control in water electrolysis. They compare three types of models and stress the significance of dynamic modeling for improved understanding and performance. Majumdar et al. [76] provide an overview of modeling frameworks relevant to controller design, emphasizing the need for computationally efficient models. They discuss various control techniques, including data-driven models, nonlinear controllers, and the importance of addressing degradation mechanisms.

2.2.1 Electrochemical models and over potentials

To determine cell voltage "V_{cell}" and account for various losses in a PEMWE system, additional considerations are required. These voltage losses should be added to reversible voltage "V_{rev}" to result in an approximation of cell voltage. In the next sections, the reversible voltage will be discussed comprehensively. Four major categories of losses are commonly considered: ohmic losses "U_o", activation losses "U_a", concentration losses "U_c", and Bubble overpotential "U_b". These losses contribute to the overall voltage increase in a PEMWE system as shown in Equation 1. This concept is obvious in Figure 2-1, which is a polarization curve of PEMWE.

$$V_{cell} = V_{rev} + U_a + U_o + U_c + U_b \qquad \text{Equation 1}$$

Ohmic losses, due to the electrolyte's resistance and ion movement, are a primary source of irreversibility. Activation losses arise from the high activation energy needed for electrochemical reactions at the electrodes, reducing efficiency. Concentration losses result from reactant and product concentration gradients, affecting mass transport within the cell. Bubble overpotential models the irreversibility of bubble formation at the electrodes and membrane. While these losses increase overall voltage, researchers may focus on specific losses based on their model's complexity. Sometimes, only activation and ohmic losses are considered for simplicity [77].

A PEMWE's reversible potential (Vref) voltage is the minimum voltage required to initiate it from a thermodynamic standpoint. Various over potential areas and V_{ref} are shown in Figure 2-1. It is common for studies to take into consideration the constant reversible voltage, typically around 1.229 at standard temperature and pressure as it is called standard reversible voltage "$V_{rev,s}$". Reversible standard voltage $V_{rev,s}$ is sometimes called reference voltage or standard voltage and shown by "E_{rev}^0", "E_0" or "V_0" in different sources. In this table whenever there is an amount it is directly expressed in the "$V_{rev,s}$" column, "V_0" stands for the assumption of the author without an amount, "E_0" is alternative forms such as Equation 2 or Equation 3 [78].

$$V_{revs} = 1.229 - 0.9(\mathrm{T} - 298) \times 10^{-3} \qquad \text{Equation 2}$$

$$V_{revs} = -T(\int_{T_0}^{T} \frac{V_{th}}{T^2} dT) \qquad \text{Equation 3}$$

Reversible voltage can be more accurately calculated using the Nernst equation, which relates the cell potential to the standard cell potential. It also relates the activities of the reactants and products involved in the electrochemical reaction. "V_{rev}" in any temperature (T) in Kelvin can empirically expressed for PEMWE at constant atmospheric pressure as Equation 4 [79, 80]. However, in some references reversible voltage is introduced as open-circuit voltage "V_{OC}" [78].

$$V_{rev}(T) = 1.5184 - 1.5421\, T \times 10^{-3} + 9.523\, T\, \ln T \times 10^{-5} + 9.84\, T^2 \times 10^{-8}$$

Equation 4

Furthermore, in more intricate models, an additional term is incorporated to accurately account for reversible voltage fluctuations under diverse operating conditions. This adjustment becomes necessary as Equation 5 shown the Nernst equation, which is widely used to quantify "V_{rev}" change, considers temperature and pressure as variables.

$$V_{rev} = V_{revs} + \frac{RT}{2F} \times \ln(\frac{P_{H_2} P_{O_2}^{0.5}}{\alpha_{H_2O}}) \qquad \text{Equation 5}$$

"R" stands for the universal gas constant, and "T", the cell stack temperature. Additionally, the partial pressures of hydrogen "P_{H_2}" and oxygen "$P_{O_2}^{0.5}$" contribute significantly to the calculation. Exponents are determined by their stoichiometric coefficients in the full electrolysis reaction.

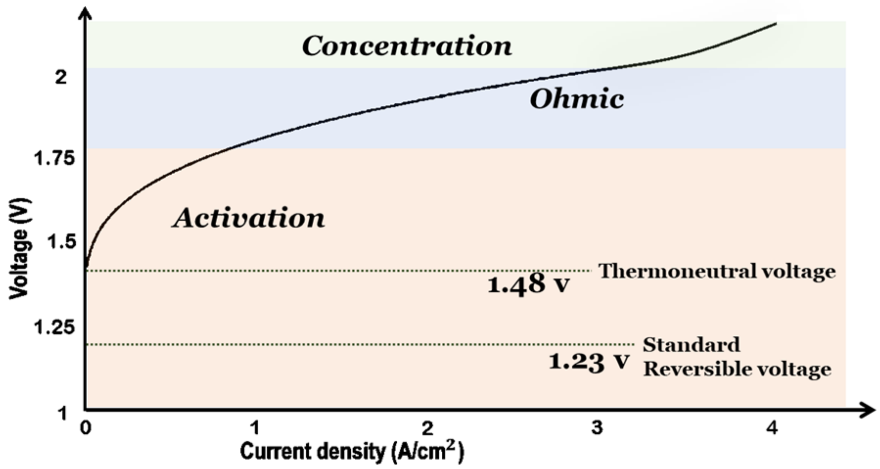

Figure 2-1 Polarization Curve and Distinct Zones of it for a PEMWE Cell

Recent studies in V_{ref} equations have predominantly focused on the logarithmic type, incorporating variables such as temperature (T), pressure (P), activity (a), voltage (v), current (i), and Gibbs energy (G). Notably, references [15, 78-153] have extensively explored logarithmic equations, often emphasizing the importance of T, P, and G in various combinations. Exceptionally, reference [154] introduced the logarithmic integral equation, adding enthalpy (H) to the mix. In contrast, references [155-157] diverged from this trend by investigating linear and polynomial equations, with reference [158] focusing solely on temperature. The constant type equation, another significant area, has been addressed in references [74, 159-169], while references [75, 170-175] have contributed to the understanding of equations where the value is zero. This research collectively deepens our understanding of the diverse nature and key factors of V_{ref} equations.

Activation overpotential "U_a" directly reflects the reaction rate and consists of two components: "$U_{a,a}$" representing the activation overpotential at the anode, and "$U_{a,c}$" representing the activation overpotential at the cathode as shown in Equation 6. Various formulations have been proposed in the literature to calculate the activation overpotential necessary for both the anode and cathode. However, in some references, it has been assumed that the cathode side is negligible [81, 176]. Each of the anode and cathode can be placed in place of "j" and the formulas from Equation 7 to Equation 10 to can be personalized for each. These formulations are derived from the simplified Butler-Volmer equation, which is specifically applicable to the oxidation reaction at the anode and reduction reaction at the cathode [78, 80, 83, 89, 90, 93, 95, 97, 98, 100-102, 106, 107, 110, 119, 120, 122, 124, 126, 129, 132, 133, 136, 137, 140, 144, 150, 154, 155, 164].

$$U_a = U_{aa} + U_{ac} \qquad \text{Equation 6}$$

One of the widely used expressions for calculating activation overpotential Equation 7 , which has been employed by numerous authors in the development of electrolyzers models [85, 109, 113, 114, 117, 118, 121, 123, 138, 141, 145, 147, 152, 153, 156, 166, 170, 173].

$$U_{aj} = \frac{RT_j}{\alpha_j F} \text{Sinh}^{-1}(\frac{i_j}{2i_{0j}}) \quad \text{Equation 7}$$

where R represents the universal gas constant, 8.314 J/mol·K. T denotes the Kelvin temperature (K). α is the symmetry factor that accounts for the additional energy fractions involved in the reduction (anode) and oxidation (cathode) processes. In Equation 8 "z" represents the stoichiometric coefficient of the number of electrons involved [15, 84, 135, 142, 143, 146, 151, 175].

$$U_{aj} = \frac{RT}{\alpha_j zF} \text{Sinh}^{-1}(\frac{i_j}{2i_{0j}}) \quad \text{Equation 8}$$

For simplicity, it is common in many references to use a stoichiometric coefficient of 2 as it is rewritten in Equation 9. This choice reflects the fact that water electrolysis involves the simultaneous oxidation of two water molecules and the reduction of two hydrogen ions. This leads to the production of one oxygen molecule and two hydrogen gas molecules [74, 79, 81, 86, 88, 92, 94, 96, 99, 104, 108, 125, 127, 128, 130, 134, 139, 148, 157, 158, 160, 172, 177].

$$U_{aj} = \frac{RT_j}{2\alpha_j F} \text{Sinh}^{-1}(\frac{i_j}{2i_{0j}}) \quad \text{Equation 9}$$

According to Chandesris et al.'s [81] electrochemical model, Equation 10 describes activation overpotential [75, 91].

$$U_{aj} = \frac{RT}{\alpha_j zF} \ln(\frac{i_j}{i_{0j}\gamma_j}) \quad \text{Equation 10}$$

The model proposed by Jing and Liu [91] differs slightly using electrical equivalents. It establishes a relationship between the anode and cathode overvoltage in a PEMWE stack, which is influenced by the electrical charge transfer occurring on the electrodes. The rugosity factor, γ_j, represents the effective surface area of the electrode in relation to its geometric area, accounting for the micro-structural characteristics and porosity [117].

Ohmic overpotential can be mathematically described using Ohm's Law, where the voltage drops "U_o" is equal to the product of the current "I" and the total equivalent resistance "Ω_{eq}" in the system in Equation 11 [83, 84, 86, 88, 95-97, 100, 101, 103, 105-107, 110, 113, 114, 118, 121, 122, 124, 127, 128, 130-132, 134, 140, 141, 146, 151, 152, 154-157, 160, 166]:

$$U_o = I \times \Omega_{eq} \quad \text{Equation 11}$$

The equivalent resistance "Ω_{eq}" includes contributions from the electrolyte's ionic conductivity, the membrane's thickness and conductivity, and the contact resistance at the interfaces between the electrodes and the current collectors. These factors collectively determine the Ohmic overpotential in the PEMWE system. A good approximation of this this equivalent resistance is the resistances of membrane and electrodes which is shown in Equation 12.

$$\Omega_{eq} = \Omega_M + \Omega_E \qquad \text{Equation 12}$$

According to Equation 12, "Ω_E" stands for electric resistance in electrodes. Drawing upon analogous systems from the literature, the electrode resistance "Ω_E"is approximated at 0.05 ohm·cm2, recognizing that variations can arise due to factors like catalyst choice and system age [178, 179]. Electric resistance in membrane is demonstrated by "Ω_M" and can be calculated by Equation 14.

$$U_o = I \times \Omega_M \qquad \text{Equation 13}$$

However, some researcher considers just thickness and conductivity of membrane as illustrated in Equation 13 [15, 78, 79, 81, 82, 89, 90, 92-94, 98, 99, 102, 104, 115, 116, 119, 123, 125, 126, 129, 133, 135-139, 142, 145, 147, 150, 158, 170, 174, 175]

$$\Omega_M = \frac{\theta}{\mho} \qquad \text{Equation 14}$$

In the Equation 14 "θ" is the thickness of the membrane and "$\mho$" represents the conductivity of the membrane.

Concentration overpotential adversely affects PEMWE performance. Firstly, it increases the energy consumption of the electrolyzer, as more electrical energy is required to overcome the additional resistance caused by concentration gradients. This translates into reduced energy efficiency and higher operating costs. Secondly, concentration over potential can lead to uneven current distribution and localized pH changes. This can negatively impact the durability and stability of the electrodes, leading to degradation over time. Generally, concentration overpotential refers to the sum of concentration overpotentials between the anode and cathode, respectively "$U_{C,a}$"and "$U_{C,c}$" as shown in Equation 15.

$$U_C = U_{Ca} + U_{Cc} \qquad \text{Equation 15}$$

One of the most common methods of calculation concentration overpotential is the Nernst equation in literature [89, 93, 95, 97, 98, 110, 129, 136, 137, 141, 146, 147, 158, 174].

$$U_{C,j} = \frac{RT}{z_j F} \ln\left(\frac{con_j}{con_{j,0}}\right) \qquad \text{Equation 16}$$

It should be noted that "con_j" refers to the concentration of oxygen at the membrane-anode interface when j=a, and that of hydrogen at the membrane-cathode interface when j=c [78]. Anode and cathode sub-reactions have different stoichiometric coefficients, "z_j". Based on chemical reactions, "z_a" on the anode side is 4, and "z_c" is 2 for the cathode.

In literature, an alternative model for calculating the concentration overpotential is described by Equation 17, which involves an empirically derived coefficient represented as "β" and the limiting current density "i_l" determined by the diffusion capabilities. Based on the experimental data mentioned in [134], these specific values were obtained through curve fitting [84, 99, 102, 160].

$$U_C = \frac{RT}{\beta zF}\ln(1 + \frac{i}{i_l}) \qquad \text{Equation 17}$$

The concentration overvoltage in PEMWEs can also be described by a model that incorporates the limiting current density, "i_l", in equation (2). In this model, the coefficient "β_1" is dependent on oxygen temperature and pressure, while "β_2" remains constant [151].

$$U_C = i(\beta_1 \frac{i}{i_l})^{\beta_2} \qquad \text{Equation 18}$$

The literature has made significant strides in understanding the fundamental principles of PEMWE operation; however, a distinct research gap remains concerning the unique challenges associated with modular PEMWE configurations. Although various models have been developed for standard PEMWE systems, these models often do not account for the complexity and specific requirements inherent in modular setups. This oversight limits the application of existing models to modular systems, where factors such as independent control of individual modules and dynamic power allocation are crucial for achieving optimal efficiency and operational stability. Addressing this gap necessitates dedicated studies that explore how modularity affects key performance indicators, including efficiency, degradation, and the system's adaptability to the fluctuations inherent in RESs.

This thesis consists of a comprehensive benchmarking of electrochemical models, assessing their strengths, limitations, and applicability to modular PEMWE configurations. Existing models provide insights into factors like concentration overpotentials and limiting current density, yet they often lack specificity for modular applications where segmented control and adaptability are critical. Modular designs present unique optimization challenges, such as balancing power and workload distribution across multiple stacks—an approach that directly influences both efficiency and lifespan. This benchmarking effort aims to identify which electrochemical models are most suited to modular configurations, providing clarity on which models offer the best performance under various operational conditions. Such an evaluation is crucial for establishing the reliability and scalability of PEMWE technology in modular formats.

This thesis addresses these identified gaps by advancing a model-based approach specifically tailored to modular PEMWE configurations. The following sections build on these insights by presenting targeted strategies for dynamic energy management, degradation mitigation, and control optimization that are uniquely suited to modular structures. Through empirical analysis and comprehensive model validation, this work aims to develop energy management guidelines for implementing effective, scalable modular PEMWE systems that can efficiently integrate with RESs. By establishing a framework for selecting and optimizing electrochemical models, this thesis seeks to ensure that modular PEMWE technology is positioned to contribute meaningfully to the broader objectives of sustainable and scalable hydrogen production.

2.3 Modular PEMWE structure

The modular PEMWE structure has gained significant attention in renewable HyPro, particularly due to its inherent flexibility, scalability, and efficiency advantages over conventional single-stack configurations. Throughout this thesis, degradation models and energy management techniques have been examined, emphasizing the need for structural designs that support these approaches to be optimized.

Because it allows for adaptive scalability and adaptable operational tactics, the modular approach stands out as being especially well-suited to managing intermittent renewable energy sources. Although modular PEMWE systems have many advantages, the existing literature offers limited guidance on how to scale them effectively. This is particularly true as regards the details of structural design and their associated impacts on the performance and durability of the system. To address this gap, the following subsection includes a detailed comparative study published in Energy, which empirically and theoretically evaluates the structural and operational performance of singular versus modular PEMWE configurations. Based on the results of this comparative research, the larger thesis goals of enhancing energy management, efficiency, and long-term system viability can be achieved.

2.3.1 Comparative analysis of singular and modular structures

Journal: Energy (Elsevier)

Publication date: 1 November 2023

Energy 282 (2023) 128911

Contents lists available at ScienceDirect

Energy

journal homepage: www.elsevier.com/locate/energy

A comparative analysis of single and modular proton exchange membrane water electrolyzers for green hydrogen production- a case study in Trois-Rivières

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A R T I C L E I N F O

Keywords:
Renewable energy
Hydrogen production
Modular PEMWE
Energy efficiency
Degradation

A B S T R A C T

Proton Exchange Membrane Water Electrolyzers demonstrate significant potential for hydrogen production from renewable energy sources. Addressing the inherent intermittency of these sources, a modular design for the electrolyzers emerges as an essential avenue of research. This study delves into potential solutions and strategies for harnessing renewable energy efficiently to fuel these electrolyzers and presents a comparative analysis between single-stack and modular designs based on a hypothetical scenario. Using experimental data, the research projects the hydrogen output derived from solar energy in Trois-Rivières. Machine learning techniques are employed to forecast available energy from photovoltaic panel datasets. A strategic power allocation mechanism is introduced to regulate input current across each electrolyzer, aiming to optimize system performance. Experimental evaluations on a purpose-built test bench validate the conversion efficiency of the electrolyzer. Notably, the results suggest that embracing a modular design can amplify hydrogen production by over 33% annually while concurrently minimizing system degradation.

1. Introduction

Nowadays, global energy consumption is steadily increasing due to population growth and rising standards of living. In this context, reliance on fossil fuels has resulted in heightened environmental pollution, exacerbated global warming, and numerous other crises. Given these circumstances, the development of renewable energy sources (RESs) appears imperative. Therefore, enhancing the efficiency of production, storage, and transfer of renewable energy is pivotal for harnessing these vital resources. The potential synergy between RES and hydrogen offers a promising avenue towards sustainability. Hydrogen (H_2) can serve as an energy carrier in almost all applications where fossil fuels are currently utilized, such as in automotive and stationary applications, without producing harmful emissions [1]. Thus, giving special attention to H_2 is essential for achieving zero-emission technologies [2]. For example, electrolyzers show promise for H_2 production (HyPro) in renewable energy storage applications. Hassan et al. offer a detailed review of green H2 production technologies, touching upon their technical, economic, ecological, and social facets, and emphasize the pressing research requirements to integrate renewable energy, cut production costs, and fill the void of environmental and techno-economic analyses of renewable H_2 pathways [3].

The proton exchange membrane water electrolyzer (PEMWE) is distinguished from other electrolyzers by its unique characteristics, including high efficiency [4], rapid response [5], flexibility, and scalability [6]. It has also garnered significant interest as an emerging technology for standalone systems in remote locations [7]. Consequently, PEMWEs are being deployed globally, continually setting new benchmarks in capacity and efficiency for the production of green H_2 using clean energy. For instance, the installation of an 8.75-MegaWatt (MW) PEMWE in Wunsiedel, Germany, is projected to cut Carbon Dioxide (CO2) emissions by 13,500 tons [8]. Meanwhile, in Bécancour, Canada, a 20 MW PEMWE generates 8.2 tons of green H2, mitigating the release of approximately 27 thousand tons of CO2 [9]. While PEMWE

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https://doi.org/10.1016/j.energy.2023.128911
Received 27 January 2023; Received in revised form 18 August 2023; Accepted 24 August 2023
Available online 26 August 2023
0360-5442/

possesses several advantages as mentioned above, it also comes with certain limitations. These encompass relatively high production costs, shorter lifespans, sensitivity to impurities, and vulnerability to extreme flow frequencies. However, these challenges are actively being addressed through continuous research and development in the field.

PEMWEs have garnered significant attention in both industrial and academic realms. This growing interest is manifested by the burgeoning body of scientific literature and research endeavors aimed at advancing the technology and its applications in green HyPro. Khelfaoui examined the performance of a solar photovoltaic (PV)-PEMWE system for HyPro in the Algerian Sahara region. The study encompasses PV module characterization and validation, as well as the exploration of the effects of ambient temperature and solar radiation on PV performance. The research also evaluates the system's performance under various weather conditions and documents a high HyPro yield of 284 L in a single day [10]. Cai et al. [11] constructed and analyzed a PV system directly coupled to a PEMWE, employing a genetic algorithm to design a working condition boasting 98.8% coupling efficiency. The researchers discovered that fluctuations in PV conditions led to more significant irreversible damage and degradation, attributed to an increased charge transfer impedance (Rct) and ion pollution. Zhang et al. devised a renewable energy utilization model for HyPro and power generation by amalgamating PV, electrolyzer, and fuel cell (FC) modules. The system's efficiency oscillated between 6% and 7% under varying environmental conditions. With a 28 m^2 PV array, the system could produce over 4100 kWh of electricity, satisfying 70% of a household's annual electricity needs, thus showcasing the viability of the PV-electrolyzer-FC configuration for efficient and eco-friendly solar energy harnessing [12].

The application of PEMWE technology has the potential to revolutionize the Power-to-Gas (PtG) process and optimize the use of RES for HyPro. Kotowicz et al. introduce a methodology to ascertain the efficiency of an H2 generator that incorporates a PEMWE, accounting for the power needs of its auxiliary systems. The authors share findings from laboratory experiments conducted on an H2 generator across a spectrum of device loads. They put forward generalized metrics for H2 generator efficiency, applicable in analyzing a PtG system paired with a 40 MW wind farm having a predetermined annual power distribution. A strategy for evaluating the thermodynamic and economic attributes of a PtG setup is presented. The authors further illustrate that the nominal power of H2 generators, the extent of their nominal power utilization, and the economic facets of the PtG setup are all influenced by the level of storage [13,14].

The intermittent nature of renewable energy sources poses challenges in the development of various green energy solutions [15]. For example, supplying PEMWE with fluctuating power stemming from the variable behavior of RES can lead to degradation and corrosion, which notably shortens its lifespan [16]. Razzhivin et al. suggest the employment of synthetic inertia for wind power plants. This aims to enhance the dynamic stability of the power system and, by extension, the wind energy H2 system through tuning the parameters of the synthetic inertia [17]. Frensch et al. have delved into PEMWE performance and degradation under seven distinct operating conditions [18]. Their research indicates that the dynamic operation of electrolysis accelerates the deactivation rate of the catalyst. Moreover, the efficiency of electrolysis is intrinsically linked to input power and current [19]. As a result, the electrical power supply process of PEMWE warrants particular consideration [20].

Numerous solutions have been advanced by experts from varied backgrounds and domains to address the unpredictability and inconsistency of renewable energies. Honsho et al. assess the resilience of a PEMWE cell against wind power voltage variations. They formulated an accelerated potential fluctuation test protocol, drawing on wind power voltage fluctuations spanning a 24-h period. The findings suggest that both reversible and irreversible losses resulting from the degradation of anode catalyst layers can be mitigated by incorporating rest intervals during operation [21]. Various approaches to these solutions can be pursued either individually or synergistically. Addressing these challenges can occur at multiple stages, such as at the power source, during the processing of incoming electricity, and throughout the electrolysis phase. Fig. 1 offers a schematic representation of potential strategies to counteract the detrimental impacts of renewable energy at different stages. From this illustration, it is evident that the obstacles tied to using RES for PEMWE can be tackled in multiple ways. Proposals encompass hybrid energy sources, power conversion and control strategies, forecast and optimization using machine learning (ML) algorithms, and flexible, multi-functional structures. Importantly, contemporary HyPro systems frequently merge these techniques at varying phases. The choice of suitable solutions for a venture depends on regional geography, existing resources and infrastructure, potential, logistical considerations, and financial limitations. Continued research, such as delving into modular PEMWE and predictive RES models, is crucial for crafting more proficient and dependable HyPro frameworks. Despite burgeoning interest, a pronounced research gap persists, primarily concerning predicting available energy for green HyPro in PEMWE setups powered by RESs. This uncertainty complicates assessments of this technology's sustainable HyPro potential. This research, therefore, endeavors to bridge this lacuna by probing the feasibility of utilizing ML to predict the efficacy of solar power-driven PEMWE systems, bolstering green and efficient HyPro. A comparative review of modular versus standalone PEMWE systems is vital to gauge their performance and delineate their respective pros and cons. The absence of such juxtapositions in current literature is striking. Such analysis can shed light on efficiency, longevity, cost-benefit, and scalability — all pivotal for the widespread adoption of PEMWE systems. Consequently, a thorough exploration of the performance metrics of both modular and standalone PEMWE units can substantially aid the evolution of enhanced and sustainable HyPro solutions.

Given the topics previously addressed, this study offers insights into potential solutions for challenges associated with the coupling of RESs and PEMWE systems for HyPro. Specifically, we delve into the advantages of deploying a modular PEMWE configuration in contrast to a singular stack system. The central objective is to assess the viability of facilitating green and efficient HyPro in Trois-Rivières by leveraging RESs. To gauge the practicality of RESs for HyPro, meteorological data alongside solar energy readings from Trois-Rivières are gathered. Subsequently, an artificial neural network (ANN) is utilized to project future energy viability. Drawing on this data, we conceive an experimental PEMWE blueprint for HyPro that aligns with the observed renewable energy trends. The projections for the PEMWE HyPro model are informed by the available energy data and prevailing operating conditions. Preliminary findings suggest that transitioning to a modular PEMWE design can notably augment HyPro while simultaneously

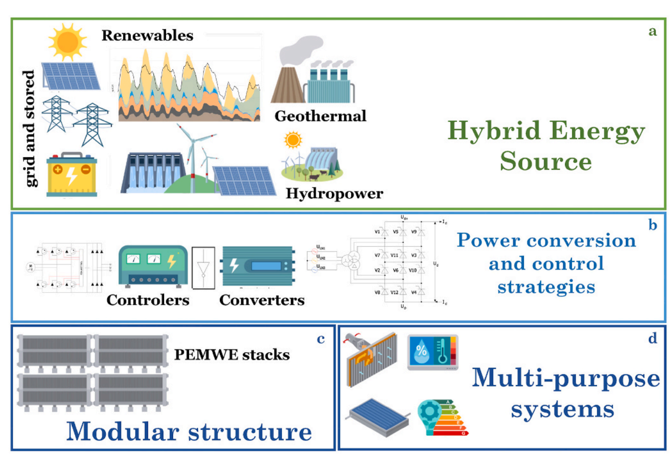


Fig. 1. Frameworks for applying possible solutions to RES utilization challenges in PEMWE.

diminishing degradation and wear, particularly when juxtaposed with traditional singular stack configurations.

The subsequent sections of this paper are structured as follows: Section 2 encapsulates a succinct literature review on existing solutions pertinent to the complexities of harnessing RESs for PEMWE operations. Section 3 outlines a comparative analysis of H2 production employing both singular stack and modular PEMWE setups. Section 4 showcases the garnered results, and Section 5 draws the paper to its conclusion.

2. Possible solutions to the challenges of using RES for PEMWE

Fig. 1a illustrates that by utilizing multiple RESs or integrating RESs with other energy sources, enhanced power and diversity in the electrolyzer power supply can be achieved. This solution encompasses increasing the capacity of the power plant, adding different types of energy sources, and incorporating batteries [22] or supercapacitors [23] for backup. The second stage, depicted in Fig. 1b, involves powering the electrolyzer with processed electricity and transferring it from the source to its input. In this stage, converters, regulators, and electrical controllers play a significant role [24,25].

The third stage, depicted in Fig. 1, addresses the effects of fluctuations and the periodicity of renewable energy. This stage involves the system's structure and complexity, in which the electrolyzer may be a component. PEMWE's modular structure stands out due to its capability to incorporate various features such as power sharing, conversion, and energy management. Power sharing or energy management can entail mechanisms, switches, or controls that utilize the appropriate amount of power at the right moments to enhance the overall efficiency of the electrolyzers, ensuring they are not subjected to high currents and voltages that could harm them. An example of this approach includes power allocation and optimal switching control strategies among system components [26]. Employing hybrid or multi-purpose systems also proves beneficial for this objective, as they stabilize input power for electrolysis [27,28].

2.1. Hybrid energy source

Using multiple energy sources can yield continuous electricity. The concept of utilizing various energy sources to provide uninterrupted electricity isn't novel. However, it gains significance with RES [29]. Given the intermittent and irregular nature of RESs, there is a general need for a consistent electricity supply. Thus, the interplay of various RESs to achieve relative sustainability is intriguing, and substantial progress has been made in this area [30].

For instance, a case study in Ref. [31] elucidates how renewable energy sources can complement each other in Brazil. Fig. 2 illustrates the complementarity between solar and wind energy, particularly from mid-spring to late autumn. The figure also highlights how solar and wind energies can offset hydropower's deficiencies during the latter half of the year. The averaged graph indicates that the synergy among these

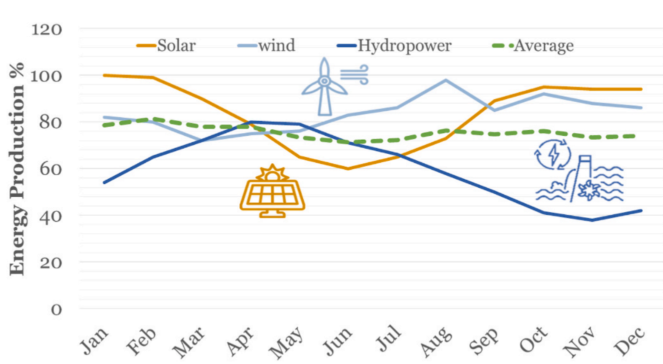


Fig. 2. A case of complementarity of RES [31].

energy sources results in relatively consistent production year-round. Globally, various RESs can be combined to yield a reasonably stable and reliable energy output. Additional RESs, like geothermal, wave, and tidal energies, can be incorporated. Li et al. [32] explored multi-energy HyPro systems and termed them "multi-energy complements." Consequently, multi-energy H2 complementary systems can draw from a plethora of renewable sources, including solar, hydro, wind, tidal, biomass, and others. Kojima et al. [33] postulate that large-scale PV and wind power plants, which benefit from smoothing effects, could be a primary solution to RES challenges. A study by Serdar Genç et al. on wind energy conversion systems (WECS) exemplifies how RES power plants might cater to PEMWEs [34]. Zaik & Werle [35], after a mini-review of RESs as PEMWE energy sources, assessed an electrolyzer paired with solar panels and wind turbines. Their findings suggest that wind and solar energies can compensate for each other's seasonal shortfalls. Moreover, utilizing a buffer battery allows the system to harness the optimal energy amount, preventing overcharging or activation losses.

In scenarios where one or multiple power sources function erratically, batteries typically serve as storage units to ensure consistent voltage. Stand-alone renewable energy systems aptly illustrate this application [36]. In certain systems, supercapacitors can assume a similar role [37]. Conversely, when there is a surplus of renewable energy, it can either be fed into the grid or used by other systems via the multidirectional H2 conversion system [38]. This not only protects PEMWE from potential damage due to excess electricity but also facilitates its effective utilization or storage. Koponen et al. [39] evaluated PEMWE's performance in the context of RES. They analyzed dynamic functional properties and operational constraints from a renewable energy standpoint, suggesting supercapacitors or batteries for uninterrupted electrolysis based on a 10-h test with a 1 Nm3/h PEMWE powered by a 5 kW solar PV. They concluded that the peak HyPro in a PEMWE system, without separate post-electrolysis compression, is achieved when the H2 outlet pressure closely aligns with storage pressure.

2.2. Power conversion and control strategies

Scaling up and enhancing PEMWE to the MW scale poses substantial challenges for both the existing components and the power management of the input. PEMWE input power managers encompass appropriate source selection, power allocation, control of power fluctuations, start-stop switching [40,41], power conversion [42], and prolonged high-power operation (Fig. 1b).

From the electrical perspective described in the prior section, the WECS highlighted the pivotal role of converters in the optimal power delivery to the PEMWE. For hydrogen generation from deionized water, electrolyzers necessitate a very low DC voltage, prompting the common use of step-down converters [43]. Yodwong et al. examined the AC-DC converters currently employed for power transmission from renewable energy conversion systems and the grid for both PEMWE and alkaline electrolyzers. Their research primarily addressed converters centered on thyristor rectifier bridges and chopper-rectifiers [24]. They probed into challenges concerning specific energy consumption, current ripple, reliability, efficiency, and power quality associated with these converters. While the application of thyristor-based rectifiers in high-power contexts has been showcased, the integration of active and passive filters becomes imperative to elevate power quality. Their findings also indicated that amalgamating a chopper with a rectifier can boost power quality by eliminating the need for sizable active and passive filters. Nonetheless, employing a basic chopper (buck converter) is not devoid of downsides, especially in terms of reliability, energy efficiency, voltage ratio, and current ripple. To counteract these pressing challenges and uphold the sustainability of HyPro, the deployment of novel DC-DC converters aligned with the emergence of new power sources is essential. As per Wang et al. [44], a solar energy-driven fast charging and

HyPro system can be regulated through a semi-decentralized control strategy for a DC microgrid. This undertaking segregates the PEMWE energy control into decentralized and power-based modes, with the PEMWE controller dictating the system mode by referencing the day's lowest network cost. Similarly, Gu et al. crafted a system marrying PV power generation with proton exchange membrane water electrolysis for green HyPro. They proposed an energy management strategy to ensure consistent HyPro throughout the day and enhance energy utilization efficiency. Validated via Matlab/Simulink-based simulation, the results underscored that integrating a battery for energy storage markedly uplifts the system's energy efficiency and trims the light discard rate [45]. Moreover, Vudata et al. unveiled a multi-software power control approach built on an electrochemical dynamic stack model. This model delineates the potency of electrolyzers in tempering PV signals to bolster grid stability and adaptability. Alongside highlighting HyPro and electrolyzer efficacy, the study also offers insights on electrolyzer sizing as a tactic to curtail short-lived power surges prompted by cloud cover [46]. Finally, Crespi et al. examined a 60 kW PEMWE setup to introduce a dynamic model for a large-scale PEM electrolysis system, delving into its adaptability during inconsistent and partial load operations. Experimental validation affirmed the model's forecasts with a deviation of less than 4%, pinpointing an elevated specific consumption at diminished current densities. The investigation inferred that this performance decrement predominantly stems from the conventional plant control methodology, power uptake of auxiliaries, and hydrogen utilization for dryer rejuvenation. The implementation of astute control strategies, like modulating the water flow rate and PSA columns' rejuvenation, slashed the net specific consumption by 21% and 50%, respectively [47].

2.3. Prediction and optimization of PEMWE with machine learning

Using Machine Learning (ML) algorithms in engineering modeling for HyPro can facilitate the optimization and study of key components and materials in PEMWE. This can substantially reduce the associated costs and expedite the conventional trial-and-error multivariate experimental optimization process [48]. Günay & Tapan employed ML techniques to explore the connection between descriptor variables and outputs in PEMWE, pinpointing the influence of particular materials and operational characteristics on current density, power density, and polarization. Their findings indicate that ML methodologies can assist in identifying optimal conditions for the design of a PEMWE for HyPro. Moreover, the Bayesian optimization algorithm can achieve peak performance more efficiently in terms of time and effort compared to traditional research methods [49]. Additionally, ML-based simulation models can predict the HyPro rate and cell current density for PEMWE cells given varying design parameters [50]. Salari et al. highlighted the optimization of a solar-based PEMWE utilizing machine learning and animal-inspired algorithms. They achieved a maximum HyPro rate of 5.44 mol h^{-1} m^{-2} and identified solar radiation as the most significant

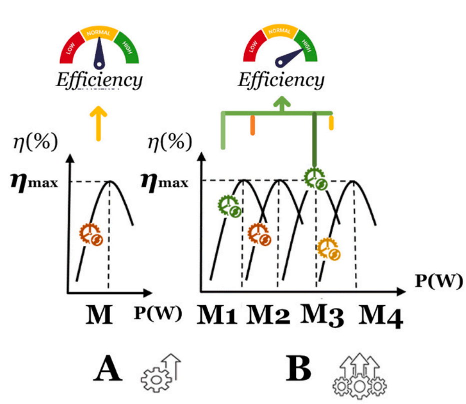


Fig. 3. Efficiency curves of single (A) and modular (B) resources [53].

determinant of the HyPro rate. This was followed by factors such as ambient temperature, inlet temperature, working fluid mass flow rate, and wind speed [51]. Meanwhile, Hai et al. delved into a solar-geothermal energy system comprising three turbines for power generation, a PEM electrolyzer for HyPro, and a thermoelectric module for converting excess heat into electricity. This system is capable of generating 3.8 MW of electricity and producing 8 g of H2 fuel per second at the operational point. To optimize design parameters, ML methods were implemented, and the optimal operating point for maximizing power and stored fuel flow rate was ascertained using a genetic algorithm. Their results revealed that the total power output at this optimal point would exceed the standard operational point by approximately 500 kW. Moreover, the H_2 production rate was projected to be nearly 29 g per second at this optimized juncture [52].

2.4. Modular and multipurpose structures

Beyond the points discussed in the previous subsection, the adaptability of electrolyzers to renewable energy can be enhanced through modifications in their structural design (as depicted in Fig. 1b). This section aims to delve into how modular and multipurpose structures assist various systems in addressing their constraints. Insights from modular energy systems (MES) can offer invaluable guidance for PEMWEs, enabling them to refine existing configurations by leveraging the merits and drawbacks of MES. Illustratively, an MES consists of several autonomous power sources capable of collective operation. In such a system, power distribution spans across components and/or energy storage is apportioned into multiple standardized modules, paving the way for a plethora of economic and technical benefits [53].

Employing MES can bolster the overall system efficiency, especially pertinent in high-power scenarios where the power supply might not perpetually function at its peak efficiency. Fig. 3 illustrates that while each module exhibits a unique efficiency, the cumulative efficiency of the modular system (B) surpasses that of individual modules. Contrasted with a single-stack FC, a modular hybrid system encompasses numerous optimal operational points. The right side of the figure (B) plots the efficiency curves for four distinct power sources, ranging from M1 to M4, equipping the system to operate at consistently high efficiency levels. Owing to this characteristic, MESs grant increased operational flexibility, presenting superior power distribution choices across diverse load scenarios.

Moreover, the availability and durability of modular systems can be enhanced through diligent performance monitoring and management. Such systems can also offer redundancy, ensuring continued operation even if one component fails. By identifying each component and efficiently delegating tasks, the system's lifespan and responsiveness are augmented [54,55]. Another durability enhancer is that the MES components, like FCs and batteries, typically operate at their optimal efficiency levels to deliver peak power. Thus, if lesser power is needed, a single module or a few can function independently, sparing unused modules from wear and tear, extending system longevity.

Architectural flexibility is a further merit of MES, crucial for ensuring system stability and safety. Modular setups offer a plethora of design avenues, allowing for innovative control strategies [56].

A standout advantage of MES is the capability to amplify capacity, bound only by the constraints of the infrastructure, due to the repetitive nature of the modules. However, the capital expense of a modular system might surpass that of a comparable MES with identical power, due to the distinct components. Nonetheless, replacing a low-power component is substantially cheaper than its high-power counterpart. Plus, modular systems stand to benefit from economies of scale.

To expedite the progression of PEM electrolyzers, insights from PEMFCs—which share analogous structure, materials, and processes—can be invaluable. Notably, the evolution of modular FC systems has been a focal point of extensive research [57–61]. Literature posits that modular FC systems, fashioned either by amalgamating multiple stacks or by segmenting a single one, hold promise for the future. These FCs have been devised with diverse electrical and fluidic designs, with their performance contingent on these frameworks. System reliability in a degraded mode is also influenced by its architecture. Moreover, select designs facilitate individual stack control to enhance power output. Depending on the architecture employed, a more robust system can be realized by integrating degraded mode functionality. The insights derived from modular FCs can significantly inform the management of input energy for electrolyzers, given the striking similarities between the study of modular FCs and electrolyzers [62].

2.5. Modular PEMWE

Generally, Modular structures for electrolyzers can generally be categorized into three groups: Multi-electrolyzers [63], segmented electrolyzers [64], and modular electrolyzers. Transitioning from single to modular electrolyzers provides technical and productivity enhancements, along with notable cost savings in HyPro [65]. Depending on system constraints and advantages, various architectural designs may be employed. Table 1 presents several modular designs for PEMWEs. An overview of the essential steps in designing and determining modular PEMWE architecture systems is depicted in Fig. 4.

Given that PEMWEs typically harness surplus energy from one or multiple sources, or from Renewable Energy Sources (RES) where input energy can fluctuate considerably, the potential input energy significantly shapes the design of modular PEMWEs. For optimal system efficiency, it is imperative to understand the peak input power and the specific average power rate. Subsequently, other relevant parameters should be factored in when deciding on the type, size, and quantity of stacks.

Three critical areas must be extensively evaluated in subsequent steps: gas, water, and electricity architectures. Decisions regarding gas architecture encompass gas transfer and storage, potential water separators or dryers, the dimensions of H2 tanks, and possibly H2 compression. For water architecture, choices revolve around storage tank specifications and the temperature of the water before it enters the electrolyzer, which may necessitate a preheater. Since the water supply must be deionized, additional considerations might be essential for system design. Lastly, considerations related to electricity architecture involve the power allocation pattern, power conversion framework, and potential control strategies for the system's input power.

Wirkert et al. [69] introduced a novel modular PEMWE termed "multistack." This design operates uniformly and boasts an efficient heat management system. In their research, a flexible container was fashioned for internal cell components by combining monopolar flat plates with plastic frames. Beyond enhancing heat management and media transfer, this fully modular stack design also presents a more compact form and straightforward stack size adjustments in comparison to traditional models. The capability of this new design for high-efficiency operation, dynamic high-pressure HyPro, and heat management that is independent of process water, has been experimentally validated.

Guilbert & Vitale [67] delved into two primary concerns associated with electrolysis' specific energy consumption: Faradaic efficiency and converter design. To address these issues, they explored a modular setup of PEMWE powered by a wind turbine conversion system. Stacking DC-DC buck converters is employed both for the electrolyzers and wind turbine conversion systems to mitigate ripple and sustain reliability. This converter is orchestrated in a manner that enables faster dynamic behavior than the wind turbine, thereby averting transient overvoltages that could harm the PEMWE. The wind turbine's output power is synchronized with the 400 W-rated power of the PEMWE. In their energy management strategy, if the power surpasses 400 W, the electrolyzer operates at its rated power, and the excess power is channeled to the next unit, as depicted in Fig. 5. This sequence persists until three electrolyzers are engaged. In particular scenarios where energy production exceeds 1200 W, a battery is also activated. Fig. 5's vertical graph displays the output power in watts every half hour (H/2). The four sections, differentiated by varying shades of green, denote the operating regions corresponding to the number of activated electrolyzers. These regions expand with the augmentation of input energy.

The architecture of the wind system for HyPro in the research by Lu et al. [68] differs. In their setup, wind power input is paralleled to the modular PEMWE array through a DC bus, and the power allocation is managed by the control module. When power allocation information for each PEMWE stack is gathered, the execution module sends the power allocation signal to the control module. This control module, which governs each PEMWE stack, will also manage the start-stop function during power outages when an external power supply isn't available. Owing to the power allocation control module, the wind H2 system achieves a cumulative energy efficiency of 61.65%, comparable to a power allocation strategy prioritizing optimal efficiency. Using a genetic algorithm method, Cai et al. [11] optimized the coupling parameters between PV and PEM electrolyzers, observing variable conditions when directly coupled.

The advantages of employing a modular structure in sizable HyPro applications become more evident. One key benefit is the ability to replace a production part if it degrades to a point where it is no longer advantageous to maintain within the system. Conversely, degradation occurs when a PEMWE stack is in operation. By restricting the activity of a segment of the system, degradation in that segment is reduced. Thus, a modular structure curtails the rate of degradation both in individual stacks and across the entire system. Fig. 6 highlights the pronounced impact of degradation on efficiency and demonstrates how a modular setup can mitigate it. Fig. 6 a illustrates that by implementing a power allocation strategy, only some of the PEMWE stacks operate concurrently, significantly reducing degradation. If all PEMWE stacks were active simultaneously, all degradation curves would look alike, with heightened degradation observed in the 2nd, 3rd, and 4th PEMWEs. As seen in Fig. 6,b, the efficiency of an electrolyzer diminishes markedly as it degrades. In this instance, there is roughly a 7% efficiency difference between a fully functional stack and one degraded by 0.2-V [68].

2.6. Multi-purpose systems and combination of different strategies

Intermittent effects of RES can be alleviated through hybrid or multi-objective systems, occasionally with a combination of input sources, multiple processes, tasks, or both. Alirahimi et al. delved into a solar thermal power plant integrated with PEMWE for co-generating power, H2, Oxygen (O2), and hot water. Their proposed system yields 2.906 kg of H2 per hour. A thermoelectric generator, used to draw off heat from the Organic Rankine Cycles (ORC) condenser, supplies the PEMWE with additional electricity, as depicted in Fig. 2-A [70]. They also explored a hybrid source multi-objective design powered by geothermal and solar energy. This design employs an ORC and Parabolic Trough (solar) Collectors (PTCs) to generate H2 with PEMWE, achieve water desalination, and also facilitate an absorption cooling system, as illustrated in Fig. 2-B [71]. To enhance HyPro, they utilized the steam generator's waste heat to pre-heat the PEMWE's deionized water. Pirom & Srisiriwat [72] integrated PEMWE and PEMFC with a PV array for a residential house, achieving a system efficiency ranging from 1.75% to 7.66%. Such net-zero emission residential houses also have freshwater as a byproduct of PEMFC. Dong et al. assessed a renewable generation system integrating a solar-geothermal driven PEM electrolyzer with ORC, ERC, and RO subsystems. Their analysis spanned energetic, exergetic, economic, and exergoeconomic aspects, optimizing the system with multi-criteria decision making and the Gray Wolf Optimizer technique [73]. Escobedo et al. outlined the design, construction, and performance assessment of a PEMWE, characterized by computational fluid dynamic analysis, CNC milling, and electrospray deposition of electrocatalysts. This system achieved a peak efficiency of 59.65% and a HyPro rate of 42 NL•h^{-1} at 15 V and 70 °C with a 132 Wh power draw [74]. Hasani et al. examined the thermoeconomic feasibility of a renewable production unit. This unit combined a geothermal-based PEMWE with the ORC. Their optimization focused on NPV, cost rate, exergy efficiency, and HyPro rate employing techniques like LINMAP, TOPSIS, Shannon Entropy, VIKOR decision-making, and Gray Wolf Optimizer. Their findings indicated an optimum payback period of 5.07 years and a total destruction of 599.13 kW achievable with ORC/IHE-PEM operating with R113. This setup yielded optimal rates: a cost rate of 26.32 $/hr, HyPro rate of 4.202 kg/h, and an exergy efficiency of 40.66% [75].

Sun et al. present a non-dimensional model of a renewable generation system that integrates a solar-geothermal driven PEMWE with the Kalina cycle, single-effect absorption refrigeration cycle, and RO unit. This system was optimized using response surface methodology, resulting in a unit cost of products of 1.75 $/GJ and an exergetic efficiency of 31.71% [76]. Seyedmatin et al. propose a new cooling cycle for a scramjet designed for co-production of electricity and H2 via a PEMWE. They conducted energetic and exergetic analyses to gauge the system's performance and the ramifications of multi-expansion. Their results indicated that the PEMWE experienced the highest exergy destruction ratio. Multi-expansion systems offered significant benefits over single-expansion systems in terms of electricity, cooling, and HyPro. Additionally, increasing the pump's back pressure yielded more electricity and HyPro, and as the freestream Mach number increased, so did the power, H2 production, and cooling load capacity [77].

Ahmadi Boyaghchi et al. introduce a multi-generation system integrating a dual ORC, biomass gasification, and a PEMWE to produce syngas, power, refrigeration effect, heating load, H2, and O2. Their optimization showed that using R600-R290 as the organic working fluid group resulted in maximum energy and exergy efficiencies of 79.35% and 67.64%, respectively. Additionally, they achieved the minimum total product cost and environmental impact rates of 152.7% and 485.1 Pt/h, respectively [78].

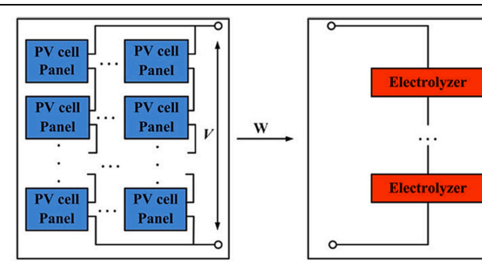
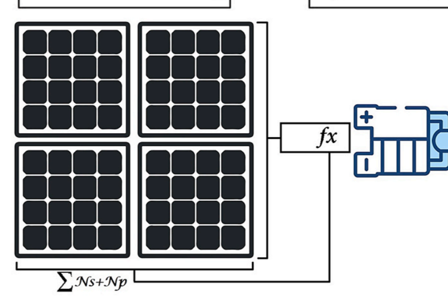
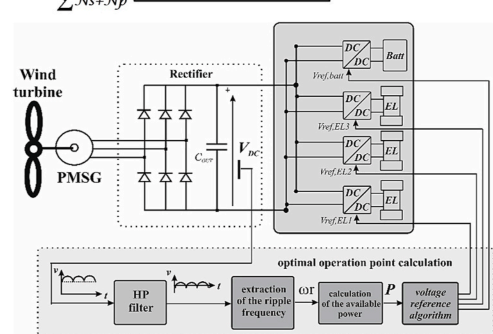
Mohammadi et al. put forth a novel combined biomass-driven cogeneration system comprising a PEMFC and a dual-ejector organic flash cycle. This system aimed to generate clean power while recovering waste heat. It was assessed technologically, economically, and environmentally, with a two-criteria optimization targeting lower costs and emissions alongside higher efficiency. Their findings pinpointed a solution with a net output power of 2.66 MW, a total cost rate of 5.39 $/h, and energy and exergy efficiencies of approximately 37.65% and 23.77%, respectively. They also identified components with the highest exergy destruction, suggesting areas for improvement [79].

Ghorbani et al. crafted an integrated structure for H2 and O2 liquefaction cycles that utilized wind turbines, the Kalina power generation cycle, and electrolyzers. This system could produce 2100 kgmol/h of liquid H2 with specific energy consumption, coefficient of performance, and energy efficiency of 5.462 kWh/kgH2, 0.1384, and 14.06%, respectively. The hybrid system's exergy efficiency stood at 58.73%. Notably, the most significant exergy destruction occurred in electrolyzers (83.13%) and heat exchangers (5.93%) [80].

Yilmaz et al. conducted a thermodynamic evaluation of geothermal energy-powered HyPro via PEM water electrolysis. They found that H2 could be produced at a rate of 0.0340 kg/s with energy and exergy efficiencies of 6.7% and 23.8%, respectively, at a geothermal resource temperature of 160 °C. Both efficiencies increased with the electrolysis and geothermal water temperatures [81].

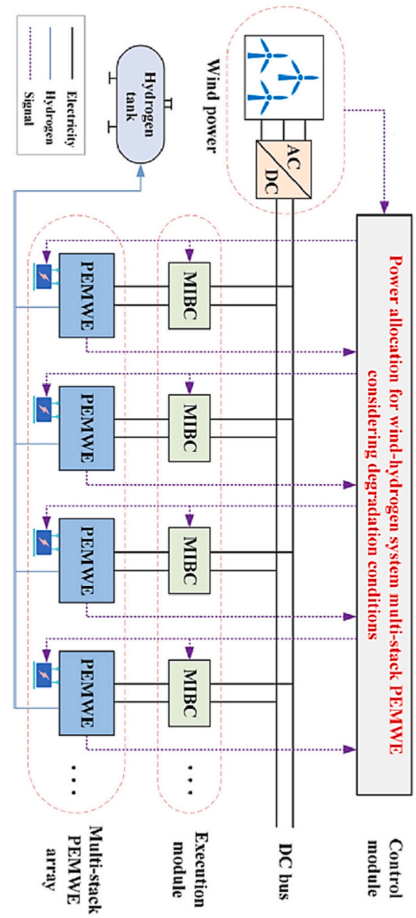
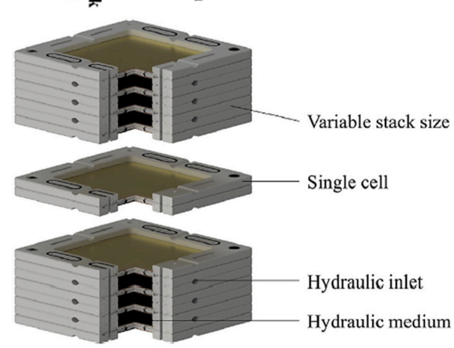
Temiz et al. proposed a unique ocean and solar-based multi-

Table 1
Successful examples of modular structure in PEMWE.

Reference	Modularity (Strategy)	Superiority and creativity	Schematic
[66]	Modular direct coupling with PV (With optimization calculations)	• higher HyPro efficiency • more leakage resistance • No converter • Compact	
[11]	Single-stack direct coupling with PV (With optimization calculations)	• No need for electrical converters • More compact • Less connections	
[67]	Modular (Control and conversion)	• Eliminating the intermittency of input energy • Faster dynamic behavior than the wind turbine • Avoiding overvoltage during transients • The operation of each converter in the mode of maximum efficiency	

(continued on next page)

Table 1 (*continued*)

Reference	Modularity (Strategy)	Superiority and creativity	Schematic
[68]	Modular (Power allocation Optimization)	• PEMWE Maximum efficiency • Lower degradation • Shortened control transient time	
[69]	Multistack (flexible pocket)	• Dynamic high-pressure HyPro • Compact structure and easy stack adjustment and size upgrade • Improved heat management • Direct current and media conduction • Full flexibility	

generational system utilizing various renewable sources in a self-sufficient manner. The overall energy and exergy efficiencies were 16.28% and 36.35%, respectively, with the system generating 25.16 GWh of electricity and 283 tons of H2 annually via PEMWE. This system also encompassed a fish farm, greenhouse, and food drying facility, producing 7.9 tons of vegetables and 374 tons of fish annually, presenting a potential remedy for Arctic communities' energy and food challenges [82].

Holmes-Gentle et al. developed a dynamic non-linear process model for a thermally-integrated concentrated PV-electrolysis system. The system exhibited a hysteresis effect in response to perturbations, and the potential for co-generating H2 and heat appeared promising [83].

Zhao et al. formulated an electrolysis power allocation and alternative control method [84], combining an optimized control strategy to forecast the peak wind power at specific times. To stabilize the power output of a wind farm, Muyeen et al. generated a reference for line power, developed a switching strategy, and produced H2 gas to absorb fluctuating wind farm outputs [85].

Shakibi et al. investigated a multi-generation system based on wind turbines and PTCs. This system incorporated a PEMWE for HyPro and utilized an ML-based optimization approach. Their optimal scenario achieved 6.20 MWh of energy and saved 1.26 tons of CO2 per year. Their study also emphasized the influence of parameters like electricity and H2 prices on the system's total cost and exergy efficiency [86].

3. Comparative study of hydrogen production

A green HyPro system based on RES demands foresight and meticulous evaluation of two processes to ensure stable, continuous, and reliable production. These processes encompass the assessment of electricity production from renewable sources and the scrutiny of HyPro with the chosen electrolyzer. In Section 3.1, the energy available from

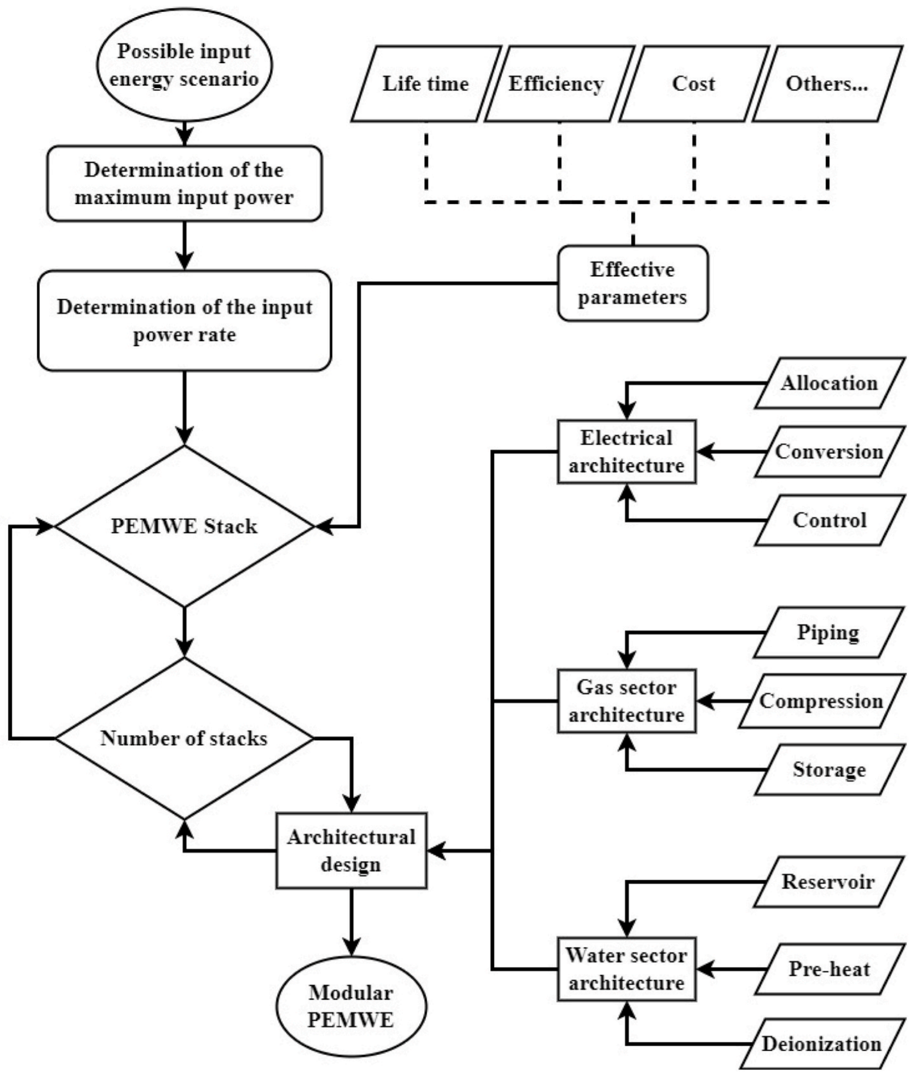


Fig. 4. Schematic of PEMWE modular design.

the PV array in Trois-Rivieres is evaluated. The experimental data for a PV panel is first gathered. Subsequently, a predictive ANN model is developed using meteorological data and energy production records. This model is then utilized to forecast the amount of energy expected to be available in the future, based on atmospheric conditions and the local climate. Section 3.2 uses the experimental energy production to power a PEMWE stack and assess its performance. In this context, HyPro in Trois-Rivieres is examined by analyzing and scaling the data. Based on the available solar energy, an optimized modular structure is proposed, which is subsequently compared to a conventional system in Section 3.3.

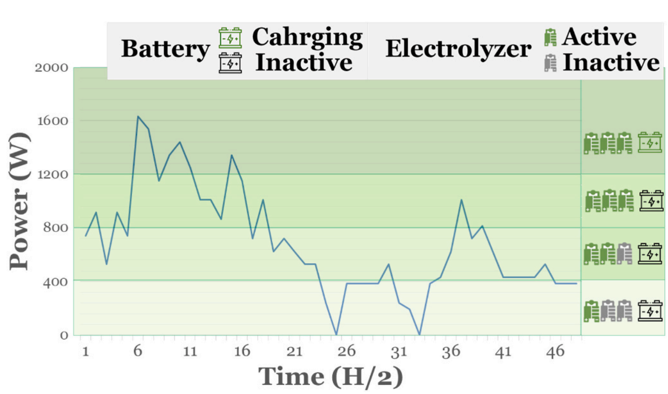


Fig. 5. Power-sharing strategy according to the available power from the wind turbine.

3.1. Available energy

PV energy production largely depends on the array placement, surrounding climate, particulate matter, and industrial emissions. Therefore, detailed and long-term information about a region's weather conditions can enhance the accuracy of energy production forecasts, especially when compared to experiences drawn from a small PV unit. Given sufficient long-term data, ANNs are an invaluable tool for creating reliable predictive models that surpass those generated by current simulations or nominal models. As such, a suitable ANN model, paired with local environmental and climate data, can effectively estimate the solar energy available in Trois-Rivières. As indicated in Eq. (1), the PV output power is predominantly influenced by solar radiation and geographical location; thus, local weather conditions play a significant role [87]. Factors such as cloud cover, atmospheric clarity, temperature, air pressure, and wind are all pivotal parameters that affect the received energy.

$$P_{pv} = \Upsilon \alpha_{PV} G_{nr}\left[1 - B_r\left(T_{pv} - T_r\right)\right] \quad (1)$$

This formula is typically used to calculate the output power (P_{pv}) of

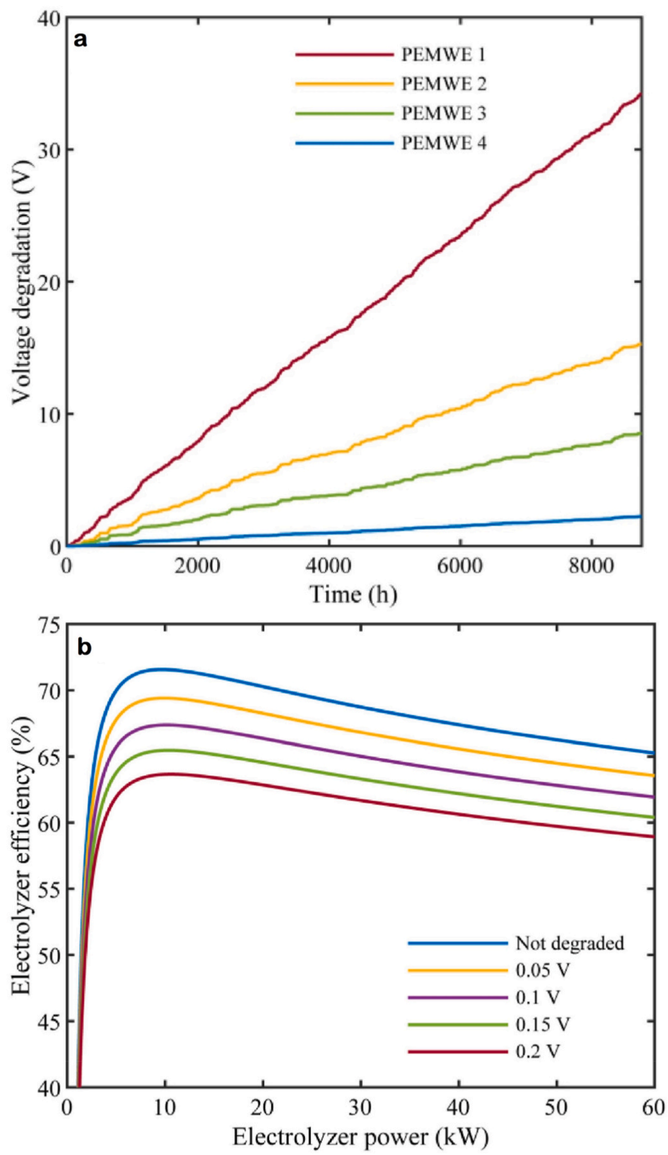


Fig. 6. Comparision of degradation in Modular and single-stack PEMWE [68].

the PV panel. G_{nr} represents solar irradiance, α_{PV} denotes cell efficiency, T_r indicates the operating reference temperature, and B_r is the temperature coefficient. Additionally, Υ stands for the surface coverage ratio, which is the module surface area that can be covered by sun irradiation relative to the total area occupied by the array. Solar dynamical positions directly influence Υ, while earth's atmospheric conditions—such as pressure, humidity, atmospheric dust, wind, and transparency—affect G_{nr} directly. Other vital parameters impacting the nominal output power of PV include panel position, soiling, shading, snow, losses, and aging [88].

Given these factors, one of the most accurate methods to determine received solar energy involves collecting experimental data from a PV panel positioned identically as depicted in Fig. 7. The University of Quebec in Trois-Rivières presents an ideal site for solar array implementation. The southern face of the university building (Albert-Tessier building) is oriented southward, with a slight 5-degree deviation to the west—optimal for the northern hemisphere. Given the arrays' elevated installation, shading is minimized. Additionally, the window architecture is slightly angled inward, complementing the PV plate's inclination. This setup mitigates several efficiency-reducing factors, including surface shading, snow accumulation (in winter), dust buildup, and high temperatures (in summer). The location also offers convenient access due to the building's windows. These features render this facade suitable for PV array installation, as illustrated in Fig. 8. Aesthetically, it enhances the building's appearance. Specifications for the PV panel utilized in the experimental tests are provided in Table 2.

Data were collected for a year, from 2021 to 2022. Since the PV output is in direct current (DC), it is directly routed to the battery after maximum power point tracking (Fig. 6) using a charge controller. Additionally, voltage and current measurements are relayed to the system via an RS-485. This procedure is depicted in Fig. 6. Maximum Power Point Tracking (MPPT) is commonly employed to regulate the electrical energy generated by PV arrays. This energy is then channeled to the PEM electrolysis through a DC-DC converter. In this state, the current remains relatively stable. Nonetheless, the high expense of electronic control equipment and efficiency losses due to multiple energy conversions have prompted the exploration of alternative methods. One such method, which can decrease both the number of energy conversions and equipment costs, is direct coupling. This method involves a direct connection between the power source and the electrolyzer. By adjusting the number of solar cells in series and parallel configurations, the system's power level can be kept close to its maximum. Consequently, the HyPro estimation will be grounded on the direct coupling method.

A promising method for estimating future available energy employs ML techniques to discern available energy for specific times or extended durations. An accurate and reliable ANN model is essential for predicting the available energy from PV panels. To realize this, input parameters must be judiciously chosen based on their marked impact on PV panel output. As indicated by Eq. (1), temperature, visibility, humidity, air pressure, wind speed, and hourly solar irradiation are chosen as input parameters, illustrated in Fig. 9, due to their strong correlation with the performance of PV panels. Furthermore, factors like azimuth and tilt angle, capacity factor, efficiency, cover ratio, system losses (including mismatch, wiring, and connections), power control, ageing, and light-induced degradation will be inherently incorporated into the outcome when training the ANN with experimental data. To guarantee model precision, genuine data gathered from a solar panel over a year was employed for both training and validation. A feed-forward neural network was adopted to forecast future electricity production from a PV system based on historical data. This neural network was preferred because of its proficiency in accurately depicting intricate nonlinear associations between input and output data, making it ideal for solar energy production prediction. The dataset was divided into training, validation, and test sets using a 76/12/12 ratio. The training set enabled the NN's education, the validation set fine-tuned the NN hyperparameters and curbed overfitting, while the test set gauged the performance of the finalized model. Data processing comprised feature selection, normalization, and standardization, which bolstered the NN model's precision. Furthermore, early stopping during training and regularization approaches like L1 and L2 regularization, which penalize hefty weights, helped mitigate overfitting. In sum, based on its adeptness in precisely modeling complex nonlinear relations and the training, validation, and testing methodologies adopted, the feed-forward neural network emerged as the most fitting NN for this undertaking.

Fig. 9 illustrates that this ANN has six inputs, two hidden layers, and one output layer. Pertaining to the model's design, a neural network structure featuring two hidden layers was chosen, grounded on past studies vouching for its efficacy in accurately forecasting PV panel output [89]. Deciding on the number of hidden layers in an ANN is pivotal for attaining supreme prediction accuracy. Generally, two hidden layers are employed as they have proven to strike an equilibrium between overfitting and underfitting. Moreover, the neuron count per layer ought to be carefully determined based on the problem's intricacy and the dataset's volume. Upon evaluating diverse algorithms, the Conjugate Gradient with Powell-Beale Restarts emerged as the most adept for training this predictive PV production model. It was chosen since it converges more swiftly and yields more precise outcomes

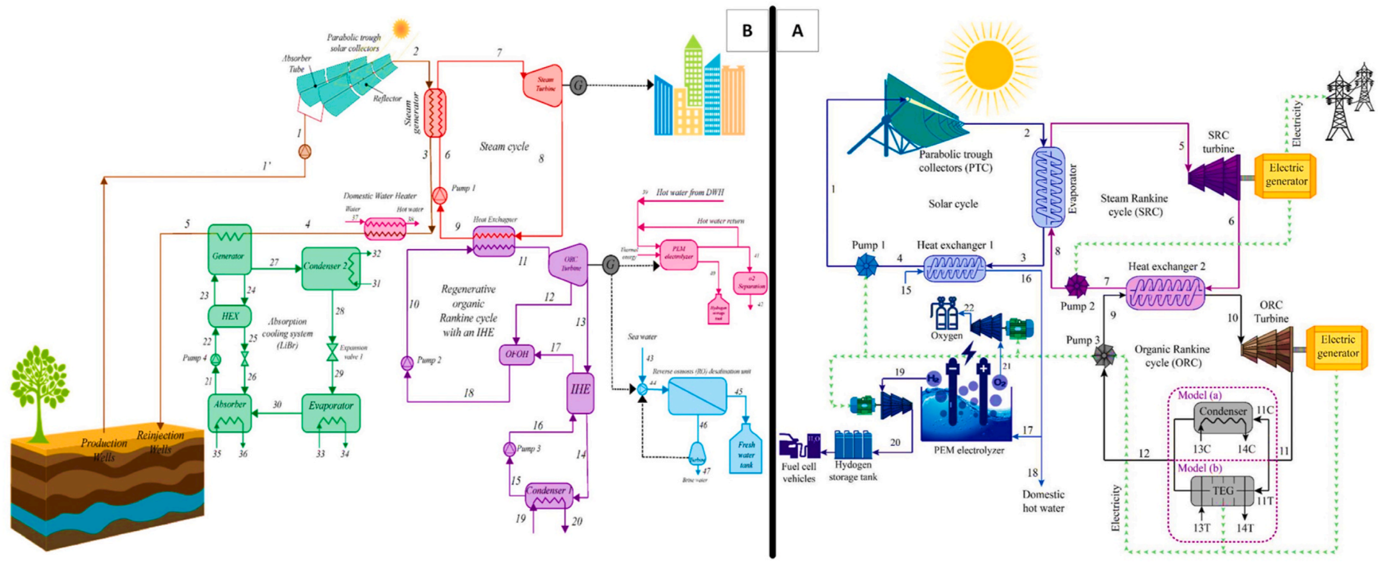


Fig. 7. The Multi-objective design for multi-generation energy systems based on renewable sources.

compared to other optimization algorithms. The conjugate gradient method occasionally readjusts its search direction to the negative gradient. Ultimately, a standard reset point is achieved when the iteration count matches the network parameters [90]. As tested with Eq. (2), where 'g' symbolizes the gradient, meeting this condition signifies that the search direction will revert to its negative counterpart.

$$\left|g_{k-1}^{T}g_{k}\right| \geq 0.2g_{k}^{2} \tag{2}$$

In summary, the chosen input parameters, data preprocessing methods, and the neural network architecture combined with its algorithm are anticipated to offer a strong and efficient solution for forecasting the potential available energy of PV panels. This approach also aims to sidestep overfitting while maintaining high prediction accuracy.

Eq. (3) assists in estimation and scaling in relation to Eq. (7) through Eq. (10). Upon examining models related to PV output DC power, both Eq. (3) and Eq. (4) underscore that maintaining the PV at its optimal efficiency point significantly influences the energy harvested.

$$n_p.P_{pv}.\eta_{array} \approx n_{el}.P_{el} \tag{3}$$

In these equations, n_p and n_{el} denote the number of panels and electrolyzers, respectively, while P_{pv} and P_{el} represent the output power of a PV panel and the required power for PEMWE, respectively. Additionally, the overall efficiency of the PV array (η_{array}) should be taken into account.

$$\alpha \text{HyPro}_S = \alpha PV_{max} \times \alpha \text{PEM} \times \text{CP}_{PV} \tag{4}$$

$$\text{CP}_{PV} = (\text{Output}_{\text{PV}} \,/\, \text{Output}_{\text{max}}) \tag{5}$$

According to Eq. (4), enhancing the efficiency of both the PV and PEMWE will elevate the overall efficiency of HyPro. However, there is a coefficient that is contingent upon the structure and design. By refining the design of a PEMWE, an increase in HyPro efficiency is projected. In Eq. (4), αHyPro_S represents the efficiency of the HyPro system within a stack. This efficiency is influenced by the combined efficiencies of the PV and PEMWE, and it incorporates a coefficient of performance (CP_{PV}). Thus, an optimal design enhances the performance of auxiliary systems, facilitating synergy between electrolysis and PV, and ultimately boosting the efficiency of the entire system.

3.2. Hydrogen production

The energy pattern identified in the previous section should be employed to evaluate an electrolysis system for HyPro utilizing solar energy. To compute the HyPro, a PEMWE model is developed based on experimental data gathered from a setup depicted in Fig. 10. The specifications of this electrolyzer, along with its environmental attributes, are detailed in Table 3. As seen in Fig. 10, one side of the PEMWE is connected to the deionized water supply, while the other is linked to a power supply. An Ethernet network enables a computer to monitor and regulate a programmable power source. Moreover, the electrolyzer's output is attached to a flowmeter before it feeds into the H2 tank, where a data logger captures its real-time information. Consequently, by controlling and recording the input electricity and the output H2, and by monitoring the cell data, the performance of the electrolyzer models can be comparatively assessed.

3.2.1. Basics

HyPro occurs within the cells of the PEMWE. This process not only offers an efficient and clean method of producing H2 from water, but it also yields O_2 as a byproduct. In a stack section, a zero-gap cell fitted with a solid polymer electrolyte facilitates proton conduction, separates the produced gases, and electrically insulates the electrodes. H_2 and O_2 are produced through reactions in the cathode (Eq. (7)) and anode (Eq. (6)) sides, as well as the catalyst layers. The role of electricity in this process is evident in Eq. (8).

$$H_2O = \left(\frac{1}{2}\right)O_2 + 2H^+ + 2e^- \tag{6}$$

$$2H^+ + 2e^- = H_2 \tag{7}$$

$$H_2O + \text{electricity} = H_2 + \left(\frac{1}{2}\right)O_2 \tag{8}$$

The voltage and current of this electricity are influenced by various parameters. If the process takes place under reversible conditions, implying that no exergy or enthalpy is consumed and no losses occur, then the potential difference at the electrodes would be 1.229 V. This is referred to as the reversible cell voltage (V_{rev}^0). Without an external heat source, the total energy required for the reaction (ΔH_R^0) must come from electrical energy. However, when the necessary thermal energy contribution is available, only minimal electrical work is needed to split the

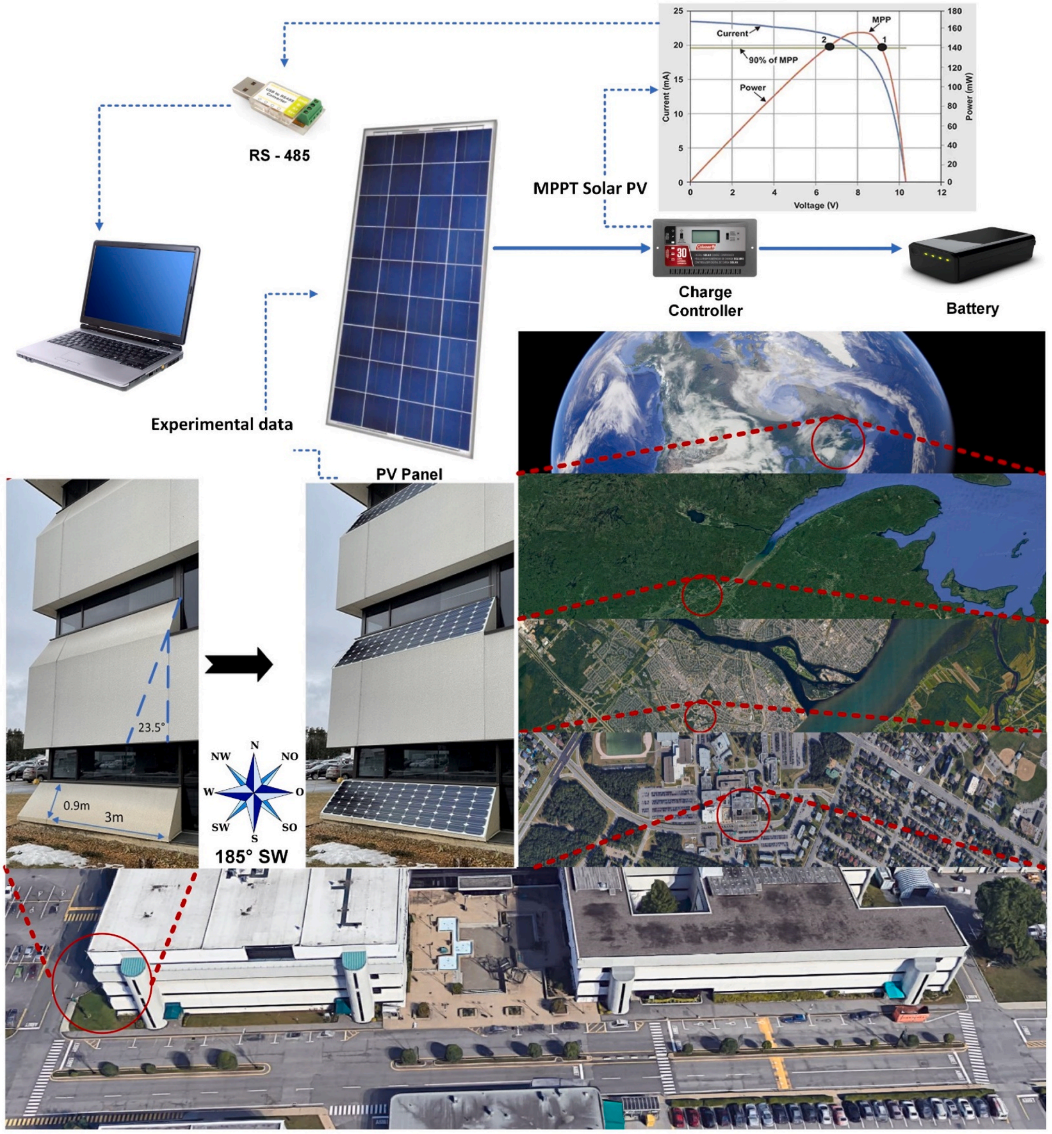


Fig. 8. The PV location, direction and position.

Table 2
The reference PV panel characteristics.

Location	Trois-Rivières, Canada
Latitude	46.35° N
Longitude	72.58° W
Module Type	Polycrystalline
Array Type	Fix tilted
Array Azimuth	185°(South-West)
Capacity Factor	12.5%
Array Tilt	66.5°
DC System Size	150 W
Maximum current	8.7 A
Dimensions	149 * 66.5 * 3.5 cm
Number of PV for the estimated array	80
Total effective area of the array	79.268 m2

water. As a result, the required voltage exceeds V_{rev}^0 and is termed the thermoneutral voltage V_{th}^0 in its standard state, as described in Eq. (9). Additionally, the Higher Heating Value of Hydrogen (HHVH) remains constant, approximately 3.54 kWh/Nmˆ3 [92–94].

$$V_{th}^0 = \frac{\Delta H_R^0}{z.F} = 1.481\ V \tag{9}$$

where z represents the number of moles of electrons transferred in the reaction and F denotes the Faraday constant, with a value of $9.6485 \times 10^4\ C/mol$. For an accurate estimate, the precise cell voltage (V_{cell}) is necessary. This voltage is determined by dividing the thermoneutral voltage by the cell efficiency (η_c), as indicated in Eq. (10). The electrical work can be derived from Eq. (11), where η_f represents the faradaic efficiency. This value approximates 285.8 J/mol or 0.08 Wh/g.

$$V_{cell} = \frac{V_{th}^0}{\eta_c} \tag{10}$$

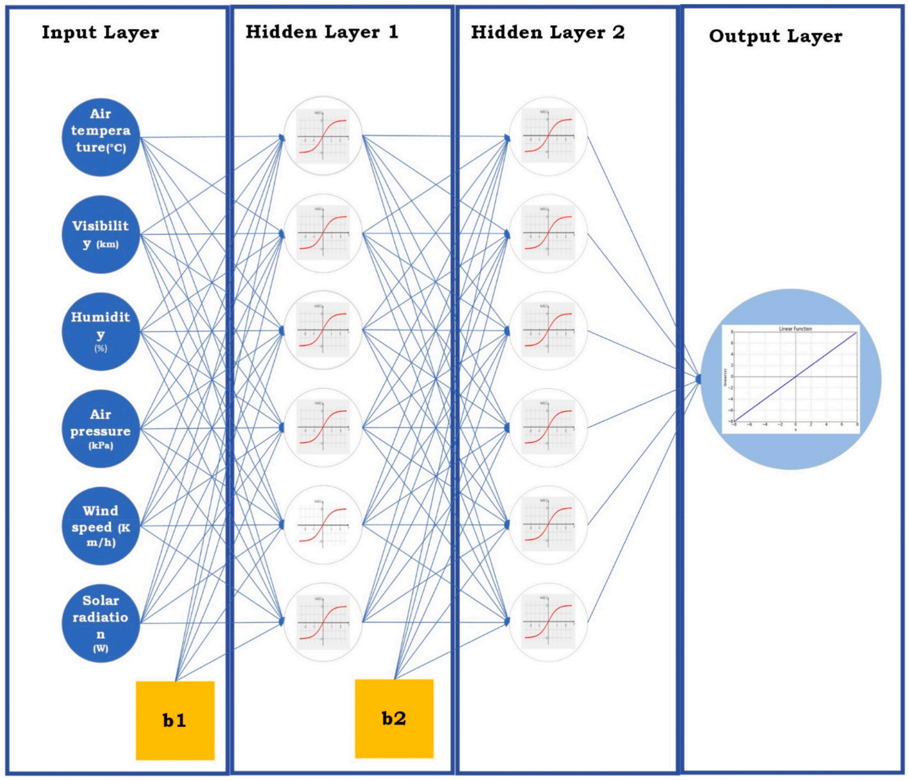


Fig. 9. The ANN design for the predictive PV production model.

$$W = zF\frac{V}{\eta_f} \tag{11}$$

3.2.2. *Performance and efficiency of PEMWE in experimental tests*

Generally, the performance of the electrolyzer is represented through the use of polarization curves. Polarization curves provide valuable insights into the performance of the electrolysis system under various operating conditions. They illustrate the relationship between cell potential and current density, aiding in the identification of optimal operating conditions. In this study, experimental data from the PEMWE (Proton Exchange Membrane Water Electrolysis) were collected to generate efficiency and polarization curves.

As shown in Fig. 11, the voltage and efficiency of the PEMWE stack are illustrated based on the current. The blue axis (left side) represents efficiency as a percentage, while the red axis (right side) indicates the voltage level. These curves were plotted using experimental data, which have been deemed a reasonable and reliable approximation for the behavior of the electrolyzer.

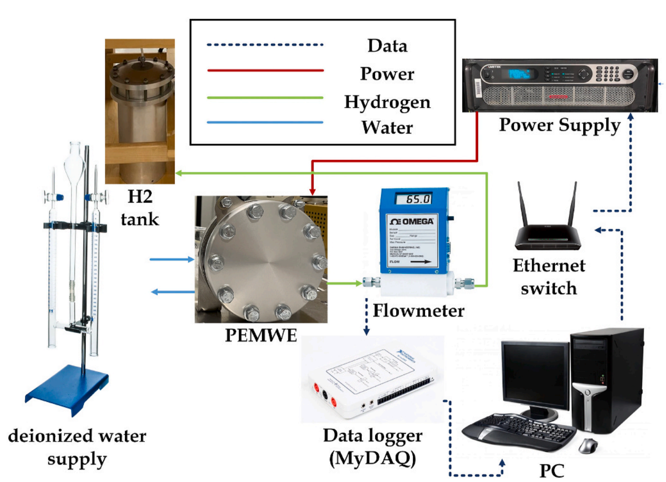


Fig. 10. PEMWE, auxiliary and connections testbench.

Observations from the literature indicate that the actual cell voltage (V_C) of a PEMWE, as measured experimentally in this specific case, is the cumulative result of its reversible (open circuit) voltage (V_o) and various overvoltages [95]. These overvoltages, termed activation (U_{ac}), ohmic (U_{oh}), and concentration (U_{co}) as per Eq. (13), significantly influence the polarization curve of the PEMWE. Each of these overvoltages impacts different segments of the polarization curve. However, it is important to note that, in this instance, the concentration overvoltage has not been factored into the calculation and scaling, including its corresponding area.

$$P_c = I_C \times V_C \tag{12}$$

$$V_C = V_o + U_{ac} + U_{oh} + U_{co} \tag{13}$$

Equation (12) is formulated for an individual cell; however, the current and voltage of a stack depend on the configuration of the system. Equation (14) illustrates the relationships for stack current (I_S) and voltage (V_S). In the case of an array connected in series, as shown in Equation (15), the voltage at the terminals of the stack is the accumulation of voltages across the series connections (with each cell's current being I_{cn}). Conversely, when the array is connected in parallel, as demonstrated in Equation (16), the stack current equals the sum of currents flowing through the parallel-connected cells (with each cell's voltage being V_{cn}) [96].

$$P_s = I_s \times V_s \tag{14}$$

$$P_s = I_s \times \sum_{n=1}^{N} V_{cn} \tag{15}$$

Table 3
Working and environmental characteristics of the PEMWE.

Lab. Location	Institut of Hydrogen Research (IHR) Trois-Riveres, QC, Canada
Lab. Average temperature	24.4 °C
Water Average temperature	24.2° W
Electrolyzer Type	PEMWE
PEMWE Manufacturer	Shandong Saikesaisi Hydrogen Energy [91]
model	QLC-1000
Number of cells	4
Input voltage	12 V
Input current	36 A
Max. voltage	15 V
Max. current	40 A
H2 Production	1 L/min
O2 Production	500 ml/min
Operating temperature	5–45 °C
Output-pressure	0-145 psi
Stack Diameter	13.8 cm
Power supply (DC)	100 V * 100 Amper (Programmable)

FLOW METER		**Storage Tank**	
Flow range	10 L/min	Capacity	10 L
Accuracy	±1%	Material	steel
Maximum Gas Pressure	250 psig	Max. Working Pressure	200 psi

$$P_s = V_s \times \sum_{n=1}^{N} I_{cn} \tag{16}$$

Utilizing these relationships, the variable quantity of HyPro can be described using Equation (17). Within this equation, 'N' represents the number of cells, while ' η_e' signifies the dynamic amount of PEMWE efficiency as determined by Equation (18), and this efficiency is linked to the current.

$$\int_0^t f_{H2}.dt = \frac{\int_0^t N \times I \times V \times \eta_e \times dt}{HHVH} \tag{17}$$

$$\eta_e = 0.00293 I^2 - 0.667 I + 85.333 \tag{18}$$

To estimate the efficiency of the electrolyzer (η_e) using Equation (18), based on the current from the solar panel, a second-order polynomial equation is employed from Fig. 11. The equation is interpolated using experimental data and applied through approximation in this context.

Building upon the experimental outcomes of a small-scale electrolyzer, the behavior of an electrolyzer with a different number of cells can be predicted by maintaining the actual cell ratio. Various scaling formulas can be utilized to extrapolate the behavior of large-scale electrolyzers from the experimental findings of smaller-scale counterparts. Equation (19) offers a summarized illustration of size conversion within the calculations. When upscaling the production of a small electrolyzer, determining the suitable size for a larger system can be facilitated by calculating the required increase in the number of cells. However, it is crucial to highlight that scaling laws may not consistently yield accurate results due to variations in operating conditions, materials, and other contributing factors. Experimental validation is necessary for confirming the outcomes of scaled-up systems [97,98].

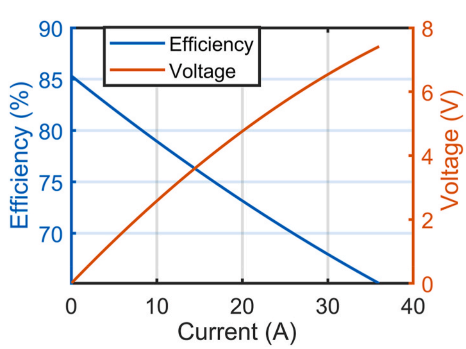


Fig. 11. PEMWE polarization and efficiency curves.

$$V_S = N(V_o + U_{ac} + U_{oh}) \tag{19}$$

The energy efficiency coefficient of an electrolysis system quantifies the effectiveness of converting electrical energy into H_2 and O_2 gases through water electrolysis, as depicted in Equation (20). It is formulated as the ratio of the energy content of the produced H_2 and O_2 gases (W_{rev}) resulting from electrolysis to the overall energy input into the system (W_{irrev}), encompassing all associated losses (such as energy and current losses, heat dissipation, etc.) occurring within the electrolysis unit cell/stack and supplementary subsystems (e.g., heat exchangers, pumps, etc.).

In practical and industrial contexts, this definition is commonly employed. Conversely, in academic and scientific research, the focus often centers on the water electrolysis reaction exclusively, within the confines of constant temperature and pressure conditions. The energy efficiency coefficient of an electrolysis system takes into consideration all parasitic losses, amalgamating them as the denominator of the equation. The numerator comprises the energy content of H2/O2 gases produced by electrolysis. This coefficient is determined as the ratio of the energy content of the products obtained at the exhaust of the system to the overall energy supplied [99].

$$\varepsilon_{PEMWE} = \frac{W_{rev}}{W_{irrev}} \tag{20}$$

3.2.3. Degradation

PEMWE degradation can be characterized by voltage decay over time under constant operating conditions. The simplest model to describe this behavior is based on empirical observation. This assumes that the voltage loss is proportional to the logarithm of the operating time [100]:

$$V_t = V_0 - d \ln (t / t_r) \tag{23}$$

Here, V_0 represents the initial voltage, 't' stands for the operating time, t_r is a reference time, and ' d ' represents the degradation rate constant. According to Voronova et al.'s research [101], under solar fluctuating conditions, this degradation rate can be approximated as 3.5 mV/h. Various degradation mechanisms are accounted for in more intricate models, encompassing catalyst degradation, membrane degradation, and issues related to water management. Typically, these

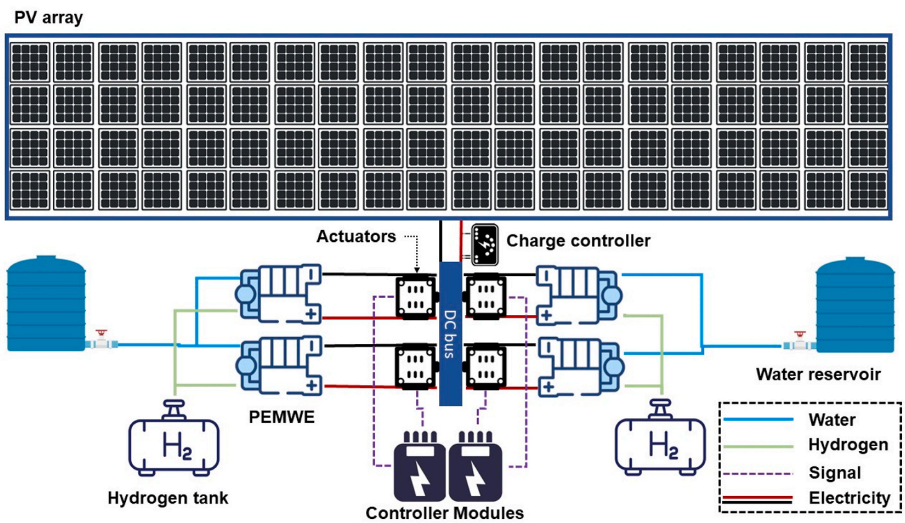


Fig. 12. Proposed structure for modular PV and electrolyzer.

Table 4
Power allocation strategy based on available energy.

Scenario	P	PEMWE 1	PEMWE 2	PEMWE 3	PEMWE 4
1	2.5 kW > P	On	Off	Off	Off
2	5 kW > P > 2.5 kW	On	On	Off	Off
3	7.5 kW > P > 5 kW	On	On	On	Off
4	P > 7.5 kW	On	On	On	On

models entail a higher number of parameters, necessitating a more comprehensive dataset from the experimental phase to accurately calibrate the model's parameters [102,103].

3.3. Modular PEMWE

As elucidated in Section 2, the utilization of modular systems plays a highly effective role in both controlling and enhancing the operational conditions and efficiency of the HyPro system. Their inherent structure not only facilitates system capacity expansion, but also significantly simplifies energy management and control, resulting in heightened efficiency. Furthermore, the integration of diverse and capable auxiliary systems is viable, as detailed in Section 2.3.

In this work, the structure employed for the proposed modular PEMWE system is depicted in Fig. 12. Since the intended placement is within a university building, specific limitations and opportunities have arisen. Although space is confined, the availability of internal building facilities and water access remains convenient. Given that the primary focus of our project centers around comparing single-stack and modular PEMWE systems in terms of HyPro, other parameters such as cost and size are not extensively discussed in this study. The architectural layout is divided into two accessible buildings, accommodating two water reservoirs and H_2 tanks to enhance safety and compactness.

In the ANN model, the proposed array can generate a maximum energy output of around 10 kW. To compare the HyPro system using both a modular PEMWE setup and a single-stack configuration, we investigate two cases in this study.

In the first case, a single-stack 10 kW electrolyzer with 80 cells is used for the HyPro application. In the second case, four medium-sized electrolyzers with a maximum input power of 2.5 kW and 20 cells each are employed. The generated energy is then transferred to a DC bus through a charge controller designed to maximize solar energy utilization, as depicted in Fig. 8. Subsequently, the controller modules determine the distribution of electrical current among the PEMWEs. The power-sharing strategy implemented follows the principles outlined by Guilbert and Vitale [67].

Table 4 presents four distinct scenarios that cover the range from zero to the maximum available energy from the PV array. In scenario 1, if the available energy is less than 2.5 kW, only one PEMWE will be responsible for HyPro. In scenario 2, when the available power falls between 2.5 and 5 kW, two of the PEMWEs will be activated. For scenario 3, if the total power output surpasses 5 kW but remains below 7.5 kW, three PEMWEs will be operational. Finally, in scenario 4, if the available energy exceeds 7.5 kW/h, all of the electrolyzers will be engaged for HyPro.

4. Results and discussion

In the preceding section, the process of predicting the HyPro amount was outlined. This involved initially deriving the available energy quantity through a precise model reliant on environmental conditions, coupled with experimentation on a control sample panel, as discussed in Section 3.1. Subsequently, an evaluation of the actual HyPro amount derived from solar energy was conducted, as detailed in Section 3.2. As the concluding step, the HyPro values for the theoretical project were juxtaposed for both the proposed single PEMWE configuration and the modular PEMWE setup, elucidated in Section 3.3.

4.1. Available energy by ANN model

The assessment of the ANN's performance encompassed three distinct stages: training, testing, and validation, as illustrated in Fig. 13. The training phase involved fine-tuning the ANN's parameters using a subset of the available data. In the subsequent testing phase, the model's capacity for generalization was appraised by applying it to a distinct dataset. The validation phase, on the other hand, gauged the model's efficacy in handling newly acquired and previously unseen data.

The performance of the ANN model was remarkably robust, exhibiting accuracy across all phases. Specifically, the performance metrics were calculated as 0.9994 for the training phase, 0.99941 for the testing phase, and 0.99944 for the validation phase. These results strongly indicate the ANN's ability to effectively learn from the input data and generalize its insights to various contexts.

The trained ANN effectively demonstrated its capability to predict solar energy levels in Trois-Rivières, grounded in the chosen input variables and reference data. The features selected, encompassing aspects such as sun irradiation quality and the influence of temperature on

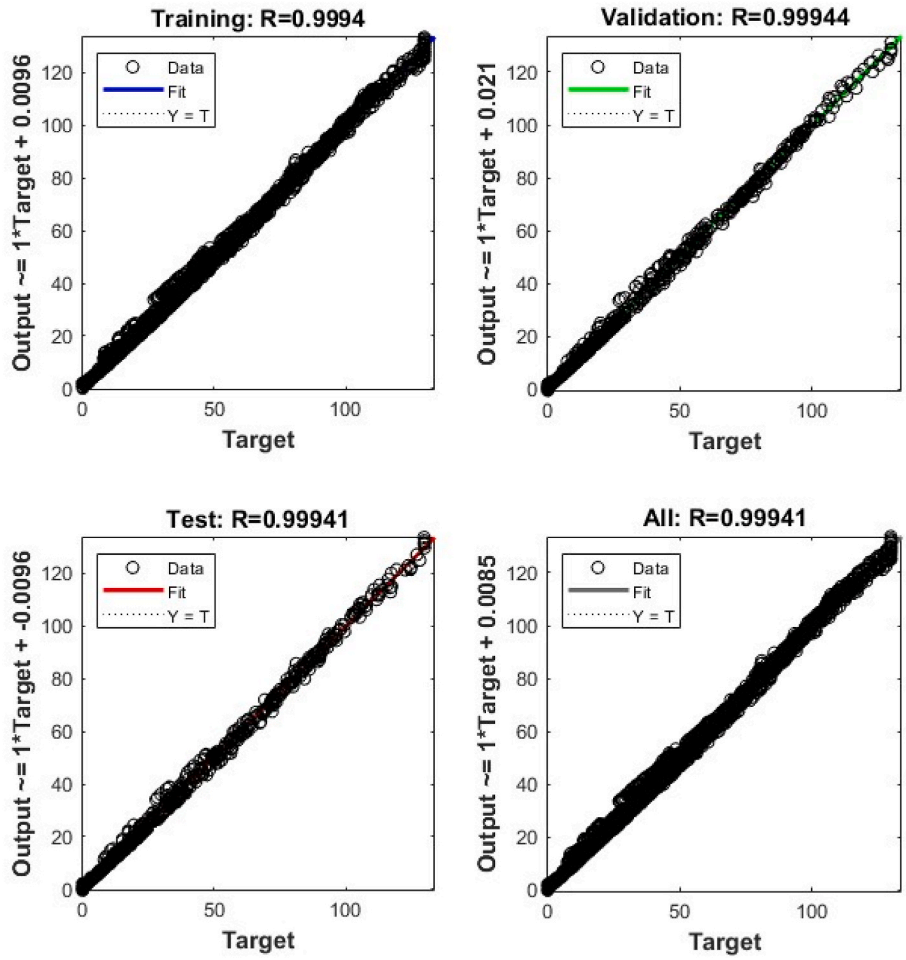


Fig. 13. PEMWE ANN model regression.

photovoltaic (PV) efficiency, proved pivotal in accurately forecasting available energy. Rigorous validation against experimental data confirmed the reliability of the ANN model, yielding outcomes that closely aligned with actual measurements, differing by a mere 6.3%.

These findings underscore the ANN model's potency as a robust tool for solar energy prediction, offering substantial implications for the strategic planning and operational efficiency of PV systems. On the whole, these results exemplify the potential harnessed by machine learning methodologies within the realm of renewable energy. Additionally, they underscore the critical role played by judicious selection of input variables and meticulous calibration of model parameters, both instrumental in attaining precision in predictions.

4.2. Hydrogen production using a single-stack system

In this section, we present the daily HyPro amount based on observations derived from laboratory tests. Fig. 14 illustrates solar radiation levels in Trois-Rivières, along with the energy harvested and the resulting H2 production. This dataset stems from a sunny day's (approximately 15 h) experimentation conducted in July 2022. For this test, the energy generated by two panels, as detailed in Table 2, powered a 1000 ml per hour electrolyzer. Notably, the HyPro algorithm closely mirrors the anticipated solar energy production pattern. Consequently, the HyPro output for this specific test day and power supply configuration reached a cumulative total of around 4.27 L.

It is imperative to factor in the disparities in performance and efficiency between a singular PEMWE stack and an upscaled version when evaluating the overall electrolyzer performance. Precise utilization of scaling factor coefficients assumes paramount importance to ensure exact calculations. Moreover, incorporating experimental data from an electrolyzer possessing the same dimensions as the scaled-up stack would undoubtedly enhance the result accuracy.

4.3. Hydrogen production using a modular structure

As described by Equation (18), the efficiency of the PEMWE is variable, contingent on the current density. This dynamic characteristic can be adeptly managed and optimized by judiciously distributing input power within a modular framework. To achieve this, a power allocation strategy is employed to ensure a consistent power supply to the PEMWE,

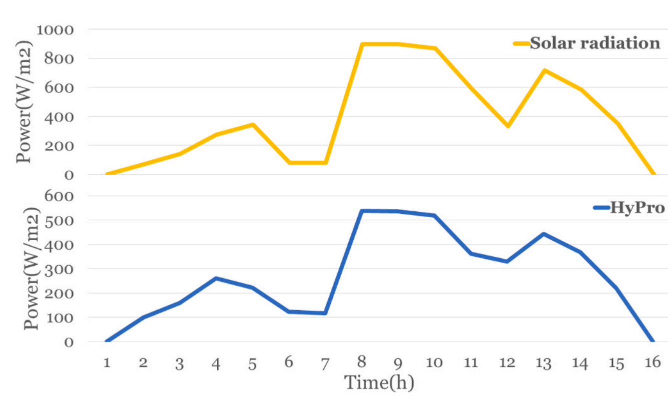


Fig. 14. HyPro with a single-stack PEMWE supplied by PV in a day.

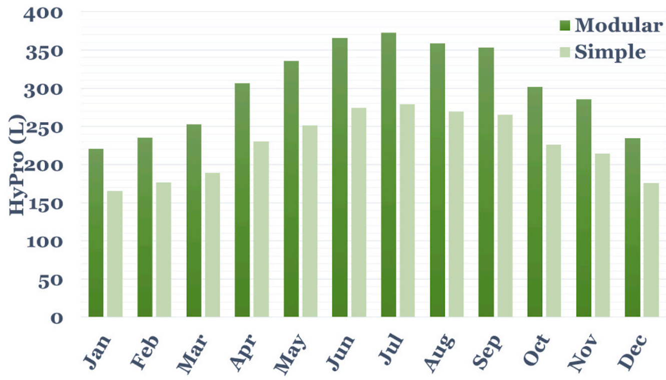


Fig. 15. Comparision of HyPro with a modular and simple system.

thereby maintaining efficiency at its peak potential, as indicated in Table 4. This approach yields two key advantages: firstly, by turning off specific PEMWE stacks, system degradation is mitigated; secondly, HyPro benefits from leveraging the complete range of optimized stacks. This intricate interplay is illustrated in Fig. 11, where the relationship between current density and PEMWE efficiency is depicted. Observing the PEMWE polarization and efficiency curves presented in Fig. 11, it is discernible that PEMWE efficiency can exceed 70% when current remains below 27 A. Notably, in three of the scenarios, at least one PEMWE is inactive, thereby preserving its integrity and decreasing overall system degradation.

With this insight, HyPro estimation in Trois-Rivières is undertaken for a year, comparing the outcomes with a single-stack PEMWE operating at high capacity and direct current from the PV array, against a modular structure employing a control strategy for maintaining constant current to the PEMWE. Fig. 15 vividly showcases the substantial impact of implementing a modular structure with controlled current allocation on HyPro. This approach is projected to yield remarkable improvements in HyPro throughout the year, with a pronounced effect during the elongated days of summer. AI-assisted estimates suggest that PV panel installation, coupled with solar energy conversion to H2, can yield over 2716 L of H2 annually. However, when factoring in the modular structure and energy control strategy, this figure escalates by 33.36% to reach 3622 L annually. Moreover, the modular structure not only curtails system degradation but also enhances capacity by boosting overall system efficiency, leading to an additional production of approximately 906 L compared to conventional methods.

Fig. 16 presents the available solar energy for the proposed PV array on a sunny summer day, elucidating the contrasting impacts of the modular system and the single-stack HyPro configuration. The modular power allocation scheme is adept at optimizing solar energy utilization. Notably, the green electrolyzer icon signifies the PEMWEs that are operating at efficiency levels exceeding 70%, consistently maintained in the modular structure, whereas this uniformity isn't realized in the case of a single PEMWE.

Furthermore, Fig. 16 also visualizes the degradation rates. Intriguingly, the likelihood of degradation for PEMWEs one through four stands at 1, 0.75, 0.5, and 0.25, respectively. This finding is noteworthy due to the inherent ease of replacing electrolyzers within modular systems.

The graphical representation in Fig. 16 effectively underscores the advantages conferred by the modular setup, particularly in terms of efficiency maintenance and degradation management, both of which contribute significantly to enhanced system performance.

The computation of total efficiency, as expressed in Equation (17), incorporates the consideration of both the scaled-up coefficient and the efficiency associated with scaling up the system. Scaling up a PEMWE encompasses several intricate adjustments, including augmenting the active surface area of the electrodes, calibrating catalyst loading, modulating electrolyte and cooling water flow rates, and potentially adapting the membrane thickness to maintain the overall current density of the electrolyzer.

Moreover, in the process of enlarging the PEMWE system, the escalated power requirements must be taken into account, given that they may increase proportionately with the system's dimensions. In essence, optimizing the scale-up of a PEMWE necessitates a meticulous examination of multiple factors, requiring a comprehensive approach to ensure consistent or even enhanced system performance. The successful execution of this scale-up strategy hinges on a thorough understanding of these considerations and their seamless integration into the design and operation of the larger system.

Comparing the voltage degradation of a single PEMWE stack and a modular PEMWE system over a span of 7000 h offers valuable insights into the relative robustness of these configurations. The collected data reveals that the single PEMWE stack exhibited a higher voltage degradation rate, with a reduction of 37.4 V over the 7000-h period, equating to a degradation of 15.58%. In stark contrast, the modular PEMWE system displayed notably lower voltage degradation rates. Specifically, PEMWE 1 experienced a 5.9 V reduction, PEMWE 2 saw a 5.3 V decrease, PEMWE 3 registered a 4.1 V decrease, and PEMWE 4 exhibited a mere 3.8 V reduction. These degradation rates translate to 10%, 8.8%, 6.8%, and 6.3%, respectively. Remarkably, the average degradation across the modular system is approximately 7.6% lower than that of the single-stack setup.

This data underscores the potential of the modular PEMWE system to exhibit greater durability and resistance to voltage degradation in comparison to the traditional single-stack arrangement. Thus, the

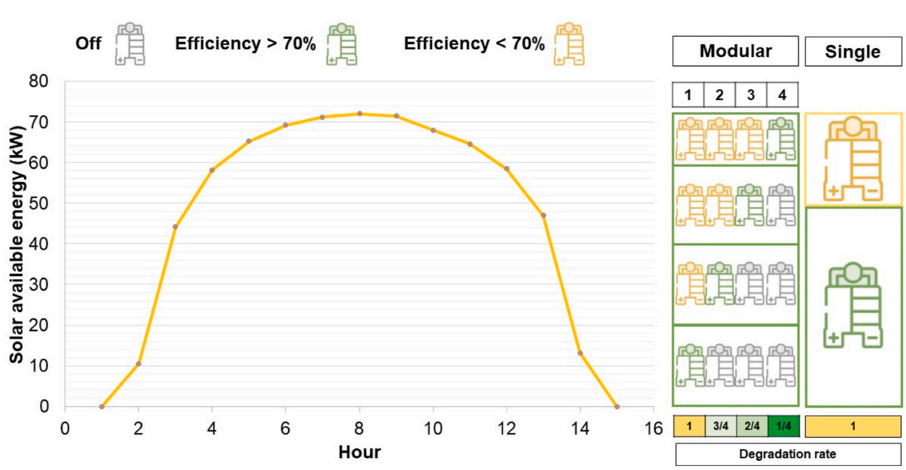


Fig. 16. Comparing the performance of using modular and conventional systems for HyPro from solar energy graph.

adoption of a modular structure coupled with strategic power allocation emerges as a compelling approach to elevate HyPro, extend the lifespan of PEMWEs, and mitigate degradation. It is imperative to note, however, that further exploration is warranted to pinpoint the root causes of degradation and validate the accuracy of the estimated outcomes. Additionally, it is crucial to acknowledge that the rate of degradation is influenced by an array of factors, encompassing operating conditions, design parameters, and the materials employed. Consequently, meticulous consideration and optimization of these variables hold paramount importance in enhancing the overall durability and performance of the PEMWE system.

5. Conclusions

Renewable energies are becoming increasingly appealing in conjunction with PEMWEs due to their capacity to store energy as environmentally friendly, efficient, and potent hydrogen (H2). However, a significant challenge associated with Renewable Energy Sources (RES) is their inherent intermittency, which can substantially impact the performance and efficiency of PEMWE systems. This intermittency not only undermines the efficiency of the PEMWE system but also accelerates its degradation and diminishes its operational lifespan. Consequently, optimizing the power supply to PEMWEs becomes paramount in mitigating degradation and enhancing the overall energy efficiency of the system.

The present study employs a machine learning-based approach to predict HyPro via solar energy in the city of Trois-Rivières. It further compares the outcomes of a conventional PEMWE system with those of a modular design. The predictive model, trained using experimental data collected from PV panels and neural networks, investigates the viability of converting solar energy into H2 through a PEMWE model validated by experimentation. A comparison between the HyPro outputs in normal and modular modes is conducted by regulating input energy. Control over the PEMWE system's input current is attained through a power allocation mechanism.

The results obtained underscore the significant benefits of a modular structure for HyPro, manifesting in an approximate 33% surge in HyPro. Moreover, the proposed modular configuration holds the potential to curtail electrolyzer degradation by around 7.6%, ultimately extending its operational lifespan.

Further research endeavors are imperative to enhance PEMWE efficiency through RES and to delve deeper into optimizing arrangements for green HyPro. Additionally, it is vital to account for PEMWE efficiency across various scales and systems, given its susceptibility to variations under diverse operating conditions.

Declaration of competing interest

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

Data availability

The data that has been used is confidential.

Acknowledgements

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC) (2018–06527)

Nomenclature

A_L	Active large surface area (mm)
A_S	Active small surface area (mm)
B_r	temperature coefficient
CP_{PV}	Coefficient of Performance
G_{nr}	Solar irradiance (W/m^2)
I_C	cell current (A)
I_S	stack current (A)
I_{cn}	each cell current (A)
P_C	cell power (W)
P_{el}	electrolyzer required power
P_{pv}	PV Power (W)
T_{pv}	PV temperature(°C)
T_r	operating reference temperature (°C)
U_{ac}	Activation overvoltage (v)
U_{co}	Concentration overvoltage (v)
U_{oh}	Ohmic overvoltage (v)
V_C	cell voltage (v)
V_O	reversible (open circuit) voltage (v)
V_S	stack voltage (v)
V_{cell}	cell voltage (v)
V_{cn}	each cell voltage (v)
V_{rev}^0	reversible cell voltage (v)
V_{th}^0	thermoneutral voltage (v)
n_{el}	number of electrolyzers
n_p	number of PV panels
t_r	reference time
$\alpha HyPro_S$	HyPro system (in a stack) efficiency
α_{PV}	PV cell efficiency (%)
η_{array}	PV array efficiency
η_c	cell efficiency (%)
η_e	Electrolyzer efficiency (%)

A	Area (square meter, m^2)
E	Energy ($Wh \approx 3600\, joules$)
f	gas flow rate (Normal Meter Cubed per Hour Nm3/hr)
F	Faraday constant (C/mol)
g	gradient
$HHVH$	Higher Heating Value of Hydrogen (kWh/Nm^3)
P	Power (W)
Rct	charge transfer impedance (Ohm)
t	Time (h and H/2)
W	electrical work of electrolysis (J/mol)
W_{irrev}	Irreversible energy (J/mol)
W_{rev}	Reversible energy (J/mol)
Υ	surface coverage ratio (/)
ΔH_R^0	Electrolysis required energy (J/mol)

Abbreviations

AC	Alternating Current
ANN	Artificial Neural Network
CNC	Computer Numerical Control
CO_2	Carbon Dioxide
DC	Direct Current
e	electron
ERC	Ejector Refrigeration Cycle
FC	Fuel Cell
H_2	Hydrogen
HyPro	Hydrogen Production
kW	Kilo Watt
L	Liter
MES	Modular energy system
ML	Machine Learning
MW	MegaWatt
NPV	Net present value
O_2	Oxygen
ORC	Organic Rankine Cycle
PEMFC	Proton Exchange Membrane Fuel Cell
PEMWE	Proton Exchange Membrane Water Electrolyzer
PTC	Parabolic Trough (solar) Collector
PtG	Power-to-Gas
PV	Photovoltaic
RES	Renewable Energy Source
RO	reverse osmosis
WECS	wind Energy Conversion System

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The empirical findings from the comparative study presented above significantly enhance the overarching research framework of this thesis. According to this study, modular PEMWE systems can substantially improve hydrogen production efficiency, over 33% more than single-stack systems, and effectively mitigate degradation through optimized dynamic power allocation strategies by systematically evaluating singular and modular systems.

The outcomes from this comparative analysis align closely with the thesis's primary objectives of integrating robust structural insights with advanced energy management strategies. Notably, the findings provide concrete evidence supporting the scalability and adaptability benefits of modular PEMWE systems in industrial applications, where renewable energy availability fluctuates widely. Furthermore, the introduced design process mapping serves as a practical framework to guide engineering practices, directly bridging the previously identified knowledge gap.

Further discussion of the correlation between modular PEMWE configurations and effective energy management will be presented in subsequent chapters. Specifically, detailed discussions will follow regarding the role of structural optimization in minimizing degradation, enhancing operational stability, and maximizing system efficiency. By integrating these insights, we can eventually advance modular PEMWE technology and its practical application in large-scale renewable hybrid power systems.

2.4 Energy management of Modular electolyzer

Energy consumption in a PEMWE system is a critical factor in determining the efficiency and economy of hydrogen production, which confirms the necessity of appropriate energy management. As shown in the figure, the modular PEMWE system consists of several subsystems that have specific energy requirements that contribute to the overall energy consumption of the system. Each of these subsystems has its energy demands, which are shown in the figure.

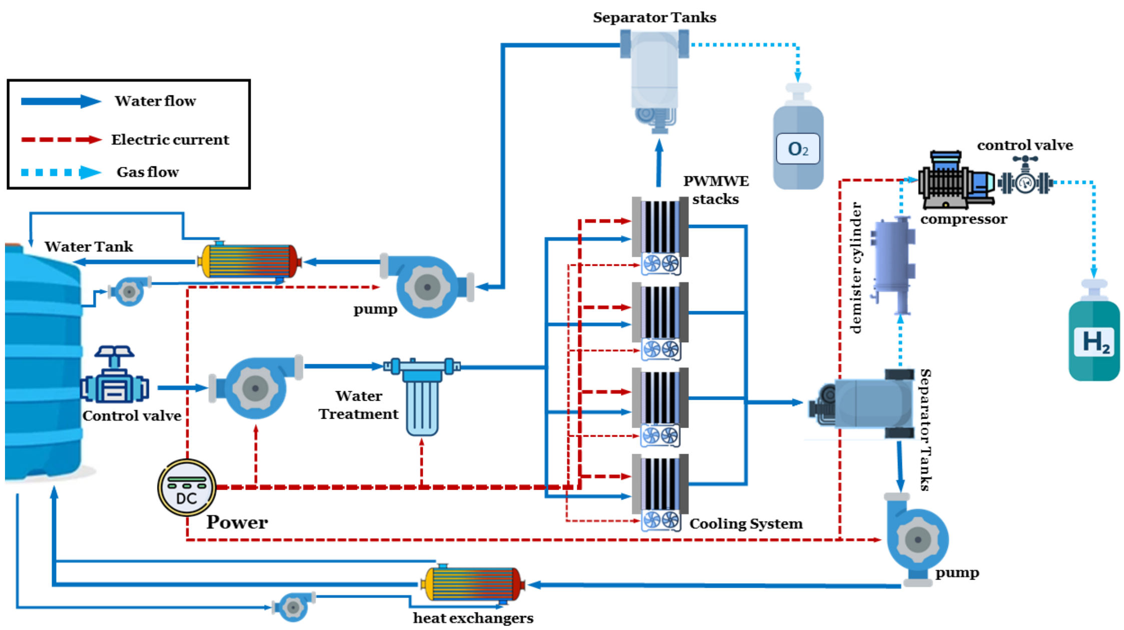

Figure 2-2 Modular PEMWE system and subsystems

The modular PEMWE system comprises several key subsystems. The water supply system includes components such as the water tank, control valve, water pump, and water treatment unit, with energy consumption primarily associated with pump operation and water treatment processes. The power supply, which provides the necessary DC electrical energy for the electrochemical reactions in the PEMWE stacks, is the most significant energy consumer within the system. The PEMWE Stacks, where water is electrolyzed into hydrogen and oxygen, consume energy based on electrochemical reactions, influenced by the applied current and stack efficiency. The cooling system, consisting of heat exchangers and pumps, uses energy to maintain optimal operating temperatures by dissipating excess heat from the PEMWE stacks. Lastly, the Gas Separation and Purification subsystem, which involves separator tanks, demister cylinders, and compressors, consumes energy during the separation, compression, and cooling of gases to achieve the required purity standards.

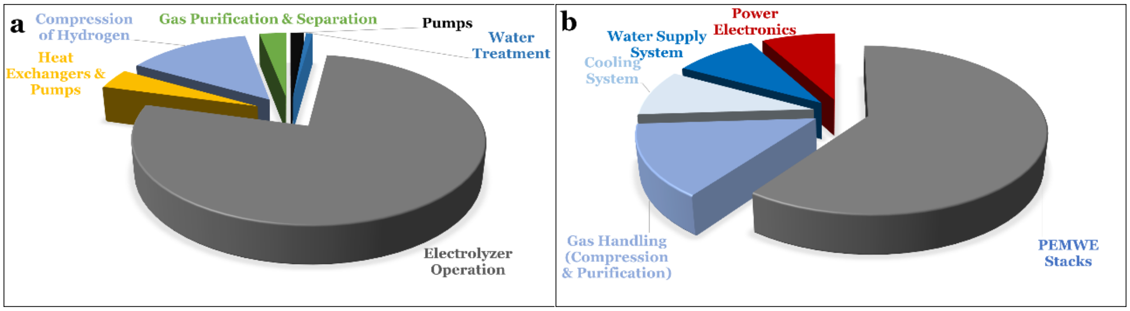

Figure 2-3 a) Energy consumption and b) Costs breakdown in Modular PEMWE Systems

A clear understanding of energy consumption is crucial for developing effective EMS that targets high-demand areas, especially within the PEMWE stack. Most studies on the energy management of electrolyzers systems focus on optimizing the energy use of PEMWE stacks as they are the most significant energy consumers, accounting for approximately 70-85% of the total energy consumption. As shown in the pie chart in Figure *2-3*-a, the energy consumption distribution across different subsystems according to the findings in the literature. The PEMWE stacks dominate energy usage, while the other subsystems, such as gas handling (compression and purification), water supply, and cooling systems, contribute smaller, but still notable portions of the total energy consumption. Specifically, the gas handling subsystem, including compression, can account for 10-15% of the energy use, while the cooling system and water management subsystems together typically represent around 4-10% of the total energy consumption. These are close approximations based on extensive studies and simulations from various sources in the field.

1. Simple energy management for renewable systems

Sharifzadeh et al. [180] and Chandrasekar et al. [181] examine the integration of wind energy and hydrogen production, but they approach the issue differently. Sharifzadeh et al. [180] explore alkaline and PEMWE, using a mixed-integer linear programming (MILP) approach to optimize operational strategies, focusing on cost-effectiveness and minimizing the levelized cost of hydrogen. This method significantly enhances economic feasibility by promoting sustainable and flexible operations. On the other hand, Chandrasekar et al. [181] investigate using wind energy curtailment to power both PEMWE and solid oxide electrolytic cell (SOEC) electrolyzers. Their study highlights the efficiency differences between low-temperature (LTE) and high-temperature electrolyzers (HTE), with an emphasis on the slower thermal response time of HTE, which impacts their operational efficiency in fluctuating power environments like those provided by wind. Salman [182] addresses the integration of wind energy into power grids, focusing on frequency stabilization amidst wind speed fluctuations. The author developed a control method that uses a Matlab/Simulink model to simulate a combined wind power and power-to-hydrogen system, showing successful management of power output and frequency maintenance within desired parameters, which enhances grid reliability.

Several systems have been presented for utilizing solar energy in the production of hydrogen and electricity. Alirahmi et al. [183] introduce a novel solar-driven system using parabolic trough collectors (PTCs) integrated with steam and organic Rankine cycles (SRC and ORC), and a thermoelectric generator (TEG) to enhance efficiency. The implementation of a multi-objective genetic algorithm optimizes system parameters, resulting in improved energy efficiency and hydrogen production rates. Conversely, Zhang et al. [184] studies a renewable energy system comprising photovoltaic, electrolyzer, and fuel cell modules. Their results demonstrate how system efficiency oscillates with changes in environmental conditions, emphasizing the need to manage efficiency and output based on solar radiation intensity. Abolfazl Shiroudi et al.'s evaluation [185] of a direct-connected PV electrolyzer system for hydrogen generation in Iran highlights the system's potential for solar energy conversion while also analysing its efficiency. The study highlights how important it is to have high-efficiency systems for Iran to be able to afford the substantial upfront costs associated with solar technology.

Ziogou et al. [62] presents the development and implementation of a flexible EMS for a small-scale solar-powered hydrogen production unit. The EMS is based on a finite-state machine combined with propositional-based logic to optimize the operation of the hydrogen production system. Central to the EMS is the use of a smart microgrid and supervisory controls, alongside a finite-state machine (FSM) that utilizes propositional-based logic to manage transitions between various operational states. The system's performance was evaluated through both short-term and long-term operations, showing smooth and efficient hydrogen production. The optimization results include achieving a mean electrolyzer efficiency of 73% during a sunny day, with hydrogen production reaching 14.3 Nm^3. The EMS successfully maximized hydrogen production while maintaining system reliability, demonstrating its effectiveness in managing the varying input power from the solar array and the interaction among subsystems.

2. ***Grid and Hybrid Systems:***

The efficiency and sophistication of such systems are increasing, as seen by recent advancements in EMS for microgrids. A two-layer EMS with a power-to-gas configuration is presented by Kumar and Bae [186]. Power converters and supervisory fuzzy logic control work together to distribute and stabilise electricity. It has been demonstrated that this technology improves microgrid power management while preserving fuel cell and electrolyzer efficiency. Kumar et al. [61] have directed their attention towards PEM technologies. They have integrated many control systems, such as Model Predictive Control (MPC) and Equivalent Consumption Minimization Strategy (ECMS), to guarantee robustness and high operating efficiency in the face of fluctuating loads. Numerical results indicate varying efficiencies for different control methods, with system efficiencies reaching up to 80.5% under optimal control settings, and operational costs being minimized significantly in most cases.

An optimisation plan for a DC microgrid with a PEMWE combined with RESs is presented by Jin et al. [187]. Their study emphasizes the importance of a coordinated control method that optimizes hydrogen production efficiency as well as energy storage systems to maintain system stability and extend device life. An EMS that optimises solar panel power using MPPT algorithms is described by Djoudi et al. [188]. This reduces voltage dips in electrolyzers and improves system resilience overall. Simulation results underscore the strategy's effectiveness, showing a consistent reduction in the electrolyzer voltage drop by 0.19 mV over 168 hours under fluctuating power conditions. Moreover, the integration of photovoltaic and electrolyzer systems through a DC bus facilitates enhanced control over power flow, contributing to an overall improvement in system efficiency and resilience in facing load variability. Using a model predictive power controller to optimise energy distribution based on market dynamics, Hossain et al. [189] built an EMS for an offshore hybrid energy system with an emphasis on hydrogen co-production. This increased both economic returns and the utilisation of RESs. To stabilise decentralised power networks, Tesfamariam et al. [190] investigate the integration of electrolyzers with RESs, presenting control algorithms that enhance network-wide frequency and voltage stability.

Assareh et al. [191] suggest an enhanced hybrid PV/thermal system that balances power output and cost-effectiveness by utilising cutting-edge optimisation techniques. Their method demonstrates a major leap in sustainable energy management by efficiently meeting home energy demands while minimising environmental impacts. It is demonstrated that the proposed energy model provides an energy efficiency of 19.1% and a cost rate of 1.299 USD/h, demonstrating its effectiveness in meeting the power, cooling, and heating demands of residential buildings while optimizing energy management and reducing greenhouse gas emissions at the same time. Manuel Agredano-Torres et al. [192] propose a dynamic power allocation control methodology for hybrid electrolyzer systems that combines the rapid response capabilities of PEMWEs with the cost-efficiency of AWEs. This approach enhances grid stability by dynamically adjusting power outputs between the different types of electrolyzers based on real-time demand and system conditions. The methodology not only leverages the distinct advantages of each electrolyzer type but also provides a comprehensive solution for managing energy in systems heavily integrated with renewable sources.

Researchers provide comprehensive insights into the integration of electrolyzers into virtual power plants (VPPs) and their operational dynamics within renewable energy systems. Each study focuses on different aspects of system integration and optimization, contributing to enhanced grid flexibility and efficiency. Antonella Maria De Corato et al. [193] examine the integration of PEMWEs and AWEs into VPPs, demonstrating that PEMWEs can operate effectively at low power levels (0-10% of nominal power). This capability is crucial for managing the variability of RESs, allowing VPPs to stabilize voltage profiles across the network effectively. The research underscores the importance of strategic placement and dynamic response of electrolyzers within the grid to optimize the feasible operating envelope of VPPs.

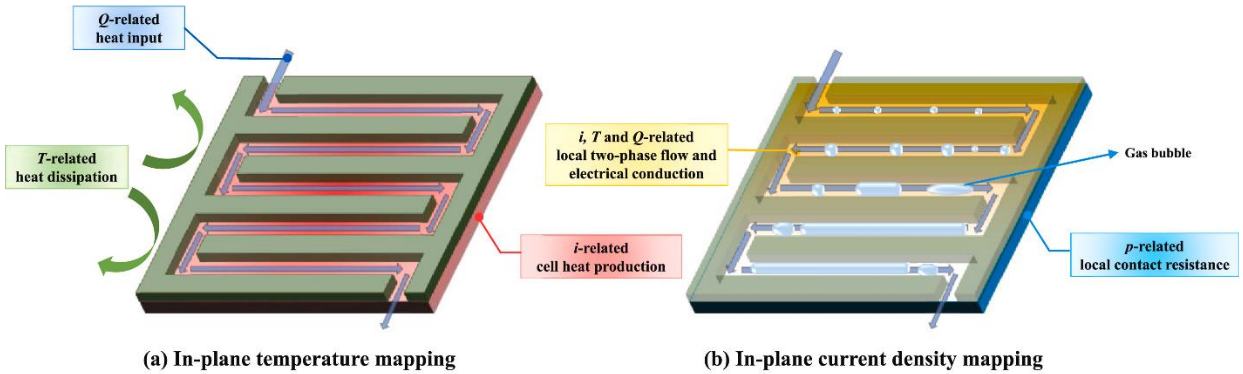

Figure 2-4 Factors influencing the in-plane distribution (a) Temperature and (b) current density [194]

3. *Optimization and Control Strategies and Specific Research:*

Following the original research of Abomazid et al. [84], additional investigation into the optimisation of PEMWEs can dig into sophisticated control mechanisms, according to the ongoing literature study on optimisation and control strategies and specific research. For example, using machine learning algorithms with real-time data could improve prediction accuracy and dynamically change operational settings to maximise durability and performance. Furthermore, studies might examine how well these models scale, evaluating their suitability for use with various PEM system designs and sizes. Research of this kind would improve the theoretical foundations supporting parameter identification and system optimisation in intricate, variable contexts, in addition to expanding the actual uses of PEM technology in industrial settings. Majumdar et al. [195] emphasize the importance of robust control systems to cope with the variability of RESs. Throughout the study, various model approaches, including electrochemical, thermal, and mass transport, are reviewed to highlight the crucial role dynamic control strategies play in optimizing operational efficiency. It explores several control techniques ranging from traditional to advanced nonlinear methods, aimed at dynamically adjusting operating conditions to improve the efficiency, reliability, and durability of PEMWEs.

A unique Equivalent Electrical Circuit (EEC) model for PEMWE is proposed by Koundi et al. [196] to improve forecasting accuracy in smart grid integrations. The main invention is a PEMWE emulator that mimics the dynamic responses and nonlinear polarisation curve of electrolyzers by using a DC/DC boost converter. With this workable and affordable option, PEMWE incorporation into smart grids may be evaluated without incurring the high expenses of direct hardware implementations. This emulator's ability to accurately simulate the behaviour of electrolyzer points to its potential for enhancing operational and management methods in smart grid systems.

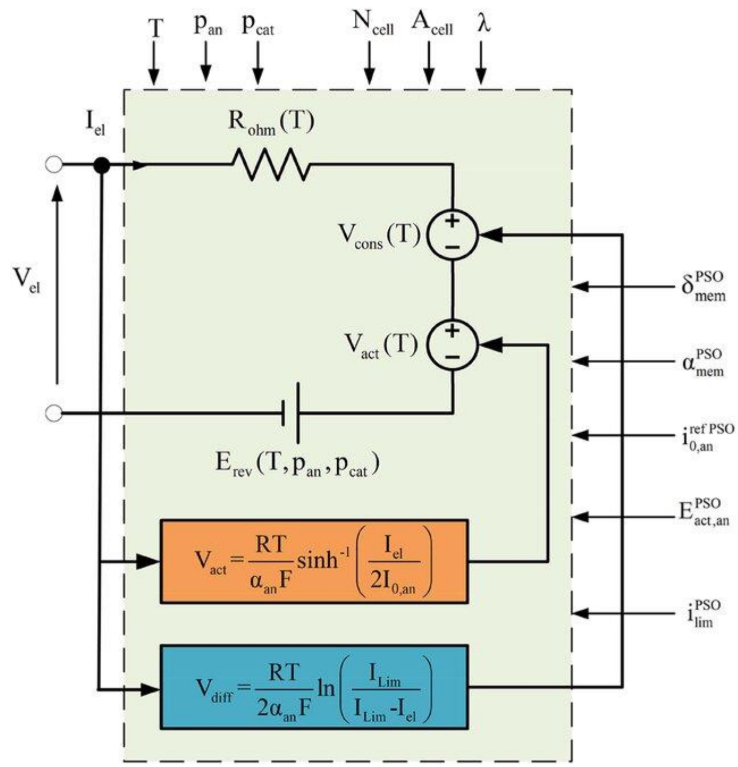

Figure 2-5 PEM electrolyzer equivalent electrical circuit [196]

Nguyen et al. [197] investigated integrating large-scale PV systems with PEMWEs. They focused on challenges caused by partial shading, system faults, and component degradation. The research used Particle Swarm Optimization (PSO) to optimize the sizing and operation of the electrolyzer. Their findings demonstrate that directly coupling PV systems to PEMWEs can significantly improve system efficiency, from as low as 0.17% to 4.47% under various conditions.

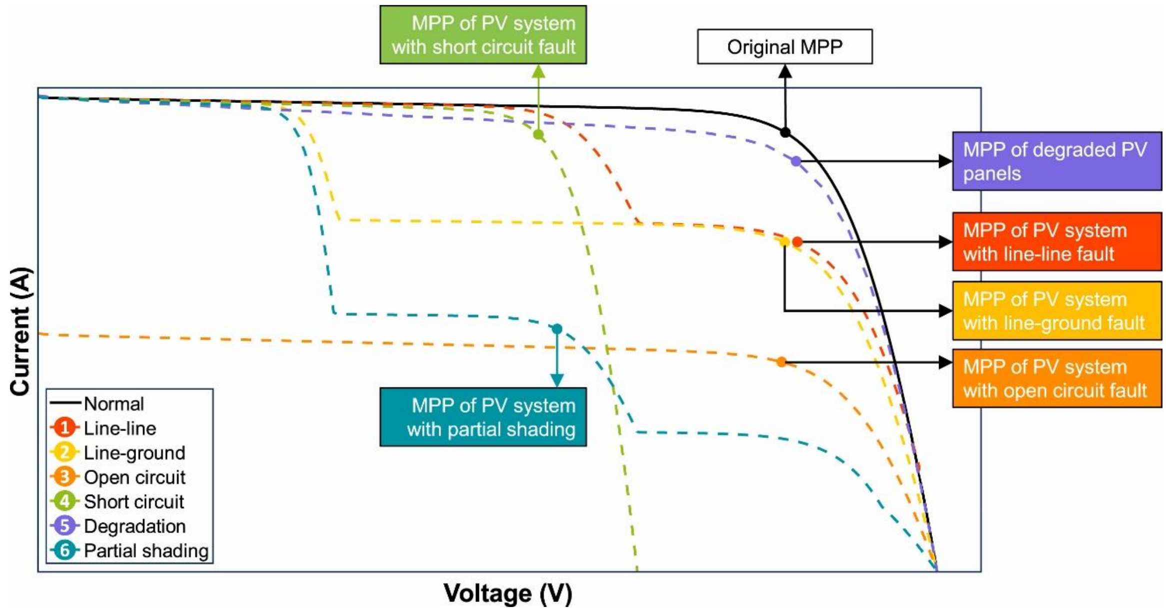

Figure 2-6 A representation of the I-V curve under typical fault conditions, partial shading, and PV panel degradation [197]

Liu et al. [198] introduce a variable-period sequence control strategy that employs multi-layer DC-DC converters to dynamically manage power distribution, significantly reducing the standard deviation of operation durations by up to 51.3%, enhancing system stability and efficiency under variable solar intensities. Stansberry and Brouwer [199] and Agredano-Torres et al. [200] examine dynamic operation and frequency regulation in systems that integrate PEMWEs. Stansberry and Brouwer [199] discuss the rapid adaptation of PEMWEs to fluctuations in renewable energy outputs, which improves operational efficiency and reduces losses. In contrast, Agredano-Torres et al. [200] detail a decentralized dynamic power-sharing control that utilizes both PEMWEs and AWEs to optimize grid frequency response, demonstrating enhanced capacity for managing frequency deviations and increasing system reliability and scalability. It has been demonstrated that dynamic operating conditions have a significant effect on the durability and economic performance of PEMWEs by Li et al. [201] and Flamm et al. [202]. Li et al. [201] investigate the effects of low and high-load cycling on PEMWE's operational stability, noting that high-load cycling can paradoxically improve performance by reducing ohmic resistance, despite potential long-term stability risks. Flamm et al. [202] optimize hydrogen production at a refuelling station through model-based optimal control, adjusting operations based on varying electricity prices and solar inputs to minimize costs, showcasing the practical benefits of integrating predictive control in renewable energy systems.

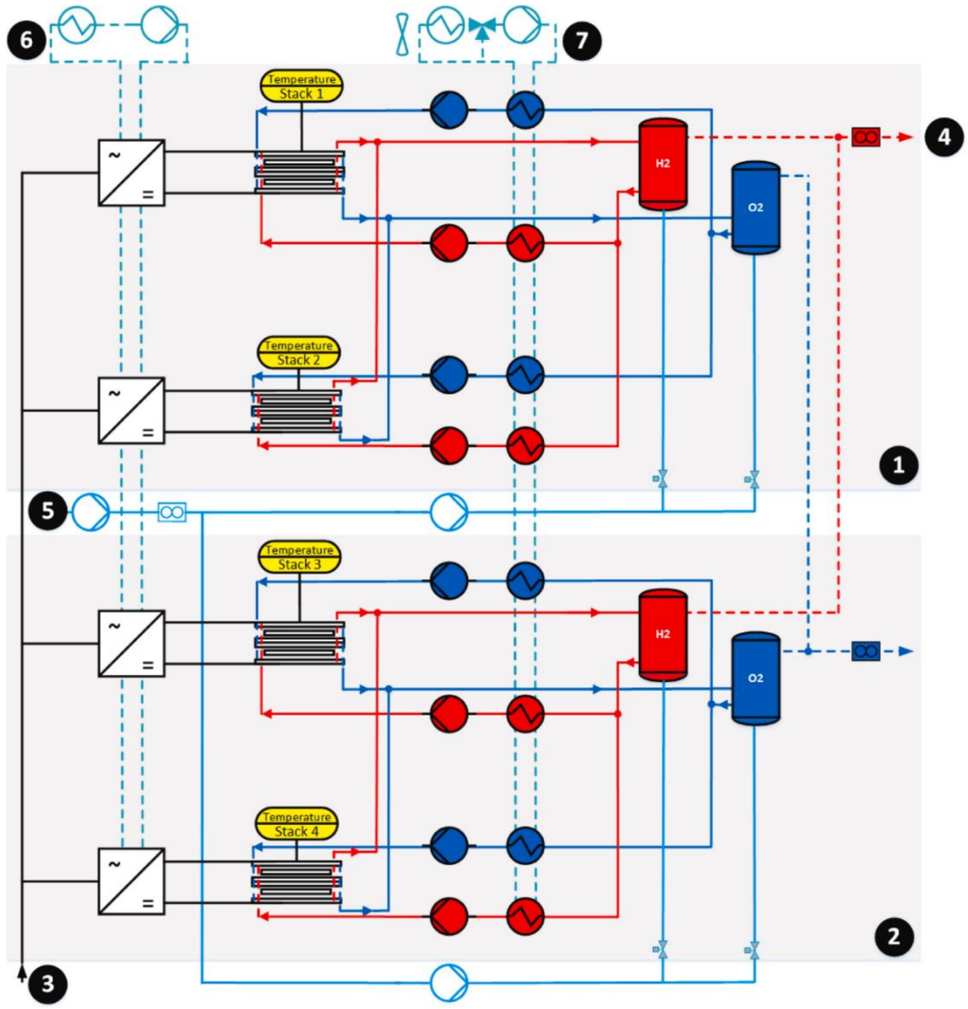

Figure 2-7 The simplified piping and instrumentation diagram for the Siemens SILYZER 100 electrolyzer includes several key components: a subsystem consisting of stacks 1 and 2, a second subsystem with stacks 3 and 4, an electrical grid connection for system power [202]

Maaruf and Khalid [203] present a comprehensive energy management strategy for an all-electric ship propulsion system that combines solar power, PEM fuel cells, and water electrolyzers. This approach effectively manages the balance between the production of energy from solar panels and the power demand, ensuring optimal performance under varying operating conditions, which has a significant impact on the development of sustainable maritime technologies.

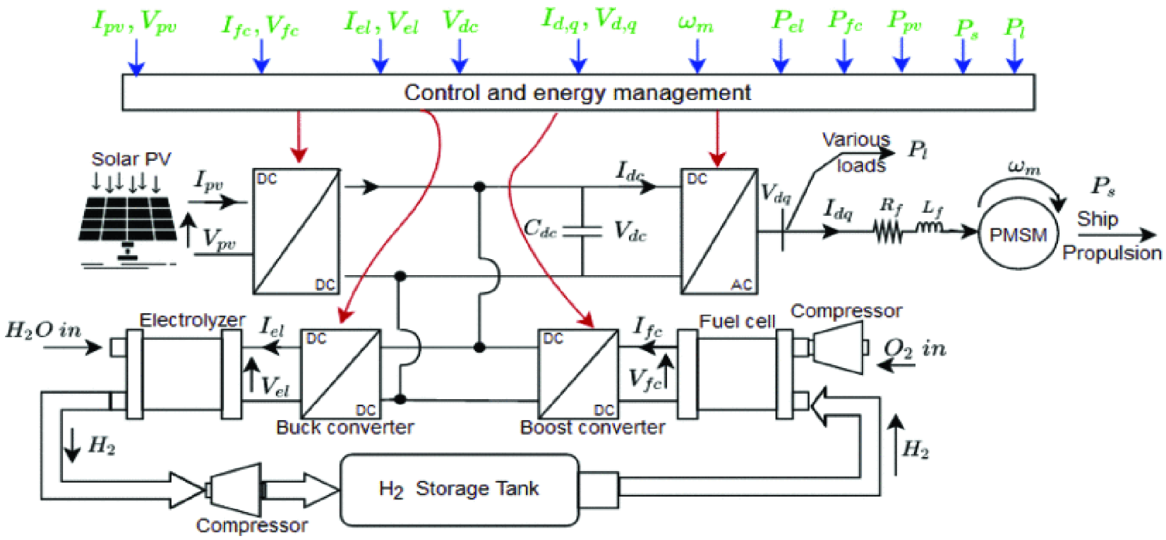

Figure 2-8 Microgrid structure of the all-electric ship and its energy management [203]

High-temperature PEMWE cells (HT-PEMWEs) have made considerable strides recently that increase their viability for integration with variable RESs. To investigate these developments, Zhao et al. [204] explore these advancements by presenting a hierarchical modelling approach that intricately combines detailed multiphysics simulations with system-level analyses. This comprehensive strategy allows for enhanced control over the dynamic behaviour of HT-PEMWEs, particularly under variable power inputs, enhancing both the efficiency and stability of these systems. The integration of such advanced electrolyzer technologies into smart grids and industrial-scale operations further highlights their potential to contribute effectively to sustainable energy applications.

Temperature optimisation is investigated by Fabian Scheepers et al. [143]to increase PEMWE ef ficiency.The study shows that temperature control, together with pressure modifications, may gr eatly improve system efficiency and safety by efficiently balancing electrochemical and mechani cal factors. This is accomplished by creating an ideal stack temperature model.

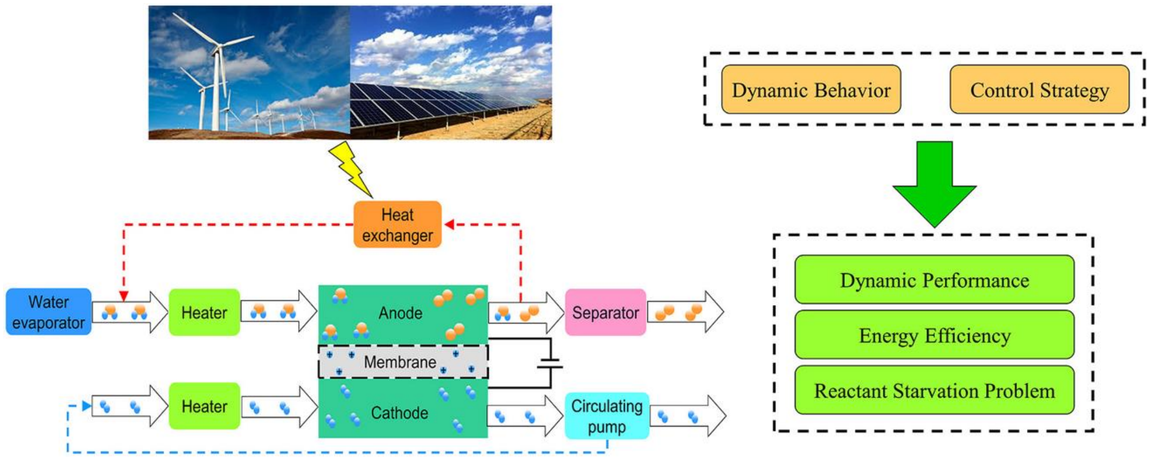

Figure 2-9 A strategy for controlling high temperature PEMWE system [204]

Continuing technological advancements are centred around developing and optimizing converters for PEMWE applications by Damien Guilbert et al. [205] and Rebah Maamouri et al. [206] focus on the design and optimization of converters for PEM applications. Guilbert developed a stacked interleaved DC-DC buck converter to minimize output current ripple and improve energy efficiency, which is crucial for the reliable performance of electrolyzers in renewable energy systems. Similarly, Maamouri et al. [206] employ advanced DC-DC converters and PID controllers to enhance the dynamic performance and hydrogen production efficiency of PEMWEs, validated through comprehensive modelling and experimental results.

4. ***Energy Management of Modular PEM Electrolyzer:***

Wang et al. [207] introduce a control strategy named "step-by-step start" for integrating PEM water electrolyzers with batch reverse osmosis desalination using wind energy. This approach effectively manages power fluctuations, improving hydrogen production by up to 17.75% and optimizing energy utilization, which underscores the feasibility of coupling RESs with water desalination and hydrogen production. Hamid Shakibi et al. [208] detail a novel hybrid system utilizing geothermal sources in Australia to simultaneously produce power, cooling, freshwater, and hydrogen. Optimized using artificial neural networks and Grey Wolf Optimization, this system achieves remarkable exergy efficiency and a rapid payback period, demonstrating the efficacy of machine learning in optimizing complex energy systems. The development of a system that can produce 1263 kW of net power with a 39.89% energy efficiency and a quick 2.13-year payback period is one of the study's major discoveries. By combining energy, exergy, and economic perspectives, multi-objective optimisation scenarios are employed to optimise this system and provide an ideal design.

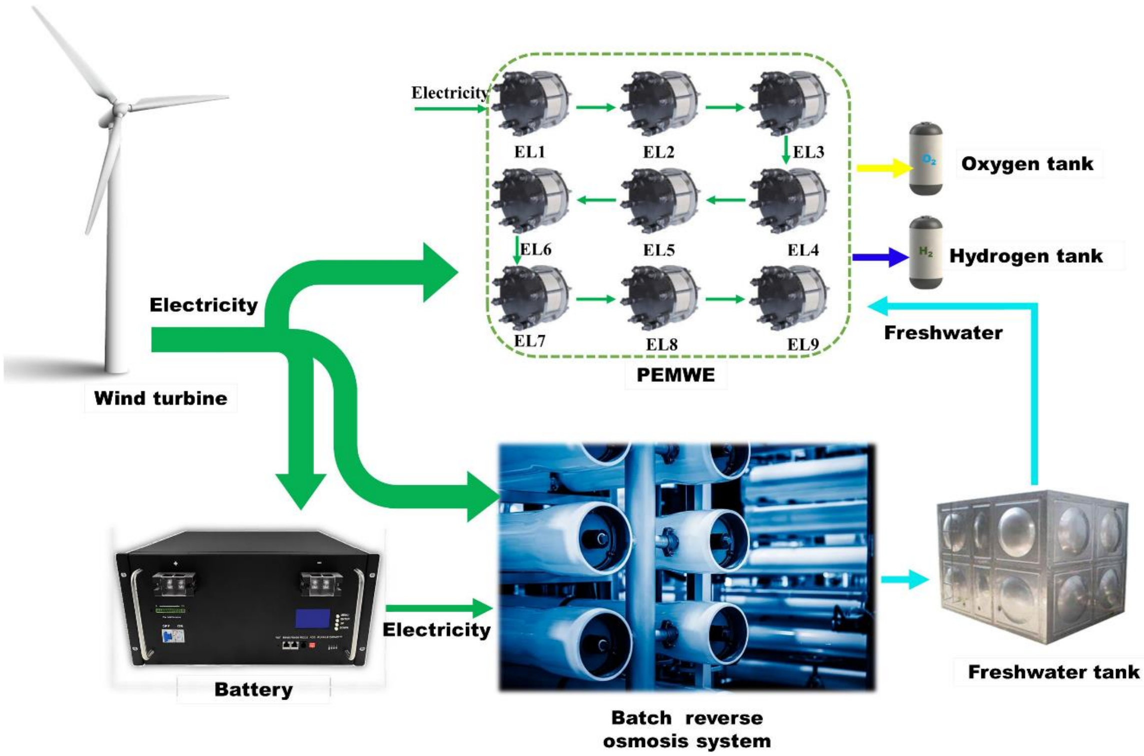

Figure 2-10 An integrated wind-hydrogen-desalination system for off-grid applications [207]

Landin et al. [209] address the integration challenges of PEMWEs with renewable energy, proposing a comprehensive system model that includes a balance of plant components. By increasing energy conversion efficiency and adapting to the variable conditions related to renewable sources, this model seeks to greatly increase the affordability and sustainability of hydrogen as a source of sustainable energy.

Rizwan, Kumar et al., and Nguyen and his colleagues focus on optimizing these integrations through innovative design and control strategies. Rizwan [210] explores design considerations for industrial water electrolyzer plants, particularly the trade-offs between shared and separate balance of plant (BoP) and power systems. The study reveals that shared systems can substantially reduce capital expenditures, although they may compromise operational expenditure efficiency under variable loads. This innovation entails the implementation of variable lye flow rates, which has been shown to result in an increase in hydrogen production of 8-13%. Kumar et al. [211] examine a grid-connected system that combines photovoltaic cells, fuel cells, and an electrolyzer, employing a modified Least Mean Square (LMS) algorithm to enhance power flow management. With this strategy, carbon-neutral energy generation for a 38-kW commercial load is achieved in addition to improved power quality at the point of common connection. Through in-depth simulation and experimental analysis, the study validates the system's capacity to maintain stability and efficiency even under variable solar irradiation and load circumstances.

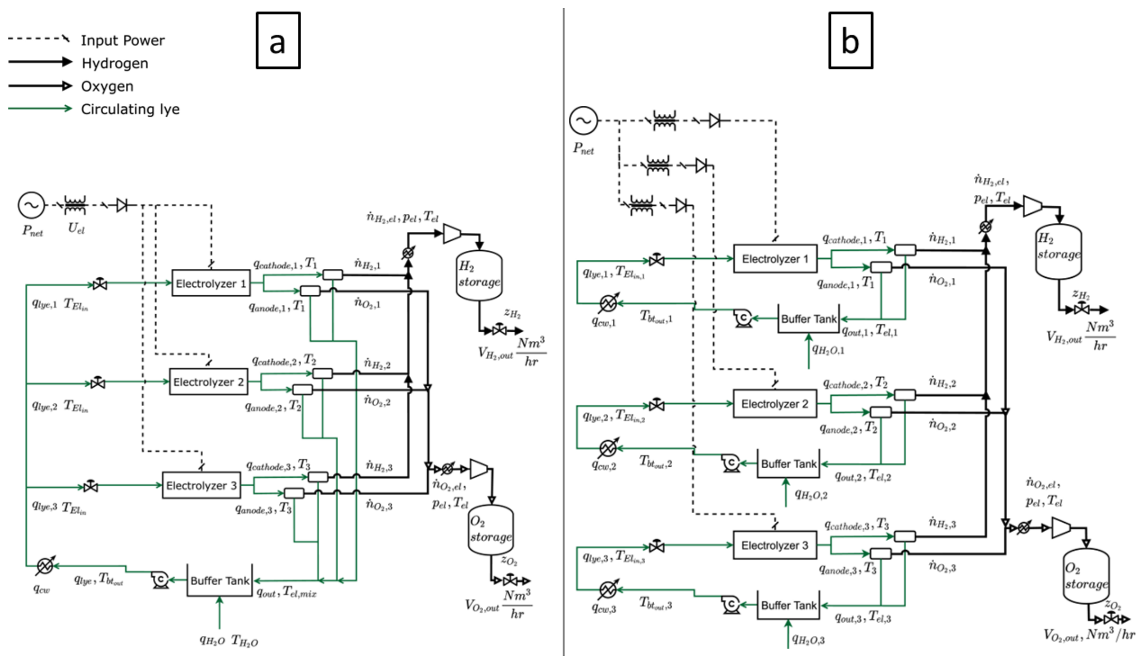

Figure 2-11 Different flowsheet designs, the impact of (a)shared versus (b)separate BoP [210]

The operational difficulties of PEMWEs are examined by Wang et al. [194], who focus on the uneven distribution of temperature and current density within the cells. They develop innovative measurement techniques using temperature measurement endplates and segmented printed circuit boards (PCBs) to monitor these variations accurately. Their findings highlight the significant impact of operational parameters on the thermal and electrical uniformity within the cells, affecting overall efficiency and longevity.

Certain research endeavours concentrate on enhancing hydrogen generation using sophisticated energy management tactics and technical advancements. Cooper and colleagues [212] introduce a Hydrogen Electrolyzer Plant Design Framework (HEPDF) that employs bi-level optimization to address both module and system levels within modular PEMWEs. This framework is applied across various power supply scenarios to determine the most effective operational strategies, ultimately achieving a cost-effective hydrogen production rate of 4.73 to 4.82 V/kg. The adaptability of this framework demonstrates significant advancements in minimizing the levelized cost of hydrogen according to different energy supply conditions.

Hammou Tebibel [30] explores the integration of wind energy for decentralized hydrogen production using water electrolysis, employing a dynamic power and hydrogen management strategy (PHMS). This system includes wind turbines, a water electrolyzer, battery storage, power converters, and a hydrogen storage tank, optimized to enhance system reliability and efficiency. The results indicate that strategic optimization can reduce the cost of hydrogen production to $33.70 per kg while maintaining 100% production reliability, emphasizing the system's capability to effectively manage energy fluctuations in low wind conditions.

Guilbert and Vitale [43] focus on optimizing hydrogen production from wind energy using a novel power management strategy for modular PEMWE system. They implement a multi-stack configuration of PEMWEs paired with a wind turbine, controlled via a stacked interleaved DC-DC buck converter (SIBC). This configuration helps minimize current ripple and enhance system reliability by dynamically responding to the wind turbine's output, preventing potential overvoltage issues. Experimental validation confirms the system's stable operation under both steady-state and transient conditions, proving its effectiveness in optimizing hydrogen production with minimized energy loss.

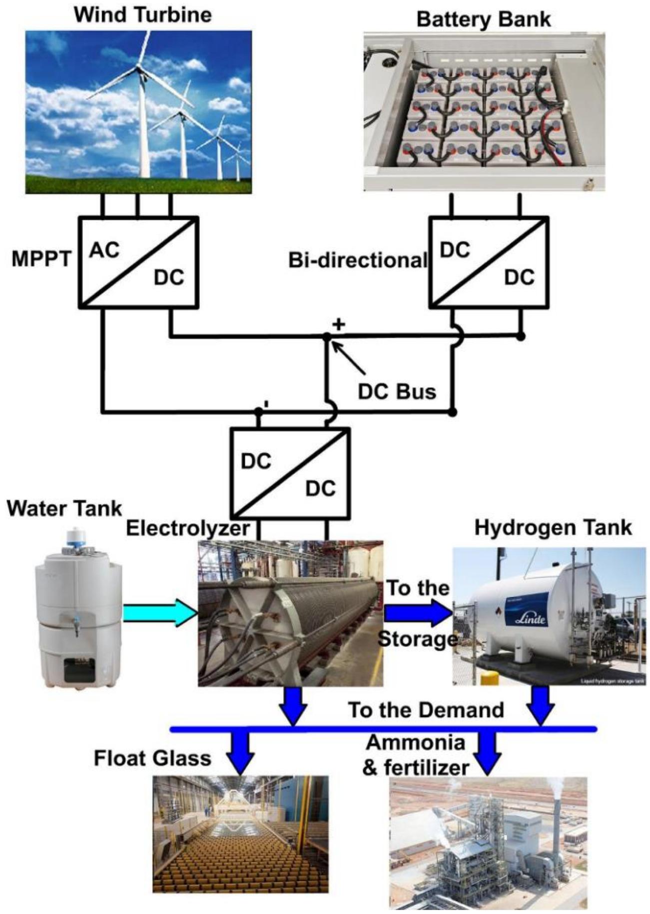

Figure 2-12 Schematic diagram of the studied WHPS by Hammou Tebibel [30]

Xiaoou Liu [213] introduces a layered power scheduling optimization methodology that effectively balances the electrolyzer's performance with a battery energy storage system. By leveraging MATLAB+Gurobi for upper-layer optimization and integrating advanced algorithms like NSGA-II and the Firefly algorithm for lower-layer adjustments, this strategy minimizes degradation and operational costs, even under fluctuating power conditions. The comprehensive model developed captures the degradation costs associated with variable power inputs, providing a sophisticated framework that enhances hydrogen production efficiency and system sustainability.

Lu et al. [46] present an optimized power allocation strategy for wind-hydrogen systems utilizing multi-stack PEMWE. Their work uses advanced thermal management techniques and a robust multi-physics model to analyse the relationship between electrolyzer efficiency and operational degradation. Their control and execution modules, employing an extended duty cycle interleaved buck converter and fuzzy PID control, ensure high-quality power delivery and lower current ripple. They demonstrate significant improvements in energy efficiency—up to 61.65% over a year, with reduced voltage degradation.

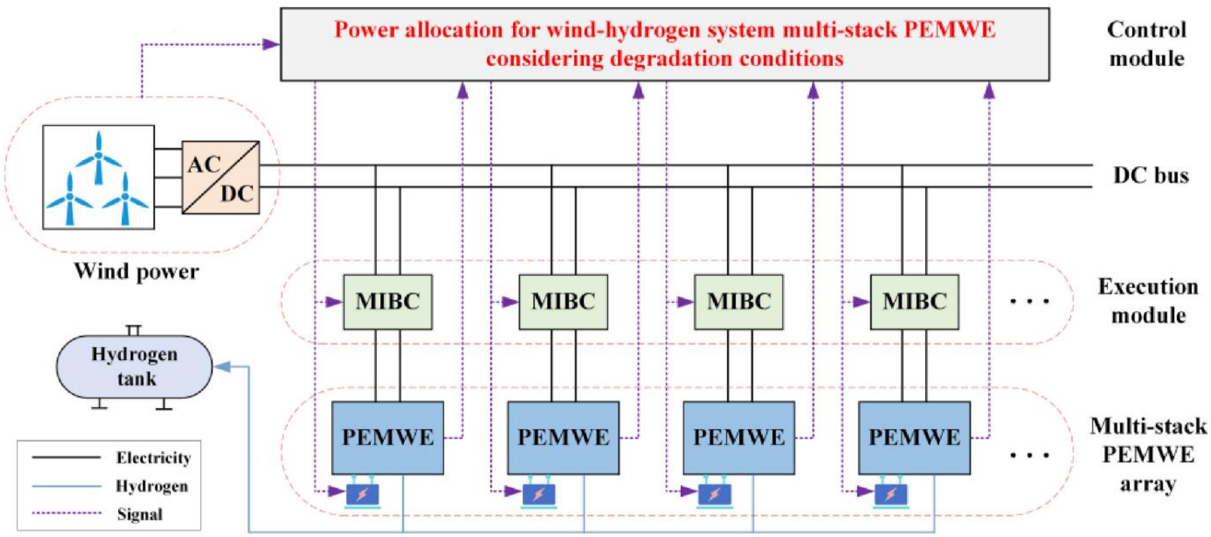

Figure 2-13 Basic architecture of the Lu et al. [46] wind-hydrogen system

Zheng et al. [214] delve into the energy management of modular electrolyzers in off-grid wind-powered systems. They introduce a rolling optimization-based operational strategy that surpasses traditional methods by significantly enhancing system efficiency and hydrogen production. Their approach reduces the levelized cost of hydrogen to 3.89 €/kg while producing 311,297 kilograms of hydrogen annually, illustrating a notable increase in both efficiency and cost-effectiveness due to the innovative management of load variations and thermal dynamics.

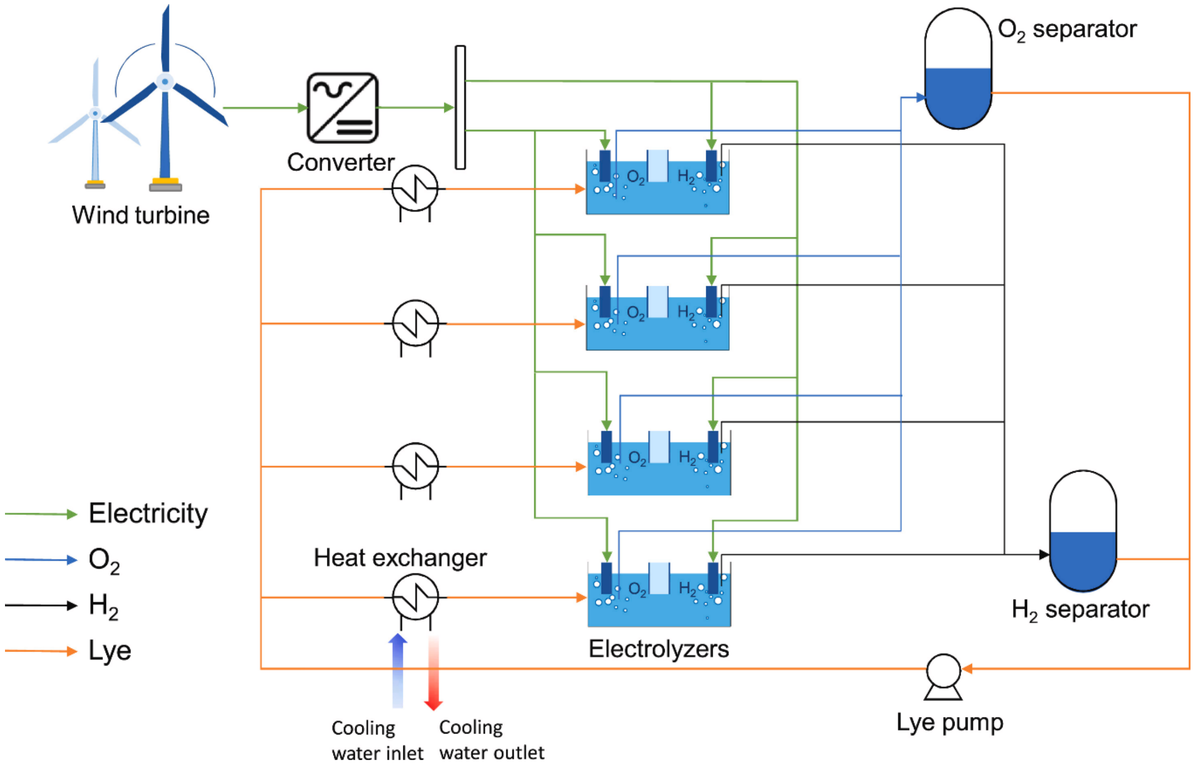

Figure 2-14 Wind/hydrogen off-grid system with four stacks of electrolyzers by Zheng et al [214]

He et al. [215] introduce a control strategy that effectively eliminates voltage overshoot by 100% during high-power operations, thereby stabilizing the hydrogen production process. This strategy significantly reduces the polarization voltage by 7.6% to 13.5%, ensuring stable and efficient hydrogen production across various operational phases. The adjustment to real-time electricity market signals and power fluctuations not only maintains consistent hydrogen production rates but also extends the longevity and performance of the electrolyzers. Zheng et al. [216] explore a dynamic optimization approach tailored to the intermittent nature of RESs. They implement a predictive control strategy that adjusts the hydrogen production rate based on real-time power input variations. This method reduces energy waste by 15% compared to static management approaches and enhances the electrolyzer's operational efficiency by 20%. By leveraging machine learning algorithms to predict energy availability and demand scenarios, Zheng et al. provide a robust framework for optimizing energy utilization and minimizing waste in hydrogen production.

Winter et al. [217] develop a sophisticated control strategy to dynamically allocate power in electrolyzers, particularly those powered by volatile RESs. This approach adapts electrolyzer operations to fluctuations in energy availability, which not only increases green hydrogen production efficiency but also significantly reduces voltage drop and operational costs. The simulation results demonstrate a notable improvement in operational efficiency, enabling better integration of electrolyzers into energy systems and optimizing their response to market signals and power availability. Table 2-1 encapsulates a diverse array of energy management strategies implemented across multiple research efforts aimed at optimizing the performance and cost-efficiency of PEMWE. Notably, the strategies range from the application of advanced control algorithms to dynamic power management systems, highlighting significant improvements in hydrogen production efficiency and reductions in operational costs.

Table 2-1 Overview of reference management strategies and key outcomes in modular PEM electrolyzer energy management

Reference	**Management Strategy**	**Key Outcomes**
Wang et al. [207]	Step-by-step start	Improves hydrogen production by up to 17.75%, optimizes energy utilization
Hamid Shakibi et al. [208]	Hybrid system with artificial neural networks and Grey Wolf Optimization	Increases exergy efficiency, achieves 2.13-year payback period
Landin et al. [209]	Comprehensive system model including balance of plant components	Increases energy conversion efficiency
Rizwan [210]	Variable lye flow rates	Increases hydrogen production by 8-13%
Kumar et al. [211]	Modified Least Mean Square (LMS) algorithm	Enhances power flow management, maintains stability and efficiency
Cooper et al. [212]	Bi-level optimization	Minimizes the levelized cost of hydrogen
Hammou Tebibel [30]	Dynamic power and hydrogen management strategy (PHMS)	Reduces hydrogen cost to $33.70/kg, maintains 100% production reliability
Guilbert and Vitale [43]	Multi-stack configuration controlled via a stacked interleaved DC-DC buck converter	Optimizes hydrogen production with minimized energy loss

Xiaoou Liu [213]	Layered power scheduling optimization	Minimizes degradation and operational costs
Lu et al. [98]	Advanced thermal management and multi-physics model	Enhances energy efficiency up to 61.65%, reduces voltage degradation
Zheng et al. [99]	Rolling optimization-based operational strategy	Reduces the levelized cost of hydrogen to 3.89 €/kg, increases efficiency
He et al. [215]	Control strategy to eliminate voltage overshoot	Reduces polarization voltage by 7.6% to 13.5%
Zheng et al. [216]	Dynamic optimization with predictive control strategy	Reduces energy waste by 15%, enhances operational efficiency by 20%
Winter et al. [217]	Dynamic power allocation strategy	Increases green hydrogen production efficiency, reduces operational costs

3 Benchmarking and selection of models for energy management

3.1 Electrochemical model

The electrochemical model forms the foundation for understanding the operational efficiency and potential of PEMWE. The importance of energy management in HyPro was discussed in earlier sections, with special attention paid to the growing need for green hydrogen and the crucial part PEMWEs play in scalable and effective hydrogen generation systems.

This section builds upon that context by providing a more detailed exploration of the electrochemical processes driving PEMWE's performance, particularly the models and variables that influence energy efficiency, degradation, and output capacity.

A thorough examination of the electrochemical processes in PEMWE systems is critical for advancing the energy management strategies discussed earlier. To achieve efficient and scalable HyPro, an accurate representation of the electrochemical model is required, enabling the optimization of operational parameters like current density, temperature, and pressure. The purpose of this section is to provide an overview of the electrochemical framework, focusing on key modelling approaches to understand overpotential, cell voltage, as well as associated losses, which will serve as a foundation for improving energy management solutions in modular PEMWE systems.

With a focus on the transition of PEMWEs from theoretical constructs to practical applications, specifically in energy management, the benchmarking study "Model benchmarking for PEM Water Electrolyser for energy management purposes" offers a thorough assessment of several theoretical models for PEMWEs.

This integration into the "Electrochemical Model" section is essential to establish a solid foundation for comparing theoretical models and optimizing energy management in modular PEMWE systems.

The study first highlights the importance of accurate modelling in predicting PEMWE system behaviour, which is critical for optimizing energy efficiency and reducing degradation. It categorizes the models into key electrochemical components, including reversible potential, activation overpotential, ohmic overpotential, and concentration overpotential. The models are evaluated based on their ability to predict voltage losses across these parameters, using both theoretical and empirical approaches. Using this comprehensive approach, it is possible to identify models that are most consistent with the operational needs of PEMWE systems while maintaining computational efficiency.

The creation and verification of a test bench especially intended to gauge the PEMWE models' performance under varied operating circumstances constitutes a significant methodological addition to the research. We can evaluate model correctness by comparing the system's actual performance with its expected performance using a test bench.

To evaluate the models' practicality, this empirical validation is essential. For example, the study finds that some models, like Model 4, are the best fit for real-world energy management applications since they continually show the lowest error rates and closely match experimental data.

The methods section of the study is robust, employing a combination of statistical metrics (MSE, RMSE, MAE, and R^2) to rigorously evaluate the predictive accuracy of each model. In addition to improving the precision of the models, the use of a GA for parameter optimization enhances the accuracy of the model by fine-tuning key variables such as membrane thickness and current density. This approach not only improves the accuracy of the models but also ensures their adaptability to different operating scenarios, which is critical for scalable and efficient PEMWE energy management.

As a result of the benchmarking study, a systematic framework for selecting electrochemical models that strike a balance between complexity and accuracy is provided. Through this integration, the thesis can go beyond theoretical discussions of model components and explore real-world, data-driven assessments that have direct relevance to modular PEMWE systems' energy management. The study's focus on empirically supported customised model selection fits in nicely with the thesis's overarching goals of improving the scalability and operational effectiveness of PEMWE systems for green HyPro.

The methodological rigour of the study is evident in its comparative analysis of eight distinct electrochemical models, each varying in complexity and computational requirements. Experimental validation is carried out on a custom-built test bench, ensuring that the models are evaluated under real-world conditions, allowing for a solid basis for practical application. The results demonstrate that models incorporating a balance of theoretical accuracy and empirical adaptability, such as Models 4 and 7, offer the best performance in terms of error rates and alignment with experimental data.

Additionally, the study includes a multi-objective optimization approach that employs a GA to minimize discrepancies in system performance between the predicted and actual values. This technique works especially well for adjusting model parameters, like overpotential losses and reversible potential, to improve the models' accuracy. The findings emphasise the need of accurate model calibration in energy management applications by clearly demonstrating a relationship between optimised parameters and increased system efficiency.

To sum up, this benchmarking study offers important information about how to choose and improve electrochemical models for PEMWE systems, with an emphasis on energy management. Its incorporation into the thesis closes the gap between theoretical concepts and real-world applications by enabling a more thorough assessment of model performance. This study lays the groundwork for the following chapters, which will examine how model selection affects the scalability and energy efficiency of modular PEMWE systems.

3.1.1 Model Benchmarking for PEM Water Electrolyser for Energy Management Purposes

The discussion thus far has delineated the critical role of electrochemical modeling in optimizing energy management within modular PEMWE systems, highlighting the significance of precise overpotential characterization and rigorous experimental validation. A forthcoming paper entitled "Model Benchmarking for PEM Water Electrolysers for Energy Management Purposes" is discussed in this context. This study systematically evaluates various electrochemical models through empirical benchmarking, thereby bridging the gap between theoretical constructs and practical implementation. An integrated framework supports the selection of models that enhance PEMWE operational efficiency by linking the preceding theoretical discourse with its practical application.

Journal: Energy Conversion and Management (Elsevier)

Published date: November 2024

Energy Conversion and Management 323 (2025) 119203

Contents lists available at ScienceDirect

Energy Conversion and Management

journal homepage: www.elsevier.com/locate/enconman

Research paper

Model benchmarking for PEM Water Electrolyzer for energy management purposes

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ARTICLE INFO

Keywords:
PEMWE
Electrochemical models
Energy management
Overpotential
Hydrogen production
Model benchmarking

ABSTRACT

This research conducts a comprehensive evaluation of various Proton Exchange Membrane Water Electrolyzer (PEMWE) models through a test bench, optimizing parameters and comparing obtained models against real-world data. Key operational factors such as reversible potential, activation overpotential, ohmic overpotential, and concentration overpotential are examined through experimental data. This study addresses critical gaps in current PEMWE research by reviewing modelling approaches, introducing a novel classification of models, and proposing an integrated approach that combines experimental validation with comprehensive model analysis. A novel, systematic methodology for model and submodel selection is presented, enabling practitioners to identify models that balance computational efficiency and predictive accuracy tailored to specific energy management and power allocation needs. This approach bridges the gap between complex modelling and industrial applications, enhancing the practical implementation of PEMWE systems in sustainable hydrogen production. Enhances model reliability for operational and manufacturing differences, provides invaluable guidance for improving the design and operation of these systems, and promotes a more robust and efficient hydrogen energy infrastructure.

1. Introduction

As the world continues to seek out sustainable energy sources, hydrogen is increasingly being viewed as a potential pathway for the future [1]. Hydrogen is a clean-burning fuel that emits only water vapour when burned, making it an attractive option for reducing greenhouse gas emissions [2,3]. Moreover, it can also be considered zero-emissions when it is utilized in Fuel Cells (FC) [4,5]. In addition to its role as a fuel, it is crucial in other industrial processes, including refining [6], steel production, and ammonia synthesis [7], demonstrating its versatility and essential role in a variety of industrial processes [8]. However, the challenges of hydrogen production and storage remains a significant barrier to widespread adoption [9,10]. One promising technology in this regard is the Proton Exchange Membrane Water Electrolyzer (PEMWE), which utilizes renewable energy sources (RES) such as solar, wind, or hydro power to produce green hydrogen from water [11,12]. PEMWE is a popular choice for hydrogen production due to its high operational efficiency in low operating temperatures [13]. Furthermore, the scalability of PEMWE systems is a significant advantage, allowing for flexible adjustments in capacity to meet diverse application requirements [14,15].

PEMWE's installed capacity has grown significantly between 2019 and 2023, and this issue is depicted in Fig. 1. According to predictions, the pace of this growth will continue to accelerate in the coming years [16]. The growth of hydrogen production in megawatt (MW) and gigawatt (GW) scale has become increasingly important in recent years due to the need for sustainable energy patterns and the drive towards achieving zero-emission goals [17]. The use of modular structures and power allocation strategies has become essential for efficient green hydrogen production in large-scale applications. These modular structures allow for easy scalability of the system and enable the efficient allocation of power based on the fluctuating demand for hydrogen production. Effective energy management is also crucial for the efficient operation of large-scale hydrogen production systems. The optimization of parameters such as operating current density, temperature, water

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https://doi.org/10.1016/j.enconman.2024.119203
Received 4 September 2024; Received in revised form 17 October 2024; Accepted 25 October 2024
Available online 11 November 2024
0196-8904/

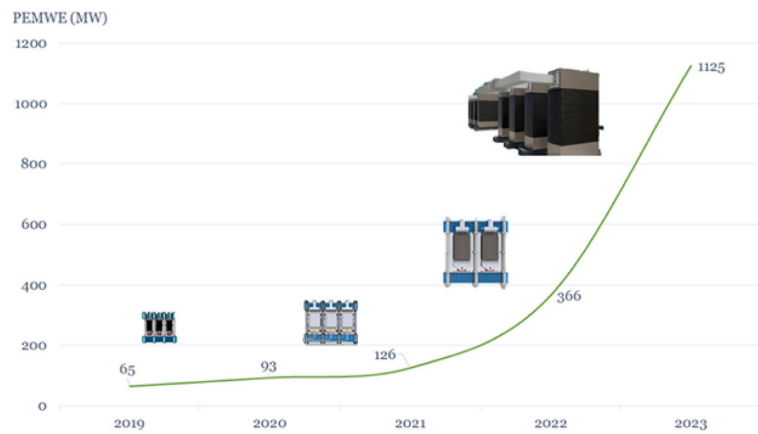

Fig. 1. The total installed capacity of PEMWE in the last four years [20].

and air flow rates, and material selection can significantly improve the energy efficiency of the system, reduce operating costs, and increase the overall sustainability of hydrogen production [18,19].

As the usage of large-scale PEMWEs increases, it becomes imperative to have accurate and practical models for them and algorithms for feeding electrolysers which can affect the behaviour of these systems across different scales [21]. The development of such models can facilitate a better understanding of PEMWE's behaviour and enable efficient design, operation, and control of these systems [22]. It is particularly relevant to increase PEMWE's scale using giant stacks or modular designs. Despite the challenges, modelling studies are crucial to developing efficient and effective electrolyzer systems for hydrogen production. Accurate models can provide insights into maximizing production, minimizing degradation, and increasing system lifespan [23]. Therefore, developing reliable and scalable models for PEMWE inputs (energy and water) is crucial to enable widespread adoption and unlock their potential as a critical technology for sustainable energy conversion and storage [24].

PEMWE modelling reviews are crucial for assessing current models, highlighting strengths, weaknesses, and research needs [25]. Lamy and Millet's analysis of energy efficiency in water electrolysis cells underscores the importance of these coefficients for evaluating performance and cost-effectiveness [26]. Olivier et al. offer an overview of low-temperature electrolysis, including PEM and alkaline, identifying key research areas and using a comparative approach [27]. Falcao and Pinto focus on PEM electrolyzer modelling, discussing prediction equations for cell voltage and performance expectations [28]. Hernandez-Gomez et al. explore the electrical aspects of PEMWEs, suggesting empirical models to enhance electrolyzer performance [29]. Majumdar et al. discuss dynamic models and control techniques for PEMWEs, stressing the significance of data-driven models and degradation-aware control algorithms [30].

Effective energy management within PEMWE systems is paramount, not only to optimize performance but also to ensure economic viability and environmental sustainability [31]. Integrating intelligent Energy Management Systems (EMS) that can dynamically adjust to varying renewable energy inputs and operational demands is crucial [32,33]. These systems help balance hydrogen production rates and energy consumption, optimizing overall efficiency and reducing costs. However, selecting the appropriate models for these EMSs can be challenging due to the many available models, each with its strengths and weaknesses [34]. Selection becomes even more complex when considering the variations and iterations within a single type of model. Various models can provide different insights and results, which can significantly affect the understanding of PEMWE system performance and consequently decision-making in EMS.

This diversity of models creates a special issue when determining which model is most appropriate for a certain application. The choice of model affects not only the accuracy of predictions and optimizations but also the practical feasibility of implementing solutions at scale. Given that every system has its character, operational condition, and performance metrics, it is not feasible to universally recommend a single model as the optimal choice across different systems. To address this challenge, introducing a systematic method for comparing and choosing a benchmark model tailored to each specific system could prove invaluable. Researchers seeking the most appropriate models for energy management and power allocation as well as industry professionals seeking robust, application-specific models would benefit from this approach.

Prior research has explored various PEMWE models, including complex multidimensional analyses [24], integration with RES [31–33], and control-oriented methods [30,34]. Other studies have examined temperature-dependent models to assess operating condition impacts [27,35,36] and employed simulations to investigate PEMWE behaviour under diverse scenarios [25,37–39]. While electrical domain models focus on efficiency and energy consumption [29,37,40], empirical studies gauge hydrogen production rates and system efficiencies [29,37,39,41,42], demonstrating the broad array of modelling techniques in use [28,43,44].

Despite these developments, there is a notable lack of comprehensive comparison or benchmarking among models tailored for PEMWE applications, a gap this study aims to fill. It benchmarks a wide array of electrochemical models, providing a structured framework to assess their complexity, performance, and applicability to energy management—critical for enhancing green hydrogen production at scale. This study addresses existing gaps in PEMWE research by conducting a comprehensive evaluation of modelling approaches geared towards power allocation and energy management. It introduces a novel classification of models and integrates rigorous experimental validation with in-depth analytical review, offering practitioners a method to select and validate models that balance computational efficiency with predictive accuracy, tailored to unique system requirements.

In summary, this paper provides essential comparisons and guidelines for model selection, substantially aiding the advancement of large-scale green hydrogen production through refined PEMWE modelling strategies.

This research aims to establish a practical method for selecting an appropriate model among the myriad available, tailored to the unique characteristics and operational conditions of each system. Section 2 provides a rapid analysis of model types and introduces the domains of PEMWE from an energy management perspective. Section 3, aligned with energy management principles, selected overpotentials are chosen, and a novel method for comparing and selecting the most appropriate models is introduced. Section 4 describes a test bench setup developed for validation and for comparing theoretical predictions with practical outcomes. Section 5 presents the test bench used for models

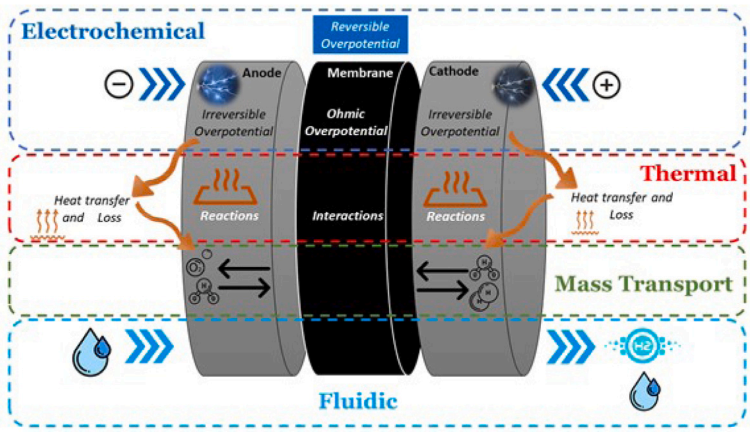

Fig. 2. Coupling of different domains for PEMWE modelling.

validation. Section 6 presents the results and discussions, providing a comprehensive evaluation of the proposed methodology.

2. PEMWE models for energy management

A PEMWE consists of interconnected domains: electrochemical, mass transport, fluid flow, and heat transfer, as shown in Fig. 2. Changes in one domain affect others, necessitating coupled sub models. In electrochemical reactions, the anode and cathode are involved, and catalysts play a role in these reactions. Overpotentials and voltage losses influence these reactions. Mass transport involves the diffusion and convection of reactants and products through the membrane and gas diffusion layers, requiring accurate modelling of species distribution and concentration profiles. Fluid flow involves water supply to the anode and gas generation, with models considering flow rates and pressure differentials [45]. Heat transfer involves thermal effects from electrochemical reactions, requiring models for heat generation and loss.

Understanding electrolyzer performance through polarization and voltage modelling is crucial for energy management. The cell voltage provides insights into hydrogen production efficiency. Variations in voltage can help identify different modes of operation, assess ageing, and determine degradation rates. It is first necessary to determine the cell voltage, considering voltage and overvoltage. Although this section primarily focuses on energy management, all domains indirectly impact overvoltage and are considered in experimental tests. The primary direction is electrochemical analysis.

PEMWE behaviour is complex, with changes in one domain impacting others. Coupled sub-models in physics-based models are essential. For example, electrochemical performance variations affect species concentration and transport, while fluid flow adjustments alter reactant and product concentrations. Thermal effects influence electrochemical kinetics and species transport properties. Accurate simulation requires integrated models to capture these interactions. As this complex phenomenon is approached from a variety of perspectives, it becomes important to adopt a modelling approach.

Models that link the practical operational system with various parameters and variables underpin PEMWE's EMSs. Several factors, such as hydrogen production rates and overall system efficiency, require the implementation of models that can accurately predict and manage these factors, such as voltage models. Various modelling approaches exist, each with distinct strengths and weaknesses, categorized based on the level of understanding of the system's physical or mathematical structure. Determining the superior model type — whether empirical, theoretical, or mathematical — hinges on the specific requirements and constraints of the PEMWE system.

As shown in Fig. 3, three primary modelling categories can be distinguished: white box, grey box, and black box. Empirical models, or black-box models, are constructed based on experimental data and observations. In general, they require fewer computational resources and are easier to develop but may not generalize beyond specific conditions. Theoretical mathematical models, or white-box models, are built on underlying physical and chemical principles and offer insights into the internal workings of the system. These models can be extrapolated to different operating conditions but are often complex and computationally demanding. Grey-box modelling, combining elements of both empirical and theoretical approaches, is particularly suitable for energy management in PEMWEs where both predictive accuracy and computational efficiency are critical. Thus, grey-box modelling is a preferable strategy for effective energy management in PEMWE systems, offering a pragmatic blend of detail and applicability.

For finding electrochemical voltage equation PMWE overall reaction, which is illustrated in (1), can be the first step. It shows how water is split into hydrogen and oxygen [43]

$$2H_2O \rightarrow O_2 + 2H_2 \tag{1}$$

This reaction occurs at the electrodes: the anode handles the OER given by (2) and the cathode handles the HER expressed by (3)

$$2H_2O \rightarrow O_2 + 4H^+ + 4e^- \tag{2}$$

$$4H^+ + 4e^- \rightarrow 2H_2 \tag{3}$$

In a PEMWE cell, water splits into hydrogen and oxygen (1), requiring electricity for electrolysis. The standard reversible cell voltage, $V_{(rev,s)}$ can be calculated by considering the maximum heat energy input of 48.6 kJ/mol, as outlined in (4) [46]

$$V_{rev,s} = \frac{\Delta G}{n_e F} = 1.23\,V \tag{4}$$

where the change in Gibbs free energy (ΔG) is 237.22 kJ/mol for the reaction, n_e the number of electrons transferred, typically 2 for water splitting and F is the Faraday constant, approximately 96485 C/mol, representing the charge of one mole of electrons.

The theoretical voltage V_{th} for water splitting in a PEMWE cell can be calculated using the enthalpy (ΔH) which is expressed by

$$\Delta H = \Delta G + T\Delta S \tag{5}$$

where T is the cell temperature in Kelvin and (ΔS) is the entropy change. Under standard conditions, the change in enthalpy (ΔH) is 285.84 kJ/mol. Using this information, the minimum voltage for water electrolysis, represented as V_{th} can be calculated as follows [41]

$$V_{th} = \frac{\Delta H}{n_e F} = 1.48\,V \tag{6}$$

The cell voltage V_{cell} is determined by taking into account various losses in a PEMWE system, additional considerations are required. These voltage losses should be added to reversible voltage V_{rev} to result

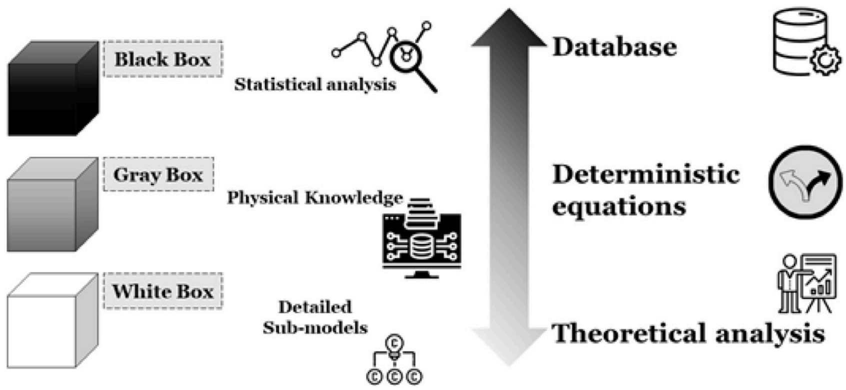

Fig. 3. Different types of models from the point of view of origin.

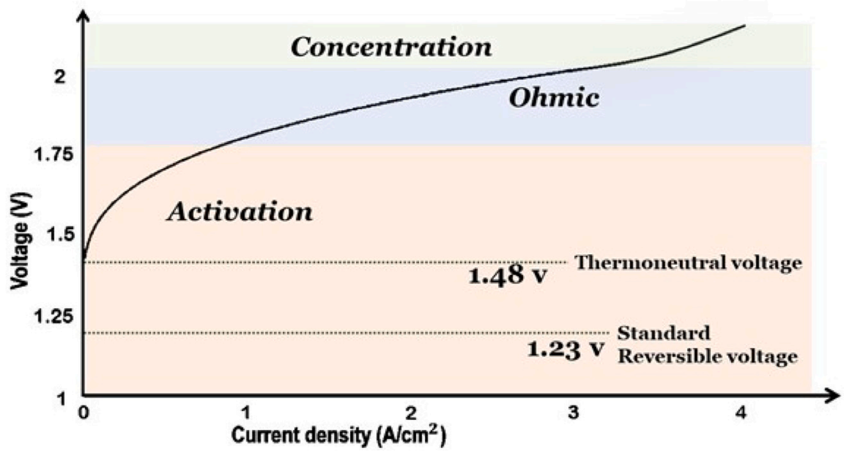

Fig. 4. PEMWE cell polarization curve [49].

in an approximation of cell voltage. By considering the four major voltage loses, the cell voltage V_{cell} is expressed by [47]

$$V_{cell} = V_{rev} + U_a + U_o + U_c + U_b \tag{7}$$

where U_a is concentration losses, U_o is ohmic losses, U_c is concentration losses and U_b is bubble overpotential.

Activation losses U_a arise from the high activation energy needed for electrochemical reactions at the electrodes, reducing efficiency. Ohmic losses U_o, due to the electrolyte's resistance and ion movement, are a primary source of irreversibility. Concentration losses U_c result from reactant and product concentration gradients, affecting mass transport within the cell. Bubble overpotential U_b models the irreversibility of bubble formation at the electrodes and membrane. While these losses increase overall voltage, researchers may focus on specific losses based on their model's complexity. Sometimes, only activation and ohmic losses are considered for simplicity [48].

A PEMWE cell polarization curve, shown in Fig. 4, illustrates the relationship between cell voltage and current density during water electrolysis. This curve is crucial for assessing the system's efficiency and performance, helping researchers identify voltage losses and determine optimal operating conditions.

The variable quantity of HyPro can be described using (8)

$$\text{HyPro} = \int_0^t f_{H_2} \mathrm{d}t = \frac{\int_0^t N.I.V.\eta_e.\mathrm{d}t}{HHV_{H_2}.\rho_{H_2}} \tag{8}$$

where N is the number of cells, and η_e is the PEMWE efficiency determined by (9), which is linked to the current [44,50].

The higher heating value of hydrogen HHV_{H_2} is a crucial thermodynamic property indicating the energy liberated when hydrogen is combusted, quantified here as approximately 39 400 J/g. The density of hydrogen, ρ_{H_2} under standard conditions is around 0.8988 g/L.

The energy efficiency coefficient of water electrolysis η_e can be calculated in function of current by [50]

$$\eta_e = -0.0786I^3 + 1.167I^2 - 7.365I + 84.44 \tag{9}$$

3. Overpotential model selection for a PEMWE

A balance is achieved between transparency and flexibility in this study of PEMWE by using grey box models. They provide a satisfying balance between the comprehensiveness of white box models and the simplicity of black box models by integrating theoretical principles with empirical data. A focus is placed in this section on the precision modelling of voltages applied to electrodes, a critical factor in considering energy management and power allocation in PEMWE systems. The voltage across a PEMWE cell, designated as V_{cell} in (7), is subject to various losses and irreversibility. These influences, along with diverse modelling strategies documented in the literature, are comprehensively examined. Moreover, the section emphasizes that models should be designed with a balance of simplicity and adaptability, ensuring they are both easy to integrate into the system and sufficiently accurate for the goal of efficient energy management. The focus is on achieving fast and straightforward operation while maintaining a high degree of precision in tracking and responding to real-time conditions. Such adaptability not only aligns with ongoing technological developments but also supports the integration of PEMWE systems into broader energy frameworks, thereby enhancing scalability and operational efficiency. This discussion sets the stage for subsequent sections, which will compare experimental outcomes with theoretical predictions, further analysing and optimizing various identified models based on their operational parameters and utility.

3.1. Reversible potential

A PEMWE's reversible potential voltage is the minimum voltage required to initiate it from a thermodynamic standpoint. It is common for studies to take into consideration the constant reversible voltage, typically around 1.229 V at standard temperature and pressure as it is called standard reversible voltage $V_{rev,s}$ as shown in (4). Reversible standard voltage $V_{rev,s}$ is sometimes called reference voltage or standard voltage and is expressed in various forms E^0_{rev}, E_0 or V_0 and also is calculated through different simple and complicated formulas [37]. The standard reversible potential represents an ideal scenario under standard conditions.

In contrast, the reversible potential in PEMWE reflects actual operating conditions, incorporating variations such as temperature, pressure, and reactant concentration. Various equations in the literature estimate this potential, each varying in complexity and operational detail. The empirical linear model simplifies calculations by directly correlating voltage to deviations from the standard temperature of 298 K, making it practical and predictable for conditions close to the norm but less effective outside this range. Conversely, the thermodynamic integral-based approach caters to a more extensive temperature spectrum, though its reliance on comprehensive data adds complexity.

Other strategies include polynomial models which, by incorporating terms up to T^3, effectively manage higher-order temperature impacts but increase computational demands. Linear models provide ease and efficacy under near-standard conditions but falter when broader applicability is required. The logarithmic model offers a mid-ground by balancing simplicity with a detailed representation of non-linear temperature effects, although its accuracy may diminish at extreme values.

Enhanced adaptability to varied operational scenarios is achieved by adding additional models that consider temperature, pressure, enthalpy, and entropy, or that utilize reference pressures. Selecting the right model balances computational efficiency with the precision required for PEMWE systems, ensuring alignment with operational demands and energy management limitations. Among them (10) stands out for its effective balance between simplicity and complexity, making it particularly suitable for practical energy management applications. It efficiently integrates key parameters, enabling quick and accurate calculations of cell voltage under non-standard conditions. By using logarithmic terms to account for pressure and concentration effects, (10) offers a tailored approach to the dynamic environments of PEMWEs. Furthermore, the factors considered in this formula such as temperature and pressure are typically measured within an energy management system, aligning with practical application needs [51].

$$V_{rev} = V_{rev,s} + \frac{RT}{2F} \times \ln\left(\frac{P_{H_2} P_{O_2}^{0.5}}{\alpha_{H_20}}\right) \tag{10}$$

where water activity α_{H_20} assumed to be 1, R is universal gas constant, and P_{H_2} is partial pressure of hydrogen and P_{O_2} is partial pressure of oxygen; and also the standard potential $V_{rev,s}$, which is represented by (4) and can be calculated accordingly [52].

3.2. Activation overpotential

In PEMWE electrochemical modelling, activation overpotential is the extra voltage required to initiate an electrochemical reaction at the electrode–electrolyte interface. It drives a Faradaic current and decreases with rising operating temperature due to increased exchange current density, which enhances the reaction. This overpotential arises from kinetic barriers such as reactant adsorption/desorption, charge transfer, and reactant diffusion. Factors influencing it include temperature, pressure, catalyst activity, and reactant concentration. Understanding activation overpotential helps optimize PEMWE design and operation, improving performance and energy efficiency, crucial for energy conversion and storage applications.

Activation overpotential, U_a reflects the reaction rate and consists of anode $U_{a,a}$ and cathode $U_{a,c}$ components as shown in (11). Some studies consider the cathode side negligible [35]. Each of the anode and cathode can be placed in place of j and the formulas from (121) to (14) can be personalized for each. calculate these overpotentials, applicable to oxidation at the anode and reduction at the cathode. This concept links the electrical current through an electrode to the voltage difference between the electrode and electrolyte for a single-molecule redox reaction involving both anodic and cathodic reactions. Various U_a equation forms exist in the literature shown in Table 1 along with their estimated computational speed.

One of the widely used expressions for calculating activation overpotential U_a is (12), which has been employed by numerous authors in the development of electrolysers models [53]. The parameter α is the symmetry factor that accounts for the additional energy fractions involved in the reduction (anode) and oxidation (cathode) processes. i_j represents the current density at the jth electrode, which is a measure of the electric current per unit area of the electrode. $i_{0,j}$ refers to the exchange current density at the jth electrode, indicating the rate of the electrochemical reaction when there is no net current flow (i.e., when the electrochemical reaction is at equilibrium). In (13), z represents the stoichiometric coefficient of the number of electrons involved. The rugosity factor γ_j in (14) represents the effective surface area of the electrode in relation to its geometric area, accounting for the microstructural characteristics and porosity [54]. (15) uncovers the effects of double-layer capacitors with shunt capacitors $C_{dl,j}$. In this equation, the current density flowing through the PEMWE stack is represented by i. The parameters ρ_j and τ_j are determined based on empirical functions that correlate to temperature.

3.3. Ohmic overpotential

Overpotential in the PEMWE electrochemical model refers to the resistance to electric current flow. It is linked to the ionic conductivity of the electrolyte and resistance of cell components, including electrodes, current collectors, and membranes. An external voltage is applied to drive the electrochemical reaction, but a voltage drop, called ohmic overpotential U_o, occurs due to resistance, reducing the effective potential for reactions. Ohmic overpotential U_o can be mathematically described using Ohm's Law, where the voltage drops U_o is equal to the product of the current density i and the total equivalent resistance Ω_{eq} in the system as illustrated in (16). Two frequent equations in the literature are shown in Table 2.

The equivalent resistance Ω_{eq} includes contributions from the electrolyte's ionic conductivity, the membrane's thickness and conductivity, and the contact resistance at the interfaces between the electrodes and the current collectors. These factors collectively determine the Ohmic overpotential in the PEMWE system. A good approximation of this equivalent resistance is the resistances of membrane Ω_M and electrodes Ω_E which is given by

$$\Omega_{eq} = \Omega_M + \Omega_E \tag{18}$$

According to (18), Ω_E stands for electrical resistance in electrodes. Membrane resistance Ω_M is given by

$$\Omega_M = \frac{\theta}{\mho} \tag{19}$$

where θ is the thickness of the membrane and $\mho$ represents the conductivity of the membrane expressed as follows

$$\mho = (0.005139\lambda - 0.00326)\exp\left(1268 \times \left(\frac{1}{303} - \frac{1}{T}\right)\right) \tag{20}$$

where λ refers to membrane humidification [59].

Table 1
Different versions of the literature's activation overpotential equations.

Equations		Parameters involved	Computational speed
$U_a = U_{a,a} + U_{a,c}$	(11)	Anode and cathode potentials	Fast
$U_{a,j} = \frac{RT_j}{\alpha_j F} \sinh\left(\frac{i_j}{2i_{0,j}}\right)^{-1}$	(12)	Temperature, symmetry factor and current density	Moderate
$U_{a,j} = \frac{RT_j}{z\alpha_j F} \sinh\left(\frac{i_j}{2i_{0,j}}\right)^{-1}$	(13)	Includes valence	Moderate
$U_{a,j} = \frac{RT_j}{z\alpha_j F} \ln\left(\frac{i_j}{\gamma_j i_{0,j}}\right)^{-1}$	(14)	Rugosity factor	Moderate
$\frac{dU_{a,j}}{dt} = \frac{\rho_j}{C_{dl,j}}\left(1 - \exp\left(\frac{U_{a,j}}{N\tau_j}\right)\right) + \frac{i}{C_{dl,j}}$	(15)	Dynamic components including capacitance and resistance	Very slow

Table 2
Ohmic overpotential formulas in scholarly works.

Ohmic overpotential equations		References
$U_o = i \times \Omega_{eq}$	(16)	[41,52,55–57]
$U_o = i \times \Omega_M$	(17)	[35,37,38,58]

Table 3
Distinct concentration overpotential formulas in scholarly works.

Concentration overpotential equations		References
$U_{c,j} = \frac{RT}{Z_j F} \ln\left(\frac{con_j}{con_{j,0}}\right)$	(21)	[36,42,56,64–67]
$U_c = \frac{RT}{\beta Z F} \ln\left(1 + \frac{i}{i_l}\right)$	(22)	[55,58]
$U_c = i\left(\beta_1 \frac{i}{i_l}\right)^{\beta_2}$	(23)	[68]
$U_c = \frac{RT}{\beta Z F} \ln\left(\frac{\frac{i}{i_l}}{1 - \frac{i}{i_l}}\right)$	(24)	[39,64]

Additionally, there are other approaches to calculation that include more details and can be chosen for various applications or research but are not necessary for energy management purposes. For instance, Correa et al. [60] note that membrane conductivity is influenced by its prior state, the activation energy for proton transport, and temperature [40]. Jing et al. [61] discuss the concept of equivalent resistance, which is calculated based on the area-specific resistance and the cell's surface area [62]. This resistance is impacted by various factors including temperature, with different components of the electrolysis cell showing varying degrees of temperature dependency [63].

3.4. Concentration overpotential

Concentration overpotential, labelled U_c, results from concentration gradients at electrodes during electrochemical processes like PEMWE water electrolysis. It increases due to mass transport issues, leading to higher energy use, lower efficiency, and more operating costs. This phenomenon also causes uneven current distribution and pH changes, which affect electrode life and stability. U_c sums up the individual overpotentials at the anode $U_{C,a}$ and cathode $U_{C,c}$.

The Nernst equation calculates concentration over potential as shown in (21) in Table 3. It uses con_j to denote the concentration of oxygen at the anode or hydrogen at the cathode, depending on whether $\varepsilon j \varepsilon$ equals $\varepsilon a \varepsilon$ or $\varepsilon c \varepsilon$ [37]. $con_{j,0}$ represents the reference concentrations of oxygen and hydrogen at the anode and cathode, respectively. Stoichiometric coefficients vary, with z_a being 4 at the anode and z_c being 2 at the cathode.

In literature, an alternative model for calculating the concentration overpotential is described by (22), which involves an empirically derived coefficient represented as β and the limiting current density i_l are determined by the diffusion capabilities. Based on the experimental data mentioned in [69], these specific values were obtained through curve fitting. The concentration overvoltage in PEMWEs can also be described by a model that incorporates the limiting current density i_l in (23). In this model, the coefficient β_1 is dependent on oxygen pressure and temperature, while β_2 remains constant. As noted in (24), bubble overpotential is sometimes included in concentration overvoltage studies. A limiting current density i_l causes bubbles to form, resulting in efficiency losses. At low current densities, concentration overpotential is often neglected due to the prominence of ohmic and activation overpotentials. However, its impact can vary significantly depending on the system's parameters and conditions [66]. To mitigate concentration overpotential and improve PEMWE performance, strategies focus on enhancing mass transport, optimizing flow fields, increasing electrode surface area, and selecting high-activity, stable catalysts to improve reaction kinetics and reduce overpotential.

Bubble overpotential U_b arises when gas bubbles, mainly hydrogen, accumulate on the electrode surface during electrolysis, impeding reactant transport and lowering electrochemical activity. This phenomenon is influenced by current density, electrolyte composition, and electrode design. High current densities or low reactant concentrations can worsen this effect, leading to increased polarization and reduced cell performance [70]. While some studies treat bubble overpotential as negligible, others acknowledge its role, particularly in non-uniform gas bubble distribution and the disruption of fluid flow patterns, which reduce mass transport and performance. In some models, bubble effects are considered by adjusting Butler–Volmer equations to incorporate nonlinearity; however, these considerations are not always considered in the context of broader system models. Ex-situ and system-wide models often overlook bubble overpotential despite its significance in some contexts [71].

4. Towards tailored overpotential model selections in PEMWE systems

The study utilized a systematic method to identify the most effective electrochemical model from eight variations (M_1 to M_8), each defined by different overpotential combinations. The identified eight models are expressed as follows

$$M_1 = V_{rev} + U_{a,1} + U_{o,1} + U_{c,1} \quad (25)$$

$$M_2 = V_{rev} + U_{a,1} + U_{o,1} + U_{c,2} \quad (26)$$

$$M_3 = V_{rev} + U_{a,1} + U_{o,2} + U_{c,1} \quad (27)$$

$$M_4 = V_{rev} + U_{a,1} + U_{o,2} + U_{c,2} \quad (28)$$

$$M_5 = V_{rev} + U_{a,2} + U_{o,2} + U_{c,1} \quad (29)$$

$$M_6 = V_{rev} + U_{a,2} + U_{o,2} + U_{c,2} \quad (30)$$

$$M_7 = V_{rev} + U_{a,2} + U_{o,1} + U_{c,1} \quad (31)$$

$$M_8 = V_{rev} + U_{a,2} + U_{o,1} + U_{c,2} \quad (32)$$

Table 4
Overpotential models selection for energy management in PEMWE systems.

Overpotentials	Abb	Eqs	Parameters: All/Known constant/Estimated/Measured	Rationale/Notes
Reversible	V_{rev}	(10)	7/5/1/1	Balances precision and responsiveness
Activation	$U_{a,1}$	(13)	7/3/2/2	Known temperature relationships
Activation	$U_{a,2}$	(14)	8/3/3/2	Current interplays
Ohmic	$U_{o,1}$	(16)	3/0/2/1	General applicability
Ohmic	$U_{o,2}$	(17)	4/0/2/2	Requiring comprehensive modelling
Concentration	$U_{c,1}$	(22)	7/3/2/2	Known limiting currents
Concentration	$U_{c,2}$	(23)	4/0/3/1	Non-linear response traits

Table 4 compares sub-models' side-by-side, highlighting their composition, parameters, and approach. This comparative analysis not only assessed each model's accuracy against experimental data but also their computational needs and practicality. Although this method provides a framework for selecting appropriate models for various electrolyzers, it should be noted that it proposes a hypothesis rather than conclusive results, serving as a preliminary guide in model selection across different scenarios.

Striking an optimal balance between computational efficiency and parameter detail is crucial in selecting sub-models for each component of these eight electrochemical models. Unlike other models, where two are chosen for comparison, the reversible overpotential V_{rev} specifically employs the logarithmic temperature–pressure dependency model. This model is well-documented in the literature and is an effective choice from an energy management perspective, particularly in controlled systems where pressure and temperature are routinely monitored.

The comparative analysis of (13) and (14) highlights their integration of critical parameters within electrochemical model benchmarking. (13) employs the $\sinh^{-1}$ function to depict rapid activation overpotential changes, albeit with potential numerical instabilities at high current densities. (14) introduces a rigidity factor, connecting the logarithm of current density to electrode characteristics and potentially simplifying reaction kinetics. These equations provide a balance between detailed accuracy and computational efficiency, vital for the effective evaluation of model performance.

(16) and (17) are selected for their straightforward yet comprehensive modelling capability, expedite and refine computation, critical for model assessment. (16) directly relates current to total system resistance, mapping out voltage variations across components. Concurrently, (19) evaluates membrane resistance considering membrane thickness and conductivity, vital for detailed energy loss analysis in electrolyzer systems.

Lastly, (22) and (23) effectively model concentration overpotentials. (22) is logarithmic formulation responsively mirrors concentration variations due to mass transport limits in electrochemical processes. (23) introduces a power-law dynamic to address non-linear outcomes at elevated currents, ensuring alignment with practical PEMWE operational scenarios and boosting the model's application relevance.

In the development of overpotential models for PEM water electrolysis, the inclusion of factors such as bubble overpotential is not universally necessary. This exclusion depends on the specific focus of the study and the anticipated operational conditions of the system. In scenarios where the primary overpotentials activation, ohmic, and concentration predominantly influence system performance, incorporating bubble overpotential may introduce redundancy. Often, the effects attributed to bubbles are implicitly accounted for within the concentration overpotential, particularly when models are calibrated with experimental data in specified operational ranges. By simplifying the model to exclude less impactful factors, computational efficiency is enhanced, allowing a sharper focus on the most critical elements that determine the electrolyzer's efficiency and effectiveness.

Table 5
Constant parameters for PEMWE model simulation and benchmarking.

Parameters	Value	Unit	Used in Eq
Standard reversible voltage $V_{rev,s}$	1.229	Volts	(10)
Universal gas constant R	8.314	J/(mol K)	(10) (13) (14) (22)
Faraday's constant F	96 485	C/mol	(10) (13) (14) (22)
Water activity α_{H_2O}	1	N/A	(10)
Temperature T	Variable	K	(10) (13) (14)
Pressure P	1.5	atm	(13) (16) (23)
Hydrogen pressure P_{H_2}	1	atm	(10)
Oxygen Pressure P_{O_2}	1	atm	(10)
Electrolyte conductivity ℧	1	S/m	(19)
stoichiometric coefficient z	2	N/A	(13) (14) (21) (22) (24)

4.1. Estimation of model overpotential parameters

For evaluating PEMWE models M_1 to M_8, the estimation of the key parameters are essential in simulation and benchmarking. These parameters listed in Tables 5 and 6[1] are critical across (10) to (24) and influence the accuracy and performance of the simulations by specifying their units and equations of application.

As a result of a better understanding of parameters, it is possible to simulate real-world conditions more accurately and enhance the design of the PEMWE system. The use of a Genetic Algorithm (GA) can facilitate parameter estimation, allowing the model to reflect real-life scenarios more accurately. Setting up a fitness function in GA for PEMWE systems minimizes differences between model outputs and experimental data, involving meticulous parameter adjustments like membrane thickness and electrolyte concentration. Iterative adjustments optimize PEMWE models, which are validated against additional datasets to ensure accuracy and reliability. This tailored approach balances computational efficiency and accuracy, vital for real-time operations or precise applications.

The objective function for each of the models (M_1 to M_8) is aimed at minimizing the sum of squared differences between experimentally measured and model-predicted voltages. This optimization method, particularly well-suited to addressing complex problems characterized by multiple local minima, is implemented in MATLAB to enhance computational efficiency and reproducibility [72]. The objective function is expressed by

$$J = \sum_{i=1}^{n} \left(V_i - M_k(p_k) \right)^2 \tag{33}$$

where V_i is the experimental voltage at the ith data point. $M_k(p_k)$ is the voltage predicted by model M_k using parameters p_k at the ith data point for $k = 1, 2, \ldots, 8$. The total data points are n.

[1] *These parameters are estimated by GA; however, parameters may have various amount in different equations in a model due to operational modes like temperature or pressure in different situations.

Table 6
Estimated parameters for PEMWE model simulation and benchmarking.

Parameters	M_1	M_2	M_3	M_4	M_5	M_6	M_7	M_8
Exchange current density i_0*	$1.2e^{-3}$	$1.4e^{-3}$	$1.5e^{-3}$	$1.6e^{-3}$	$1.7e^{-3}$	$1.8e^{-3}$	$1.9e^{-3}$	$2.3e^{-3}$
Limiting current density i_l* A/m^2	1.63	1.79	1.69	1.77	2	1.53	1.78	1.91
The effective surface area γ_j* m^2/s	$2e^{-5}$	$5e^{-6}$	$1e^{-5}$	$2.5e^{-5}$	$2.6e^{-5}$	$7.5e^{-5}$	$2.8e^{-5}$	$2.9e^{-5}$
Charge Transfer Coefficient α*	0.08	1.14	0.18	0.2	2.19	0.27	1.32	0.35
Concentration constant β*	0.7	5.2	3.1	2.8	3.3	4.6	3.9	3.8
Concentration constants β_1*	0.01	0.18	0.23	0.36	0.23	0.52	0.06	0.41
Concentration constants β_2*	0.17	0.47	0.94	0.66	0.83	0.48	0.37	0.54
Thickness of the membrane θ*	185.3	125.6	263.9	307.4	139.2	98.4	317.8	349.6
Membrane humidification λ*	52.4	33.7	78.5	58.9	97.3	99.4	38.7	67.1
Ohmic resistance Ω_M*	0.13	0.05	0.1	0.34	0.21	0.24	0.36	0.12
Ohmic resistance Ω_E*	0.32	0.19	0.14	0.23	0.08	0.23	0.31	0.45

Table 7
PEMWE technical specifications.

Parameters	Specifications
Model	QLC-1000
Number of cells N	4
Operational current range	0–36 A
Active area	50 cm^2
Operational voltage range	DC 12–15 V
Hydrogen production rate	1000 ml/min
Operational temperature	5–40 °C
Feed System	Gravity-fed

Optimization of the model is carried out using a Genetic Algorithm (GA), which is well suited to complex optimization problems with multiple local minima. The optimization process is initiated by randomly generating potential solutions within defined limits. Each solution undergoes evaluation, and selections are made for further breeding through methods such as tournament or roulette wheel selection. Crossover produces offspring, and mutations are introduced to increase diversity and enhance exploration of the search space. This cycle repeats until the predefined stopping criteria are met, such as reaching a maximum number of generations or observing minimal changes in the best solution. Constraints are applied to ensure that the solutions remain realistic and relevant [73].

5. PEM electrolyzer test bench and operational conditions

The study uses a PEMWE test bench equipped with current, voltage, and gas flow measurement instruments, integrated with software for data handling via the electrolyzer's digital controls. The system is calibrated before experiments to ensure data consistency and repeatability. After achieving steady state, data is refined to eliminate transient anomalies and then compared with electrochemical models to assess the PEMWE system's performance and pinpoint discrepancies between theoretical predictions and actual results. Fig. 5(a) shows the PEMWE test bench setup. Specific operational parameters and hydration control methods are detailed in Table 7.

Table 8 outlines the Balance of Plant (BOP) technical specifications for the electrolyzer, featuring a programmable power supply for precise input control tailored to the dynamics of PEM electrolysis. The test bench is equipped with a Labview suite for real-time data management and high-resolution flow meters to monitor hydrogen and oxygen production rates.

Fig. 5 details the key electrical components of the PEMWE test bench, which ensure both smooth operation and safety. The architecture includes a main switch that toggles between operational and standby modes, optimizing energy use and system readiness. An emergency push-button facilitates rapid shutdown in an emergency to protect both equipment and operators. Fuse protection also protects against electrical surges, which is essential for the protection of sensitive components. The power source is finely calibrated to meet PEMWE's specific energy demands, ensuring optimal performance and longevity. The precision of PEMWE test bench results hinges on maintaining strict operational conditions that mimic real-world environments for detailed system evaluation. Key to this is a stable temperature, consistently maintained at approximately 24 °C to optimize hydrogen production and minimize fluctuations. The test setup measures hydrogen flow at atmospheric pressure to maintain stable output and avoid pressure-related discrepancies. A gravity-fed water system ensures continuous water flow, preventing concentration overpotential. The bench's electrical setup prioritizes safety with streamlined controls, including a single switch-off and an emergency push-button as depicted in Fig. 5(b), ensuring operational safety and data integrity. At the heart of operations is a computer-controlled programmable power source that adjusts electrical parameters dynamically, capturing real-time data for subsequent analysis against established electrochemical models.

6. Results and discussion

The performance of various predictive models for PEMWE was assessed using four primary statistical metrics: Root Mean Error (MSE), Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and Coefficient of Determination (R^2), as outlined in Fig. 6. Based on the different models evaluated M_1 through M_8, different approaches to the simulation of PEMWE are explored, with varying degrees of mathematical integration and complexity. The performance of each model across four critical statistical measures shown in Fig. 6; model M_1 exhibited moderate performance with an MSE of 0.093, RMSE of 0.305, MAE of 0.234, and an impressive R^2 of 0.99076. Model M_4 showed the best overall performance with the lowest MSE (0.039), RMSE (0.199), and MAE (0.101), along with the highest R^2 (0.996), indicating a highly accurate model. Model M_3, designed to address complex dynamics, had the highest errors with MSE of 0.179, RMSE of 0.423, and MAE of 0.373, but still managed an R^2 of 0.982, reflecting reasonable model fit despite high variability in predictions.

While these metrics indicate that most models are quite robust, capturing the underlying dynamics of the PEMWE differences in error metrics largely demonstrate that model selection is influenced by the characteristics of the experimental data as well as the electrolyzers operational settings. Fig. 7 depicts the models' performance across the polarization curve. The line graph, representing voltage against current density, illustrates how closely each model M_1 through M_8 follows experimental data. Models M_4 and M_7 track the experimental curve closely, indicating their effective capture of the physical and chemical processes within the PEMWE under varied operating currents.

6.1. Comparison of hydrogen production

This section evaluates eight electrochemical models (HyPro1 through HyPro8) for their accuracy in predicting hydrogen generation at different current densities. 'HyPro' represents the estimated hydrogen production by each model, derived from (8), resulting in individual outputs like HyProx. The main objective is to determine which model aligns best with the test bench data, aiming to find the models'

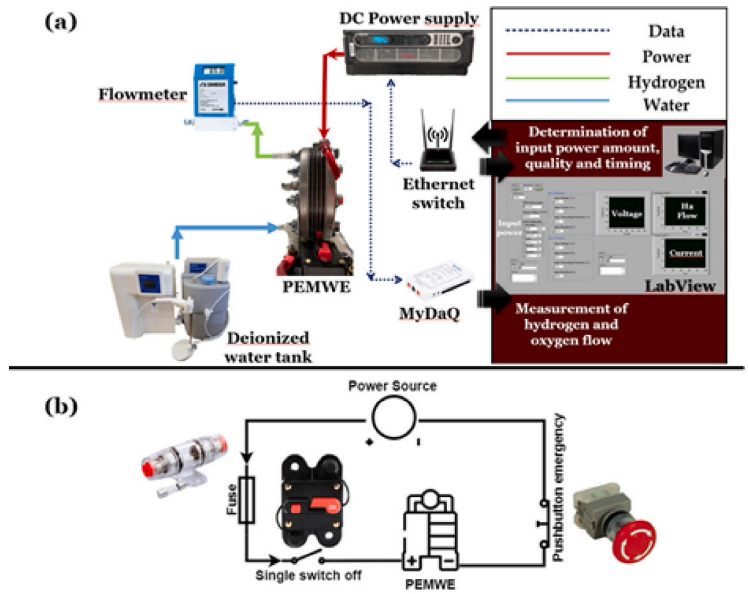

Fig. 5. (a) PEMWE test bench and its BOP, (b) schematic diagram of electrical safety and control components in PEMWE BOP.

Table 8
BOP technical specifications.

Component	Specification	Description/Function
Power supply	0–100 V and 0–100 A	Provides controlled DC power
Data acquisition	myDAQ (National Instruments) system interfaced with LabVIEW	Collects and processes real-time data from the test bench
H_2 flow	Omega FH	Volumetric emanation rates of hydrogen
Control mechanism	PC-controlled power supply	Provides control over the power delivered to the PEM electrolyzer through LabVIEW
Feed water reservoir	Elevated for gravitational flow	Stores and feeds deionized water to the electrolyzer using gravity
Temperature measurement	Precision thermocouples/sensors	Monitors and records the operational temperature of the PEM electrolyzer during the testing process

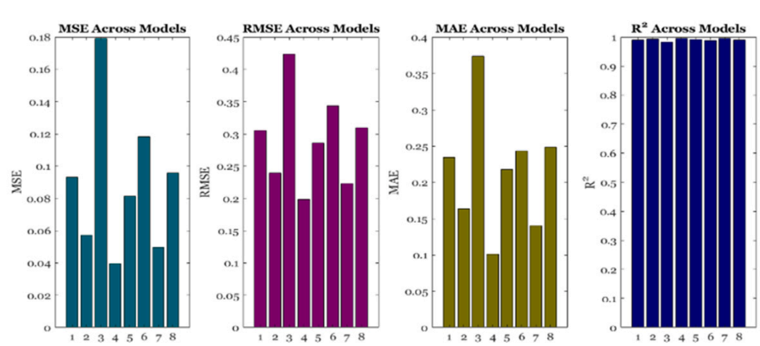

Fig. 6. Performance metrics comparison across models.

predictive capabilities for the model benchmark of PEMWE systems. This evaluation is crucial for exploring operational performance and developing appropriate EMSs. Fig. 8 displays hydrogen production rates at various current densities, juxtaposing actual data (black circles) with model predictions (coloured lines). The graph indicates that models HyPro2, HyPro4, and HyPro7 closely align with actual data, showing high accuracy, while HyPro3 and HyPro6 exhibit significant deviations, particularly at higher current densities.

Error analysis, detailed in Fig. 9, shows that M_4 consistently has the lowest error rates across all densities, highlighting its accuracy. Conversely, M_3 exhibits significant errors at higher densities, suggesting it requires refinement.

Fig. 10 measures errors in millilitres per minute (ml/min), with M_4 maintaining the lowest average error at about 14 ml/min, confirming its precision. Models M_3 and M_6, with average errors of 45 ml/min, indicate a need for adjustment to better match experimental conditions.

The analysis provided in both Figs. 9 and 10 are crucial for evaluating the relative performance of different models in consistent experimental settings. It allows identifying which models frequently deviate from observed measurements and points out the necessity for ongoing refinement. This approach is valuable for monitoring long-term trends in model performance and underscores the need for developing precise models. It also provides a critical evaluation of model performance, for

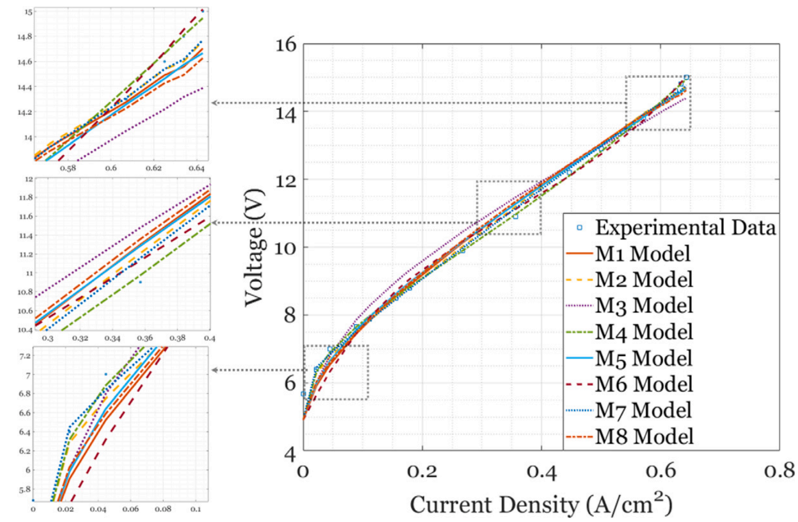

Fig. 7. Voltage–current characteristic comparison of PEMWE models with experimental data.

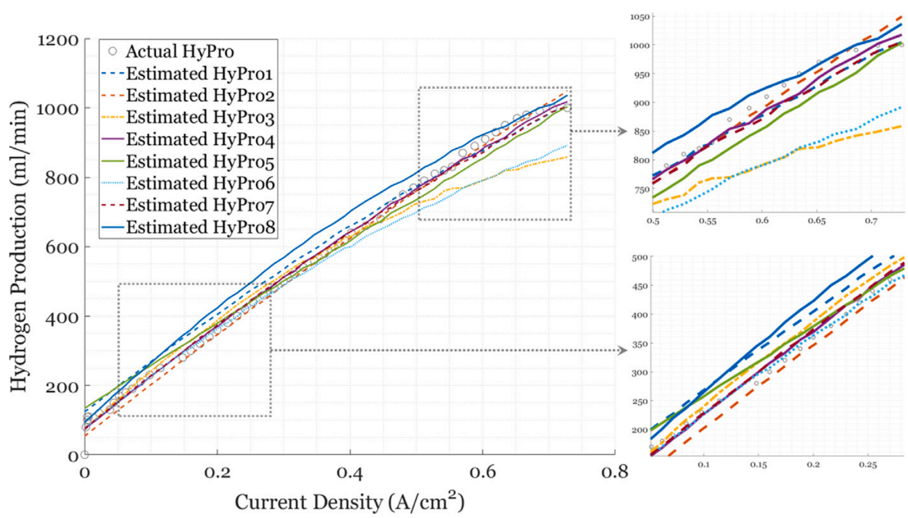

Fig. 8. Actual vs estimated hydrogen production models.

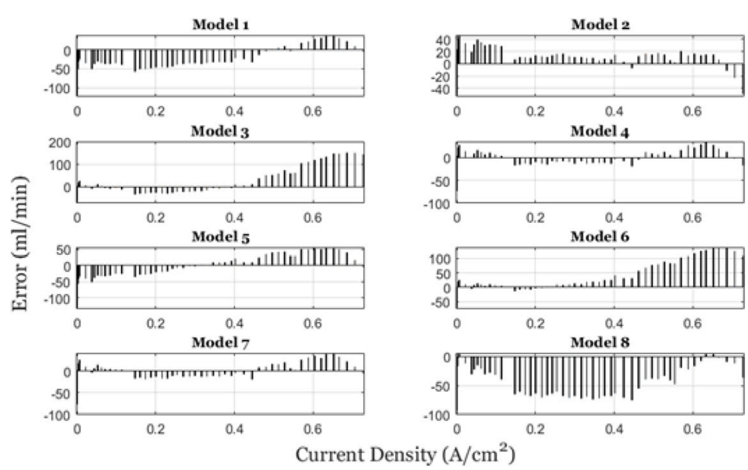

Fig. 9. Error analysis across current density for models.

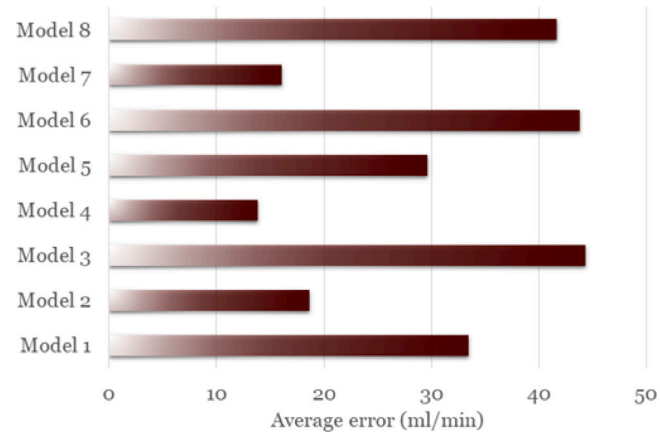

Fig. 10. Average error of model predictions for hydrogen production in PEMWEs.

identifying models like M_3 and M_3 that may need further tuning to enhance accuracy.

6.2. Comparative analysis of model complexity and performance

This section presents a comparative analysis of model complexity and performance. It enables the assessment of eight models based on their parameter configurations categorized into total, estimated, constant, and measured parameters as depicted in Fig. 11. The radar chart in this figure visually compares the models across these parameter categories to highlight their respective complexities and capabilities.

The comparison of models is categorized into four key parameter types: total, estimated, constant, and measured. The total parameters (a) encompass all parameters utilized within each model, offering a comprehensive view of the model's overall complexity. Estimated parameters (b) refer to those that are inferred rather than directly measured; a higher count of these parameters can lead to reduced predictive accuracy due to inherent uncertainties in the estimation process. Constant parameters (c), on the other hand, remain unchanged across various operational scenarios, playing a crucial role in maintaining the stability of the model's predictions. Finally, Measured parameters (d) are directly obtained from experimental data, and their inclusion can significantly enhance the model's robustness, ensuring that simulations are closely aligned with real-world operational conditions.

The analysis highlights that the selection of an appropriate model depends significantly on the balance between complexity and performance. Models with many estimated parameters might offer flexibility but at the risk of lower accuracy, while those with more measured parameters are likely more reliable but could be complex to implement. This benchmarking facilitates the choice of an optimal model for specific electrolyzer systems, aiming to improve simulation fidelity and operational efficiency.

6.3. Discussion

The discussion surrounding the performance evaluation of various predictive models for PEMWE systems reveals several critical insights into the selection and application of these models. The analysis of four primary statistical metrics (MSE, RMSE, MAE, and R^2) indicates that while models like M_4 exhibit superior overall accuracy, the choice of model must consider the specific operational and experimental conditions. The results demonstrate that models with lower error metrics are generally better suited to accurate simulations, but the variability in performance across different scenarios underscores the importance of tailoring model selection to the unique characteristics of the system being studied.

Furthermore, the comparison of hydrogen production models highlights the importance of aligning predicted data with experimental results. Models such as HyPro2, HyPro4, and HyPro7, which closely match the actual hydrogen production data, suggest that accurate modelling of PEMWE systems requires a careful balance between complexity and empirical validation. The deviation observed in models

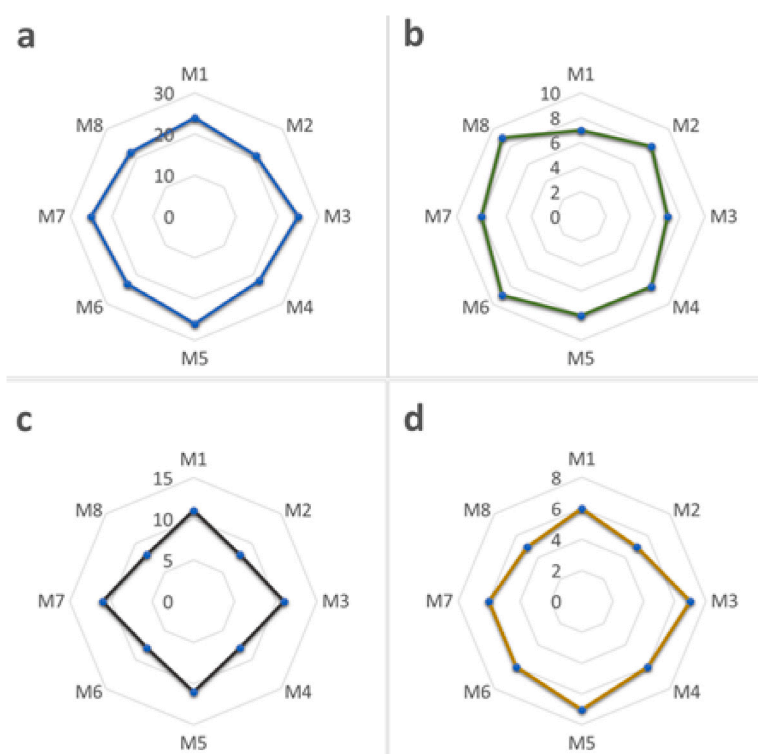

Fig. 11. Parameters comparison of models M_1 to M_8 (a) Total (b) Estimated (c) Constant (d) Measured.

like HyPro3 and HyPro6 at higher current densities indicates that further refinement is necessary to improve their predictive capabilities, particularly under more demanding operational conditions.

The discussion herein extends beyond mere model performance evaluation to explore the practical implications of the findings for real-world energy management. This study provides essential insights into selecting the most suitable models for specific applications by demonstrating how different models perform under various conditions. This serves the scientific community by outlining clear, actionable guidance and assists industry professionals in making informed decisions that enhance the operational efficiency and sustainability of PEMWE systems.

In the context of model complexity and performance, the radar chart comparison of parameters provides a comprehensive view of each model's strengths and weaknesses. Models with a higher count of measured parameters tend to be more robust and accurate, as they align more closely with real-world conditions. However, the increased complexity associated with these models may present challenges in implementation. This discussion emphasizes that achieving an optimal balance between model simplicity and accuracy is crucial for effective energy management in PEMWE systems, and this benchmarking approach serves as a valuable tool for guiding model selection and refinement.

7. Conclusion

An extensive benchmarking of PEMWE models is undertaken in this study, proposing grey-box approach, and employing a novel method for comparing submodels in different configurations. The analysis singles out Model M_4 for its exceptional performance, demonstrating the lowest error metrics like MSE, RMSE, MAE, and R^2, affirming its strong alignment with experimental data and high reliability in forecasting hydrogen production rates.

While Model M_4 proves superior in many scenarios, this study reveals that no single model achieves universal applicability. Certain models, such as M_3, exhibit elevated error rates at higher current densities, suggesting a need for targeted refinement to enhance their predictive accuracy. This variability underscores the necessity of customizing model selection based on the specific operational requirements and experimental conditions of the PEMWE systems in question.

Additionally, the research identifies the importance of a systematic approach to selecting and validating PEMWE the most appropriate models for specific applications. It illustrates that choosing the right model involves balancing computational simplicity with the depth of accuracy needed for effective energy management. In addition to facilitating the selection of the most appropriate model for specific applications, this comprehensive comparison provides a foundational framework for the development of scalable and efficient energy management strategies and power allocation.

Conclusively, the insights garnered from this benchmarking provide valuable guidelines for future enhancements in model precision and practical deployment. Beyond enriching the theoretical landscape of PEMWE modelling, this study bridges the gap between complex modelling and industrial applications, offering actionable knowledge that can significantly contribute to the advancement of sustainable hydrogen production technologies and the optimization of PEMWE systems for energy management.

CRediT authorship contribution statement

Ashkan Makhsoos: Writing – original draft, Visualization, Methodology, Formal analysis, Data curation, Conceptualization. **Mohsen Kandidayeni:** Writing – review & editing, Validation, Supervision, Data curation. **Meziane Ait Ziane:** Writing – review & editing, Writing – original draft, Validation, Formal analysis, Data curation. **Loïc Boulon:** Writing – review & editing, Supervision, Project administration, Funding acquisition. **Bruno G. Pollet:** Writing – review & editing, Supervision.

Declaration of competing interest

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

Acknowledgement

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC) (2018-06527).

Data availability

The data that has been used is confidential.

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In the aftermath of the benchmarking study, the thesis reorients its focus toward the broader implications of energy management in PEMWE systems. The empirical findings and model selection criteria articulated in the paper substantiate the theoretical models examined previously, thereby reinforcing the connection between experimental validation and operational performance. These insights enable a nuanced understanding of degradation mechanisms and inform strategies for multi-stack energy management. By assessing the creation of scalable and effective hydrogen production systems based on reliable, data-driven methodologies, the benchmarking study ultimately advances the dissertation's main goal.

3.2 Contribution of the research

This research makes significant contributions to the field of PEMWE by addressing key challenges in energy management, system design, and operational efficiency in modular configurations. Each objective of the study provides novel insights and practical tools that contribute to the advancement of both theoretical understanding and practical application in this field.

Benchmarking and Selection of Models for Energy Management

The first contribution is the development of a comprehensive test bench for benchmarking and selecting electrochemical models suitable for energy management in modular PEMWE systems. This involves an extensive review of all existing models in the field, followed by the selection and comparison of several promising candidates. A systematic selection method is introduced, filling a notable gap in the literature regarding model choice for modular systems. Additionally, degradation models are reviewed in-depth, and their relationships with various operational modes are analyzed and classified. This analysis provides critical insights into how degradation affects system performance over time, enabling more accurate simulations and predictions. Through the presentation of a clear methodology for model selection as well as an understanding of degradation effects, this contribution lays a foundation for improving power allocation in modular PEMWEs and energy management strategies.

Introduction of a design process map for modular PEMWE configuration

The second major contribution is the creation of a detailed design process map specifically for modular PEMWE configurations. This map serves as a practical guide for engineers and researchers, outlining the steps necessary to design efficient and adaptable modular systems. The research includes an analysis of a modular PEMWE equipped with a simple energy management system, which is then compared with a traditional single-stack PEMWE. This comparative study highlights the advantages and potential trade-offs of modular designs over conventional systems. It provides valuable insights into the design and implementation of next generation electrolyzer systems by demonstrating how modular PEMWEs can achieve better scalability, flexibility, and performance.

Development of an advanced energy management system

The third contribution is the development and implementation of an advanced energy management system tailored to modular PEMWEs. Building upon the insights and models identified in the previous objectives, this system optimizes the balance between energy efficiency and system degradation under varying conditions of renewable energy supply. The performance of this advanced system is compared with that of a simple linear modular PEMWE, showcasing improvements in operational efficiency and system longevity. By addressing the dynamic nature of renewable energy inputs and the specific needs of modular configurations, this contribution offers a robust solution that enhances the practical viability of PEMWEs in real-world applications. It offers a strategic framework that improves current operations while providing a basis for future innovations in energy management for HyPro systems.

Collectively, these contributions address critical gaps in existing research and offer practical tools and methodologies for advancing the field of PEMWE technology. The study enhances the understanding of model selection and degradation impacts, provides a structured approach to system design, and introduces an effective energy management strategy.

3.3 Selection of parameters for analysis of comparison results

The choice of parameters for analyzing the performance of PEMWE plays a critical role in ensuring effective energy management and system optimization. The utilisation factor that balances energy input with hydrogen output, as well as efficiency and degradation, was covered in earlier sections as key issues in PEMWE operations. Although efficiency models and equations are well-established, the operational sensitivity of degradation models necessitates a more targeted strategy for their classification and deeper comprehension. This section attempts to give a dedicated analysis of PEMWE degradation, which is frequently associated with different operating modes and has an impact on energy management.

Efficiency, degradation, and utilisation variables are among the metrics chosen for this research since they are essential to comprehending and contrasting system performance. Efficiency is modelled based on electrochemical principles, considering both cell voltage and energy efficiency. The utilization factor accounts for how well the system harnesses input power for HyPro, which is particularly important in modular PEMWE setups where power allocation can vary between stacks. Degradation, however, needs special attention due to its non-linear and multi-faceted nature. This section explores degradation phenomena by classifying models according to their operational modes and identifying degradation mechanisms that affect long-term system performance.

This dedicated study of degradation stems from the realization that operational modes such as dynamic cycling, constant load, or intermittent power supply significantly affect PEMWE components differently. Key components such as the membrane, catalyst layers, and porous transport layers degrade at varying rates due to the distinct stress conditions introduced by each operating mode. To derive a thorough understanding of how deterioration impacts total energy management in PEMWE systems, this section classifies degradation models based on these types.

The attached study on degradation models offers a detailed examination of PEMWE's degradation mechanisms and their implications for energy management. The paper thoroughly investigates how degradation accelerators such as temperature, current density, and intermittent RES affect the performance of PEMWEs. The methods used in the study include both empirical and theoretical approaches to capture the complex dynamics of degradation. With an emphasis on the membrane and catalyst layers, the review divides deterioration into three categories: mechanical, chemical, and thermal. Low humidity and high pressure were found to worsen the membrane's mechanical degradation, causing thinning and the creation of pinholes. Thermal degradation further erodes membrane integrity by desulfonating the polymer chains, while chemical degradation, which is fuelled by the oxidation of membrane components and the entry of contaminants, speeds up at high temperatures.

Several important facts are highlighted by the study's results. First, membrane degradation was found to occur more rapidly on the cathode side, influenced heavily by current density and temperature. The study successfully developed models that account for the non-linear relationship between operational parameters and degradation rates. It also establishes that catalyst layers, particularly the anode, suffer from dissolution and agglomeration of catalyst particles, reducing their effective surface area over time. According to the study, system performance may be preserved more successfully by integrating these degradation models into a comprehensive energy management plan, with power distribution being dynamically modified to reduce degradation.

3.3.1 PEMWE degradation models review: Implications for power allocation and energy management

In the preceding sections, the selection of key parameters—namely efficiency, degradation, and utilization—was identified as critical to the formulation of effective energy management strategies for modular PEMWE systems. The investigation clarified how varying operating modes, such as dynamic cycling and continuous loading, affect how system components degrade.

Building on these fundamental considerations, the subsequent study offers an in-depth exploration of PEMWE degradation models. By combining empirical and theoretical approaches, this study thoroughly investigates degradation events and explains the complex effects of temperature, current density, and the intermittent nature of renewable energy inputs.

The insights provided serve to bridge the gap between theoretical model development and practical energy management applications.

Journal: Journal of Power Sources (Elsevier)

Submission date: 19th September 2024 (Under review)

Proton Exchange Membrane Water Electrolyzers Degradation Models Review: Implications for Power Allocation and Energy Management

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Abstract

Proton Exchange Membrane Water Electrolyzers (PEMWEs) are central to the shift toward sustainable Hydrogen Production (HyPro), utilizing Renewable Energy Sources (RESs) to convert water into hydrogen and oxygen efficiently. Despite their high operational efficiencies and adaptability to varying pressure conditions, PEMWE systems face significant challenges due to component degradation in dynamic operating environments. This review comprehensively explores the intricacies of degradation phenomena within PEMWE systems, emphasizing the crucial role of advanced Electrochemical Degradation Models (DMs) in predicting and mitigating these effects. Through a detailed examination of the empirical and theoretical aspects of PEMWE operations, this paper highlights the integration of rigorous energy efficiency calculations, degradation mechanism studies, and the application of sophisticated modelling techniques to enhance the durability and performance of PEMWEs. The synthesis of findings from varied studies underscores the necessity of a systematic approach to PEMWE design and operation, which includes understanding key degradation accelerators such as temperature, pressure, and intermittent renewable energy utilization. By leveraging advanced DMs and innovative mitigation strategies, this review suggests pathways to optimize system performance and extend the lifecycle of PEMWE installations, thus contributing to the global endeavour for clean and sustainable energy solutions. Besides providing an overview of the current state of PEMWE technology, this study lays the groundwork for future innovations in HyPro by PEMWEs.

Keywords: Green Hydrogen; PEMWE; HyPro; Degradation; Renewable energy; Energy Efficiency; Energy Management

'word count [9813]

1. Introduction

In the pursuit of sustainable energy solutions, hydrogen emerges as a compelling alternative, offering a clean combustion process that releases only water vapour [1, 2]. Yet, the production and storage of hydrogen represent considerable challenges that hinder its broader adoption [3-9]. PEMWEs, leveraging RESs like solar, wind, and hydro, present a promising avenue for efficient hydrogen generation from water [10, 11]. Characterized by high efficiency, low operating temperatures, rapid response times, and versatile pressure operations, PEMWEs are increasingly favoured for HyPro, allowing scalable solutions tailored to specific needs [12-14].

Despite the advantages of PEMWE technology in fostering sustainable HyPro, it is crucial to confront its inherent limitations, including cost, materials, system efficiency, water quality demands, durability, and susceptibility to degradation processes [15]. Addressing these issues through ongoing research and development is vital for enhancing PEMWE performance and reliability [16-18]. Degradation phenomena pose significant challenges to the efficiency, reliability, and lifespan of PEMWEs, necessitating a deep understanding of these mechanisms and the development of strategies for mitigation [19, 20]. Although Electrochemical Degradation Models (DMs) offer insights into these complex processes, their computational intensity often limits their applicability in real-time energy management.

With the increasing capacity of PEMWE production systems to meet the demand for sustainable HyPro, as illustrated in Figure 1-1 [21], the scalability of PEMWE technology underscores the urgency of addressing degradation-related challenges [22]. The expansion of PEMWE installations enhances the significance of robust and accurate DMs in ensuring system reliability and performance over the long term, amidst predictions of continued growth [23]. The transition to larger-scale PEMWE systems introduces novel challenges, particularly in managing degradation impacts on system efficiency and durability. Consequently, a comprehensive understanding of degradation mechanisms and the application of precise DMs are indispensable for optimizing system performance and sustainability.

The significance of precise and efficient energy efficiency calculations in water electrolysis cannot be overstated, with key contributions from scholars like Lamy and Millet, who critically assessed energy efficiency coefficients under various conditions, laying foundational understanding [24]. Olivier et al. and others continue to explore low-temperature electrolysis system models, PEMWE modelling, and the electrical domain of PEMWEs to gain a more complete understanding of how these systems operate and degrade [25]. It is evident from the above reviews that PEMWE operations are complex, involving thermodynamics, kinetics, RESs, as well as power electronics and power transmission, also dynamic of system [26, 27]. Several aspects of performance and degradation are explored, including fundamental energy efficiency considerations and dynamic models that address power electronics control in PEM electrolysis [28-31].

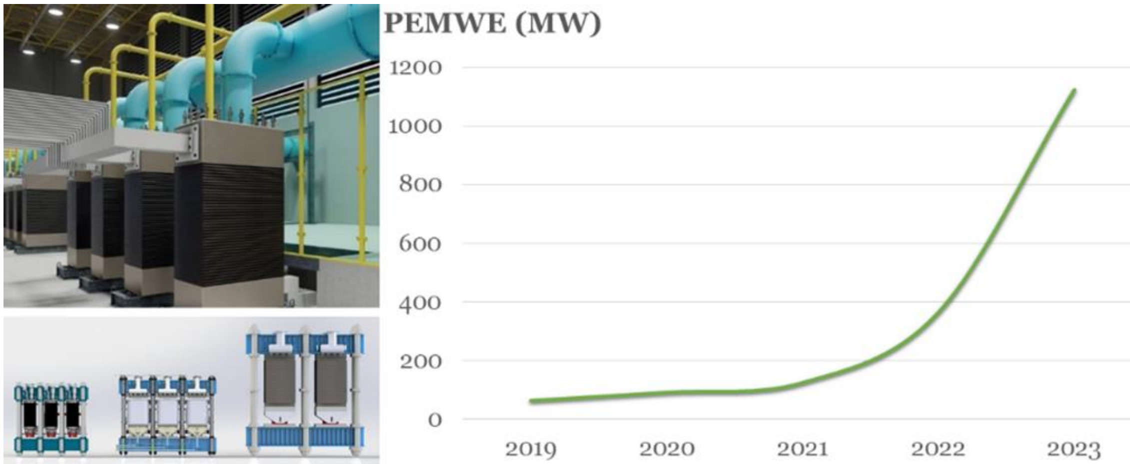

Figure 1-1 The total installed capacity of PEMWE in the last four years

The increasing adoption of large-scale PEMWEs underscores the essential need for advanced models and algorithms [32-34]. These tools are vital for guiding electrolyzer operations effectively across different scales, impacting overall system behaviour [35]. To investigate PEMWE systems, researchers use a variety of modelling techniques. These models vary from simple analytical to complex computational approaches, each with specific benefits and limitations tailored to different scenarios. Effective PEMWE modelling demands a thorough understanding of the physical and chemical fundamentals, alongside proficiency in numerical methods and simulation. This modelling is crucial for enhancing PEMWE design and operation, optimizing performance and efficiency.

As deployment scales up, the design, operation, and control of PEMWE systems must be optimized, highlighting the indispensable role of DMs in this process. DMs serve not just as a framework for comprehending complex degradation pathways but also as a cornerstone for developing scalable and dependable operational models. These models are instrumental in predicting and mitigating degradation impacts, optimizing operating conditions, and aiding in the strategic planning of maintenance and resource allocation. Degradation modelling is particularly critical, offering insights into longevity and performance decline factors. It is essential for robust system design, operational effectiveness, and sustainable use, enabling proactive degradation mitigation strategies. Additionally, understanding degradation processes—such as membrane, electrode, and component decay due to environmental stresses—is vital for developing maintenance strategies that extend the system's life.

The complexity and multifaceted nature of PEMWE degradation demands the development of sophisticated models for precise performance forecasting. The literature identifies key operational parameters—temperature, pressure, and current density, as well as the cyclic impact of using intermittent RESs—as significant degradation accelerators. The convergence of empirical evidence and theoretical models is crucial for enhancing the accuracy and utility of DMs, enabling strategies for predictive maintenance and the fine-tuning of operations for optimal performance. Tackling both reversible and irreversible degradation processes is critical for boosting operational efficiency, system durability, and economic viability, advancing the goal of sustainable HyPro and the adoption of green energy technologies [36].

The push towards green energy solutions, with HyPro through PEMWE at its core, necessitates the development of refined DMs and a unified approach to testing methodologies. Progress in these areas is essential to bolster the resilience of PEMWE systems, marking a significant stride towards their sustainable scale-up and the broader realization of hydrogen's potential as a clean energy vector. This holistic approach aims not only to address the immediate challenges of PEMWE technology but also to lay a foundation for its evolution, ensuring its role in a sustainable energy future.

The integration of empirical findings, such as degradation rates obtained from accelerated stress testing, into PEMWE models, marks a significant enhancement in their predictive accuracy. For example, findings that detail membrane thinning at 0.1 µm per 1000 hours and a 20% reduction in catalyst active surface area over 500 hours under certain conditions, provide invaluable insights into power allocation and energy management within PEMWE systems [37]. This quantitative approach is vital for the development of robust models that can accurately forecast system performance under varying operational scenarios.

Highlighting the work of Feng et al., the literature underscores the crucial role of understanding degradation mechanisms affecting electrocatalysts and Catalyst Layers (CLs), such as dissolution, poisoning, agglomeration, and migration. These factors critically influence PEMWE's performance and durability, emphasizing the necessity for advanced mitigation strategies, including the optimization of catalyst supports and layer structures [38]. Sayed-Ahmed et al. suggested that optimizing operational parameters could mitigate the adverse effects of load fluctuations and on/off cycles on durability and efficiency caused by PEMWE degradation under dynamic conditions [39].

Bazarah et al. contribute to the discourse by exploring how both static and dynamic factors, including stack design and operating conditions, affect PEMWE performance and durability. The review advocates innovative approaches like 3D printing and hydraulic cell compression to enhance electrolyzer efficiency, highlighting the importance of temperature, pressure, and water flow rate in system optimization [40].

Various analyses have been performed on degradation phenomena at both the micro- and macroscale, ranging from the integrity of cell components under various stresses to the performance of stacks and systems as a whole. Such comprehensive evaluations aim to elucidate the degradation processes affecting the Proton Exchange Membrane (PEM), CLs, and gas diffusion layers (GDL), alongside the broader system-level operational strategies [41, 42]. PEMWE production systems require an intensified focus on DMs to maximize efficiency and longevity. These models offer insights into degradation mechanisms such as catalyst deterioration [43], membrane ageing [44], electrode/electrolyte interface issues [45], and water management challenges. Accurately capturing degradation processes facilitates proactive measures to minimize degradation effects and ensure optimal system performance.

Despite detailed understanding of degradation mechanisms and their impacts within PEMWEs, there are significant gaps when it comes to applying this knowledge to effective power allocation and energy management practices. This disparity highlights the significance of this manuscript, which aims to merge insights from both microscale and macroscale degradation analyses. To facilitate the incorporation of advanced DMs into the design and operational protocols of PEMWEs, a comprehensive, actionable framework is being developed. This strategy is in line with practices used in the development of more mature technologies and moves the field toward improved system efficiency and reliability.

This review contributes to the existing literature by providing a detailed analysis of PEMWE degradation processes, exploring their implications for energy management, and classifying the current state of degradation modelling. By identifying operational modes that significantly affect degradation pathways and categorizing existing models, this work seeks to drive progress in HyPro on a large scale. It aims to deliver crucial insights to stakeholders in the HyPro ecosystem, highlighting the need to integrate degradation considerations into PEMWE development and operational strategies, advancing sustainable energy solutions.

By linking detailed studies of stacks and cells to their practical applications in system-wide energy management, this review offers a scientifically reliable guide to enhancing PEMWE performance and sustainability. This effort supports the ongoing development of green HyPro, envisioning a future where PEMWE technology is central to the global energy landscape.

The structure of the review is as follows: Chapter 1 discusses the fundamental components of PEMWEs and their vulnerabilities, providing a basis for understanding system susceptibility to degradation. Chapter 2 examines stack and system degradation in various studies and operational modes, revealing how different operational conditions influence degradation. In Chapter 3, the focus is on the analysis of degradation patterns and the identification of key parameters for effective energy management and power allocation in PEMWE systems. Finally, Chapter 4 synthesizes the findings and discusses future research and application directions, underscoring the need for continuous innovation and adaptation.

2. Fundamental Components of PEMWEs and Their Vulnerabilities

The PEMWE is an electrochemical device that splits water (H_2O) into hydrogen (H_2) and oxygen (O_2) gases using electricity. This process involves water oxidation at the anode, which produces O_2 and isolated hydrogen ions (H^+). At the cathode, H^+ (protons) combine with electrons (e^-) from an external circuit to produce hydrogen gas. A PEM separates these compartments, allowing protons to migrate while blocking electrons. These reactions take place in separate compartments divided by a PEM. Once the current has been applied to the PEMWE, water molecules lose e^- at the anode while protons move to the cathode through the membrane. As a result of the combination of protons and electrons at the cathode, hydrogen gas is formed. Using the PEM, gas separation can be achieved, which enables hydrogen gas to be collected as the desired product, while oxygen gas is typically released as a byproduct. Overall, the PEMWE facilitates the efficient and controlled production of hydrogen gas through electrochemical water splitting [46].

A PEMWE structure consists of a stack made of multiple units of cells. Figure 2-1 shows a PEMWE stack and its structural configuration. The stack consists of four individual cells, distinctly numbered. The positive and negative sides of the stack are explicitly marked with plus and minus symbols. One specific cell is meticulously zoomed in to enhance the comprehension of internal dynamics within a PEMWE cell, presenting a schematic representation. Various layers are demonstrated, and material transfer is represented.

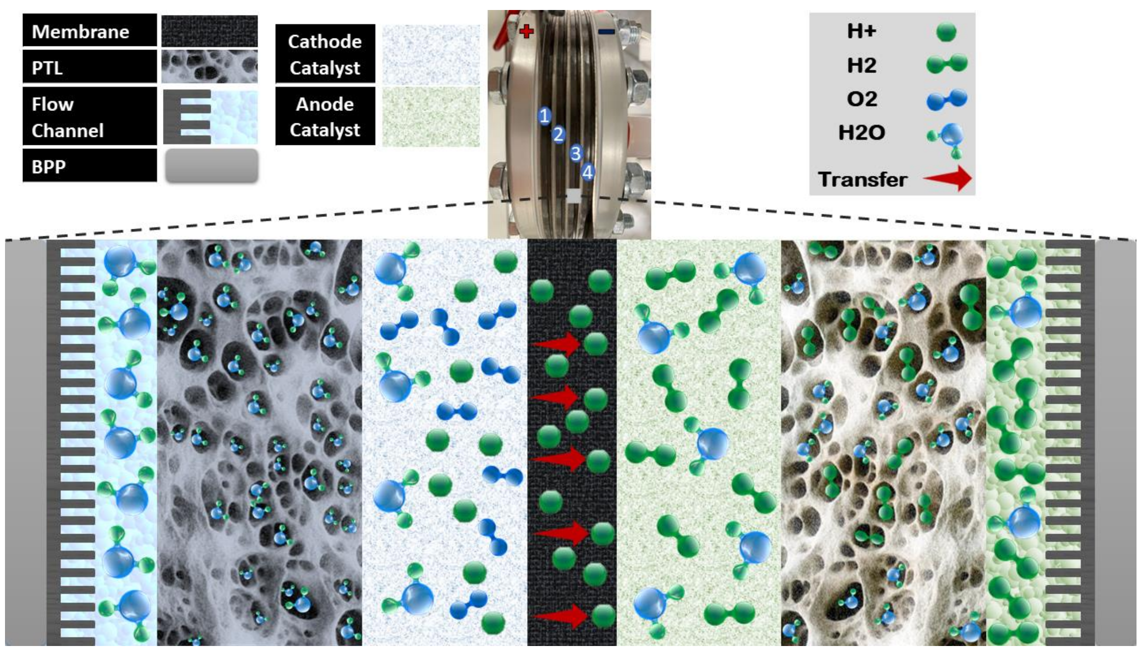

Figure 2-1 Degradation-Prone Components of a PEMWE

In PEMWEs, the membrane electrode assembly (MEA), CL, Porous Transport Layers (PTLs), and bipolar plates (BPPs) with flow channels make up the assembly (Figure 2-1). Among these components, the PTL is vital in optimizing the PEMWE system by facilitating improved utilization of the CL. The PTL serves as a conduit for efficiently transporting reactant gases and facilitates the distribution of reactants across the CL. Its porous structure allows for enhanced mass transfer, ensuring effective utilization of the catalyst material and promoting uniform electrochemical reactions [47]. By providing a favorable environment for gas diffusion and maintaining sufficient contact with the CL, the PTL contributes to the overall performance and efficiency of PEMWEs. This intricate interplay between the PTL and CL highlights the significance of their interaction in achieving optimized electrolysis processes in PEMWEs [48, 49].

In a PEMWE cell, electrolysis occurs by delivering water to the anode, dissociating into O_2, H_+, and e_-. The following equations can express the reactions taking place in a PEMWE. The overall reaction representing the electrochemical splitting of water into hydrogen and oxygen is depicted in Equation (1). It is important to note that this reaction occurs at the respective electrodes, with the anode responsible for oxygen evolution reaction (OER), as shown in Equation (2), and the cathode facilitating hydrogen evolution reaction (HER), as depicted in Equation (3) [28].

$$2H_2O \rightarrow O_2 + 2H_2 \qquad (1)$$

$$2H_2O \rightarrow O_2 + 4H_{(+)} + 4e_{(-)} \qquad (2)$$

$$4H_{(+)} + 4e_{(-)} \rightarrow 2H_2 \qquad (3)$$

As described and shown in Figure 2-1, a PEMWE cell, the layered structure, can be segmented into various components, each serving a specific function. The division of a PEMWE into these distinct layers and components allows for the precise management of reactants, efficient ion transfer, and effective separation of product gases. This intricate design is critical in optimizing PEMWE systems' performance and efficiency. However, despite their significance, these fundamental components are susceptible to diverse forms of degradation [50, 51]. For further investigation of degradation factors, the primary components can be divided as follows: *membrane, CLs, PTL, and end plates*.

Membrane

Membrane in PEMWEs serves as a critical component that allows the migration of protons while preventing the passage of electrons. It plays a vital role in maintaining reactant gas separation and facilitating ion transfer during the electrolysis process [52]. Membrane degradation in PEMWEs can be classified into mechanical, chemical, and thermal degradation mechanisms. Mechanical degradation is typically associated with early failures caused by mechanical stresses, inadequate humidification, and structural issues such as punctures, tears, and cracks. Chemical degradation occurs due to the attack of oxidizing species and metallic ions, resulting in chain scission, loss of functional groups, and reduced ionic conductivity. Thermal degradation involves the removal of sulfonic acid molecules from the membrane and is triggered by elevated temperatures [53].

To investigate the effects of temperature and current density on membrane degradation, Chandesris et al. [54] developed a 1D model. Their experimental findings confirmed that degradation primarily occurs on the cathode side and revealed the significant influence of temperature. The model effectively captured the complex relationship between current density and degradation rate, including a maximum at low current density. Furthermore, it accurately predicted the observed accelerated thinning of the membrane over time.

In the EU ELECTROHYPEM project, Siracusano et al. [55] focused on investigating membrane degradation mechanisms in PEMWE systems. Through their research, they successfully developed components with enhanced activity and stability, leading to improved durability, performance, and cost-effectiveness of PEMWEs. The optimized MEAs exhibited minimal irreversible decay and provided valuable insights into mitigating degradation under real-life operating conditions.

In their comprehensive review, Chen et al.[56] addressed the advancements and challenges in PEMWE technology, emphasising key components and their impact on performance. They highlighted the critical importance of high-performance electrocatalysts and long-term stability in PEMWEs. Additionally, they discussed strategies such as using composite materials and 3D printing to enhance the membrane and BPPs. The review offers valuable insights and directions for future research and development in PEMWEs. Mirshekari et al. [57] presents a pioneering study on high-performance, cost-effective membranes for PEMWEs. Utilizing reactive spray deposition technology, the fabricated MEAs demonstrate exceptional durability and activity with significantly reduced platinum group metal (PGM) loadings. These findings have promising implications for commercializing PEMWEs, with future research focusing on scaling up MEAs and optimizing the Pt recombination layer to further improve performance and reduce hydrogen cross-over.

Catalyst layer

Catalyst degradation in the CL of PEMWEs can have a detrimental impact on performance over time. This degradation can occur through the dissolution of catalyst materials, such as iridium and platinum, during operation. Passivation of the anode support can impede current flow, while agglomeration of catalyst particles can result in a loss of electrochemical surface area. Additionally, metallic cations can poison the catalyst, leading to increased charge transfer resistance and reduced reactivity [58]. In their mini-review, Pushkarev et al. highlight the importance of PEMWE for efficient and practical green HyPro. They emphasize the significance of OER electrocatalysts, particularly those based on noble metals like Ir or Ru, in determining the efficiency and stability of water splitting [59].

The cathode CL is responsible for HER, where protons from the membrane combine with electrons to form hydrogen gas. Similarly, the anode CL facilitates OER, where water molecules are oxidized, producing oxygen gas, protons, and electrons. Catalyst degradation in these layers can be caused by contamination, corrosion phenomena, or agglomeration of catalyst particles, resulting in reduced catalytic activity and compromised system performance [60, 61].

In their research on PEM water electrolysis, Pham et al. focus on optimizing catalyst materials and electrode structure to mitigate degradation and reduce the use of noble metals. They emphasize the importance of a holistic approach that considers all components of the electrode to enhance performance and durability. The study highlights the promising results achieved with supported iridium oxide catalysts, which exhibit improved dispersion and performance at low loadings. Critical parameters such as ionomer content, porosity, and interfacial contact are identified as significant factors in designing an optimal anodic electrode with low iridium loading. These findings offer valuable insights for future research and development aimed at addressing degradation and cost reduction challenges, with the goal of achieving widespread adoption of PEMWE technology [62].

Yu et al. conducted a comprehensive study on the degradation of a PEMWE with ultra-low catalyst loading. After a long-term test lasting 4500 hours, they proposed a mechanism for cathode degradation, involving the dissolution of platinum from nanoparticles and rapid reduction of platinum oxide. The analysis revealed that iridium dissolution and re-deposition were responsible for a significant portion of anode catalyst loss. Additionally, the distribution of platinum and iridium across the MEA was quantified, highlighting the formation of Pt-Ir precipitates in the membrane. These findings provide valuable insights into the degradation mechanisms and behavior of platinum and iridium in PEM water electrolysis systems [63].

Suermann et al. propose an electrochemical characterization protocol to investigate degradation factors in PEM water electrolyzers. They identify apparent degradation resulting from changes in catalyst oxidation states, as well as real degradation at the ohmic and mass transport overpotentials, particularly under higher current densities and longer operating times. This study offers valuable insights for the development of accelerated stress tests and the understanding of fundamental degradation mechanisms in PEM water electrolyzers [64].

PTL

The PTLs play a crucial role in PEMWEs by facilitating reactant gas transport and ensuring optimal utilization and reaction rates within the CLs. In addition, these layers help dissipate excess water generated during the electrolysis process [65].

Yuan et al. provide a comprehensive review of the PTL in PEMWEs, underscoring its significance in achieving stable electrochemical performance. The authors discuss different types of PTLs and their properties, with particular emphasis on the PTL/CL interface and its impact on overpotentials. The study investigates the influence of PTL microstructure on kinetic, ohmic, and mass transport overpotentials, providing a valuable resource for material development and quality control. The authors also emphasize the need for further research on PTL materials, interfacial properties, systematic studies, and corrosion effects to optimize PTL design and advance PEMWE technology [66].

Stiber et al. developed a PTL for PEMWE, specifically the porous sintered layer (PSL) on a low-cost titanium mesh (PSL/mesh-PTL). This novel design enabled operation at high current density (up to 6 A cm−2), elevated temperature (90 °C), and increased hydrogen output pressure (90 bar). Compared to the mesh-PTL alone, the PEMWE incorporating the PSL/mesh-PTL achieved the same cell potential but at a higher current density, resulting in 31% higher efficiency at a nominal load of 4 A cm−2. Pore network modelling demonstrated that the PSL/mesh-PTL design facilitated efficient gas and water management, eliminating the need for a complex flow field in the BPP. These findings not only enhance the economic attractiveness of PEMWE but also pave the way for large-scale integration of renewable energies with reduced CO2 emissions. The PSL/mesh-PTL developed in this study is now commercially available for interested laboratories to order from GKN Sinter Metals [67].

Rakousky et al. [68] focus on significant role of the anode's PTL and its surface condition on PEM electrolyzer performance. The document highlights that utilizing Pt-coated titanium PTLs substantially mitigates degradation, cutting down the rate to 12 mV/h compared to 194 mV/h with uncoated PTLs, primarily by preventing titanium passivation. This underscores the importance of surface coatings on PTLs for enhancing the durability and efficiency of PEM electrolyzers, suggesting a strategic approach to selecting and designing PTL materials to curb degradation rates effectively.

End Plates

Electrode/electrolyte interfaces in PEMWEs are susceptible to degradation, adversely affecting system performance and shortening lifespan. This degradation can manifest as electrochemical reactions, delamination events, or accumulation of reaction byproducts [46].

BPPs used in PEMWEs are particularly prone to hydrogen embrittlement, passivation, and corrosion. Titanium BPPs, in particular, require additional coatings to enhance their durability due to their susceptibility to hydrogen embrittlement and passivation. Corrosion can also occur due to chemical attacks from fluoride ions and hydrogen peroxide [69]. Prestat's analysis underscores the complexity of corrosion phenomena within PEMWE anodes, particularly concerning BPPs and PTL, traditionally comprised of titanium. Prestat's review elucidates the progression towards employing less costly materials, such as stainless steel, contingent on the development of effective protective coatings against the harsh oxidizing environment within the anode compartment [70].

A comprehensive analysis by Teuku et al. highlights the crucial role of BPP materials and fabrication methods in achieving optimal performance and durability in low-temperature PEMWEs. The review emphasizes the importance of corrosion and interfacial contact resistance and calls for innovative solutions to address these challenges. Notably, coating materials such as Ir, Nb, and Ta have shown promising outcomes in maintaining low interfacial contact resistance. Additionally, emerging techniques like metal 3D printing offer exciting possibilities for the cost-effective production of BPPs and corrosion mitigation in PEMWEs [71].

The shape of end plates also influences production and durability in PEMWEs. Jo et al. compared circular and square end plates in a highly pressurized PEMWE stack. They successfully designed lightweight end plates through finite element analysis and topology optimization, achieving weight reductions of 22.9% and 23.3% for circular and square end plates, respectively. Importantly, their analysis confirmed that the uniformity of clamping pressure was maintained in both end plate designs, thereby enhancing the performance of high-pressure PEMWE systems by ensuring gas-tight sealing and uniform pressure distribution [72].

In addition to BPPs, current collectors in PEMWEs, typically made of titanium, can undergo chemical degradation leading to passivation and corrosion. Mechanical degradation can also occur due to compression pressures that affect the properties of the current collectors and their interfaces with the CLs and BPPs. Compression pressure significantly influences mass transport, current transport, and overall cell performance [73].

To encapsulate the intricate dynamics of degradation across different components of PEMWEs and the innovative strategies devised to counteract these effects, Table 1 provides a succinct overview, underlining the mechanisms, pivotal discoveries, and significant contributions from various studies.

Table 1 Summary of Degradation Mechanisms and Key Findings in PEMWE Components

Component	**Degradation Mechanisms**	**Key Findings**	**Ref.**
Membrane	Mechanical, Chemical, Thermal	• Degradation occurs mainly on cathode side • Effects of temperature and current density significant • Development of components enhancing durability and performance • High-performance, cost-effective membranes developed	[52-57]

CL	Dissolution, Passivation, Agglomeration, Poisoning	• Degradation impacts performance over time • Optimization of catalyst materials and electrode structure critical • Supported iridium oxide catalysts show improved dispersion and performance • Pt and Ir degradation mechanisms identified	[58-64]
PTL	-	• Facilitates reactant gas transport and optimal utilization within CLs • PSL/mesh-PTL design enhances gas and water management • Pt-coated titanium PTLs reduce degradation rate.	[65-68]
BPP	Corrosion, Hydrogen Embrittlement, Passivation	• Titanium BPPs require coatings for durability • Shape and material of end plates influence production and durability • Innovative solutions and materials for BPPs and end plates can enhance performance.	[69, 71-73]

3. Stack degradation and Impact of operational modes

This section delves into the operational challenges and degradation mechanisms affecting PEMWEs, underpinned by recent studies. Critical factors such as electrical supply [74], suboptimal water management, elevated pressures [75], and high operating temperatures can significantly undermine the performance and longevity of PEMWE systems.

The distribution of water plays an essential role in maintaining PEMWE efficiency and mitigating component damage. A study by Frensch et al. [76] analyzed seven operation modes, including constant current and voltage, alongside current cycling, revealing that rapid current cycling enhances cell performance through ohmic resistance reduction. However, dynamic operations were associated with increased fluoride emissions and membrane thinning, highlighting the need for judicious operation mode selection and the development of strategies to foster efficient, durable PEMWE systems.

Research by Garbe et al. [77] focused on the impact of high-temperature conditions, observing that PEMWE cell operation at 100 °C led to a quicker rate of voltage loss and accelerated degradation compared to lower temperature operations. The study underscores the necessity for meticulous temperature regulation to leverage efficiency improvements against the backdrop of increased degradation risks.

Aßmann et al. [78] contributed insights into the primary degradation mechanisms within PEMWEs, such as anode catalyst dissolution, membrane chemical decomposition, and semiconducting oxides formation on metal components. These processes are exacerbated by conditions like high current density and dynamic operation, prompting the recommendation of accelerated stress testing protocols for evaluating the durability of emerging, cost-effective components and the importance of standardized testing hardware for reliable component evaluation.

The degradation of current collectors, essential for CL contact, is categorized into chemical and mechanical processes, highlighting the susceptibility of stack metallic components to degradation under pressure. The systematic examination of these mechanisms is crucial for ensuring the long-term operation and durability of PEMWEs. Figure 3-1 delineates the potential degradation mechanisms within various components of PEMWEs, including the stack, cells, and layers, illustrating the complex interplay of factors that compromise system integrity.

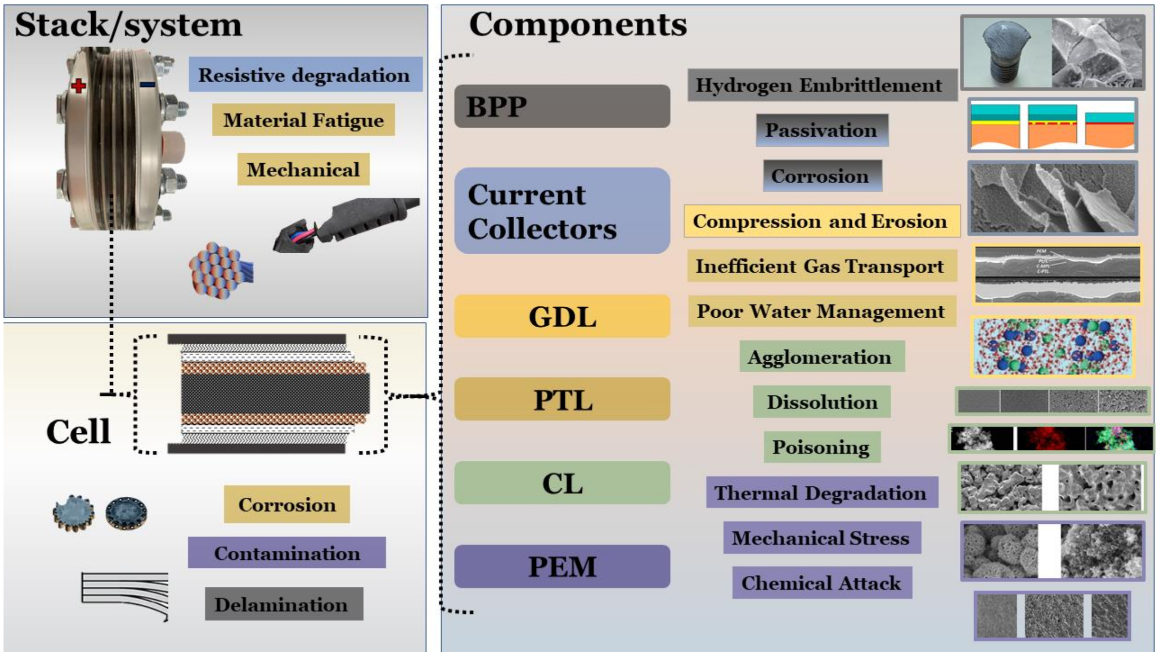

Figure 3-1 Degradation Mechanisms in PEMWE

Understanding the vulnerabilities and degradation mechanisms of PEMWE components—encompassing electrodes, membrane, catalysts, transport layers, flow channels, and BPPs—is pivotal for advancing system durability and efficiency. Strategies encompassing effective mitigation measures, material optimization, and sophisticated monitoring systems are essential for bolstering PEMWE performance and reliability. The forthcoming discussion on DMs aims to further elucidate these processes, fostering the development of precise maintenance strategies for sustaining PEMWE systems' performance over time.

Thermodynamics of the PEMWE model

As it was discussed in first Section and shown in equation (1), PEMWE splits water into hydrogen and oxygen. The water-splitting process requires energy input, typically supplied by electricity, to drive the electrolysis reaction. By considering the maximum heat energy input (48.6 kJ/mol), the resulting reversible cell voltage "V_{rev}" can be calculated, as described in Eq. (4).

$$V_{rev} = \frac{\Delta G}{n_e . F} = 1.23\ V \quad (4)$$

$$\Delta H = \Delta G + T\Delta S \quad (5)$$

Here "ΔG" is Gibbs free energy which means the change in Gibbs free enthalpy and equals 237.22 (kJ mol^{-1}). Temperature is shown by "T" and expressed in Kelvin. "ΔS" is the entropy of the reaction. "F" stands for Faraday's constant and is 96500. The quantity of involved electrons is also "n_e" [79]. Although, during the water-splitting process, entropy is generated inevitably, making it more appropriate to use enthalpy "ΔH" (5) instead of "ΔG" for potential calculations. Consequently, under standard conditions, the change in enthalpy is 285.84 $kJ\ mol^{-1}$. Therefore, we can calculate the minimum voltage required "V_{th}" for water electrolysis using Eq.(6) which represents the thermoneutral voltage.

$$V_{th} = \frac{\Delta H}{n_e.F} = 1.48\ V \tag{6}$$

It's worth noting that the thermal energy used in Eq.(4), also referred to as the Lower Heating Value (LHV), and the thermal energy expression in equation (6), known as the Higher Heating Value (HHV), play important roles in the calculations.

To accurately determine cell voltage "V_{cell}" and account for various losses, including thermoneutral voltage, additional considerations are needed. The main contributors to increased voltage in a PEMWE can be classified into three major categories as shown in (*7*): Ohmic losses "U_o", activation losses "U_a", and concentration losses "U_C". In some cases, however, only activation and ohmic losses are considered for purposes of simplifying the modelling process. Polarization curves, which depict the relationship between cell voltages and current densities, are commonly used to compare electrolysis cell performance as shown in Figure 3-2 [80].

$$V_{cell} = V_{th} + U_a + U_o + U_C \tag{7}$$

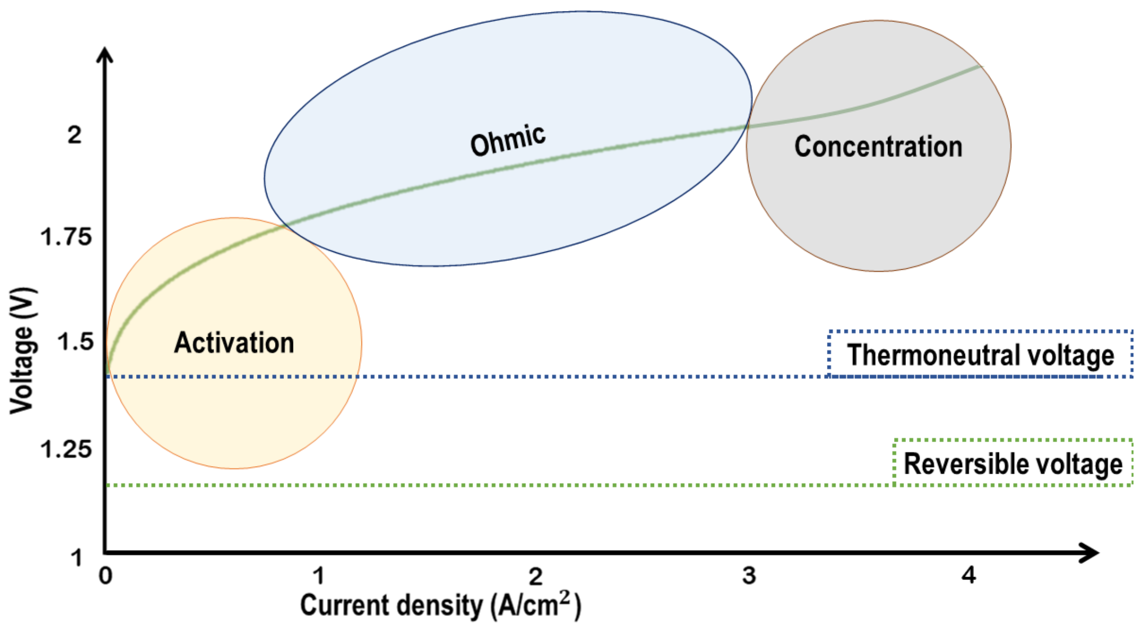

Figure 3-2 PEMWE cell polarization curve

PEMWE efficiency

In accordance with the fundamental principle of energy conservation described by the first law of thermodynamics, the conversion efficiency is determined by quantifying the amount of electrical energy converted into chemical energy. Water electrolysis efficiency is assessed using hydrogen HHV. Considering that water is supplied to the electrolysis cell in its liquid phase, the efficiency can be calculated using equation (8) provided below.

$$\eta_{el} = {}^{V_{th}}/_{V_{cell}} \times 100 \tag{8}$$

Consequently, the efficiency of a water electrolyzer can be calculated by a given current density for any given size of electrolyser.

In PEMWE, faradaic efficiency is one of the quantitative analyses which is useful in determining how many electrons are transported in the external circuit to the surface of the electrode for conducting the electrochemical reaction either OER or HER and other electrochemical reactions in the electrolytes. Therefore, the faradaic efficiency can be defined as the ratio between the experimentally evolved volume of gas value (hydrogen or oxygen) and the theoretically calculated volume of gas value, as shown in Eq. (9). The theoretical gas volume generated during electrolysis can be determined using Faraday's second law, considering the current density, electrolysis time, and electrode area. This is done assuming 100% Faradic efficiency, as described in Eq.(10). The actual amount of gas produced in experimental settings can be measured using techniques such as the water-gas displacement method or gas chromatography analysis.

$$\eta_F = {}^{\mathrm{V}_{HyPro}}\!\big/_{\mathrm{V}_{Hcal}} \times 100 \tag{9}$$

$$\mathrm{V}_{Hcal} = \frac{\mathrm{V_M}.I.t}{2F} \tag{10}$$

$$\mathrm{V_M} = \frac{R(273 + T)}{P} \tag{11}$$

Where "V_{Hcal}" shows the theoretically calculated H_2 volume. It can be calculated by Eq.(10) and "$\mathrm{V_M}$" which stands for molar volume of the gas ($Lmol^{-1}$), is the outcome of Eq.(11). "t" is time in seconds, and current is shown by "I" and in amperes (A). "T" denotes the temperature. The symbol R represents the ideal gas constant ($0.0821\ \mathrm{atm.K^{-1}.mol^{-1}}$), where "P" represents the pressure in units of atm, and F corresponds to Faraday's constant (96,485 $\mathrm{C \cdot mol^{-1}}$) [81, 82].

Yodwong et al. [83] focused on analyzing and modelling Faraday's efficiency in PEMWE based on variations in current density and hydrogen pressure. The results demonstrate that Faradaic losses are significant at low current densities. An increase in hydrogen pressure leads to a decrease in Faraday's efficiency. The findings highlight the importance of further research to investigate the model coefficients for different PEMWE and to thoroughly understand the impact of the high-pressure operation on Faraday's efficiency, thus providing valuable insights for optimizing electrolyzer efficiency in varying operating conditions.

Finally, the energy efficiency of the system, which is widely used in energy management and power allocation, can be calculated from (12) by determining the ratio between productive energy and input energy.

$$\eta_s = {}^{\mathrm{E}_{HyPro}}\!\big/_{\mathrm{E}_{input}} \times 100 \tag{12}$$

"E_{HyPro}" is productive energy, which represents the amount of hydrogen produced per unit of time, and its HHV. On the other hand, "E_{input}" stands for the input energy the multiplication of input voltage and current in terms of time. This efficiency calculation provides valuable insights into the system's ability to efficiently convert input energy into usable hydrogen energy. This makes it a crucial metric in evaluating its overall performance and utilization [84].

The overall energy efficiency of the PEMWE system can be determined by multiplying the individual efficiencies of different components as illustrated in Eq.(13). This includes cell voltage efficiency and Faraday efficiency. Additionally, the efficiency of auxiliary equipment specific to each system should also be considered.

$$\eta_{PS} = \eta_{el} \times \eta_F \times \eta_{au} \tag{13}$$

A PEMWE system's overall energy efficiency, denoted as "η_{PS}", is determined by the product of multiple individual efficiencies. One of these efficiencies is cell voltage efficiency, "η_{el}". This reflects the cell's effectiveness in converting electrical energy into chemical energy (Eq.(8)). Another important efficiency is the Faraday efficiency, "η_F", which accounts for losses resulting from gas diffusion and is closely associated with the operating pressure, p. It quantifies the extent to which the actual amount of hydrogen produced matches the theoretical amount based on Faraday's laws. Additionally, system energy efficiency should consider auxiliary equipment, "η_{au}". This is specific to each system and contributes to overall performance and energy utilization [85].

Degradation

Electrochemical models for degradation inherently involve the analysis of in situ components, wherein the degradation of specific elements plays a critical role. When it comes to PEMWE, degradation of the membrane is of the utmost importance due to its significant impact on system performance and durability. Understanding the mechanisms and factors contributing to membrane degradation is essential for developing accurate and reliable electrochemical models that can effectively predict and mitigate degradation effects in PEMWE systems.

Chandesris et al.[54] investigated the influence of temperature and current density on chemical degradation rate. They found that membrane degradation primarily occurred on the cathode side and observed a significant increase in chemical degradation with increasing temperature. The effect of current density was more complex, with a maximum degradation rate observed at low current densities. A 1D PEMWE model incorporating degradation mechanisms was developed, successfully capturing the temperature and current density effects on degradation rates. This included unexpected behaviour at low current densities. The model was further utilized to analyze the time evolution of membrane thickness under constant current density, demonstrating the acceleration of degradation over time. Equation (14) describes the temporal changes in the membrane thickness within the model. As the membrane thins, the oxygen crossover intensifies, resulting in an accelerated fluoride release and membrane degradation. Consequently, the membrane thinning process is expected to follow an exponential rather than linear time evolution, due to this acceleration.

$$\frac{d\delta_M}{d_t} = \Delta\delta_M R_f \tag{14}$$

"$\Delta\delta_M$" in this equation refers to the reduction in membrane thickness per mole of released fluoride. "R_f" represents the rate of fluoride release in moles per second, obtained from the membrane DM. To address the issue of modelling membrane thinning and its associated geometric changes, the research study implemented a change of variable in the spatial parameter "X". This variable represents the direction of membrane thickness as shown in Eq. (15). "δ_M^0" in this equation demonstrates the membrane thickness at time zero.

$$X = \frac{\delta_M}{\delta_M^0} X_0 \quad (15)$$

This approach allowed for an effective representation of evolving membrane structure and its influence on overall system dynamics. The methodology employed in the study enabled the researchers to overcome the challenge of incorporating membrane geometry changes into the modelling process.

Supply through renewable energy

Given the increasing integration of RES into power systems, efficient power allocation and energy management have become paramount. RES, such as solar and wind power, are inherently intermittent and subject to fluctuating availability. This variability poses challenges to maintaining a stable power supply and managing energy generation. To ensure optimal utilization of RES and grid stability, effective power allocation strategies need to be implemented. It is possible to balance supply and demand, maximize system efficiency, and minimize curtailment by intelligently distributing and managing RES power. Furthermore, efficient energy management plays a crucial role in mitigating RES fluctuations' impacts on system components. It also reduces the degradation of power generation and conversion devices, such as PEMWE systems. By implementing advanced control and optimization techniques, it is possible to optimize energy flow, minimize degradation, and enhance the overall performance and longevity of PEMWE systems.

In their study Lu. [85] focuses on the optimization of power allocation in a wind-hydrogen system with a multi-stack PEMWE, considering degradation conditions. As illustrated in Figure 4, degradation can have a significant impact on the efficiency of PEMWEs. The study contributes to slowing down degradation and improving the energy efficiency of multi-stack PEM water electrolyzer arrays in wind-hydrogen systems, providing practical significance for large-scale applications. They showed how researchers developed a three-dimensional multi-physics field model of PEMWE to analyze the relationship between efficiency and degradation. They proposed a power allocation strategy consisting of a control module and an execution module. The control module quantifies the electrolyzer degradation using the voltage degradation rate and determines power allocation in order to minimize degradation. The execution module utilizes an extended duty cycle interleaved buck converter controlled by fuzzy PID (Proportional-Integral-Derivative) control to supply power to each PEMWE stack. Computer simulations were conducted, and the results showed that the wind-hydrogen system achieved an energy efficiency of 61.65% over one year of operation, with a voltage degradation of 7.5 V in the PEM water electrolyzer single-stack. The proposed power allocation strategy demonstrated efficient signal-following capability with low current ripple. Dynamic operation of PEMWE leads to degradation, resulting in increased operating voltage. PEMWE voltage degradation varies under different operating conditions, with frequent start-stop switching and high constant input power causing significant degradation, while low and medium constant input power has a lesser impact on degradation rates. They demonstrate the effect of degradation on PEMWE efficiency by Figure 3-3 , it is brought here to show how the performance of PEMWE can be affected by degradation.

With the assumption that voltage degradation rates under different operating conditions are independent of each other. In addition, all cells within the same PEMWE single stack exhibit the same performance. In accordance with this assumption, the total voltage degradation "ΔV_D" of the PEMWE single stack can be expressed in Eq.(16) based on ref.[85] as the cumulative effect of individual voltage degradation contributions from each cell.

$$\varDelta V_D = n_{el} \times (V_{cr} \times t_{cr} + V_{ct} \times t_{ct} + V_{fh} \times t_{fh} + V_{fl} \times t_{fl} + V_m \times t_m) \quad (16)$$

The different operating conditions in the Eq.(16) PEMWE system can be categorized as follows: "V_{cr}" stands for constant rated power operation, "V_{ct}" refers to constant turning power operation. Similarly, "V_{fh}" represents high power fluctuation operation, "V_{fl}" corresponds to low power fluctuation operation, and "V_m" denotes maintaining operation. These categories represent various modes of operation that can have distinct effects on the voltage performance of the system. In addition, the variable "t," with the same subscript as the voltages mentioned earlier, represents the duration or time that the PEMWE system operates in the corresponding operational mode. It serves as a parameter to indicate the length of time the system remains in a specific operational situation, such as constant rated power, constant turning power, high power fluctuation, low power fluctuation, or maintaining operation. The value of "t" influences the extent of voltage degradation experienced by the system during a particular operational mode.

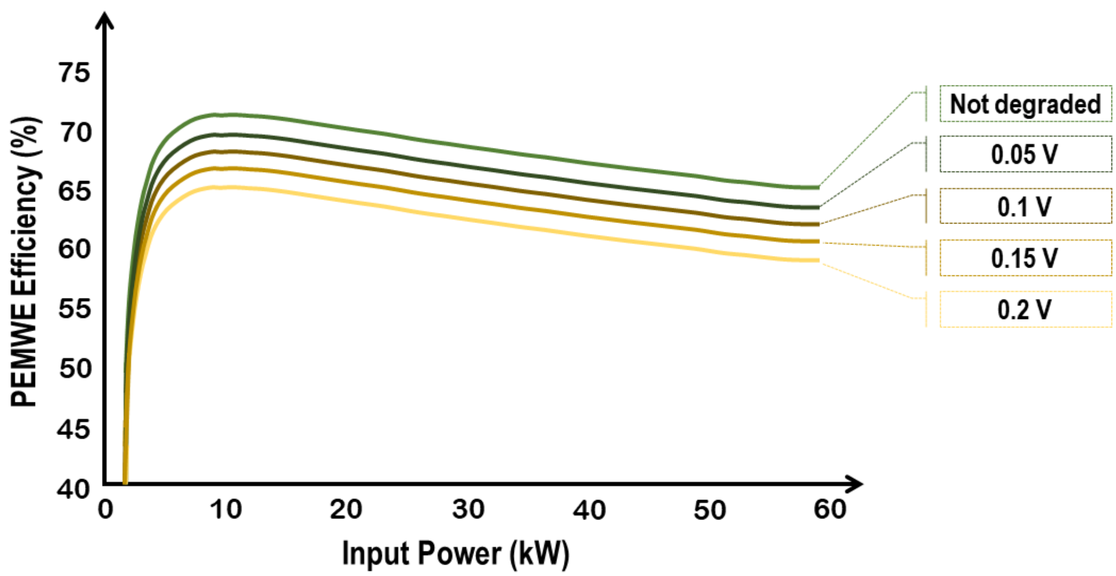

Figure 3-3 PEMWE efficiency at different voltage degradation levels [85]

Prediction of degradation is crucial for systems' long-term performance and durability. Various models and approaches have been developed to forecast degradation processes and estimate their impact on system operation. These predictive models for systems like PEMWE consider factors such as operating conditions, electrode materials, catalyst activity, water management strategies, and cell design. By analyzing degradation mechanisms, identifying key degradation indicators, and considering the interplay of multiple factors, these models provide valuable insights into degradation trends. They allow proactive maintenance and optimization strategies. By predicting degradation accurately in PEMWEs, energy management and power allocation can be improved, resulting in improved system efficiency and increased lifespan of the equipment. Furthermore, these predictive models aid in the development of advanced mitigation strategies, materials, and designs to minimize degradation effects. This will enhance PEMWE performance and reliability.

Degradation prediction in PEMWE under dynamic conditions can be achieved by considering the phenomenological dependence of current density on time. By accounting for the observed linearity of the High frequency resistance (HFR) over time, the authors derived an equation (Eq.(*17)*) that accurately describes the near-linear decrease of current density. The degradation rate of overpotential under galvanostatic conditions was also determined (Eq.(*18)*), showing a logarithmic increase with time and a slowing degradation rate. The projected average degradation rate over 100.000 hours was approximately 0.6 μV/h. These findings emphasize the significance of minimizing both HFR and the rate of change of HFR ($^{d\Omega_{HF}}/_{dt}$) to mitigate degradation and achieve desired operational targets in PEMWEs.

$$i(t) = \frac{i(t_0) \times \Omega_{HF}(t_0)}{(\frac{d\Omega_{HF}}{dt}.t + \Omega_{HF}(t_0))} \quad (17)$$

$$U_O(t) = \left(\frac{b}{2.303}\right).\log\left(\frac{d\Omega_{HF}(t)}{dt}.t + \Omega_{HF}(t_0)\right) + U_O(t_0) \quad (18)$$

In these equations "Ω_{HF}" stands for HFR ($\Omega.cm^2$), "t" is the desired time and "t_0" is the zero time (the existing situation for predictive purposes). "b" is part of the coefficients of the Tafel slope (it depends on materials and might change). "U_O" represents overpotential voltage in Volts [86].

4. The Role of Degradation in Energy Management and Power Allocation in PEMWE

The durability, efficiency, and performance of PEMWEs are critically influenced by degradation phenomena. The design of system architecture, alongside specific configurations and operational modes, plays a pivotal role in influencing the rates and patterns of degradation. Such variability necessitates careful consideration within the framework of energy management strategies and power allocation to optimize system performance and extend its lifespan. Understanding these factors is essential for developing robust PEMWE systems that can maintain high efficiency over time and adapt to varying operational demands.

This section provides a systematic review of existing literature that explores the role of degradation in the energy management and power allocation of PEMWEs. Initially, the review will highlight the importance of considering degradation in the energy management of various energy systems, particularly electric vehicles and fuel cell/battery hybrids as discussed by Alyakhni et al. [87] and Wang et al. [88]. These studies emphasize the need for health-conscious energy management systems (EMSs) to extend vehicle lifespan and reduce running costs, incorporating both electrochemical and empirical models to mitigate the degradation of key components like Li-ion batteries and proton exchange membrane fuel cells (PEMFCs).

In addition to the static DMs, Dynamic Degradation Models (DDMs) capture the time-dependent behavior of PEMFCs, taking into account factors such as the start-stop cycle and load variations that affect the system longevity. Multi-scale modelling approaches address different degradation mechanisms—from catalyst degradation to membrane deterioration—enabling targeted mitigation strategies [89-93].

Health management systems that integrate DMs are pivotal in extending the service life of PEMFCs by enabling real-time power allocation and proactive maintenance [94-99].

Operational strategies, considering load, temperature, and humidity, optimize energy usage and enhance the system's cost-effectiveness by mitigating degradation [100-117]. Figure 4-1 illustrates the key considerations in the energy management of energy systems, encapsulating the interconnected roles of system design, degradation impact analysis, dynamic and multi-scale modeling, health management systems, and operational strategies. This graphical representation underscores the integrated approach required to effectively manage and mitigate degradation across different types of energy systems, ensuring optimal performance and extended system lifespan.

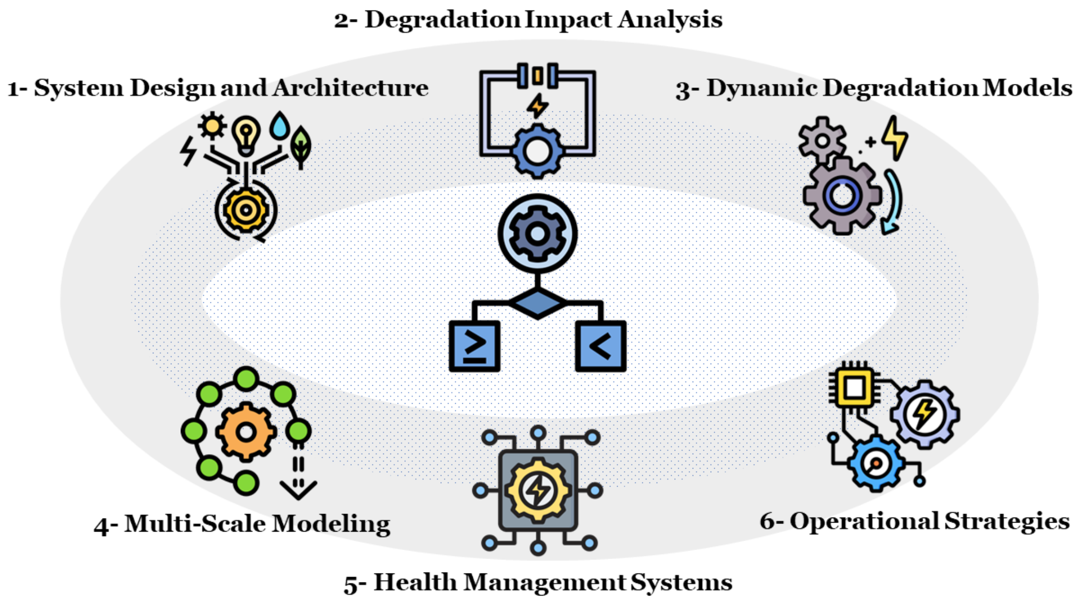

Figure 4-1 Key Considerations in Energy Management of Energy Systems

Degradation Modes in PEMWE Systems: Classification and Impact on Energy Management and Power Allocation

Building upon insight into the key considerations in energy management of energy systems, this section endeavours to classify crucial degradation modes that influence PEMWE system performance. It sets a framework for identifying and prioritizing key degradation modes, which will be instrumental in subsequent analyses to optimize power allocation and energy management within PEMWE applications.

It has been demonstrated in several studies, including one by Norazahar et al. [118], that operational variables like current density and anode water content have significant impact on PEMWE reliability, underlining their significance in terms of system performance and degradation [76]. Adverse operational conditions—such as high overpotential, acidic environments, and elevated pressure—along with factors like high current density and improper material choices, exacerbate component degradation in PEMWE systems, especially affecting membranes, BPPs, and PTLs under ***high-pressure conditions*** [73, 119].

The resilience of PEMWE systems to the intermittent nature of RESs, which leads to ***power fluctuations***, is a major degradation challenge [120]. Such fluctuations can disturb the consistent power supply to electrolyzers, leading to dynamic operating conditions that accelerate the degradation of critical components like catalysts, membranes, and electrodes [121-123], thereby reducing system performance and increasing maintenance needs [124].

High input power can also precipitate rapid component degradation due to increased stress and temperatures, which adversely affects system longevity and performance. Pham et al. [125] discussed advancements in catalyst materials and electrode structures aimed at minimizing degradation while enhancing the power density and durability of PEMWE systems.

Conversely, ***low power levels*** can cause inadequate reactant supply, leading to poor water management and decreased efficiency, thereby diminishing system performance [126]. Rapid changes in power input also introduce mechanical and thermal stress, contributing to accelerated degradation [127-130], emphasizing the importance of effective power management strategies to counterbalance these effects.

Li et al. [131] pointed out the ***economic impact of degradation*** in PEMWE systems, advocating for optimized component design and power management strategies to enhance system durability and reduce operational costs. Similarly, start-stop cycles introduce thermal and mechanical stresses that accelerate degradation [85], while Kuhnert et al. [132] identified protective strategies during shutdown periods to mitigate degradation in photovoltaic-PEM electrolyzer systems.

During normal operation, degradation occurs gradually through chemical reactions, corrosion, or impurities, affecting catalysts, electrodes, and membranes [133]. The system's pressure and temperature also influence degradation processes, with high-pressure conditions potentially introducing contaminants that can degrade catalysts and electrodes [134, 135]. Chandesris et al. [54] and Ogumerem & Pistikopoulos [136] further explored the impacts of temperature and operational strategies on membrane degradation, proposing optimized thermal management strategies to extend system life.

As PEMWE systems age, they experience a natural decline in performance due to the gradual loss of catalysts, membrane deterioration, and electrode performance [137]. By adopting advanced diagnostics, control algorithms, and maintenance strategies, these ageing effects can be mitigated, enhancing system reliability and longevity.

In sum, understanding and managing the diverse degradation modes in PEMWE systems is essential for optimizing energy management and power allocation, thus ensuring sustainable and efficient operation. Table 2 provides a classification of operational degradation modes in PEMWE systems, highlighting the effects of these modes on system performance and its components. The table categorizes and summarizes the impacts of various degradation modes, including input power variations, start-stop cycles, normal operation, pressure and temperature effects, and ageing.

Table 2 Classification of the effects of PEMWE operational degradation modes

Degradation Mode	Result
High input power	Accelerate degradation due to increased stress
	Higher operating temperatures
	Dissolution of catalyst
	Agglomeration of catalyst
	Passivation of catalyst support
	Passivation of electrode
	Dissolution of membrane
Low input power	Insufficient power may lead to stop-start
	Reactant supply issues
	Decreased efficiency
	Poor local power distribution in cell
Input power fluctuations	Induce voltage fluctuations
	Temperature variations
	Poisoning of membrane

	Accelerating degradation mechanisms in CL, membranes, and electrodes
Start-stop cycles	Thermal and mechanical stress
	Material fatigue and degradation of catalysts and electrodes
	Agglomeration of catalyst
	Poisoning of membrane
Normal operation	Extended operation can result in gradual degradation catalysts, electrodes, and membranes due to chemical reactions, corrosion
	Impurity exposure
Pressure	Degradation in catalysts (poisoning) and electrodes
Temperature	Catalysts and electrodes membrane degradation
Ageing	Gradual catalyst loss, membrane deterioration
	Decline in electrode performance and Current reversal during power off
	Decreased efficiency and performance
	Catalyst poisoning

This understanding paves the way for developing robust control strategies and energy management schemes that address the specific degradation challenges associated with PEMWE systems. Understanding and effectively managing these degradation modes is crucial for optimizing the performance, efficiency, and durability of PEMWE systems. It enables the development of robust control strategies and energy management schemes tailored to address the specific degradation challenges associated with PEMWE systems. Figure 4-2 illustrates the diverse operational conditions impacting PEMWE systems. It depicts various factors such as renewable energy inputs, power levels (high and low), power fluctuations, and operational modes like start-stop cycles. Also shown are environmental conditions like pressure and temperature, and system responses such as ageing, all contributing to the degradation dynamics of PEMWE systems.

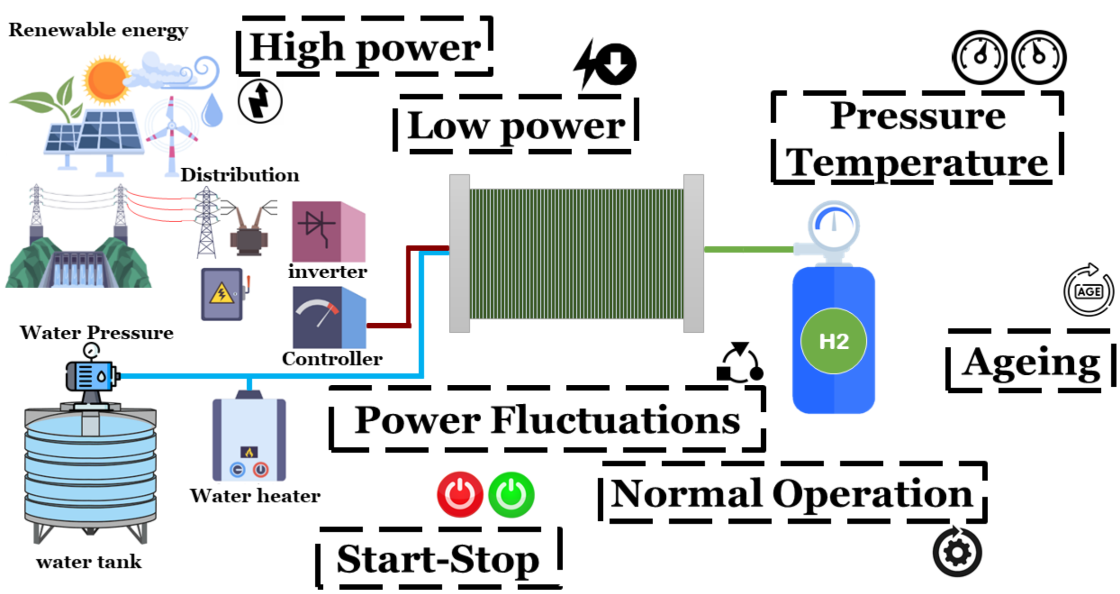

Figure 4-2 Operational Dynamics and Degradation Influences in PEMWE Systems

Based on the literature review, Table 3 presents the reported and measured degradations in PEMWE systems under various operating modes. Degradation modes classification is crucial for understanding and managing performance degradation in PEMWE systems. The importance of this is particularly apparent when it comes to energy management and power allocation. Degradation modes include low or high input power, input power fluctuations, start-stop cycles, normal operation, pressure and temperature effects, and ageing. These degradation modes have significant implications for PEMWE systems' efficiency, durability, and overall performance, and understanding them is essential for effective mitigation strategies. By comprehensively examining these degradation modes, researchers and engineers can develop effective control strategies and energy management approaches to mitigate degradation. This will optimize system performance and extend PEMWE systems lifespan.

Table 3 PEMWE degradation in various working modes

Mode	cell	Current density (A/cm^2)	T (h)	D	Unit	Ref.
System efficiency degradation	N/A	N/A	N/A	2.09	%/year	[138]
Under constant current	N/A	N/A	N/A	0 - 230	mV/ h	[133]
Normal operation	50	2	8000	1.5	μV/h	[85]
Low power fluctuation operation	50	2	8000	50	μV/h	[85]
Constant turning power operation	50	2	8000	20	μV/h	[85]
High power fluctuation operation	50	2	8000	66	μV/h	[85]
Constant rated power operation	50	2	8000	196	μV/h	[85]
Solar fluctuating condition	N/A	1	N/A	3.5	mV/ h	[127]
constant current condition	N/A	1	N/A	2.05	mV/ h	[127]
fluctuating condition (average)	N/A	1	100	7.8	mV/h	[127]
Constant Current	1	N/A	7800	35.5	μV/h	[139]
Constant Current	9	N/A	4805	589	μV/ h	[139]
continuously and a degradation rate	10	N/A	2000	1.5	μV/h	[140]
constant operation	1	2	N/A	194	μV/h	[141]
hydraulic cell compression constant current(65°C)	1	2	600	4.43	μV/h	[135]
constant current	N/A	4	400	200+	μV/h	[64]
constant current	N/A	1	400	10 ± 30	μV/h	[64]
Dynamic	1	0.75	830	35.2	μV/h	[86]
						[132]

5. Future Trends

To maximize the benefits and further the advancement of PEMWE technology, it is essential to identify and outline crucial future directions based on a comprehensive literature analysis. This chapter discusses key future trends and areas for further investigation that are critical to the advancement of PEMWE degradation research. As well as highlighting crucial steps for future research, this chapter emphasizes the essential need for ongoing innovations and explorations in the field of PEMWE degradation and energy management. These recommendations act as a blueprint for focused studies, aiming to refine and optimize the efficiency and reliability of HyPro systems through innovative degradation management and energy solutions. Figure 5-1 illustrates the key areas of technological innovation and degradation management that are essential to improving the sustainability and environmental impact of PEMWE. It emphasizes the integration of renewable energy sources with predictive degradation models and advanced diagnostic tools, highlighting future directions for enhancing system durability and energy efficiency in green hydrogen production.

Key Focus Areas for Future Research:

Standardization: Essential for consistent evaluation and benchmarking, standardization ensures uniformity in testing protocols and degradation rate measurements across different studies. This facilitates comparative analysis and fosters advancements in PEMWE technology. Tomic et al. [36] underscore the need for standardized degradation tests and proper activation procedures to ensure accurate evaluations of PEMWE durability.

Utilizing Existing FC Formulas: Adapting generalized formulas from fuel cells (FC) to fit the specific needs of electrolyzers can significantly enhance the prediction and mitigation of degradation in PEMWE systems. This approach promotes a systematic analysis of degradation mechanisms and assists in optimizing PEMWE performance and longevity.

Manufacturing Variability and Component Differences: Acknowledging the diversity in PEMWE components and manufacturing techniques is crucial for accurate degradation analysis. Tailoring studies to account for these variations ensures a deeper understanding of how different factors contribute to system degradation.

Degradation Measurement Across Operating Modes: It is critical to measure degradation under various operating conditions to fully understand how different modes impact system performance. Future research should focus on integrating comprehensive measurement techniques to develop robust maintenance strategies and optimize operational guidelines.

Green HyPro: With the integration of RESs such as solar and wind, understanding the degradation mechanisms specific to PEMWE systems used for green HyPro is imperative. Future studies should explore long-term performance and standardized testing protocols to enhance system efficiency and sustainability.

Prevention of Degradation: Prioritizing the prevention of degradation through improved fabrication techniques, optimized operating conditions, and predictive maintenance strategies is essential for enhancing the durability and cost-effectiveness of PEMWE systems. Shakhshir et al. [142] discuss the impact of clamping methods on current distribution in PEMWE cells, highlighting the need for careful selection of assembly techniques to ensure optimal performance.

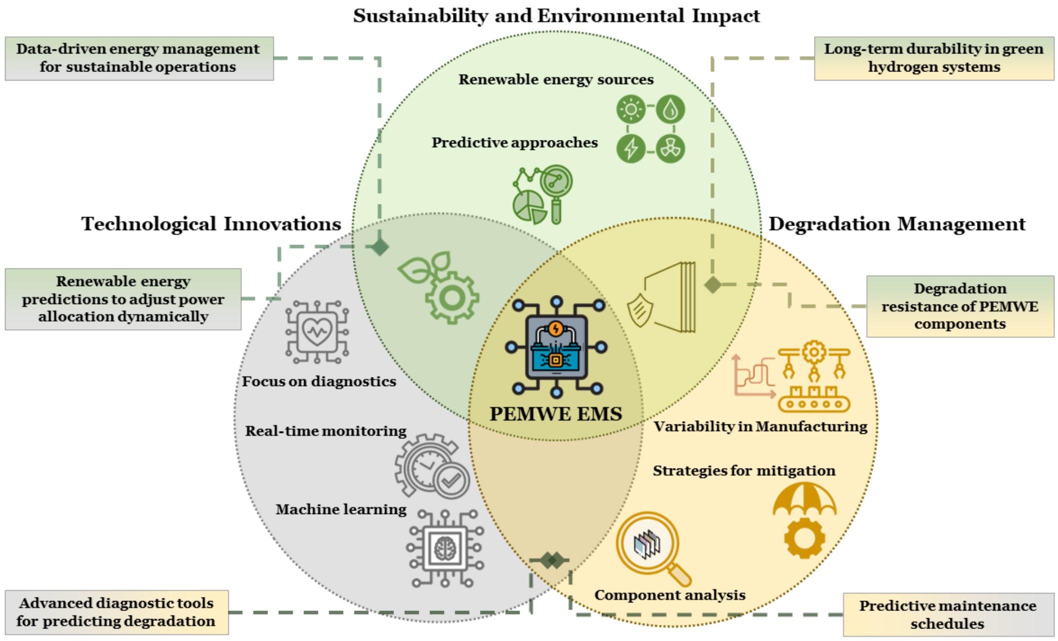

Figure 5-1 Integration of Technological Innovations and Degradation Management in PEMWE Systems for Enhanced Sustainability

Advancements and innovations:

Technological Innovations: Future trends may include the development of advanced diagnostic tools and real-time monitoring systems, utilizing machine learning algorithms to predict and mitigate degradation actively.

Material and Catalyst Development: Developing new materials and catalysts can result in significant improvements to the structural integrity and efficiency of PEMWE systems.

Energy Management and Power Allocation: Optimizing power allocation strategies for green hydrogen systems and incorporating advanced data analysis techniques could greatly enhance the operational efficiency and lifespan of PEMWE systems.

Sustainable Practices: Emphasizing sustainability, future research should also focus on reducing the environmental impact of HyPro and enhancing the integration of PEMWE systems with RESs.

Table 4 Some PEMWE degradation prevention strategies that involve power allocation and energy management

Focus	*Mitigation strategy*	*Method*	*Result*	*Ref.*
Thermal stress	Parametric optimization and control	Predictive Controller	Successful temperature control	[136]
Power allocation	Optimization	Extended duty cycle interleaved buck converter	slows down the degradation/	[85]

			improves the system energy efficiency	
High Frequency resistance	Prediction	Identifying the location of high corrosion inhibiting or long-lived species	recoverable stationary deactivation	[86]

For future studies, it is highly recommended to focus on advancing fabrication techniques, exploring novel materials and catalysts, developing real-time monitoring and control systems, and implementing machine learning algorithms for predictive maintenance and optimization. These efforts will contribute to the development of more efficient, reliable, and durable PEMWE systems, accelerating the transition towards sustainable and clean energy technologies.

Conclusions

This comprehensive review underscores the paramount significance of PEMWEs in advancing sustainable HyPro. As the adoption of large-scale PEMWEs intensifies, the development and integration of advanced DMs becomes crucial. These models are instrumental not only in enhancing our understanding of complex degradation pathways but also in ensuring the reliability and performance of PEMWE systems across various operational conditions.

Throughout this review, we have highlighted the multifaceted nature of PEMWE operations and the critical role that DMs play in optimizing system performance. Throughout the PEMWE process, each component has been shown to interact complexly within the system, with regards to the thermodynamics and kinetics of the system in addition to the integration with RESs. The degradation challenges, particularly concerning the membrane, electrode assembly, and CLs, are formidable yet addressable through innovative strategies.

Empirical studies and advanced modelling approaches have offered insights into mitigating degradation impacts, thereby enabling more sustainable and efficient operations. For instance, findings detailing the rate of membrane thinning and catalyst degradation under various conditions have provided critical data that can be used to refine power allocation and energy management within PEMWE systems. Additionally, the integration of empirical findings, such as those obtained from accelerated stress testing, into advanced DMs has significantly enhanced their predictive accuracy, marking a substantial step forward in the operational reliability of PEMWEs.

Further, the review emphasized the importance of ongoing research and the continuous refinement of DMs. As the scale of PEMWE deployment grows and the complexities of managing large-scale systems increase, the role of precise and adaptable DMs becomes even more critical. The insights derived from both microscale and macroscale degradation analyses must be effectively integrated into the operational strategies of PEMWEs to ensure their robust performance in the face of dynamic operational environments.

Even though PEMWE technology represents a promising avenue towards achieving a sustainable energy future, significant challenges remain in terms of degradation and efficiency. Addressing these challenges through enhanced understanding, innovative material use, and advanced modelling techniques is imperative. Continued research and development efforts are required to harness the full potential of PEMWEs, thereby solidifying their role in the global shift towards clean and RESs. This endeavour not only aligns with the goals of the green energy transition but also contributes fundamentally to the resilience and sustainability of future energy systems.

Nomenclature:

$\mathbf{V_{Hcal}}$	HyPro calculated volume
$\mathbf{V_{HyPro}}$	HyPro actual volume
$\mathbf{E_{HyPro}}$	Productive energy
$\mathbf{E_{input}}$	Input energy
$\mathbf{P_{el}}$	electrolyzer required power
$\mathbf{R_{f}}$	Fluor release (mol/s)
$\mathbf{T_{r}}$	operating reference temperature (°C)
$\mathbf{U_{a}}$	Activation overvoltage (v)
$\mathbf{U_{c}}$	Concentration overvoltage (v)
$\mathbf{U_{o}}$	Ohmic overvoltage (v)
$\mathbf{V_{C}}$	cell voltage (v)
$\mathbf{V_{M}}$	Molar volune
$\mathbf{V_{O}}$	reversible (open circuit) voltage (v)
$\mathbf{V_{S}}$	stack voltage (v)
$\mathbf{V_{cell}}$	cell voltage (v)
$\mathbf{V_{cn}}$	each cell voltage (v)
$\mathbf{V_{ct}}$	Constant turning power operation voltage degradation
$\mathbf{V_{fh}}$	High power fluctuation operation voltage degradation
$\mathbf{V_{fl}}$	Low power fluctuation operation voltage degradation
$\mathbf{V_{m}}$	maintaining operation voltage degradation
$\mathbf{V_{rev}}$	reversible cell voltage (v)
$\mathbf{V_{th}}$	thermoneutral voltage (v)
$\mathbf{n_{e}}$	Number of electrons
$\mathbf{n_{el}}$	number of electrolyzers
$\mathbf{t_{r}}$	reference time
$\mathbf{\Delta V_{D}}$	Total voltage degradation
$\mathbf{\Omega_{HF}}$	High frequency resistance ($\Omega.cm^2$)
$\boldsymbol{\delta_{DR}}$	Conductivity loss degradation rate
$\boldsymbol{\delta_{M}}$	Membrane thickness
$\boldsymbol{\eta_{F}}$	Faradaic efficiency (%)
$\boldsymbol{\eta_{PS}}$	PEMWE System efficiency (%)
$\boldsymbol{\eta_{au}}$	Auxiliary equipment efficiency (%)
$\boldsymbol{\eta_{c}}$	cell efficiency (%)
$\boldsymbol{\eta_{e}}$	Electrolyzer efficiency (%)
$\boldsymbol{\eta_{s}}$	System efficiency (%)
$\boldsymbol{\lambda_{age}}$	Conductivity loss degradation
$\boldsymbol{\lambda_{0}}$	Conductivity loss degradation in zero time
$\mathbf{A}$	Area (square meter, m^2)
$\mathbf{D}$	Degradation (μV/h)
$\mathbf{E}$	Energy ($Wh \approx 3600\ joules$)

F	Faraday's constant
F	Faraday constant (C/mol)
g	gradient
P	Power (W)
t	Time (h and H/2)
t	Time (h)
W	electrical work of electrolysis (J/mol)
W_{irrev}	Irreversible energy (J/mol)
W_{rev}	Reversible energy (J/mol)
Υ	surface coverage ratio (/)
$\Delta\delta_M$	Thinning of membrane thickness
ΔH_R^0	Electrolysis required energy (J/mol)
ΔT	Operating time (h)

Abbreviations:

BoL	Beginning of Life
BPP	Bipolar Plate
CL	Catalyst layer
DM	Degradation model
e-	electron
EM	Energy management
EMS	Energy management system
FC	Fuel Cell
GDL	Gas Diffusion Layer
H+	Protons (isolated hydrogen ions)
H_2	Hydrogen
H_2O	Water
HFR	High Frequency Resistance
HHV	Higher Heating Value
HyPro	Hydrogen Production
L	Liter
LHV	Lower Heating Value
MEA	Membrane Electrode Assembly
O_2	Oxygen
OER	Oxygen Evolution Reaction
PEM	Proton Exchange Membrane
PEMFC	Proton Exchange Membrane Fuel Cell
PEMWE	Proton Exchange Membrane Water Electrolyzer
PSL	porous sintered layer

PTL	porous transport layer
RES	Renewable Energy Source

Acknowledgements

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC) (2018-06527)

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The findings derived from this comprehensive degradation study are highly pertinent to the overarching objectives of the thesis. The study highlights the vital significance of adaptive power allocation strategies and clarifies the complex links between operating conditions and the lifespan of PEMWE systems by integrating sophisticated degradation models into the energy management framework.

These results significantly enhance the understanding of how degradation influences both system efficiency and long-term operational stability. Consequently, the focus shifts to the development of robust, proactive energy management strategies for optimizing power allocation, minimizing degradation effects, and improving the overall performance and durability of modular PEMWE systems. This change lays the foundation for further discussions on control strategies and dynamic adjustment tactics aimed at maintaining system performance under various operating conditions.

4 Energy management strategy

Energy management is a critical aspect of optimizing the operation of PEMWE, particularly in modular configurations, where performance, efficiency, and system degradation are tightly interrelated. This section presents an energy management approach designed especially for modular PEMWE systems, building on earlier considerations of system configuration and degradation models.

By enabling dynamic power distribution across several stacks, the modular configuration provides special optimisation options, guaranteeing balanced deterioration and increased efficiency.

It aims to bridge this gap by developing a sophisticated energy management system (EMS) that dynamically allocates power across modular stacks, taking into account RES's unique operating modes and demands.

Existing studies have largely neglected the complex interplay between energy efficiency, system degradation, and real-time power allocation in such systems. To close this gap, the study will dynamically distribute electricity among modular stacks while taking into account the distinct demands and operation modes of RESs.

The paper's methodology for designing and assessing EMS is based on empirical data and sophisticated simulation models. The main tactic is the Rotary Power Allocation Strategy (RPAS), which evenly divides power among stacks such that no stack is overloaded. By ensuring that every stack runs within its ideal efficiency range, this rotating system lessens wear and tear, which usually results in degradation. When PEMWE systems are combined with intermittent RESs like solar or wind, power input is frequently quite variable, making the RPAS especially crucial.

The EMS introduced in the paper is based on a dynamic optimization function that aims to maximize system efficiency while minimizing degradation. The core of the methodology involves solving a nonlinear optimization problem using the objective function:

$$Maximize: J = \sum_{t=1}^{T}\sum_{s=1}^{S}(\eta_s(P_{t,s}) \times P_{t,s}) - \lambda_1 \sum_{s=1}^{S} D_s - \lambda_2 \sum_{s=1}^{S}(H_s - \overline{H})^2 \qquad (19)$$

Where $P_{t,s}$ is the power allocated to stack s at time t, $\eta_s(P_{t,s})$ stands for the efficiency of stack s based on the allocated power. D_s represents the degradation of stack s. Degradation penalty coefficient (λ_1) controls the weight given to the degradation term in the objective function. The total operational hours of stack s is H_s, and $\overline{H}$ is the average operational hours across stacks. Balancing utilization penalty coefficient λ_2 ensures that the operational hours are balanced between the stacks. It penalizes situations where some stacks are overused compared to others.

Simulations are comparing the created EMS with a more straightforward rule-based system to validate the approach. The results demonstrate that the created EMS considerably raises the system's overall efficiency, sustaining an efficiency above 66% even in the face of power fluctuations. Additionally, it facilitates more equitable distribution of the operational load among stacks, which immediately lowers degradation. This balanced approach to power allocation is essential for increasing the PEMWE system's operational lifetime.

The paper also introduces a comprehensive degradation model that categorizes degradation into operational modes, such as high-power operation and start-stop cycles. These modes are incorporated into the EMS to adjust power allocation dynamically, ensuring that stacks experiencing higher degradation rates are rested while others take on the load. Using this approach not only optimizes efficiency but also maintains the system's long-term health.

According to the study, PEMWEs' modular design offers several benefits over conventional single-stack setups, including increased system robustness, scalability, and flexibility. Modularity enables more precise control over the performance of individual stacks, and the flexibility to modify operational modes in response to real-time data guarantees that power is distributed where it is most required. In real-world applications, where power availability can vary significantly, this flexibility is crucial.

4.1 Energy management of modular PEMWE

In the preceding chapters, the theoretical underpinnings and practical considerations for modular PEMWE systems were laid out, emphasizing both the scalability benefits and the inherent complexity of operating multiple stacks in parallel. By exploring electrochemical modeling frameworks, we were able to optimize performance and reduce degradation, setting the stage for a robust energy management strategy that can adapt to fluctuations in renewable energy sources in the future. Furthermore, insights gathered from various operational modes, benchmarked degradation models, and comparative analyses of singular versus modular electrolyzer structures underscore the importance of a unified approach that accounts for efficiency, durability, and cost-effectiveness.

Following these foundational insights, the following paper explores an advanced EMS specifically tailored for modular PEMWE configurations based on conceptual modeling. The interplay between real-time power allocation, stack deterioration, and operational efficiency under changing renewable power inputs is one of the crucial gaps that it fills, as previously mentioned in previous sections. The research connects our previous theoretical and benchmarking efforts with a workable, experimentally supported solution by introducing a unique RPAS and describing its effect on performance indicators. By doing this, it supports the main goal of the thesis, which is to show that industrial-scale green hydrogen production is feasible using a coherent, data-driven EMS framework.

Journal: Applied science (Elsevier)

Submission date: 09 April 2023

Energy management for modular proton exchange membrane water electrolyzers under fluctuating solar inputs: a constrained nonlinear optimization approach

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Abstract

The rapid increase in the usage of renewable energy highlights the need for dependable systems that efficiently convert and store intermittent electricity. In this regard, Proton Exchange Membrane Water Electrolyzers (PEMWEs) present a feasible method of producing hydrogen. However, fluctuations in energy input can compromise both their durability and efficiency. An advanced Energy Management Strategy (EMS) is recommended by the current study for modular PEMWEs to overcome these challenges and ensure that critical objectives, including maximum efficiency, balanced stack power consumption, and minimal degradation, are met under a wide range of operating constraints.

The EMS is methodologically described as a constrained nonlinear optimization problem parallel with a Rotary Power Allocation Strategy (RPAS). By methodically balancing loads, the proposed approach mitigates uneven wear and harnesses optimal efficiency, thus ensuring both immediate performance gains and extended system lifespans. According to an 8760-hour evaluation of a 20-kW solar plant, which was taken from a simulated power plant, the suggested EMS produces about 12% more hydrogen than conventional rule-based methods. It also decreased degradation by approximately 38.6%, raised stacks average efficiency up to 6.9%. Aside from enhancing productivity, efficiency and dropping degradation, the EMS addresses the challenges arising from partial loading, overloading, paving the way for environmentally friendly, cost-effective, and sustainable hydrogen production.

Contents

1. Introduction

Energy management is crucial to minimizing energy consumption in all sectors, as illustrated in Figure 1, to reduce expenditures, improve efficiency, and reduce environmental impact. Its applications span a variety of industries, such as manufacturing, data centers, and Renewable Energy Sources (RESs), and it involves implementing energy-saving measures and monitoring energy in real-time [1]. In numerous scenarios, including Heating, Ventilation, and Air Conditioning (HVAC) control in commercial buildings [2, 3], manufacturing production efficiency [4], and data center electrical usage monitoring, Energy Management Systems (EMS) optimize operations, enhance sustainability, and save costs. For greater power efficiency, data centers, for instance, use sophisticated server management and cooling systems [5, 6].

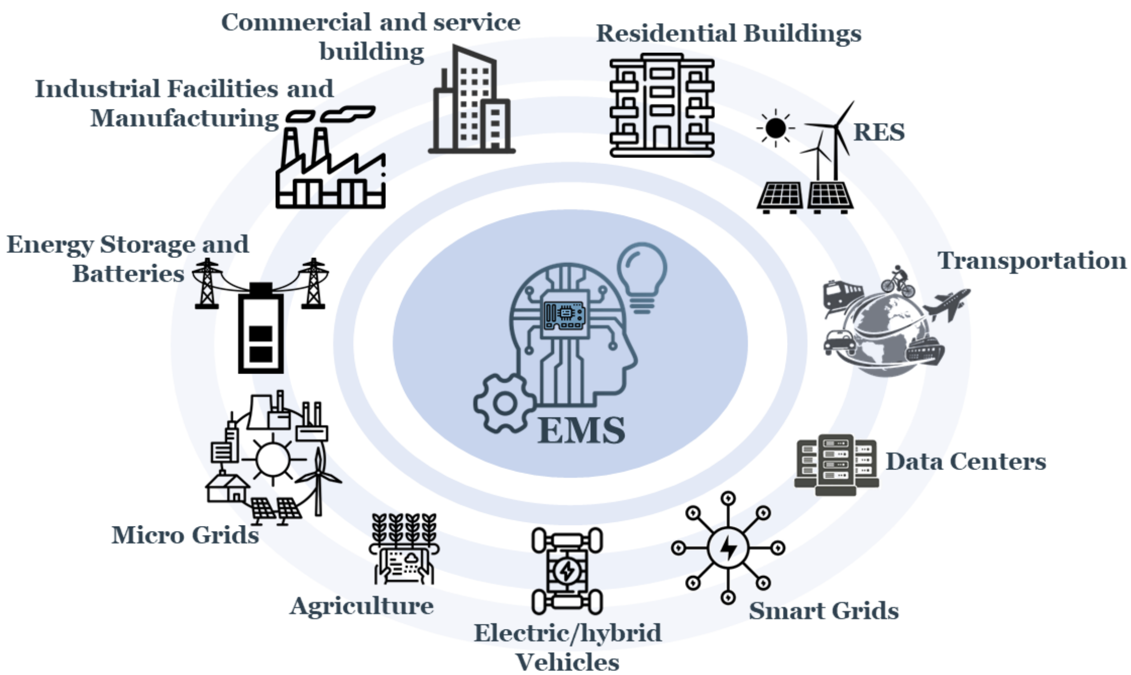

Figure 1 Utilizations of EMS

In addition to facilitating RES integration, EMS ensures consistent energy distribution while resolving intermittency issues. By combining Hydrogen Production (HyPro) with the availability of renewable energy, EMS optimizes the production, storage, and distribution of hydrogen [7]. When coupled with fuel cell systems, EMS-enabled smart grids can improve grid efficiency by dynamically adjusting load to reduce transmission losses and enhance the integration of renewable energy. For example, modifications to wind turbines and optimised solar panels can improve grid efficiency further when coordinated with fuel cell systems [8, 9]. Day-ahead scheduling and scenario clustering are innovative strategies that boost energy utilization and improve the economic viability of HyPro systems. For example, Su et al. [10] introduced a multi-state transition electrolyzer model integrated with energy storage to clearly demonstrate these benefits. While EMS oversee hydrogen fueling stations to satisfy the needs of fuel-cell vehicles, electrolyzers dynamically modify operations for sustainability and cost-effectiveness. In a comparable way, Aryan Nezhad [11] enhance energy efficiency and lower costs in renewable-rich settings by using demand response mechanisms in microgrids.

According to recent research, EMS has improved the efficiency, longevity, and grid stability of electrolyzers in hydrogen systems during HyPro operations [12, 13]. To support its function as a scalable renewable energy vector, EMS also tackles issues with hydrogen transportation and storage [14, 15].

PEMWE technology has advanced recently due to its compatibility with intermittent Renewable Energy Resources (RESs) such as solar and wind. PEMWE is a flexible, zero-emission energy storage system that solves intermittency problems and improves grid stability by effectively converting surplus renewable energy into hydrogen with rapid response times [16]. Market research indicates that the PEMWE industry will develop rapidly as governments and businesses embrace hydrogen as a crucial component of the energy revolution [17]. Europe, Japan, South Korea, and the Middle East are making significant investments in hydrogen initiatives, highlighting the relevance of PEMWE in integrating RESs to achieve carbon neutrality [18, 19]. Membrane, catalyst, and system design technological advancements have lowered PEMWE costs, increasing its economic feasibility and competition with conventional techniques. The development of efficient electrocatalysts and robust ion exchange membranes is essential if performance is to be improved and operating costs to be reduced [20-22]. Because modular PEMWE systems are flexible and scalable, they can be adapted to integrate with local renewable projects and respond dynamically to changing energy sources [23-26]. Modularity increases hydrogen generation efficiency while meeting industrial automation standards.

For scalable, high-capacity electrolysis systems, Lange et al. [27] stress the shift from monolithic to modular designs, while Chatenet et al. [28] emphasize the use of modern materials and machine learning for their selection in order to increase the durability and efficiency of electrolyzers. Schwarze et al. [29] highlight how High-Temperature Electrolysis (HTE) devices show commercial feasibility. To optimize alkaline electrolysis stacks in variable renewable conditions, Huang et al. [30] provide quantitative model that considers interrelated factors (electrode size, position and number), which increase performance by more than 6%. They have done it by decreasing the bubble coverage effect and shunt current effect.

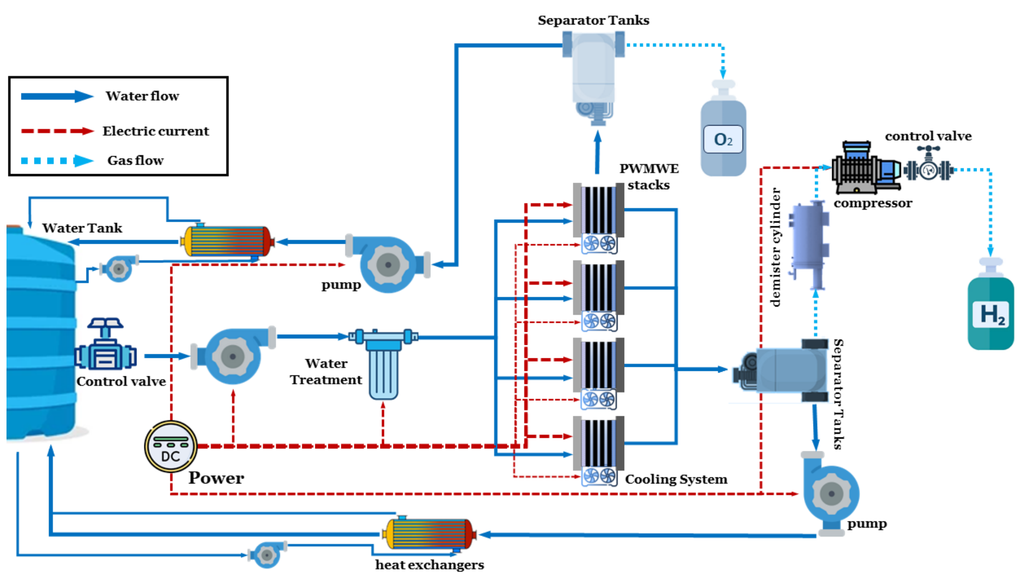

Figure 2 Modular PEMWE system and subsystems

From single-module configurations for places that are limited to scalable modules that guarantee continuity under variable energy supplies, PEMWE systems are made to be operationally flexible. These systems support a low-carbon economy by adjusting to the availability of renewable energy. It is still difficult to successfully integrate RESs because of high upfront costs and the requirement for efficient EMS.

To maximize PEMWE energy utilization, energy management is essential. Energy demands are met by the subsystems that make up modular systems, including cooling, gas separation, power supply, and water supply (see Figure 2). PEMWE stacks make up 70–85% of overall energy consumption, as illustrated in Figure 3, with gas handling coming in second (10–15%) and cooling (4–10%) [51–53].

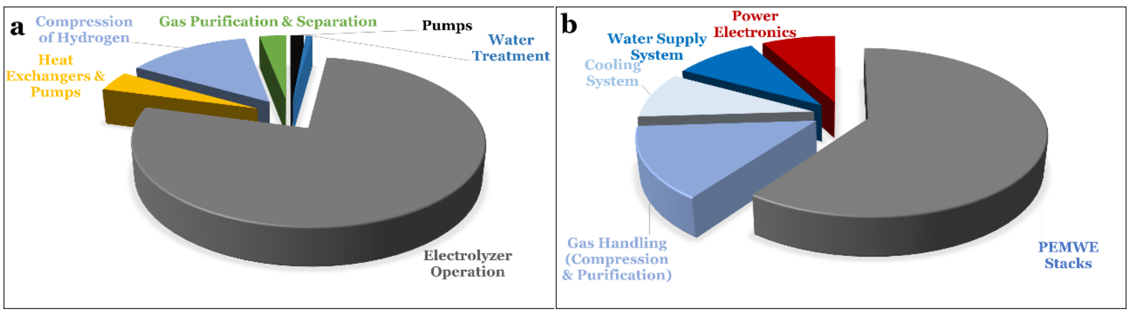

Figure 3 a) Energy consumption and b) Costs breakdown in Modular PEMWE Systems

Strategies for integrating wind energy with hydrogen generation are highlighted by Sharifzadeh et al. [23] and Chandrasekar et al. [31]. The design and operation of PEMWE and alkaline electrolysers optimised by Sharifzadeh [32] using a multi-scale, multi-period mixed-integer linear programming method to maximise economic viability. The model enhances HyPro through cost-effective supply chain solutions by integrating strategic (plant locations, capacities) and operational (process scheduling, raw material flows) decisions, while also accounting for uncertainties (feedstock availability, hydrogen demand, etc.). Chandrasekar examines wind curtailment for PEMWE and Solid Oxide Electrolysis Cells (SOEC), highlighting the efficiency disparity between low- and high-temperature electrolyzers under fluctuating power. Salman [33] uses MATLAB/Simulink to study grid stability with wind-to-hydrogen systems to achieve reliable frequency stabilization.

Using genetic algorithms for solar-powered hydrogen synthesis, Alirahmi et al. [34] suggest incorporating Parabolic Trough Collector (PTC) and thermoelectric generators to enhance the efficiency and hydrogen yield of the system. While Shiroudi [35] evaluates direct PV-electrolyzer connections for solar energy conversion in Iran, Zhang et al. [36] study PV-electrolyzer systems, highlighting efficiency fluctuations with environmental changes.

Ziogou et al. [37] develop a finite-state machine-based EMS for a solar-powered hydrogen unit, achieving 73% electrolyzer efficiency and reliable operation. In their optimization of DC microgrids combining PEMWE, Jin et al. [38] place an intense focus on energy storage and the efficiency of hydrogen production.

Modular designs for operational flexibility are among the advancements in PEMWE scalability. Guilbert et al. [39] improve energy efficiency with interleaved DC-DC converters, while Shakibi et al. [40] use neural networks to optimize geothermal hydrogen systems. Layered power scheduling is employed by Liu et al. [41] to minimize expenses and deterioration in PEMWE systems.

Grid flexibility is improved by attempts to integrate PEMWE with Virtual Power Plants (VPPs) and smart grids. PV-PEMWE systems have been improved by Nguyen et al. [42] using Particle Swarm Optimization (PSO), increasing efficiency in the presence of deterioration and shade. Winter et al.'s [43] dynamic power allocation strategies increase grid reliability and green hydrogen generation efficiency.

Even after many years of progress, scaling PEMWE to industrial grids, optimizing its lifetime, and offering reliable control and heating systems remain challenges [44-48]. Modular PEMWE applications require regulatory frameworks and lifecycle assessments to strike a balance between economic viability, sustainability, and efficiency.

Degradation in PEM water electrolyzers remains a critical challenge that directly impacts system longevity, efficiency, and operational costs. Under dynamic operation and high current density, voltage degradation is caused by numerous intertwined mechanisms, such as catalyst dissolution, membrane thinning, and PTL degradation. Empirical studies have reported voltage degradation rates ranging from a few microvolts per hour under steady-state conditions to tens of microvolts per hour in dynamic cycling, particularly in renewable energy-driven systems [49]. In particular, Siracusano et al. [50] demonstrated that thermal cycling exacerbates the degradation of membrane performance, while Frensch et al. [51] identified significant fluoride emissions at elevated temperatures, indicating membrane degradation as the dominant failure mode. In addition, Rakousky et al. [52] have demonstrated the impact of fluctuating power input on PTL oxidation and membrane stress, concluding that transient operations result in higher degradation rates than continuous ones. To address these challenges, researchers have developed degradation models ranging from empirical voltage-loss predictions to physics-based and machine-learning-enhanced approaches. Alia et al. [53] demonstrate that there is a trade-off between catalyst loading and degradation rate, demonstrating that lower Ir loadings, while cost-effective, can have a detrimental effect on performance. Similarly, Babic et al. [54] conducted comprehensive diagnostics on material aging, correlating membrane thinning with increased ohmic resistance and catalyst degradation with rising overpotential. The findings support the need for energy management strategies that mitigate degradation using load balancing, controlled ramp rates, and material innovations, which would ensure a lengthy electrolyzer lifetime suitable for large-scale hydrogen production.

The literature highlights several gaps concerning the optimization of EMS for modular PEMWE systems under fluctuating renewable energy inputs, specifically regarding efficiency optimization [49, 50, 52, 55], degradation mitigation, and adaptive operational management [28]. Existing rule-based energy management methods often lead to inefficiencies [56], uneven stack utilization, and accelerated component degradation [32, 40], particularly in situations when input conditions are extremely changeable [57].

This paper aims to provide an advanced EMS that takes advantage of real-time performance metrics, a Rotary Power Allocation Strategy (RPAS), and constrained nonlinear optimization strategies to address these challenges. Specifically, the study aims to enhance HyPro efficiency, reduce stack degradation, and improve overall operational sustainability by dynamically balancing power distribution across electrolyzer stacks.

The structure of the paper is as follows: Section 2 provides a detailed review of PEMWE technology modeling strategies. The subject of Section 3 is a detailed discussion of the experimental methodology, including the set-up of the testbench and the computational modeling techniques that have been used. The suggested EMS framework and optimization strategy are presented in Section

4. In Section 5, comprehensive analyses and comparisons between the developed EMS and traditional rule-based strategies are presented, demonstrating significant improvements in hydrogen yield, efficiency, and reduced degradation rates. A summary of the results and suggestions for more study to improve the scalability and resilience of modular PEMWE energy management systems are included in the paper's conclusion.

2. Modeling

Electrochemical cell model

PEMWE cells, uses electrical energy to split water into hydrogen and oxygen. A PEMWE system's hierarchical structure, from setup to the molecular scale, is depicted in detail in Figure 4. Initially, the diagram illustrates the system configuration, highlighting the power sources and control mechanisms, and demonstrating the modularity of the electrolyzer. Initially, the diagram illustrates the system configuration, highlighting the power sources and control mechanisms, and demonstrating the modularity of the electrolyzer. In a cross-section, key components such as anode and cathode catalysts, membranes, porous transport layers (PTLs), flow channels and bipolar plates (BPPs) are visible. The figure demonstrates the proton transfer within the membrane by illustrating the movement of protons (H_+), hydrogen (H_2), oxygen (O_2), and water (H_2O) molecules, thereby explaining how hydrogen is produced through electrochemical reactions and electrical flow.

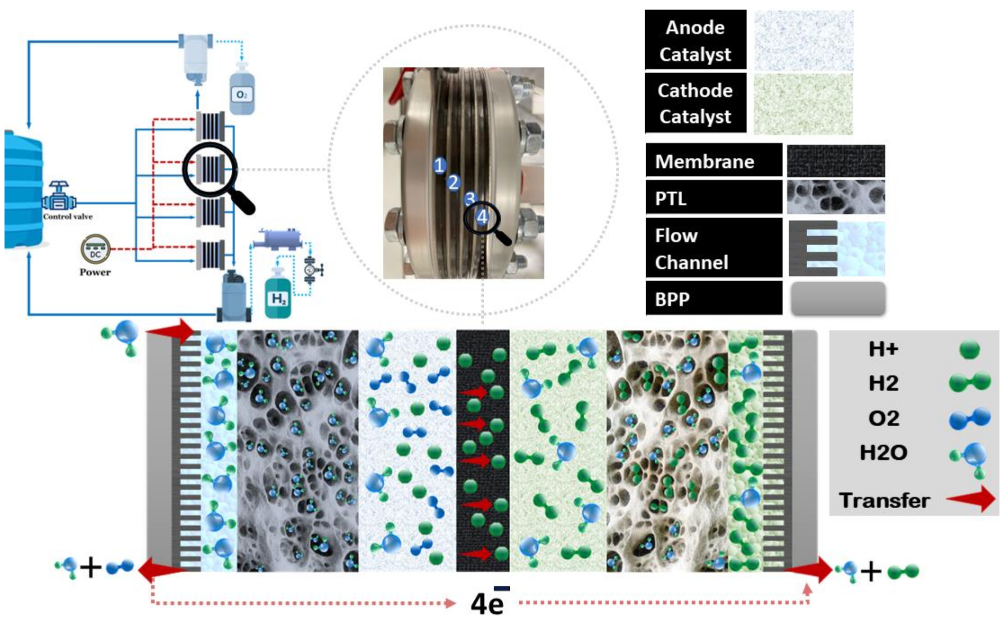

Figure 4 Integrated overview of PEMWE system, stack, and cell components and proton transfer processes

Three essential processes provide a concise description of the electrolysis of water in PEMWE cells. In reaction (1) liquid H_2O is electrolyzed, resulting in the formation of O_2 gas, H^+ in aqueous solution, and electrons (e^-). In (2) these H^+ and e^- recombine at the cathode to produce H_2 gas.

$$2H_2O\ (\mathrm{l}) \rightarrow O_2(\mathrm{g}) + 4H^+(aq) + 4e^- \quad (1)$$

$$4H^+(aq) + 4e_{(-)} \rightarrow 2H_2(\mathrm{g}) \quad (2)$$

$$2H_2O\ (\mathrm{l}) \rightarrow O_2(\mathrm{g}) + 2H_2(\mathrm{g}) \quad (3)$$

These steps are combined to demonstrate the net conversion of liquid water into equal molar amounts of hydrogen and oxygen gasses in the whole process, which is summed up in (3)[58].

The efficiency and performance of a PEMWE depend significantly on the cell voltage (V_{cell}), which is a combination of the reversible voltage and various overpotential losses as shown in (4).

Overpotentials are a result of inherent inefficiencies associated with the electrolysis process and the materials used.

$$V_{cell} = V_{rev} + U_a + U_o + U_c \quad (4)$$

The reversible voltage (V_{rev}) represents the minimum voltage required under ideal conditions to split water into hydrogen and oxygen. This voltage is derived from thermodynamic principles, specifically Gibbs free energy, and can be expressed as (5).

$$\boldsymbol{V_{rev} = V_{rev,s} + \frac{RT}{2F} \times \ln(\frac{P_{H_2}P_{O_2}^{0.5}}{\alpha_{H_2O}})} \quad (5)$$

where the standard reversible voltage "$V_{rev,s}$" is a temperature-dependent parameter, essential for electrochemical calculations. It is influenced by the universal gas constant (R=8.314 J/mol), the absolute temperature (T) in Kelvin, and the Faraday constant (F=96,485 C/mol). Additionally, the partial pressures of hydrogen "P_{H_2}" and for oxygen its "P_{O_2}". The activity of water "α_{H_2O}" is typically assumed to be 1 in liquid-phase electrochemical calculations.

$$V_{rev,s} = 1.229 - 0.9(\mathrm{T} - 298) \times 10^{-3} \quad (6)$$

Activation overpotential "U_a" arises due to the energy barrier that must be overcome for electrochemical reactions to occur at the electrode surfaces, particularly the hydrogen evolution and oxygen evolution reactions. It is possible to model this overpotential using (7) the Butler-Volmer equation, which describes the relationship between current density and overpotential. In this equation j can be anode or cathode side which the U_a will be their sum.

$$U_{a,j} = \frac{RT}{\alpha_j zF} \mathrm{Sinh}^{-1}(\frac{i_j}{2i_{0,j}}) \quad (7)$$

The charge transfer coefficient "α_j" represents the fraction of the voltage that drives the electrochemical reaction. The number of electrons transferred "z" is typically 2 for water electrolysis, indicating the participation of electrons in the reaction. The current density at electrode i_j reflects the current per unit area at the electrode surface, while the exchange current density $i_{0,j}$ is a measure of reaction kinetics at equilibrium, indicating the rate of electron transfer without any net electrolysis. At low current densities, where reaction kinetics play a more significant role, activation overpotentials are one of the major contributors to cell voltage.

Ohmic losses "U_o" occur due to resistance to ion flow through the electrolyte and other cell components. A direct cause of these losses is the electrical resistance present in the PEMWE, including the proton-conducting membrane and the conductive materials used. The equation for ohmic losses is given by (8).

$$U_o = I \times \Omega_{eq} \quad (8)$$

where "I" is the current through the cell. "Ω_{eq}" is the equivalent resistance of the cell, which can be further broken down into the main resistances which are membrane Ω_M and electrodes Ω_E resistance. It is also common for researchers to consider multiple layers (PTL, CL and...) of ohmic resistance separately or to disregard some of them, but when a model is fitted automatically, most of the resistance will be considered.

$$\Omega_{eq} = \Omega_M + \Omega_E \quad (9)$$

The Ω_M depends on its thickness and conductivity, which in turn are functions of water content and temperature. The membrane resistance can be expressed as:

$$\Omega_M = \frac{\theta}{\mho} \quad (10)$$

$$\mho = (0.005139\lambda - 0.00326)exp\,[1268(\frac{1}{303} - \frac{1}{T})] \quad (11)$$

where "θ" is the membrane thickness. "$\mho$" is the membrane conductivity, which is a function of water content "λ" and temperature and is expressed in (11). Based on this equation, it is demonstrated that as the moisture content or temperature of the membrane increases, the membrane conductivity will improve, resulting in a reduction in ohmic losses.

Concentration overpotential "U_C" occurs when there is a difference between the concentration of reactants at the electrode surface and their concentrations in the bulk solution. This overpotential is particularly significant at higher current densities, where the supply of reactants becomes diffusion limited. The U_C can be calculated by (12). The limiting current density "i_l" is determined by the diffusion capabilities of the system.

$$U_C = \frac{RT}{zF} ln(\frac{i_l}{i_l - i}) \quad (12)$$

This equation highlights how the overpotential increases as the operating current approaches the diffusion-limited current [59].

Test bench and model validation

A specialized test bench designed for PEMWE systems was used to validate this model, which is based on a benchmark developed by the team in previous research studies (see Table 1) [60]. The test bench facilitates accurate measurement of current, voltage, and gas flow rates, managed through National Instruments interfaced with LabVIEW, as shown in Figure 5. Before each experiment, the system is calibrated to ensure reliable results, with operational details provided in.

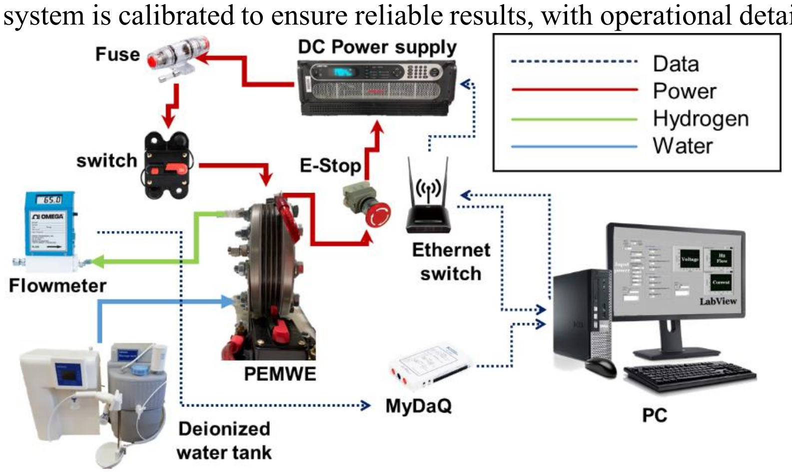

Figure 5 Setup of the PEMWE test bench: instrumentation and control system configuration

Table 1 Test bench specifications

PEMWE Parameter	Specification	BOP	Specification
Model	QLC-1000	Temperature	5-35°C
Number of Cells	4	Water/hydrogen pressure	~101.325 / 4.905 kPa
Operational Current	0-36A	Power Supply	0-100V, 0-100 A
Active Area	50 CM²	Control Mechanism	PC-controlled power supply

Operational Voltage	DC 12-15V	Data Acquisition	myDAQ / Extech thermometer
HyPro Rate	1000 ml/min	H_2 Flow Control	Omega FH

The chosen model was tuned using experimental data from the test bench, employing a Genetic Algorithm (GA) to adjust the parameters, thus minimizing the error between the calculated and experimental polarization curves. This GA-based tuning ensures that the model accurately reflects real-world performance, with the optimized parameters detailed in Table 2.

Table 2 PEMWE single-cell model parameters

Parameter	**Amount**	**Unit**
Universal gas constant ($\boldsymbol{R}$)	8.314	J/(mol·K)
Faraday's constant (F)	96485	C/mol
water activity ($\boldsymbol{\alpha_{H_2O}}$)	1	N/A
Current density (i)	Variable	A/m²
Exchange current density ($\boldsymbol{i_0}$) *	1e-3	A/m²
Limiting current density ($\boldsymbol{i_l}$)*	1.75	A/m²
Temperature (T)	Variable	K
Pressure (P)	1.5	atm
Hydrogen Pressure ($\boldsymbol{P_{H_2}}$)	1	atm
Oxygen Pressure ($\boldsymbol{P_{O_2}}$)	1	atm
The effective surface area ($\boldsymbol{\gamma_j}$)*	5.5e-5	m²/s
Charge Transfer Coefficient (α)*	1.54	N/A
Concentration constant ($\boldsymbol{\beta}$)*	3.23	N/A
Concentration constants ($\boldsymbol{\beta_{1\&2}}$)*	0.341	N/A
Thickness of the membrane ($\boldsymbol{\theta}$)*	285	μm
Electrolyte Conductivity (℧)	1	S/m
Membrane humidification ($\boldsymbol{\lambda}$)*	57	N/A
Ohmic Resistance (Ω_M) *	0.163	Ohms
Ohmic Resistance (Ω_E) *	0.054	Ohms
stoichiometric coefficient (z)	2	N/A

* These parameters are estimated by GA; however, parameters may have various amount in different equations in a model due to operational modes like temperature or pressure in different situations

The polarization curve, illustrated in Figure 6, represents the relationship between cell voltage and current density in PEMWE. It serves as a crucial tool for assessing electrolyzer efficiency and performance across various operational regimes—highlighting activation losses at low current densities, ohmic losses at intermediate levels, and concentration losses at high densities. The experimental data for this curve are derived from measurements taken on the test bench depicted in the figure, where the red curve indicates the tuned model. It has been validated that the model fits well and is reliable for use in future calculations.

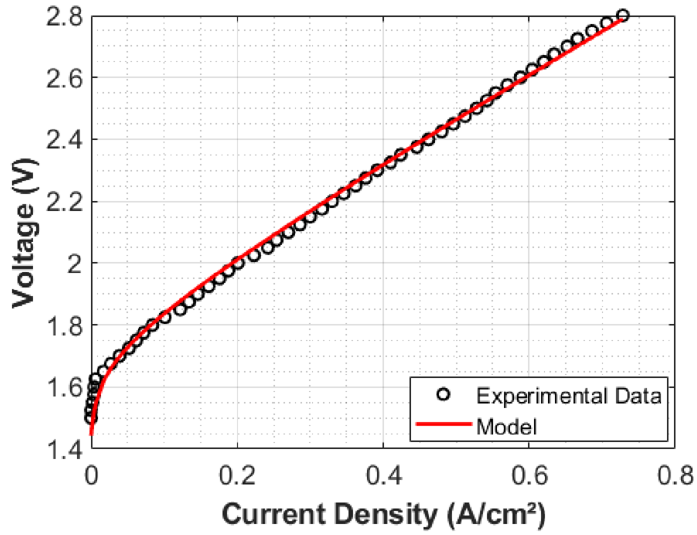

Figure 6 PEMWE cell polarization curve

Case study

This research investigates the performance and efficiency of a modular PEMWE under fluctuating solar inputs at Quebec, Canada. To be more precise, a 20-kW photovoltaic (PV) solar system located in Trois-Rivières was used as a renewable energy source to simulate real-world conditions. The PEMWE system consists of four modular 5 kW stacks, each carefully managed by an advanced Energy Management Strategy (EMS). Data from PVWatts® Version 8.4.0 [61] provided precise estimations of solar power availability throughout a year, thus allowing a comprehensive evaluation of the EMS in balancing efficiency, degradation, and power allocation across stacks. The main objective of this case study is to validate a constrained nonlinear optimization approach and RPAS under realistic, variable operational scenarios.

The validated single-stack (0.5kW) PEMWE model from the test bench was adapted for application in this case study by scaling its parameters and operational characteristics to match the modular 5 kW stacks utilized. Adjustments included increasing the number of cells, active area, and operating current range to align with stack specifications (see Table 3). Using this method, it was possible to simulate stack performance under variable solar input conditions, thus bridging the gap between experimental validation and practical application. Building on the cell model described the relationship between a single cell and a single stack in the PEMWE is illustrated in (13). As shown in Table 3, the parameters for the 5 kW PEMWE discussed in this study were derived from both simulation results and parameters of existing commercial systems.

$$I_s = i \times A_a \qquad \Big| \qquad V_s = N \times V_{cell} \qquad \Big| \qquad P_s = I_s \times V_s \tag{13}$$

Table 3 Characteristics and parameters of the PEMWE stack

Names	Parameters	Value	Unit
Rated power	P_s	5	kW
Operating voltage	V_s	15–28	V
Operating current	I_s	1–179	A
Cells number	N	10	N/A
Active area	A_a	248	cm²

Operating pressure	P	196	kPa
Temperature	T	320	K

The rate of HyPro based on Faraday's law can be described using (14), where, '$\dot{f}_{H2}$' is the HyPro flow rate in m^3/s. "ρ_{H_2}" denotes the partial pressure of hydrogen, expressed in atm [59].

$$\dot{f}_{H2} = \frac{N \times I \times R \times \mathrm{T}}{2F \times \rho_{H_2}} \tag{14}$$

3. Methodology, parameters and energy management

Efficiency

The voltage efficiency "η_v" of a PEMWE, representing membrane and heat losses, is calculated by assessing the cell voltage. It is determined using (15) and expressed as the ratio of the thermoneutral voltage (V_{th}=1.48v [62]) to the actual cell voltage "V_{cell}" [63].

$$\eta_v = \frac{V_{th}}{V_{cell}} \times 100 \tag{15}$$

The overall energy efficiency of the PEMWE system, denoted as "η_S", is calculated by multiplying the individual efficiencies, as shown in (16). This includes the voltage efficiency and Faraday efficiency "η_F", which accounts for losses due to gas diffusion. Although it is typically considered to be 1 [64], especially at standard operating pressures, it can be calculated using (17)[65]. Additionally, Balance of Plant (BoP) efficiency "η_{BoP}", which accounts for subsystems such as water and heat management, is assumed to range between 80% and 100% in literature [66, 67]. In this study η_{BoP} is 90%.

$$\eta_S = \eta_v \times \eta_F \times \eta_{BoP} \tag{16}$$

$$\eta_F = (-0.0034\text{P} - 0.001711).\, i^{-1} + 1 \tag{17}$$

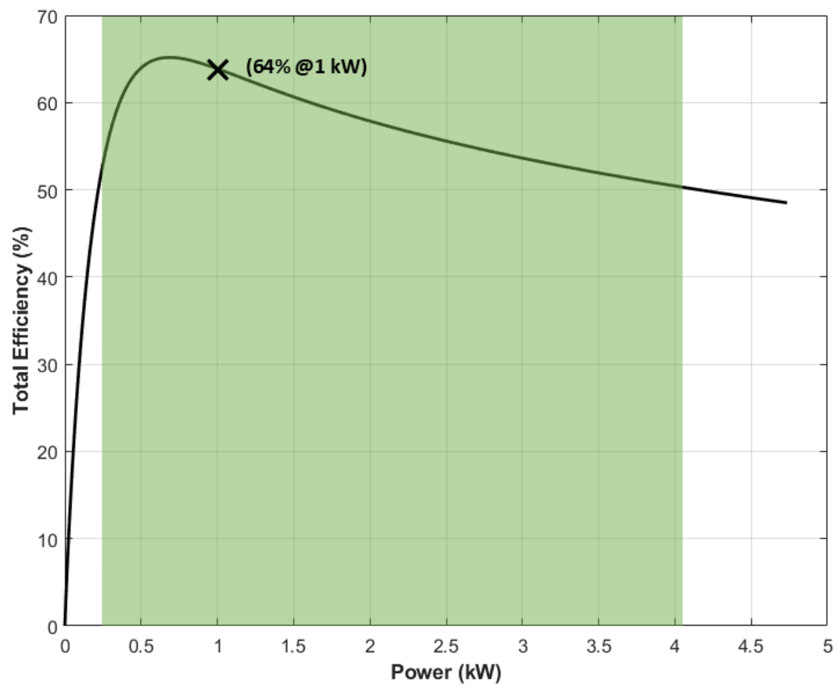

Figure 7 Total Efficiency vs. Power Curve of a PEMWE System

Figure 7 illustrates the total efficiency of the PEMWE system. As power increases, the overall efficiency reaches a peak before gradually declining due to increasing losses in the system.

Utilization factor

The utilization factor (UF) serves as a critical measure in efficient operation of a PEMWE stack, as it provides a clear indicator of how effectively the electrolyzer uses its capacity relative to its maximum potential of each stack. This evaluation helps in identifying operational efficiencies and areas for improvement. The stack utilization factor "UF_s" of a PEMWE is calculated using (18):

$$UF_s = \frac{I_S \times V_S}{I_{max} \times V_{max}} \times 100 \tag{18}$$

where I_S and V_S are the in-use capacity and is the total power of the system and I_{max} and V_{max} represent the nominal current and voltage respectively, determined by the polarization curve. UF_s is expressed in percentage and reflects the system's power utilization efficiency. Figure 8 illustrates a detailed analysis of the utilization factor for the PEMWE stack, demonstrating its performance across varying voltage, current, and power.

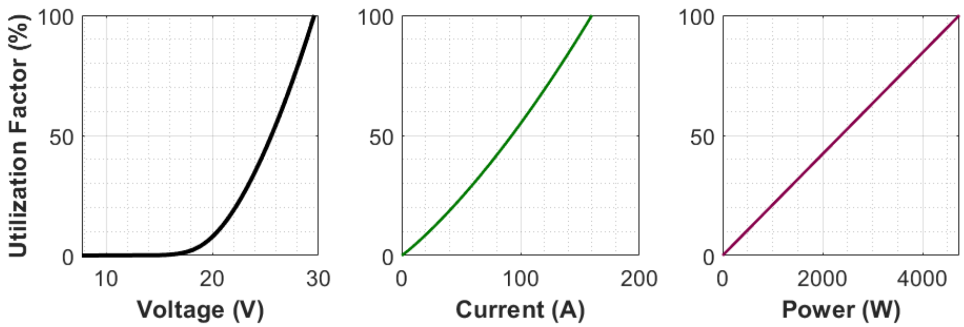

Figure 8 Comprehensive Utilization Factor Analysis of a PEMWE Stack Across Voltage, Current, and Power Dimensions

Rotary Power Allocation Strategy

Linear power allocation is a conventional, rule-based approach in modular PEMWE systems. Stack 1 is allocated power sequentially, and subsequent stacks are allocated power only when the previous stack reaches its maximum power capacity, as illustrated in Figure 9 [68]. A proposed Rotary Power Allocation Strategy (RPAS) is presented in this study and compared to the conventional rule-based allocation method.

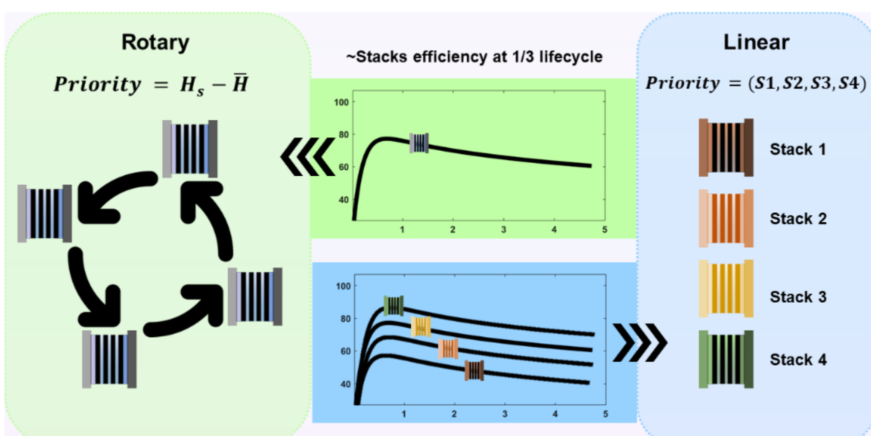

Figure 9 Power allocation strategies

RPAS dynamically distribute power among multiple stacks or modules, aiming to optimize operational efficiency and equipment longevity. RPAS, unlike linear allocation, avoids continuous stress on any single module by rotating power distribution systematically, which is more effective than linear allocation. By using this approach, degradation is significantly reduced, and overall system efficiency is enhanced, particularly when renewable energy inputs are variable.

RPAS primarily serves as a complementary strategy to the existing optimization system, ensuring correct activation and deactivation of stacks rather than introducing additional complexity to power allocation. It can ensure the equitable use of all stacks and functions more as an insurance mechanism. Consequently, it improves system durability through a balanced load distribution, increases overall efficiency through optimization of stack usage, increases adaptability to fluctuations in power availability, and reduces maintenance frequency, which contributes to an increased system scalability.

Degradation and operational modes

The dynamic operation of a PEMWE stack is a significant factor driving component degradation, particularly affecting membranes, and catalysts. This degradation compromises operational efficiency by increasing the operating voltage of the PEMWE stacks as shown in Figure 10. To quantitatively assess this degradation, voltage degradation rates are analyzed, providing a metric to monitor the wear, and ageing of PEMWE components. Based on reports in the literature, the most significant degradation in PEMWE systems typically occurs during start-stop cycles, high-rated operations, and severe fluctuations. For example, high constant input power and frequent start-stop cycles accelerate the voltage degradation rate. This study assumes that the stack is fed smoothly and steadily, so only normal phase, stop-start and rated power operations are considered. Several studies, including [69-71], have thoroughly investigated these phenomena. Table 4 summarizes the average degradation observed in different operational modes in the literature, such as rated power, normal operation [65], and start-stop cycles which is an estimation based of existing data [72].

Table 4 Average degradation rates in PEMWE cell

Operational Mode	Average voltage degradation rate
Rated power	196 (μV/h)
Normal	35.5 (μV/h)
Start-stop cycling	60 (μV/cycle)

The progression of voltage increase due to degradation is illustrated in Figure 10, which correlates increasing cell voltage with decreasing overall PEMWE efficiency. As the cell components wear down, the voltage required to maintain operation increases, thereby reducing the system's energy efficiency over time. The relationship between voltage degradation and efficiency can be seen in (15) where V_{cell} increases by adding degradation voltage rate in (μV/h).

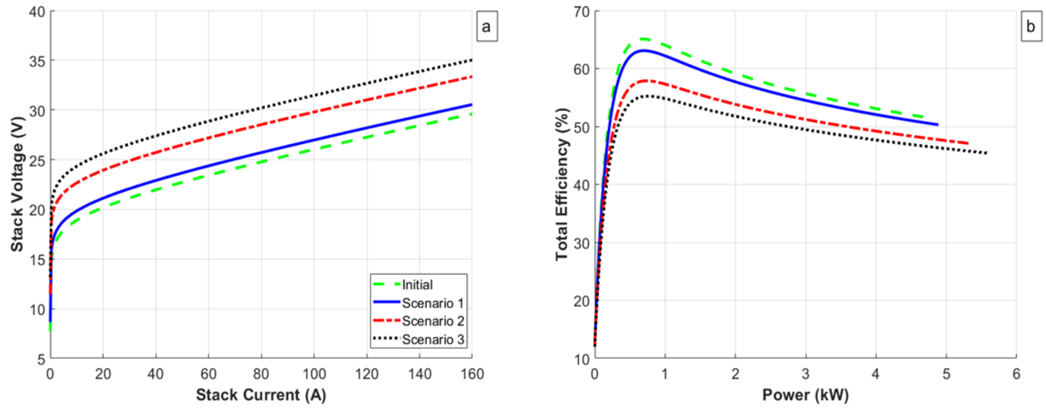

Figure 10 analyze of the effect of degradation on a) Stack voltage b) Total efficiency of stack.

Understanding and quantifying the impacts of operational modes on PEMWE degradation is critical for extending the lifespan and optimizing the performance of these systems. Eq. (19) illustrates the aggregate voltage degradation "V_d" in a PEMWE stack, factoring in each operational mode's contribution over time. based on [65] as the cumulative effect of individual voltage degradation contributions from each cell.

$$V_d = \mathrm{N} \times (\delta \mathrm{V}_R \times t_R + \delta \mathrm{V}_n \times t_n + \delta \mathrm{V}_{SSC} \times n_{SSC}) \quad (19)$$

where "$\delta \mathrm{V}_R$" denotes voltage degradation during rated power operation, while "$\delta \mathrm{V}_n$" refers to the same parameter in constant normal operation and parameter t stands for the time that each mode remains active in hours. The term "$\delta \mathrm{V}_{SSC}$" indicates each start-stop cycle, and "n_{SSC}" representing the total number of such cycles experienced. N is the number of cells in the stack.

In a multi-stack system, each stack may experience a different operating schedule and therefore incur different degradation

$$D_s = N \times (\delta \mathrm{V}_R \times t_R^{(s)} + \delta \mathrm{V}_n \times t_n^{(s)} + \delta \mathrm{V}_{SSC} \times n_{SSC}^{(s)}) \quad (20)$$

where $t_R^{(s)}$, and $t_n^{(s)}$ are the time stack (s) spends at rated and normal conditions. $n_{SSC}^{(s)}$ is the number of start–stop cycles that stack (s) undergoes.

Figure 10 illustrates three specific scenarios: In Scenario 1, the 5-kW stack is subjected to a single start-stop cycle daily and operates in normal mode for 3000 hours. Scenario 2 involves the same stack operating at rated power 70% of the time, with one start-stop cycle daily included. Finally, scenario 3 entails continuous normal operation of the stack with start-stop cycles occurring every 6 hours. These scenarios provide a comprehensive view of the stack's performance under different operational regimes.

Energy management strategy

In the quest to enhance the operational efficiency and longevity of the PEMWE, an EMS is implemented. This method utilizes a dynamic rotational strategy to optimize the allocation of power across multiple stacks, aiming to balance efficiency, degradation, and utilization effectively. There are priorities and weights for management in the following form:

i. **Maximizing total efficiency**: The power is distributed among stacks based on the highest efficiency at each moment, ensuring that stacks operate within their optimal efficiency range.

ii. **Minimizing degradation**: Degradation is managed by minimizing rated power operation and start-stop cycles and distributing operational hours equally across stacks to avoid overloading any single unit.

iii. **Balancing stack usage**: A rotational strategy ensures that all stacks are used evenly. This prevents the overuse of certain stacks while others remain underutilized, which can lead to uneven degradation.

iv. **Adhering to UF constraints**: Stacks are only turned on when the available power is sufficient to meet the minimum UF thresholds, preventing unnecessary energy losses and degradation.

Based on these objectives the optimization problem is formulated in (*21*) to maximize the efficiency while minimizing degradation and balancing stack utilization.

$$J = \sum_{t=1}^{T}\sum_{s=1}^{S}(\eta_s(P_{t,s}) \times P_{t,s}) - \lambda_1 \sum_{s=1}^{S} D_s - \lambda_2 \sum_{s=1}^{S}(H_s - \overline{H})^2 \qquad (21)$$

where $P_{t,s}$ is the power allocated to stack s at time t, $\eta_s(P_{t,s})$ stands for the efficiency of stack s based on the allocated power and D_s represents the degradation of stack s. Degradation penalty coefficient (λ_1) controls the weight given to the degradation term in the objective function. The total operational hours of stack s is H_s, and $\overline{H}$ is the average operational hours across stacks. Balancing utilization penalty coefficient λ_2 ensures that the operational hours are balanced between the stacks. It penalizes situations where some stacks are overused compared to others.

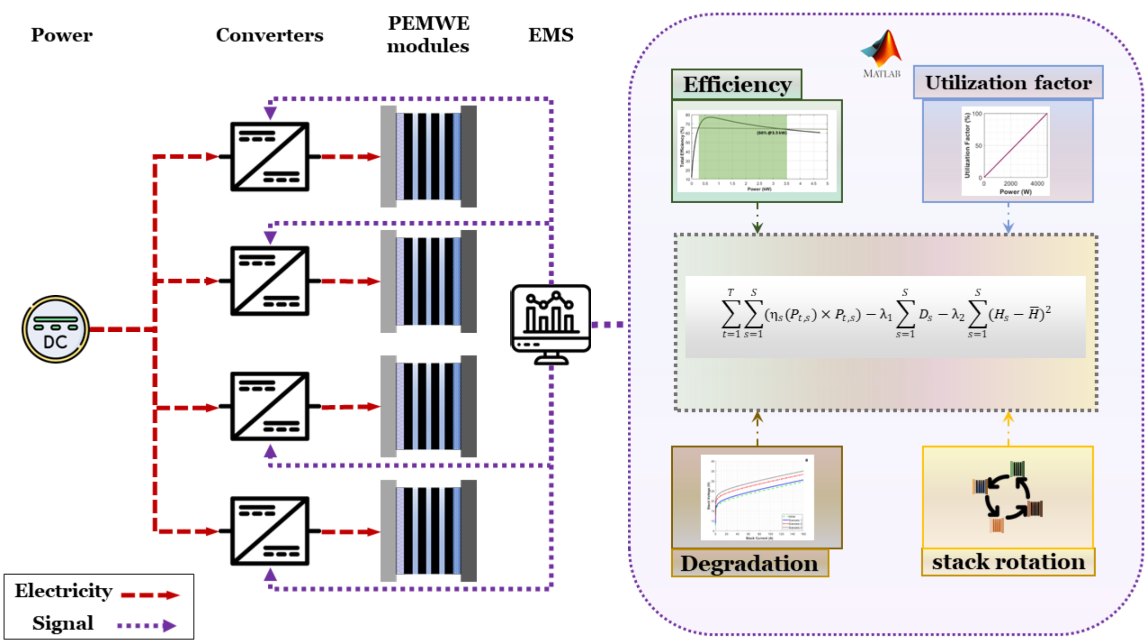

Figure 11 Schematic illustration of the developed EMS

Several constraints are integral to the model to ensure optimal performance, safety, and longevity of the system:

Stack capacity constraint: Each stack has a fixed maximum capacity (P_{max}) of 5kW. The power allocation to each stack must not exceed this limit to prevent overloading and potential damage ($P_{t,s} \leq P_{max}$).

Power allocation dynamics constraint: Ensures that the power allocated does not exceed the available power (P_{real}) from input power ($P_{t,s} \leq P_{real}$).

UF constraints: A stack is only turned on if the allocated power as a percentage of its capacity is at least 20%. This constraint ensures energy efficiency by avoiding operations under minimal load, which can be inefficient and lead to increased wear.

$$\begin{cases} UF_{on} \leq \dfrac{P_{t,s}}{P_{max}} & = turning\ on\ stack \\ UF_{off} \leq \dfrac{P_{t,s}}{P_{max}} & = keeping\ a\ stack\ on \\ where\ UF_{on} = 0.2\ and\ UF_{off} = 0.15 \end{cases}$$

Stack rotation strategy constraint: Rotate operational duties among stacks to even out wear and tear, governed by ($H_s \leq \overline{H}$) and operational thresholds.

$$\begin{cases} H_s < \overline{H} & = turning\ on\ stack\ (if\ previous\ constrains\ are\ satisfied) \\ H_s \geq \overline{H} & = keeping\ a\ stack\ on\ (if\ previous\ constrains\ are\ not\ satisfied) \\ H_s > \overline{H} & = turning\ a\ stack\ off\ (if\ previous\ constrains\ are\ satisfied) \end{cases}$$

These constraints are implemented using conditional logic within a loop over time and stack in the MATLAB code. Decisions to turn stacks on or off are based on the current power allocation relative to stack capacity and operational history, adjusting dynamically to changes in available power and operational needs. The actual efficiency and degradation computations adjust for current operating conditions using predefined mathematical formulas, ensuring the system operates within the defined constraints to optimize performance and longevity. This comprehensive approach integrates both operational and sustainability considerations, crucial for maintaining system efficiency and extending the service life of the PEMWE stacks.

Solving the objective function

Due to the inherent complexity and nonlinear characteristics of the system's operational parameters, nonlinear programming is chosen as the approach for solving the objective function for PEMWE system optimization. There are several nonlinear terms integrated into the objective function, including efficiency calculations, which entail exponential and logarithmic functions, particularly for modeling the activation, concentration, and ohmic overpotentials within the stack's electrochemical behaviour. These overpotentials depend on the current density, itself a function of the power allocated to each stack, thus introducing nonlinearity. Furthermore, constraints like the minimum UF threshold introduce conditional behavior that linear programming cannot accommodate efficiently. In addition, nonlinear programming provides a robust and precise tool for maximizing operational efficiency while balancing degradation and ensuring equitable utilization across multiple stacks by incorporating these complex relationships and varying constraints into the optimization process.

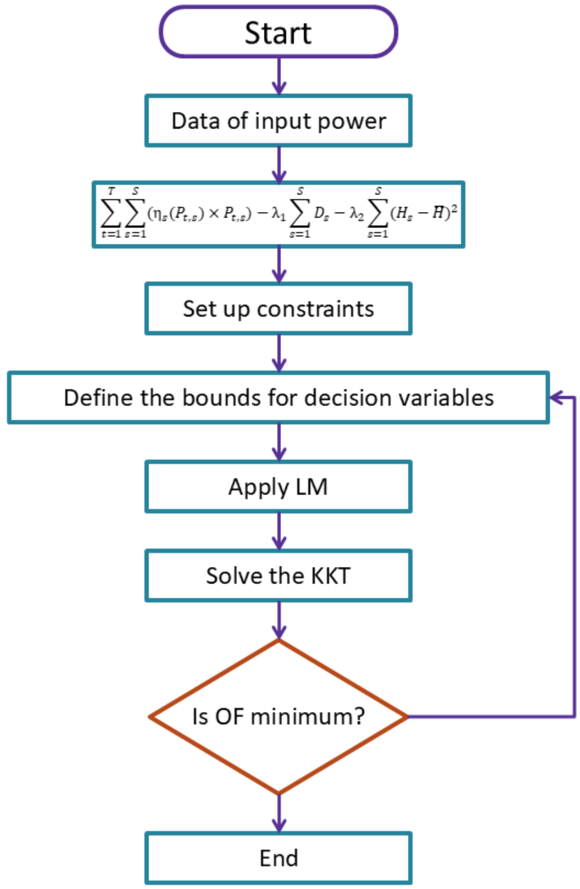

Figure 12 Solution to the objective function

The rationale for choosing nonlinear optimization over alternative techniques, such as linear programming or heuristic approaches, stems from the inherent complexities and accuracy requirements of the PEMWE system. Although linear programming is computationally simple, it is not capable of reproducing the nonlinear electrochemical relationships and operational dynamics involved, which could result in suboptimal or unrealistic solutions [73]. Meanwhile, heuristic methods, although often flexible, do not reliably ensure convergence to globally optimal solutions and typically lack theoretical optimality guarantees. Contrary to linear optimization, nonlinear optimization adheres to optimality criteria, in particular, the Karush-Kuhn-Tucker (KKT) conditions, which define the criteria for optimality [73].

At the optimal solution, the KKT conditions are satisfied via Lagrange Multipliers (LM), ensuring the solution's validity under the given constraints. As part of MATLAB's fmincon solver, the objective function and constraints are integrated into a Lagrangian function. It is then iteratively adjusted until convergence criteria (defined by gradient-based tolerances) are well achieved [74, 75]. Consequently, solutions derived from this method are mathematically rigorous, reproducible, and robust.

A numerical method (e.g., finite difference approximations) is generally used to estimate the gradients of the nonlinear objective as well as the constraints within the solver. Additionally, line search or trust-region strategies regulate the step size, ensuring the solver maintains stability and robustness over the entire optimization horizon [76]. By integrating these numerical techniques, the nonlinear optimization solver navigates the complex landscape of constraints and nonlinear objective functions inherent to energy management in modular PEMWEs, particularly under fluctuating solar energy inputs.

This combined approach—encompassing nonlinear modeling, appropriate constraints, and rigorous numerical methods—is especially well-suited to addressing the dynamic and multi-dimensional challenges of modular PEMWE energy management. The entire solution process is illustrated in Figure 12, showing how input data, constraints, and solver steps connect to find the optimal operating point for each stack.

4. Results

Using the standardized solar power dataset described in the methodology section, the modular PEMWE system demonstrated robust performance in terms of efficiency and operational reliability. Figure 13 illustrates the standardized DC input power profile, highlighting its consistency with the PEMWE's power requirements. Table 5 summarizes key technical specifications and performance metrics of the utilized PV system. It was possible to rigorously assess and validate the EMS and its effectiveness in maintaining high operational efficiency and minimal degradation under fluctuating solar inputs through these standardized inputs.

Table 5 PV System Specifications, Location and Station Identification

Category	Specifications
Requested Location	Trois-Rivieres
Weather Data Source	Lat, Lng: 46.35, -72.58 (0.7 mi)
Latitude	46.35° N
Longitude	72.58° W
DC System Size	20 kW
Module Type	Standard (Polycrystalline)
Array Type	Fixed
System Losses	14.08%
Array Tilt	66.5°
Array Azimuth	185° (South-West)
Inverter Efficiency	96%
DC Capacity Factor	13.5%

The inclusion of solar power data provides a solid basis for evaluating the PEMWE’s energy management capabilities. In addition, the dataset was standardized in accordance with our EMS approach, which involved removing long periods of zero production to ensure consistent and reliable outcomes in subsequent analyses.

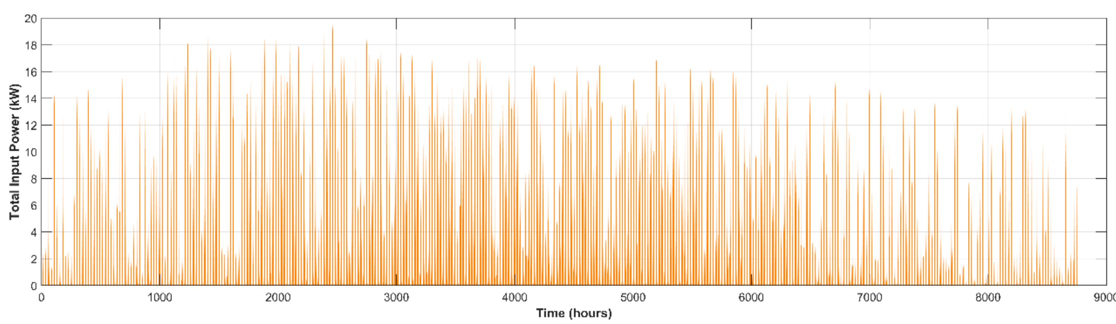

Figure 13 Total input power

The efficiency curve in Figure 14 illustrates the operational efficiency of the PEMWE system over the observed 8760-hour simulation period. This efficiency measurement integrates voltage efficiency, Faraday efficiency, and Balance of Plant (BoP) efficiency, as detailed in the methodology of this study. The efficiency generally remains consistently above 57%, with occasional peaks approaching 63%, reflecting effective EMS. The minor fluctuations depicted in the graph are attributed to variations in solar energy inputs, demonstrating the adaptive capability and robustness of the developed EMS. This performance highlights the success of the proposed EMS in maintaining optimal efficiency despite intermittent renewable energy supply, thereby significantly mitigating potential efficiency losses associated with fluctuating operational conditions and enhancing overall system resilience and longevity.

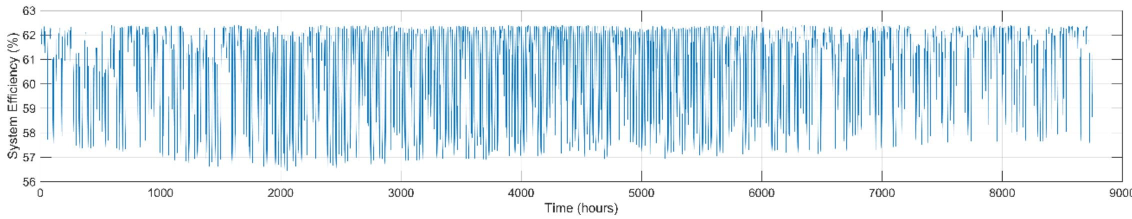

Figure 14 System efficiency over time for PEMWE

The comparison of input power allocation between a simple rule-based EMS and a developed EMS, as depicted in Figure 15, offers a revealing insight into the efficiency and effectiveness of advanced power distribution strategies. Graphs show the allocation of power for four stacks within a PEMWE system over 8760 hours.

In the simple rule-based strategy, power distribution is somewhat uniform but prone to sudden spikes and drops Figure 15.a. Each stack receives power in a fixed sequence, regardless of its current efficiency or state of degradation. Despite the simplicity of this approach, it may result in inefficiencies. For example, power may continue flowing to an almost full stack, leading to increased wear and inefficiencies because of overloading. However, the developed EMS see Figure 15.b uses an adaptive and dynamic power allocation technique which enhances the overall performance of the system as well as maintains the overall health of each stack while improving the overall operating efficiency.

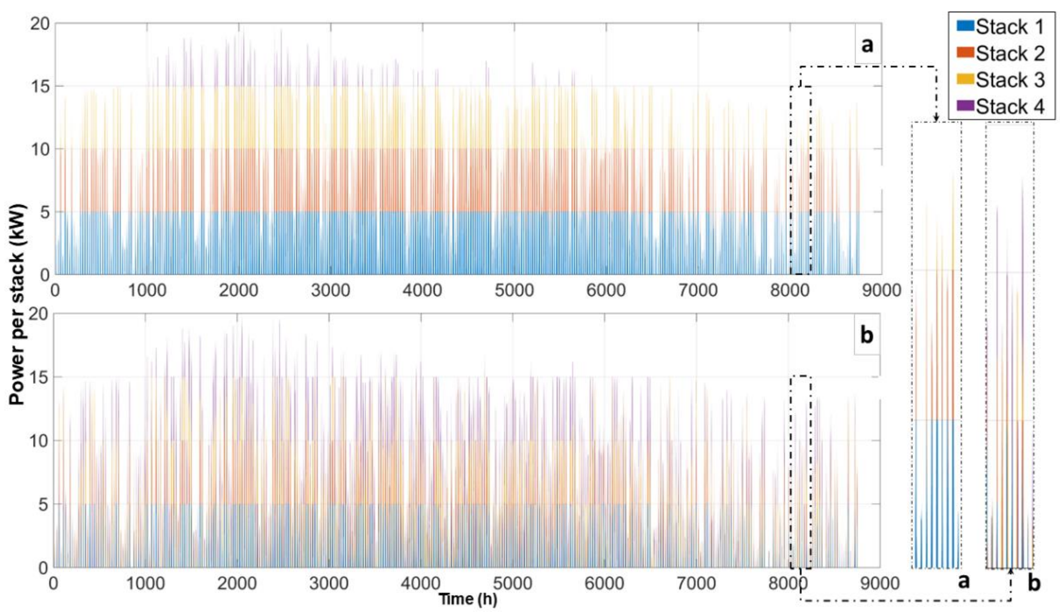

Figure 15 Input power allocation to each stack for a) simple rule-based EMS b) developed EMS

The modular PEMWE system efficiency with the designed EMS has increased compared to linear power allocation. Specifically, simulations show that the advanced EMS achieves an average efficiency of about 62%, approximately 5–6% higher than that observed with the simple approach.

It minimizes energy loss and lowers the chance of stack deterioration by allocating power based on real-time data and stack performance. Specifically, by avoiding prolonged high-power operation in any single stack, the proposed EMS significantly reduces the voltage degradation and membrane stress that drive premature stack failure. A regular rate of wear and tear is maintained by more evenly distributing the load throughout all stacks, which is essential for the system's lifetime and dependability. A regular wear and tear rate is maintained by distributing the current evenly throughout all stacks, which is essential for the system's lifetime and dependability. A designed EMS optimizes the response of the system to varying power inputs by adapting to shifting stack performance levels as well as power availability conditions.

Figure 16 provides a quantitative comparison of daily on/off cycle patterns between the developed EMS and the simple EMS. Stack on/off cycles represent the average number of times stacks are powered on and off during the day, indicating typical operational behavior. A higher mean suggests more frequent switching, potentially impacting operational consistency and component lifespan.

As indicated by the maximum daily on/off cycles chart, the highest observed number of on/off cycles in one day indicates the peak of switching activity. Frequent high peaks may stress system components and accelerate degradation.

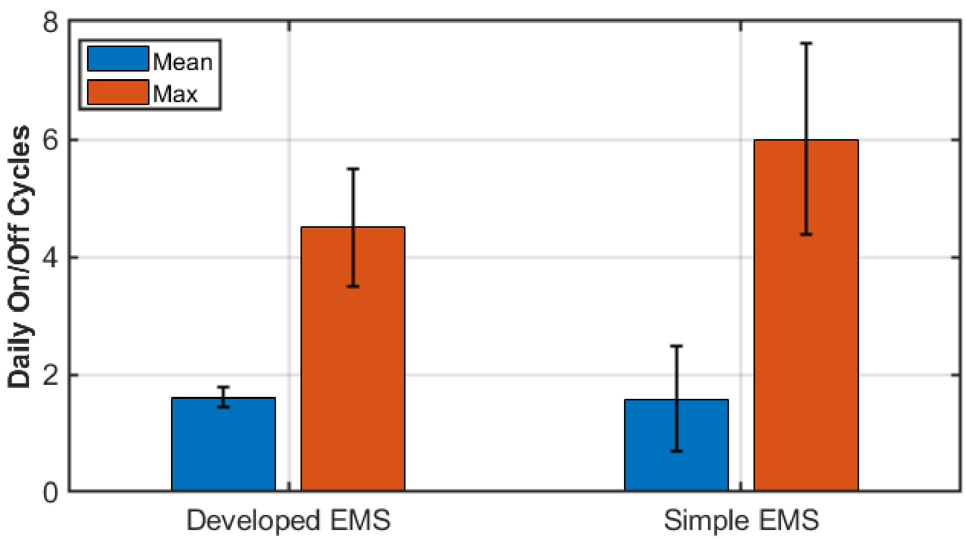

Figure 16 Overall Daily On/Off Cycle Statistics

The data (see Figure 16) indicates variations among individual stacks. For example, Stack 1 under the developed EMS has an average daily cycle of approximately 1.38 compared to 2.36 under the simple EMS. According to the developed EMS, stack 2 experiences an average of 1.62 cycles compared to 2.13 cycles with the simple EMS. Stack 3 shows a slightly higher average daily cycle with the developed EMS (1.69) than with the simple EMS (1.45). Finally, stack 4 significantly contrasts, having an average of 1.74 daily cycles under the developed EMS compared to only 0.36 cycles under the simple EMS. The differences observed between the two EMS approaches can be attributed to their respective strategies. The simple EMS distribute power to multiple stacks simultaneously, resulting in a generally lower mean daily cycle but occasionally higher peaks because it activates stacks for nearly any available power. Conversely, the developed EMS, constrained by utilization factor thresholds and designed to maintain higher operating efficiency, tends to activate stacks in a favorable efficiency region and after a certain amount of power, resulting in higher average daily cycles but lower peak cycles.

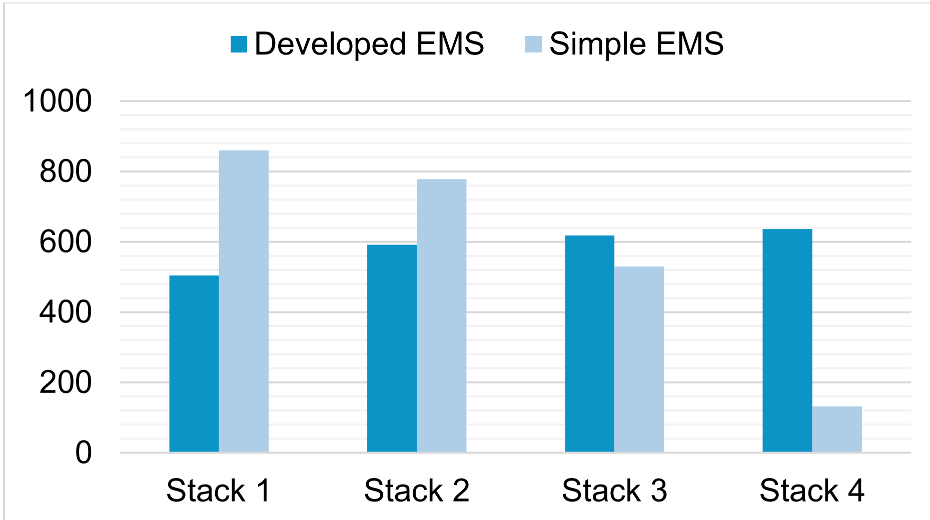

Figure 17 Total on and off for each stack separately

The maximum number of daily cycles observed also varies. The developed EMS consistently reaches a maximum 4 daily cycles for stacks 1, 2, and 3. In contrast, the simple EMS reaches 6 for stack 1, 8 for stack 2, and 6 for stack 3. According to the developed EMS, stack 4 exhibits a maximum of six daily cycles as opposed to four under the simple EMS.

Figure 17 complements this analysis by presenting the total on/off cycles per stack over the operational period. As a result of the use of this metric, insights into the operational patterns and maintenance implications of each energy management system are further enhanced.

A heatmap showing the power distribution over 8760 hours across four stacks based on the suggested EMS method is shown in Figure 18. The stack index is indicated on the y-axis, while hours are displayed on the horizontal axis. Each stack can be classified according to its power allocation by its color intensity, which ranges from yellow, indicating full capacity, to dark blue, which represents no power allocation.

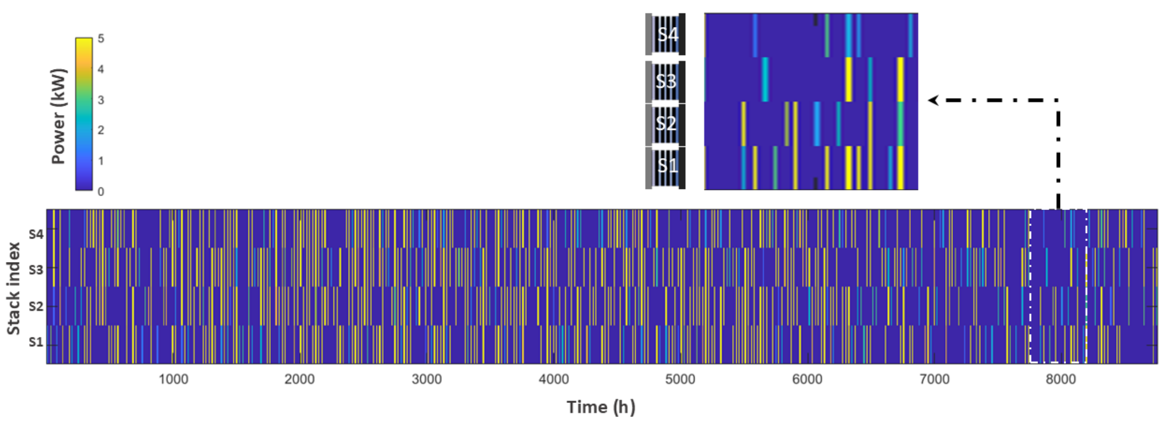

Figure 18 Heatmap of power allocation - developed EMS

As shown in Figure 18, the developed EMS is flexible and dynamic. The EMS modifies power distribution based on stack efficiency and performance in real-time, as opposed to the basic rule-based system that distributes power in a predetermined order. As indicated by the heatmap, a balanced power allocation rotation will guarantee that no stack will ever become overloaded. This strategy promotes uniform degradation, enhances system reliability, and maintains higher operational efficiency by evenly distributing the load over the system's operational lifetime. The adaptive allocation is evident from the varying intensities, demonstrating how the EMS reacts to fluctuating input power and stack conditions.

Expanding upon the improved power management features of the developed EMS, Figure 19 provides a clear visual depiction of the system's cumulative hydrogen generation over time.

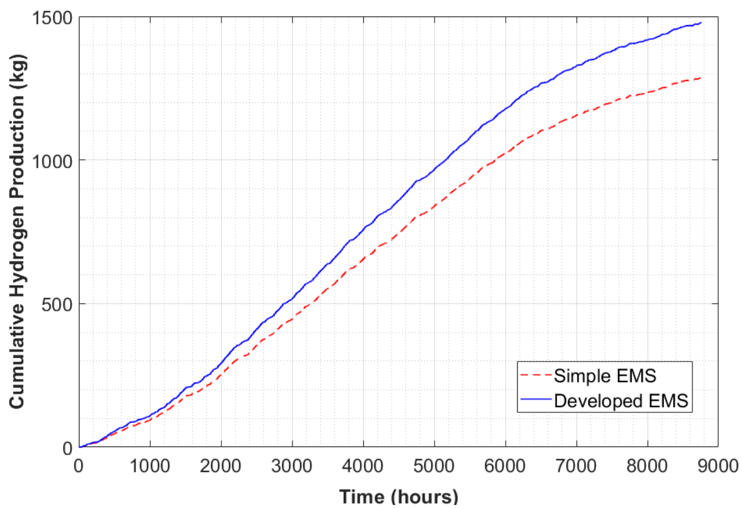

Figure 19 Comparison of cumulative hydrogen production

As compared to the Simple EMS, which generates around 1290 kg of hydrogen in the same period, the Developed EMS, represented by the blue line, generates nearly 1480 kg of hydrogen after 8760 hours. This discrepancy of almost 190 kg demonstrates how well the developed EMS performs in maximizing hydrogen generation over long operating hours. Interestingly, after 2000 hours, the difference between the two systems becomes more noticeable, highlighting the long-term benefits of employing advanced control strategies. The efficiency gains achieved by the planned EMS are illustrated by this quantitative comparison. By improving the power allocation, the hydrogen output may be raised by 12% as compared to the Simple EMS. This improvement is crucial for PEMWE systems' operational and financial viability in renewable energy scenarios with variable input power.

The basic rule-based EMS doesn't adjust to the efficiency or operational condition of the stacks; instead, it follows a set sequence. This static technique raises the possibility of rapid degradation and results in less-than-ideal power distribution, especially in situations when power fluctuates. In the absence of adaptability, stacks are worn unevenly, with those that operate consistently near their capacity limits experiencing significantly greater degradation rates.

On the other hand, Figure 20 illustrates how the developed EMS reduces deterioration. This EMS dynamically allocates power based on stack conditions, ensuring balanced utilization and reduced stress on individual stacks. Comparing cumulative voltage degradation illustrates these improvements.

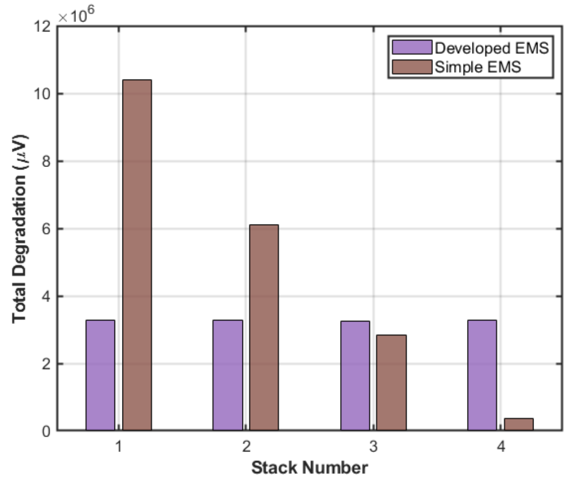

Figure 20 Comparison of degradation per stack for rule based and developed

Stack 1 experiences a degradation of 3.31 V under the developed EMS, compared to 10.44 V for the rule-based EMS. Stack 2 shows a reduction from 6.07 V with the rule-based EMS to 3.24 V under the developed EMS. A balanced allocation technique is demonstrated by Stack 3, which records 3.27 V with the created EMS, which is marginally greater than the 2.83 V with the rule-based EMS. Because of the more uniform distribution of operating stress, Stack 4 degrades 2.27 V under the created EMS as opposed to 0.35 V with the rule-based EMS. The designed EMS's cumulative values are 12.09 V, whereas the rule-based EMSs are 19.69 V, indicating a 38.6% reduction in overall system deterioration.

Figure 21 provides a detailed comparative analysis of the average efficiency across four stacks of a PEMWE, comparing the performance between a simple EMS and a developed EMS. According to the graph, the evolved EMS performs better than the simple EMS in terms of average efficiency for each stack. Efficiency is a crucial metric for assessing the effectiveness of the energy management strategies put in place since it denotes increased power and operational parameter optimization under varied loads. The bar chart compares the average efficiency percentages for the four stacks, numbered 1 through 4, under the two different EMSs—Developed EMS and Simple EMS. The efficiency achieved by both methods is shown by parallel bars for each layer.

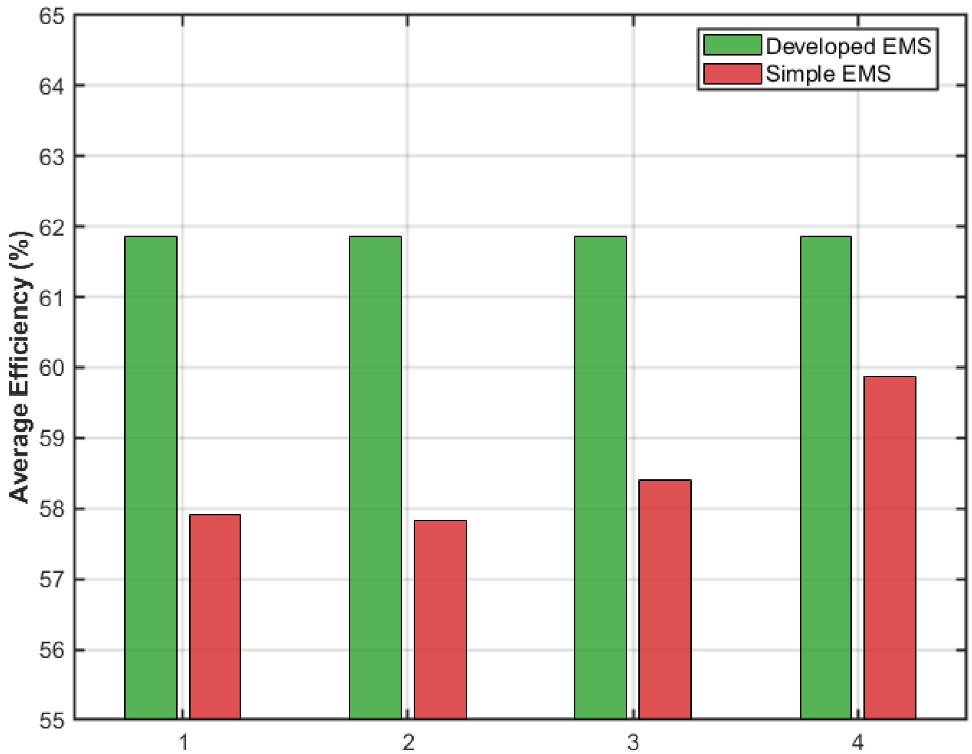

Figure 21 Comparison of stacks average efficiency of both simple and developed EMS

Across all stacks, the developed EMS achieves a consistent maximum efficiency of about 62%, with no performance variance. This implies that the management techniques used by the developed EMS are the same for all stacks, resulting in the same levels of efficiency. In comparison, the simple EMS has a slightly lower efficiency, continuously averaging around 58% for each stack, except for stack 4, which almost hits 60% since it uses significantly less labor or electricity. While performance is consistent, it is lower than that of the established EMS, indicating valid but less optimal functioning. Across all stacks, the developed EMS exhibits an efficiency increase of about 5.8% over the simple EMS (where for one-by-one stack: S1= 6.9%; S2 = 6.8%; S3=6%; S4=3.3%).

Conclusions

This work presented an advanced EMS tailored for modular PEMWEs operating under variable solar power inputs. This EMS dynamically balances power distribution, stack utilization, and degradation by integrating real-time performance metrics and optimizing control strategies, as opposed to a conventional rule-based allocation method. Specifically, the EMS optimizes voltage efficiency, Faraday efficiency, and balance-of-plant (BoP) efficiency, ensuring sustained performance even under fluctuating solar inputs.

It was demonstrated through an extensive evaluation of the developed EMS over an operational year (8760 hours) that the developed EMS had significant advantages over a traditional rule-based approach. Notably, the EMS achieved approximately a 39% reduction in cumulative voltage degradation and an approximate 12% increase in hydrogen production, reaching nearly 1480 kg compared to 1290 kg for the conventional approach. In addition, the system maintained a stable operating efficiency of approximately 62 percent, or about 5 percent higher than that of a simple rule-based EMS. The adaptive response capability of the EMS, reflected in controlled switching cycles and balanced power allocation across stacks, underscores its effectiveness in extending stack lifespan and operational reliability.

It remains important to investigate certain aspects further, however. The simplified assumptions regarding start-stop cycles and steady power transfers do not adequately represent the complex operational conditions in real-world conditions, including rapid fluctuations and transient grid disturbances. Moreover, the scalability and efficacy of the EMS in larger and more complex renewable energy systems warrant additional exploration. As a future step, advanced predictive methodologies, including machine learning and neural networks, should be explored to enhance power allocation efficiency and adaptability. Incorporating elements found in real-world operational contexts into deterioration models will greatly improve their accuracy. The degradation models can include catalyst activity losses, membrane stability, and temperature fluctuations. Multi-objective EMS frameworks should include considerations such as dynamic power prices, efficiency, and degradation. Hydrogen generation will also be safe and dependable if EMS scalability in large-scale or hybrid renewable systems is validated, and plans are in line with regulatory and standardization initiatives. These issues may be resolved to make EMS solutions more robust, economical, and sustainable, which will strengthen PEMWEs' position in renewable energy systems.

Nomenclature:

A_L	**Active large surface area (mm)**
A_S	Active small surface area (mm)
B_r	temperature coefficient
CP_{PV}	Coefficient of Performance
G_{nr}	Solar irradiance (W/m^2)
I_C	cell current (A)
I_S	stack current (A)
I_{cn}	each cell current (A)
P_C	cell power (W)
P_{el}	electrolyzer required power
P_{pv}	PV Power (W)
T_{pv}	PV temperature(°C)
T_r	operating reference temperature (°C)
U_a	Activation overvoltage (v)
U_c	Concentration overvoltage (v)
U_o	Ohmic overvoltage (v)
U_b	Bubble overpotential
V_C	cell voltage (v)
V_{OC}	Open circuit voltage (v)
V_S	stack voltage (v)
V_{cell}	cell voltage (v)
V_{cn}	each cell voltage (v)
V_{rev}	Reversible cell voltage (v)
$V_{rev,s}$	Standard reversible cell voltage (v)
V_{th}	Thermoneutral voltage (v)
n_{el}	number of electrolyzers
n_p	number of PV panels
t_r	reference time
$\alpha HyPro_S$	HyPro system (in a stack) efficiency
η_v	voltage efficiency (%)
η_c	cell efficiency (%)
η_e	Electrolyzer efficiency (%)
η_s	Electrolyzer system energy efficiency (%)
η_{BP}	Balance of plant efficiency (%)
A	Area (square meter, m^2)
E	Energy ($Wh \approx 3600\ joules$)
f	gas flow rate (Normal Meter Cubed per Hour Nm3/hr)
F	Faraday constant (C/mol)
g	gradient
$HHVH$	Higher Heating Value of Hydrogen (kWh/Nm^3)
P	Power (W)
Rct	charge transfer impedance (Ω)

$\boldsymbol{R}$	The universal gas constant 8.314 (J/mol·K)
$\boldsymbol{t}$	Time (h and H/2)
$\boldsymbol{W}$	electrical work of electrolysis (J/mol)
$\boldsymbol{W_{irrev}}$	Irreversible energy (J/mol)
$\boldsymbol{W_{rev}}$	Reversible energy (J/mol)
$\boldsymbol{\Upsilon}$	surface coverage ratio (/)
$\boldsymbol{\Delta H_R^0}$	Electrolysis required energy (J/mol)
$\boldsymbol{\Omega_E}$	Electric resistance in electrodes (Ω)
$\boldsymbol{\Omega_{eq}}$	Equivalent electric resistance in PEMWE (Ω)
$\boldsymbol{\Omega_M}$	Electric resistance in membrane (Ω)
$\boldsymbol{\theta}$	Thickness of the membrane (cm)
Ʊ	Conductivity of the membrane (umho/cm)
$\boldsymbol{\lambda}$	Humidification of the membrane

Abbreviations:

AC	**Alternating Current**
ANN	Artificial Neural Network
CNC	Computer Numerical Control
CO_2	Carbon Dioxide
DC	Direct Current
e_-	electron
ERC	Ejector Refrigeration Cycle
FC	Fuel Cell
H_2	Hydrogen
HyPro	Hydrogen Production
kW	Kilo Watt
L	Liter
MES	Modular energy system
ML	Machine Learning
MW	MegaWatt
NPV	Net present value
O_2	Oxygen
ORC	Organic Rankine Cycle
PEMFC	Proton Exchange Membrane Fuel Cell
PEMWE	Proton Exchange Membrane Water Electrolyzer
PTC	Parabolic Trough (solar) Collector
PtG	Power-to-Gas
PV	Photovoltaic
RES	Renewable Energy Source
RO	reverse osmosis

WECS	wind Energy Conversion System
SIBC	stacked interleaved buck converter
MEA	Membrane Electrode Assembly
PTL	porous transport layer
OER	Oxygen Evolution Reaction

Acknowledgements

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC) (2018-06527)

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The insights from this study are directly applicable to the broader scope of this PhD thesis, which aims to develop advanced energy management strategies for modular PEMWE systems. The findings on power allocation and degradation directly inform the development of more robust energy management frameworks. The RPAS introduced in the paper provides a practical solution for enhancing system efficiency while simultaneously managing degradation, a key concern in long-term operations.

In the context of this thesis, the study's contributions are twofold. First, it demonstrates that advanced energy management strategies can significantly enhance the operational efficiency of PEMWE systems, especially in modular configurations. This supports the broader thesis objective of optimizing the balance between efficiency and degradation in energy management systems. Second, the research provides empirical data and simulation results that validate the proposed strategies, offering a foundation for future studies and applications in industrial-scale HyPro.

The findings in this paper demonstrate the critical importance of strategic power distribution and real-time stack management in maximizing the efficiency of modular PEMWE systems. The study confirms the main contention of this thesis, which is that efficient energy management is essential to the long-term sustainability of industrial-scale HyPro, by demonstrating how an EMS, enhanced by dynamic load allocation, degradation modelling, and optimisation algorithms, can significantly increase hydrogen production while reducing wear.

As the following sections proceed, these results will be integrated into a broader framework addressing a range of scaling challenges as well as operational challenges beyond the laboratory test bench, such as real-time management of large-scale renewable inputs, industrial automation requirements, and long-term degradation control. The thesis moves closer to its goal by applying the EMS concepts discussed here to a variety of industrial settings. This is to demonstrate how a comprehensive and flexible EMS makes modular PEMWE systems dependable and effective pillars in the shift to a green hydrogen economy.

5 Conclusion

The deterioration analysis of PEMWE systems, modular design, and energy management are some of the major knowledge gaps that this thesis fills. To improve the efficiency and sustainability of HyPro systems, this work has broadened our understanding of how to optimize energy allocation, minimize degradation, and improve system scalability by concentrating on modular designs.

The first major contribution is the development of a comprehensive test bench for benchmarking and selecting electrochemical models for energy management in modular PEMWE systems. The analysis of various models has shown that tailored models, such as those integrating activation and ohmic overpotentials, provide the best balance between accuracy and computational efficiency, which is crucial for real-time energy management. This study provides a unified paradigm for comprehending how operational modes affect system lifetime by classifying degradation mechanisms and their implications on PEMWE performance.

The development of modular PEMWE system design is the second contribution. By including the chosen electrochemical models, the suggested design process map offers a useful manual for maximizing system configurations according to scalability, stability, and efficiency. According to experimental results, modular topologies perform noticeably better than single-stack systems, with HyPro enhancements and slower rates of degradation.

The final contribution is the development of an advanced EMS that dynamically allocates power among multiple electrolyzer stacks based on real-time data. By using an RPAS, this system extends system longevity under varying renewable energy sources and balances stack use by optimizing the trade-off between efficiency and degradation.

To sum up, this thesis developed a strong foundation for expanding the real-world use of PEMWE systems, especially in renewable energy settings. The development of scalable and effective HyPro technologies is greatly aided by the knowledge obtained from model benchmarking, system design optimization, and energy management techniques. This work contributes to the larger shift toward sustainable energy systems by bridging the gap between theoretical understanding and real-world application, establishing modular PEMWE setups as a feasible option for large-scale green HyPro.

5.1 Summary of Findings

This doctoral thesis provides a comprehensive exploration of the key challenges and solutions in PEMWE, with a special focus on modular configurations for enhanced energy management and operational efficiency in HyPro systems.

Model Benchmarking and Selection:

The study established a robust methodology for benchmarking and selecting electrochemical models suitable for modular PEMWE systems. It revealed that models incorporating activation and ohmic overpotentials are particularly effective, offering a balanced approach between computational efficiency and modelling accuracy. This is essential for practical, real-time energy management applications.

Degradation analysis:

Detailed degradation studies highlighted critical insights into the longevity and operational challenges of PEMWE systems. The research classified and analyzed various degradation mechanisms, emphasizing the need for robust models to mitigate these effects and improve system durability. This understanding allows for better prediction and management of system performance over time.

Energy Management Strategies:

The development and implementation of an advanced EMS was central to this research. Utilizing dynamic, rotational strategies for power allocation among electrolyzer stacks, the EMS effectively enhances overall efficiency and prolongs system lifespan by balancing energy efficiency with degradation management.

Design and structural optimization:

By integrating selected electrochemical models, the thesis proposes a detailed design process map for modular PEMWE systems. Experimental findings demonstrate that modular configurations significantly improve HyPro and reduce degradation compared to single-stack setups. This validates the modular approach as more adaptable and scalable to varying operational demands.

Comparative analysis:

A comparative analysis between single-stack and modular systems underscored the benefits of modular designs in operational flexibility and scalability. The study showed that modular systems could achieve higher HyPro efficiencies and sustain less degradation over time, making them more suitable for large-scale and diverse application scenarios.

Practical Applications and Future Directions:

PEMWE systems are poised to be significantly influenced by the findings of this thesis. By addressing the practical aspects of model applicability, energy management, and system degradation, the research provides a foundational blueprint for enhancing the scalability and efficiency of HyPro technologies.

This comprehensive summary underscores the thesis's contributions to advancing PEMWE technology, highlighting significant strides made in modelling, system design, degradation mitigation, and energy management. These achievements mark substantial progress toward developing more sustainable, efficient, and scalable HyPro systems.

5.2 Future Research Directions

While this thesis has made significant strides in understanding energy management, modular design, and degradation analysis of PEMWE systems, several areas remain open to further investigation. Advancing research in these domains will enhance the efficiency, scalability, and practical deployment of HyPro technologies, especially when integrated with RESs. The following subsections outline key directions for future research.

5.2.1 Simulation of Energy Management under Variable Operational Conditions and different renewable energies

The integration of RES like solar, wind, and hydropower introduces variability in energy supply due to fluctuating environmental conditions. This variability poses challenges for PEMWE systems, whose performance and efficiency are susceptible to power input stability. Future research should focus on simulating and evaluating energy management strategies for modular PEMWE systems operating under variable conditions driven by different renewable energy inputs.

Developing advanced strategies that optimize energy allocation, minimize degradation, and enhance overall system efficiency across diverse renewable energy conditions is crucial. A possible approach involves creating simulation models in MATLAB/Simulink that incorporate detailed electrochemical processes, dynamic energy allocation, and degradation factors. The impact of fluctuating conditions on the system can be assessed by inputting different renewable energy profiles—such as solar cycles, wind speed variations, and seasonal hydropower flows.

The expected outcomes include insights into effective energy management strategies that maintain high efficiency and minimize degradation under varying renewable energy inputs. This research will contribute to the practical integration of renewable energy with PEMWE systems, enhancing the scalability and efficiency of HyPro technologies.

5.2.2 Implementation of Machine Learning Algorithms for Enhanced Efficiency

Managing energy systems for PEMWE involves real-time adjustments to optimize efficiency, manage degradation, and accommodate varying operational demands. Traditional energy management strategies may not adequately adapt to dynamic conditions or predict future performance. Incorporating machine learning algorithms offers a promising solution by enabling predictive modelling and intelligent decision-making for power distribution and operational modes.

Future research should aim to integrate machine learning algorithms into the energy management systems of modular PEMWE setups to enhance operational efficiency and minimize degradation.

This could involve collecting historical data on PEMWE performance and renewable energy profiles and developing predictive models using techniques such as artificial neural networks, decision trees, or reinforcement learning. Implementing these algorithms within a simulation environment like MATLAB/Simulink would allow for testing and refinement of real-time adjustments to energy allocation based on predictive analytics.

The anticipated outcome is an advanced energy management system capable of dynamic, data-driven decision-making. By leveraging machine learning, the PEMWE system can optimize power allocation, improve efficiency, reduce degradation, and increase lifespan, even under fluctuating renewable energy supplies. This advancement will make the system more adaptive, scalable, and suitable for integration with RESs.

5.2.3 Strategic overview of electric ramp-up and conversion to minimize degradation and optimize EMS

Rapid changes in electric power input, known as electric ramp-up, can impose significant stress on PEMWE systems, accelerating the degradation of components like catalyst layers and membranes. Efficient energy management systems are essential for controlling the ramp-up process, minimizing sudden surges that could harm the system, and optimizing performance. Future research should develop strategies that balance the need for fast response times with the long-term reliability of the PEMWE system.

This research could involve studying degradation patterns under different ramp-up speeds and current loads, simulating various electric ramp-up profiles to identify optimal ramp-up speeds that minimize degradation while maintaining efficiency. Integrating these optimized profiles into the energy management system, possibly using advanced control strategies like model predictive control, would ensure dynamic adjustment to changing power conditions without inducing excessive stress.

The expected results include guidelines and control strategies for managing electric ramp-up and conversion in PEMWE systems. Using variable RESs, these strategies will enhance HyPro reliability and efficiency over time by reducing degradation rates and extending operational lifespans.

5.2.4 Strategic overview of electric warm-up and normalizing voltage period for EMS

Transitioning PEMWE systems from a cold start to normal operational conditions requires careful management to minimize thermal stresses and prevent accelerated degradation. The electric warm-up phase and the normalizing voltage period are critical for stabilizing electrolyzer components and ensuring efficient operation. Future research should aim to develop comprehensive strategies for managing these phases within an energy management system. Figure 5-1 illustrates the voltage profile of the PEMWE of our testbench during the initial warm-up and subsequent normalizing phases, highlighting how the voltage is carefully ramped up to operational levels and then adjusted to stabilize after fluctuations, crucial for minimizing thermal stresses and ensuring the longevity of the system. Effective management of these phases within the EMS is key to ensuring system durability and efficiency.

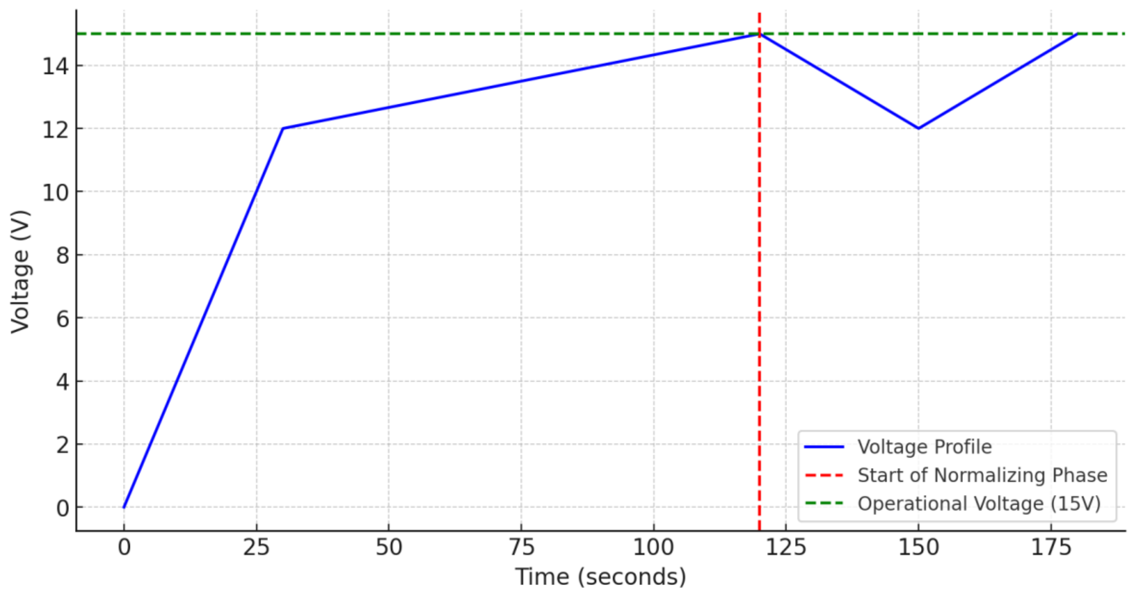

Figure 5-1 Voltage Profile During Warm-up and Normalizing Phases in PEM Water Electrolysis

This could involve analyzing the effects of different warm-up profiles on component behaviour and degradation rates, simulating gradual voltage increases and stabilization periods under various conditions, and integrating optimal warm-up and voltage normalization strategies into the EMS using control systems like model predictive control. Experimental validation would ensure the effectiveness of these strategies under real-world conditions.

By optimizing warm-up and voltage normalization protocols, this research will reduce thermal stresses, extend system lifespan, and improve operational stability and efficiency. This is particularly important in applications with variable renewable energy inputs that necessitate frequent voltage adjustments.

5.2.5 EMS dependency on the PEMWE application characteristics

The performance of EMS in modular PEMWE setups can be heavily influenced by external factors such as the type of RESs, system architecture, and environmental conditions. This dependency can lead to variability in energy management effectiveness and system performance. Future research should focus on identifying and mitigating these dependencies to achieve consistent and reliable PEMWE operation across different contexts.

This could involve analyzing external factors that influence EMS performance, simulating dependency scenarios with different renewable energy profiles and environmental conditions, and designing adaptive EMS frameworks that adjust system parameters dynamically based on real-time data. Integrating machine learning algorithms may enhance the system's ability to predict and respond to environmental changes.

The anticipated outcome is an adaptive EMS that reduces the impact of external dependencies, maintaining consistent performance and reducing inefficiencies and degradation. This advancement will enhance the long-term viability of PEMWE systems, especially when integrated with fluctuating RESs.

5.2.6 Temperature and pressure regulation in EMS

Temperature and pressure are critical parameters that significantly affect PEMWE system performance, efficiency, and longevity. Fluctuations in these variables, especially due to variable renewable energy inputs, can impact electrochemical reactions and accelerate component degradation. Future research should aim to develop energy management systems that dynamically regulate temperature and pressure to maintain stable and optimal operating conditions.

This research may involve analyzing how temperature and pressure variations affect system performance and degradation, developing control algorithms for real-time monitoring and adjustment of these parameters, and integrating these algorithms into the EMS. Simulation and experimental validation would assess the effectiveness of these strategies under various operational conditions.

By effectively regulating temperature and pressure, the EMS will improve system efficiency, reduce stress, minimize degradation, and extend its operational lifespan. This will make PEMWE systems more resilient to external variability and more effective for large-scale HyPro.

5.2.7 Cold weather effect in EMS in Canada

Cold weather conditions prevalent in regions like Canada can severely impact the performance and efficiency of PEMWE systems. Low temperatures can reduce membrane conductivity, slow electrochemical reactions, and increase mechanical stress, leading to accelerated degradation. Future research should explore how cold weather affects PEMWE performance and develop energy management strategies to mitigate these effects.

This could involve analyzing performance data from PEMWE systems operating in cold climates, simulating cold-weather operational scenarios, and developing adaptive EMS strategies that regulate system temperature and manage cold starts effectively. Experimental validation under simulated Canadian winter conditions would ensure the EMS's ability to maintain performance and minimize degradation at low temperatures.

By optimizing system performance during cold weather, this research will enhance the reliability and efficiency of PEMWE systems in harsh climates. This will contribute to the broader understanding of temperature regulation in PEMWE systems and improve their integration with RESs in variable environments.

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Appendix

I. Evaluation of High-Efficiency Hydrogen Production from Solar Energy using Artificial Neural Network at the Université du Québec à Trois-Rivières

Conference: VPPC 2022

Publisher: IEEE

Date Added to IEEE Xplore: 05 January 2023

2022 IEEE Vehicle Power and Propulsion Conference (VPPC) | 978-1-6654-7587-7/22/$31.00 ©2022 IEEE | DOI: 10.1109/VPPC55846.2022.10003314

Evaluation of High-Efficiency Hydrogen Production from Solar Energy using Artificial Neural Network at the Université du Québec à Trois-Rivières

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Abstract— **Hydrogen produced through renewable energy sources is rapidly emerging as one of the most promising ways to meet future fuel demands. Developing models that simulate the operation of this process (photovoltaic (PV) panel, electrolysis devices, etc.) is paramount to efficiently designing power generation systems, cutting manufacturing costs, and reducing resource usage. Artificial Neural Network (ANN) plays a crucial role in developing predictive models for complex systems due to their nonlinear nature. This study evaluates the solar hydrogen production in Trois-Rivières while modeling the PV by ANN and the water electrolysis process using semi-empirical equations. According to the obtained results, solar panels can be used for the annual production of more than two thousand and seventy hundred kg of hydrogen in UQTR.**

Keywords— Hydrogen Production, Solar Power, Renewable Energy, Neural Network

I. Introduction

Proton exchange membrane water electrolysis (PEMWE) can make renewable energy even more attractive. However, renewable energy sources, such as wind and solar energy, remain the most reliable alternative to fossil fuels as they are clean, accessible, and illimitable. They are also unpredictable and inevitably involve intermittency due to their variable nature. In addition, the available amount of power can fluctuate wildly, so it would be more efficient to transform it into an energy carrier [1]. This transition can also happen with surplus energy [2]. PEMWE plays a vital role in this transition. Because of the characteristics of PEMWE, it can bear a wide range of ripple energy. It is one of the best options for facing renewable power due to the wide range of changes in the amount of energy from renewable energy sources (RES). Due to PEMWE's quick response time, they can be coupled with RES to provide a 100% renewable system. Less than a minute dynamic response time, in some new technologies even sub-second response, enables PEMWE to have the wide operating range and fast kinetics of RES nature, while providing acceptable efficiency [3].

Available energy prediction is essential for planning electric power system response, restoration, and maintenance efforts. The transition section needs to understand the impact of output energy to develop appropriate maintenance and resilience measures, as they have two freedom degrees [4]. However, PEMWE providers mention the amount of hydrogen production in the instruction. For instance 4500 kg/day by a 10MW PEMWE [5]. The practical output would not always be in the maximum amount. The losses, operational conditions, and ambient features make many changes in the output. So, models are needed to predict the hydrogen flow after applying appropriate inputs. One of the best solutions for solving this problem is the neural network approach. Based on analysis of the influential variables, and performance of the PEM Electrolyser, some neural networks have already been designed in the literature [6].

The performance of electrolyzers facing renewable energy is becoming more complicated. For instance, integrated solar systems depend on the set efficiency, weather circumstance, and PV array system losses. Today, weather forecasting has become highly computerized due to human efforts. Thanks to artificial intelligence (AI) techniques, the most recent improvements in weather predictions and large quantities of machine-based forecasts have happened [7-11]. Laoun et al. modeled a direct-coupled PV and PEMWE, in which they could estimate the hydrogen production in Algeria [12].

In previous studies, the influence of location and environmental factors over the energy output has been ignored. However, these parameters have an important role in predicting the hydrogen production of PEMWEs from renewable energies. A detailed analysis of the location and environment of solar energy production is presented in this study. This paper studies the possibility of using PV panels at the University of Quebec at Trois-Rivières (UQTR) and estimates the amount of hydrogen production in the Institute for Hydrogen Research (IHR) using clean, accessible, and unlimited solar energy (Figure 1). Various methods and algorithms are employed to find the most accurate NN model of PV to determine the possible amount of available power in this particular geographical location. Then PEMWE

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performance is analyzed by a semi-empirical model, considering PV power as the input in the Trois-Rivières climate. Section II introduces the method and materials for this study. Results and analysis are in Section III. Finally, conclusions and future trends are expressed.

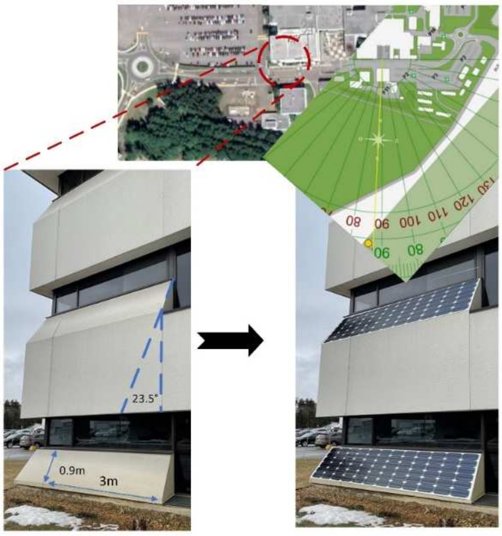

Figure 1 Appropriate tilt locations for PV on the university facade

II. METHOD

A. *General description*

As mentioned in the literature, machine learning can use the real measured data to treat the system for a more accurate forecast. Various online simulators use different formulas to predict PV output. However, they follow a program, and many tiny details are missed in their result. They are mainly focused on sun radiation which is the most vital part. Sometimes, all or part of soiling, shading, snow, losses, and aging effects are not considered.

Furthermore, temperature, air pressure, transparency, and wind also play a role in PV outputs in different circumstances [13]. So, training an ANN will teach the system how various parameters can change the PV output. The final goal of this study is to predict hydrogen production in the UQTR. So, Meteorological data of this particular region and experimental data of a photovoltaic panel in the same area are the training facts of an ANN to predict the available energy in the future by just having a weather forecast. An empirical model could then calculate the possible hydrogen production with the readily available energy (Figure 2).

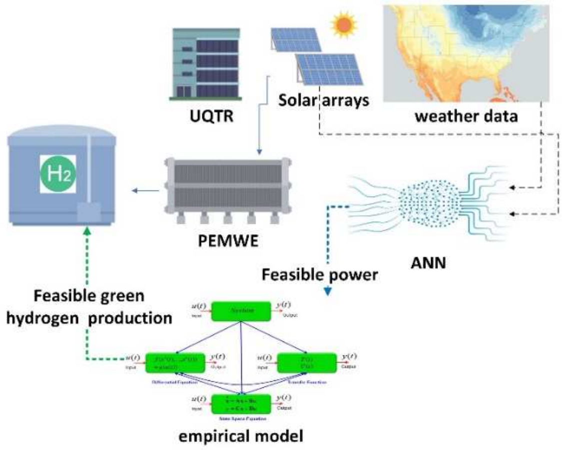

Figure 2. Schematic of the whole process

B. *PV performance and ANN*

Based on the literature, to train a NN for predicting the available energy, the input should be as close to the desired situation as possible. The data of a PV panel was collected precisely at the exact location, direction (Figure 1), and circumstance for a year from the first of January 2021 to the end of December 2021 (Table 1). In order to anticipate total harvested energy by about 250 m^2 PV panels, it was necessary to determine the impact of climatic data, radiation, and losses on the output power as well as to train a predictive model for predicting available energy for PEMWE from an observation.

Table 1 The PV System deployment status

Location	Trois-Rivières, Canada
Latitude	46.35° N
Longitude	72.58° W
Module Type	Polycrystalline
Array Type	Fix tilted
Array Azimuth	185°(South-West)
Capacity Factor	12.5%
Array Tilt	66.5°
DC System Size	0.15 kW
Maximum current	8.7 A
Dimensions	149 * 66.5 * 3.5 cm

The PV output is direct current (DC), as the input of the PEMWE stack requires the same type. An MPPT or charge controller is needed, and an AC-DC converter is unnecessary. However, to save the data history, an RS-485 was employed, and the power was stored in a battery (Figure 3).

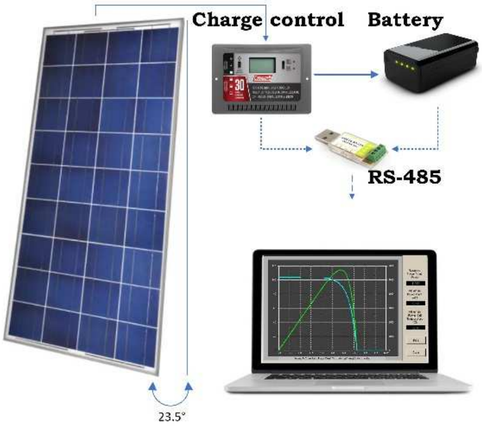

Figure 3 PV system configuration

To determine NN inputs, parameters that influence the system's performance must be diagnosed. In the same way, PV generated power depends on the following formula [14, 15]:

$$P_{pv} = \Upsilon \alpha_{PV} G_{nr}[1 - B_r(T_{pv} - T_r)] \quad (1)$$

Here γ is the coverage ratio of the PV cell, α_{pv} is the efficiency of the cell, G stands for solar irradiation, nr is the reference cell efficiency, T_r is the operating reference temperature, and B_r is the temperature coefficient. The dynamic spatial position of the sun affects Υ, and the earth's atmospheric conditions, such as pressure, humidity, atmospheric dust, wind, and transparency, directly affect G. Other effective parameters will automatically influence the NN by training with an experimental system. It includes system losses (mismatch, wiring, connections), power control, aging, and light-induced degradation. As a result, temperature, visibility, humidity, air pressure, wind speed, and hourly solar irradiation are six variables that will be considered in training NNs.

C. *PV Neural Network*

After preprocessing (normalization, standardization, and analysis) the PV data, it is realized that an MLP works better for fitting a model. So, a two hidden layer NN with six inputs is created and its details are mentioned in Figure 6. Then Root Mean Squared Error (RMSE) is used to distinguish between the predicted values by the model and the observed ones. It will describe the difference between the expected and observed values, as shown in (2): where n stands for every hour of measurement. Ai and Pi respectively introduce the actual and predicted amount of the model prediction.

$$RMSE = \sqrt{\frac{1}{h}\sum_{i=1}^{h}(P_i - A_i)^2} \quad (2)$$

This arrangement was appropriate for validating a well model by Conjugate Gradient with Powell-Beale Restarts (CGB). After analyzing various algorithms such as; Quasi-Newton backpropagation (BFG), Fletcher-Reeves updates (CGF), Polak-Ribiere updates (CGP), Gradient descent momentum & adaptive LR backpropagation (GDX), Levenberg-Marquardt backpropagation (LM), One-step secant backpropagation (OSS), Rprop (RP), Scaled conjugate gradient backpropagation (SCG). Each algorithm has been tested to find the most accurate prediction of PV output power. The best results are compared to other backpropagation algorithms to find the best performance in predicting power production. Various algorithms with the number of their layers are compared in Table 2. CGB algorithm seems to have the best ability to train the NN for this favor. Different numbers of hidden layers have been examined, where two layers have led to the best performance. A conjugate gradient algorithm periodically resets its search direction to the negative gradient (3). A standard reset point is reached when the number of iterations equals the number of network parameters [16].

$$|g_{k-1}^T g_k| \geq 0.2 g_k^2 \quad (3)$$

Table 2 The comparison of different algorithms in PV model

Algorithm	Hidden layer	validation	All
BFG	1	0.99698	0.99715
	2	0.99909	0.99919
CGB	1	0.99704	0.99702
	2	0.99941	0.99944
CGF	1	0.99686	0.99690
	2	0.99894	0.99903
CGP	1	0.99686	0.99683
	2	0.99870	0.99867
GDX	1	0.59437	0.56792
	2	0.99491	0.99480
LM	1	0.99764	0.99721
	2	0.99917	0.99923
OSS	1	0.99695	0.99678
	2	0.99692	0.99696
RP	1	0.99565	0.99590
	2	0.99930	0.99933
SCG	1	0.99677	0.99670
	2	0.99918	0.99933

D. ***PEMWE model***

If the electrolysis process occurs under reversible conditions (without losses), the potential difference at the electrodes is called the reversible cell voltage (V_{rev}^0), which equals 1.229 volts. Minimal electrical work is needed to split up water if the requisite contribution of thermal energy is present. Without having an external heat source, the total energy for the reaction to take place would be (ΔH_R^0) that must be delivered by electrical energy. Hence, the required voltage is higher than V_{rev}^0 and is called the thermoneutral voltage V_{th}^0 at a normal state [17, 18]:

$$V_{th}^0 = \frac{\Delta H_R^0}{z.F} = 1.481\ V \quad (4)$$

For an actual estimation, the accurate cell voltage (V_{cell}) is needed. It is the division of thermoneutral voltage by cell efficiency (η) [18]:

$$V_{cell} = \frac{V_{th}^0}{\eta} \quad (5)$$

Finally, the electrical work (J) can be derived from W in (5), where ε_i is faradic efficiency [19]:

$$W = 2F\frac{V}{\varepsilon_i} \quad \text{[J/mol]} \tag{6}$$

This amount is about 285.8 (J/mol) or 0.08 (Wh/g).

Hydrogen production happens in the cells of the PEMWE. The equation and the role of electricity are as follow:

$$H_2O = \left(\frac{1}{2}\right)O_2 + 2H^+ + 2e^- \quad \text{(anode)}$$

$$2H^+ + 2e^- = H_2 \quad \text{(cathode)}$$

$$H_2O + \text{ electricity} = H_2 + \left(\frac{1}{2}\right)O_2 \tag{7}$$

The electrolyzer's performance is most commonly represented through the polarization curve, which illustrates the current density and cell voltage relationship (Figure 3). It describes the current (I_C) and cell voltage (V_C) of the cell relation. According to Faraday's law, the current directly correlates with the production rate, so the polarization curve shows a correlation between the production rate and electric power. It can be expressed as (8).

$$P_c = I_C \times V_C \tag{8}$$

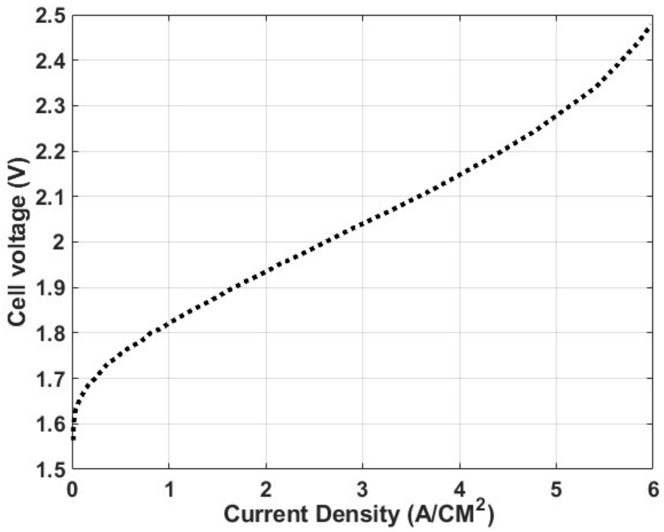

Figure 4 PEMWE cell performance polarization curve [20]

The reversible potential and overpotential sum of a PEMWE cell can be shown as the actual cell voltage:

$$V_C = \eta_a + \eta_o + \eta_c + V_r \tag{9}$$

In this equation V_r stands for the reversible potential and η_a, η_o, and η_c are activation, ohmic, and concentration overpotentials, respectively [21]. So, with having these equations and calculating the losses in voltage, it is possible to have a more accurate prediction of hydrogen production in a stack. As well as cells, the stack polarization in (10) demonstrates the stack current (I_S) and voltage (V_S) relations Whenever an array is connected in series, the voltage at the stack terminals is equal to the sum of voltages at the series connections. In contrast, when it is connected in parallel, the stack current is equal to the sum of the currents flowing through the parallel connections of the cells [22].

$$P_S = I_S.V_S \tag{10}$$

$$P_S = I_C.\sum_{n=1}^{N} V_c.n_{ss} \quad \text{Serie}$$

$$P_S = V_C.\sum_{n=1}^{N} I_C.n_{ps} \quad \text{Parallel}$$

Based on studies, the amount of produced hydrogen flow rate can be calculated by the (10):

$$\int_0^t f_{H2}.dt = \frac{\int_0^t N.I.V.\eta_e.dt}{HHVH} \tag{11}$$

In this equation, the Higher Heating Value of Hydrogen (HHVH) is 3.54 kWh/Nm^3, and 't' is the production period. In this extracted empirical model, the efficiency of the electrolyzer'η_e' is [20]:

$$\eta_e = -0.0786I^3 + 1.167I^2 - 7.365I + 84.44 \tag{12}$$

$$f_{H2} = \frac{N \times I_c}{2F} \times \eta_f \tag{13}$$

Faradays constant equals $F = 96{,}485(\frac{\text{C}}{\text{mol}})$, which is one mole of electrons, or Avogadro's number, contains one mole of electric charge, η_f is the ratio of real to ideal electricity; it represents Faraday's efficiency:

$$\eta_f = \frac{C_r}{C_i} \times 100 \tag{14}$$

In the final step, it is necessary to determine how many stacks are necessary to convert available energy to hydrogen. In this regard as this study is using a validated empirical model (11,12), according to (1) and PV power production:

$$n_p.t.P_{pv}.\eta_{array} \approx n_{el}.E_{el} \tag{15}$$

$$n_p.(\eta_c.I_c.V_c.N_c.t)_p.\eta_{array} \approx n_{el}.E_{el} \tag{16}$$

n_p and n_{el} are the number of panels and PEMWEs. η_{array} is the efficiency of the group of panels which are called array. It contains all events that penalize the available array output energy, such as linking wires, charge control and so forth. The feeding duration is shown by't'. E_{el} is the PEMWE stack energy requirements. η_c, I_c, V_c, N_c, are efficiency, current, voltage, and the number of the cells, respectively. These parameters should be considered in a panel structure which is illustrated with index 'p'.

III. RESULTS AND DISCUSSION

A. PV Neural networks algorithms

The results of estimated power production by the ANN model using CGB algorithm are pretty close to the measured one, as shown in Figure 5. The training, validation, and test output and targets are also illustrated. Best validation performance and an abstract of ANN configuration are also tagged in Figure 6.

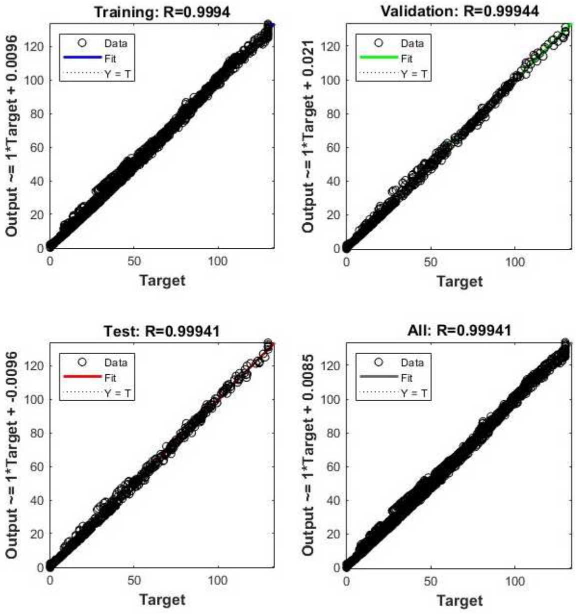

Figure 5 The regression PV NN with CGB

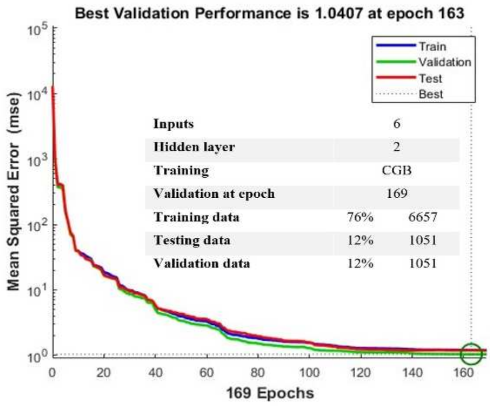

Figure 6 PV ANN performance

B. Hydrogen production in UQTR

After studying various models and finding out the feasibility of producing efficient hydrogen in UQTR, it derivates that by implementing at least 80 m^2 solar panels on the frontage of the UQTR building, at least 2,800 kg of hydrogen can be produced yearly. The details of this feasible production can be seen in Figure 7. The monthly hydrogen comparison shows that the most hydrogen is produced in March 2021 and April 2021. This result primarily relies on solar irradiation and also PV direction and angle. However, daytime and weather conditions are highly impacting the output. According to Figure 1, the implementation of solar panels can increase the beautification of the UQTR building facade. However, hydrogen production can experience a significant rise if solar energy is harvested in a solar farm or a rooftop with the azimuth direction 180 and panels implemented by 35-45 degrees instead of 66.5.

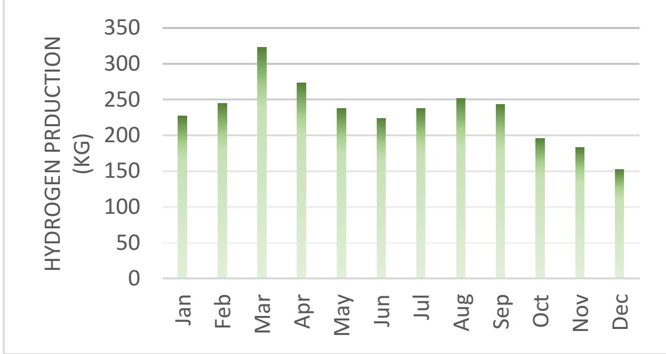

Figure 7 Hydrogen production in UQTR

Figure 8 shows the amount of produced power in the panel in January at Trois-Rivières. The yellow color illustrates the range that is not efficient for hydrogen production with the stack because of losses, activation energy, and dynamic feeding impact. The green area is appropriate for the PEMWE stack hydrogen production. The red range in this figure shows a higher amount of power which might be harmful and increase degradation in the stack. On some cloudy days, when solar radiation is significantly lower, the power production is less than optimal. This situation sometimes continues for several days. So, this optimal range in future studies should be analyzed more accurately. The possible solutions could be modular electrolyser system or integrating energy storage systems, such as supercapacitors, batteries, and appropriate energy management.

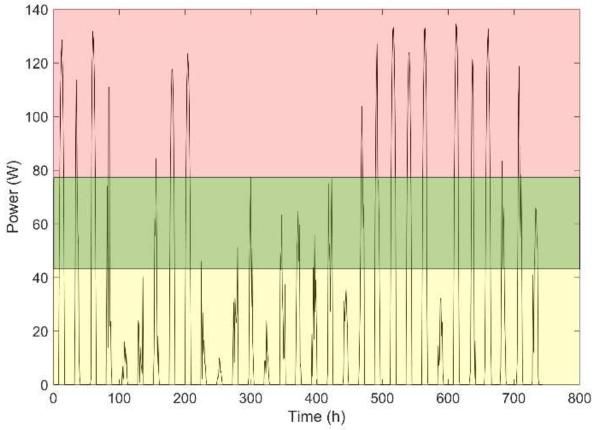

Figure 8 Optimal range of PEMWE input

CONCLUSION

In this study, the feasibility of solar-based hydrogen production in the IRH located at UQTR in Trois-Rivières has been studied. First, the production of PV power is modeled by employing various algorithms. Then an empirically validated model of PEMWE is employed to simulate its performance. Finally, it is realized that over two thousand and six hundred cubic meters of hydrogen can be produced by implementing PV arrays on the UQTR building facade.

In the future, the following efforts can be made:

- Considering some effective parameters, such as PV temperature, ground, Airborne dust, atmospheric pollutants, etc., in the training phase to enhance the modeling accuracy.

- Since the concept of the study is a prediction by local data, it would be more meaningful if a PEMWE stack is implemented in the following study and experimental data is obtained.
- Since the PEMWE required voltage is highly affected by the feeding pattern and input power, adjusting the input power in an optimal range is recommended.

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II. Estimation of increasing the solar-based hydrogen production in Trois-Rivières

Conference: The 14th International Green Energy Conference (IGEC- XIV)

Publisher: Journal of Green Energy

Date: 06 Jun 2022

Proceedings of the 14th International Green Energy Conference
IGEC 2022
July 4-8, 2022, Glasgow, UK (Virtual)

ESTIMATION OF INCREASING THE SOLAR-BASED HYDROGEN PRODUCTION IN TROIS-RIVIÈRES

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ABSTRACT

The proton exchange membrane water electrolyzer (PEMWE) is the most viable hydrogen production method from renewable energy sources (RESs). However, the efficiency of PEMWE widely varies, encountering different amounts of input currents. In addition to efficiency, intermittent input affects the durability of PEMWE and causes its cell to erode. In this direction, hybrid energy sources with energy management are becoming more popular in hydrogen production. Hybrid energy sources include two or more supplements of electrolyzers, such as the battery, wind, and solar combined. This research evaluates efficient green hydrogen production from clean, accessible, and unlimited solar energy and anticipates the possible amount of solar power by employing machine learning techniques. The PEMWE feeding configuration is analyzed to determine the most profitable feeding configuration. First, available energy is experimentally collected by a photovoltaic (PV) panel. Then an empirical PEMWE model is nominated, and the hydrogen output in the standard scenario is calculated. Afterward, the PEMWE feeding pattern is equipped with a battery, and its current is controlled. Finally, the results of different configurations are compared, and the continuous feeding seems to be more compelling.

Keywords: PEMWE, Solar Energy, Photovoltaic, Energy Efficiency.

INTRODUCTION

Nowadays, global energy consumption has gradually increased due to population growth and the standard of living. In addition, with the increase in global warming and environmental pollution, the development of renewable energy sources (RESs) is becoming more and more essential. Thus, increasing the efficiency of the production, storage, and transfer of renewable energies play a crucial role in using these beneficial resources. The potential synergy between RES and hydrogen provides an exciting prospect in terms of sustainability. Hydrogen can be used as a fuel in almost any application where fossil fuels are used today (vehicular and stationary applications) without harmful emissions [1]. In addition, hydrogen can be converted into proper forms of energy more efficiently than fossil fuels. PEMWE is emerging today as a straightforward way for hydrogen production and a viable key to transitioning from fossil fuels to RES [2, 3]. High efficiency, compactness, and high output pressure are PEMWE's upper hands in competition with its rivals. Furthermore, their fast response time made them a great pairing with RES to bring the world's energy sector closer to its zero-emission targets [4].

RES is not without its challenges, mainly due to its intermittent nature. Feeding PEMWE with such s dynamic power leads to degradation and corrosion, and its efficiency and lifespan decrease significantly [5-7]. So the combination of RES and PEMWE needs to be carefully examined [8]. Feng *et al.* [9] have published a review article on the degradation mechanisms. Mainly focused on the effect of degradation on the important components of PEMWE with accelerated stress tests and protocols. They concluded that evolving markets related to the implementation of RES require PEMWE systems that can tolerate more aggressive operating conditions, namely the temperature, pressure, and power loads of different magnitudes and frequencies. Such cycles can have devastating effects on the performance and durability of cell components. Finally, it is mentioned that PEMWE technology will be incredibly advanced and commercialized through codes and standards development. Parache et al. [10] surveyed how ripple currents harm the PEMWE. Their research found an increase in ohmic resistance, titanium mesh corrosion, passivation, and mass transport limitations, and these effects appear to be intensified by triangular current ripples.

Koponen *et al.* [11] analyzed the performance of the PEMWE encountering RES. They assessed functional dynamic properties and operational limitations with a renewable energy approach. They recommend the use of a supercapacitor or battery for continuous electrolysis; based on a ten-hour test featuring a 1 Nm^3/h PEMW powered by 5 kW solar PV. The highest hydrogen production achievable in a PEMWE system without a separate post-electrolysis compression occurs when the hydrogen outlet pressure is adjusted to the storage pressure as close as possible. Zaik & Werle [12] evaluated an electrolyzer coupled with a solar panel and wind turbine after a minireview on RES as a PEMWE energy source. Their study shows that wind and solar energy can compensate for each energy shortage at certain times of the year. In addition, charging a buffer battery gives the system freedom to use the optimal amount of energy and avoid overcharging or activation losses. Pirom & Srisiriwat [13] combined PEMWE & PEM FuelCell with a photovoltaic array for a residential house with a system efficiency between 1.75 and 7.66%. Net-zero emission residential houses also had freshwater available as a byproduct of PEMFC.

This paper discusses the possibility of green, efficient hydrogen production in Trois-Rivières using renewable energy. Based on the literature, input power plays a critical role in hydrogen production. So this study will propose the best scenario for achieving maximum hydrogen from solar energy. First, the amount of solar energy is recorded in Trois-Rivières, and a neural network (NN) estimates feasible future energy. PEMWE models are then analyzed, and the basis of performance formulas in PEMWE is discussed. An empirical model is nominated, and the hydrogen production based on available energy and operational conditions is estimated. Finally, the suggestions for improving efficiency and achieving the highest amount of green hydrogen are presented.

Materials and methods

Available energy

The available solar energy in Trois-Rivières is annually measured. From Eq.(1), the PV output power is mainly related to solar radiation and geographical location, so local weather situations significantly impact it [14]. So the placement of clouds in the sky, transparency, temperature, air pressure, and wind are all critical parameters that make differences in the received energy.

$$\mathrm{P}_{\boldsymbol{pv}} = \Upsilon \alpha_{\mathrm{PV}} \mathrm{G}_{\mathrm{nr}} [1 - \mathrm{B_r}(\mathrm{T}_{pv} - T_r)] \quad (1)$$

Solar irradiation is represented by $\mathrm{G_{nr}}$, cell efficiency by α_{PV}, operating reference temperature by T_r, and temperature coefficient by $\mathrm{B_r}$. In addition, Υ stands for the surface coverage ratio is the module surface area that can be covered by sun irradiation to the area that the array occupies. Solar dynamical positions directly affect Υ, and the earth's atmospheric conditions, such as pressure, humidity, atmospheric dust, wind, and transparency, directly impact $\mathrm{G_{nr}}$. The panel position, soiling, shading, snow, losses, and aging are other crucial parameters affecting the nominal output power of PV [15]. Thus based on these facts, one of the best ways to find out the received solar energy is by collecting the experimental data from a PV panel in the same direction and location as illustrated in Figure 1. The University of Quebec at Trois-Rivières is a feasible site for implementing solar arrays.The university front wall is directed to the South (with a slight angle to the west, approximately 5 degrees). It is the best situation in the northern hemisphere. In addition, since arrays will be installed relatively high, the possibility of shading is limited. Due to the tilt position snowing and dust effect is pretty slight. The accessibility of this area is also fair due to the windows of the building. These advantages make this facade appropriate for the installing PV array, as shown in Figure 1. Also, from an aesthetic point of view, it will have a better view. The PV panel data is listed in Table 1.

Table 1 The reference PV panel characteristics

Location	Trois-Rivières, Canada
Latitude	46.35° N
Longitude	72.58° W
Module Type	Polycrystalline
Array Type	Fix tilted
Array Azimuth	185°(South-West)
Capacity Factor	12.5%
Array Tilt	66.5°
DC System Size	0.15 kW
Maximum current	8.7 A

Dimensions	149 * 66.5 * 3.5 cm
Number of PV for estimated array	80

Data was collected for a year from 2021 to 2022. Since the PV output is direct current (DC), it is directly passed to the battery after maximum power point tracking by a charge controller. Besides, the voltage and current are measured and transferred to the system by an RS-485. This process is shown in Figure 1.

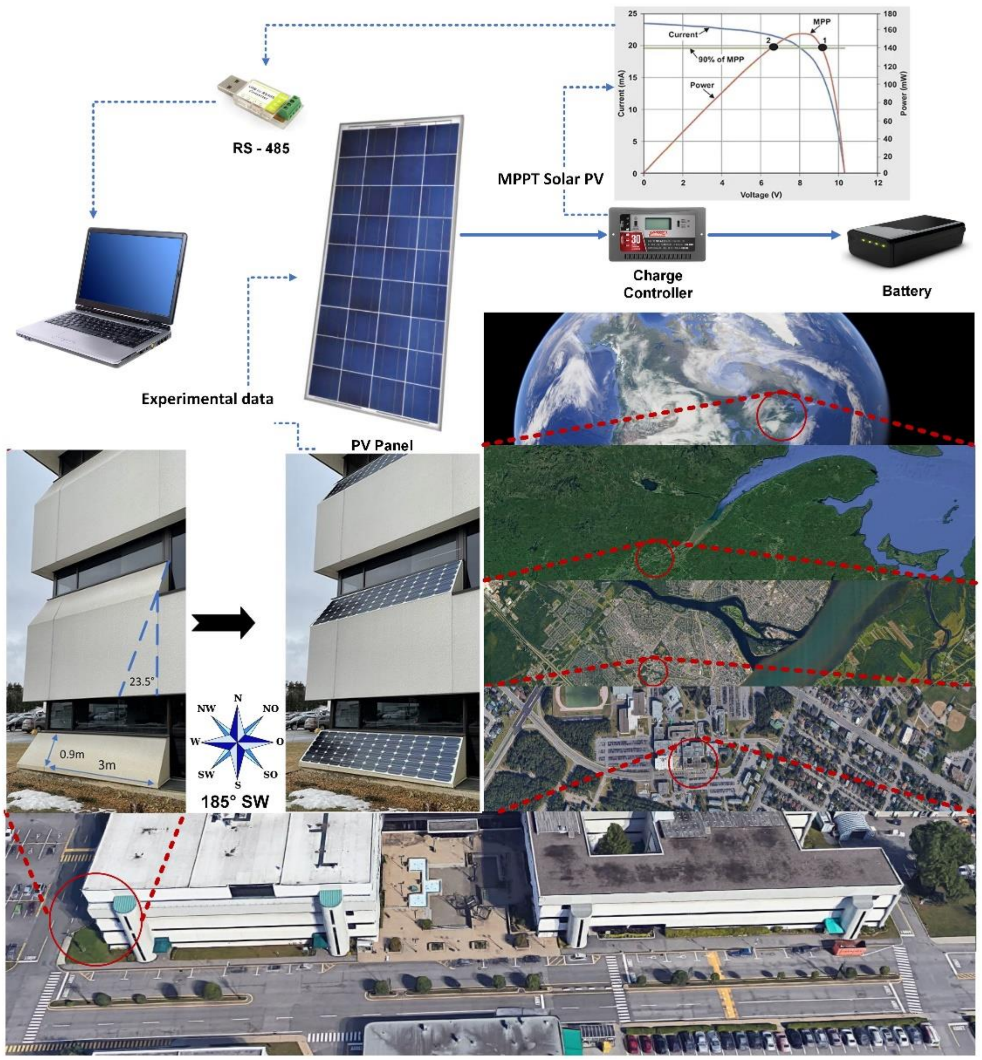

Figure 1 The PV location, direction and position [16]

Estimating available energy in the future needs machine learning to find out available energy for a particular time or a more extended period. By having the PV output power and using the meteorology data of the location, it would be possible to train a predictive model with ANN. According to Eq.(1), temperature, visibility, humidity, air pressure, wind speed, and hourly solar irradiation are effective parameters in the output of PV panels. So they will be considered in training ANN as input variables, as demonstrated in Figure 2. In addition, azimuth and tilt angle, capacity factor, efficiency, cover ratio, system losses (mismatch, wiring, connections), power control, aging, and light-induced degradation will be automatically inserted into the result by training ANN with experimental data. As shown in Figure 2, this NN has six inputs, two hidden layers, and an output layer. After analyzing various algorithms, Conjugate Gradient with Powell-Beale Restarts seems to have the best ability to train this NN. The method of a conjugate gradient algorithm is a way that periodically resets its search direction to the negative gradient Eq.(2). Finally, a standard reset point will be reached when the number of iterations equals the network parameters [17].

$$|g_{k-1}^{T}g_k| \geq 0.2g_k^2 \quad (2)$$

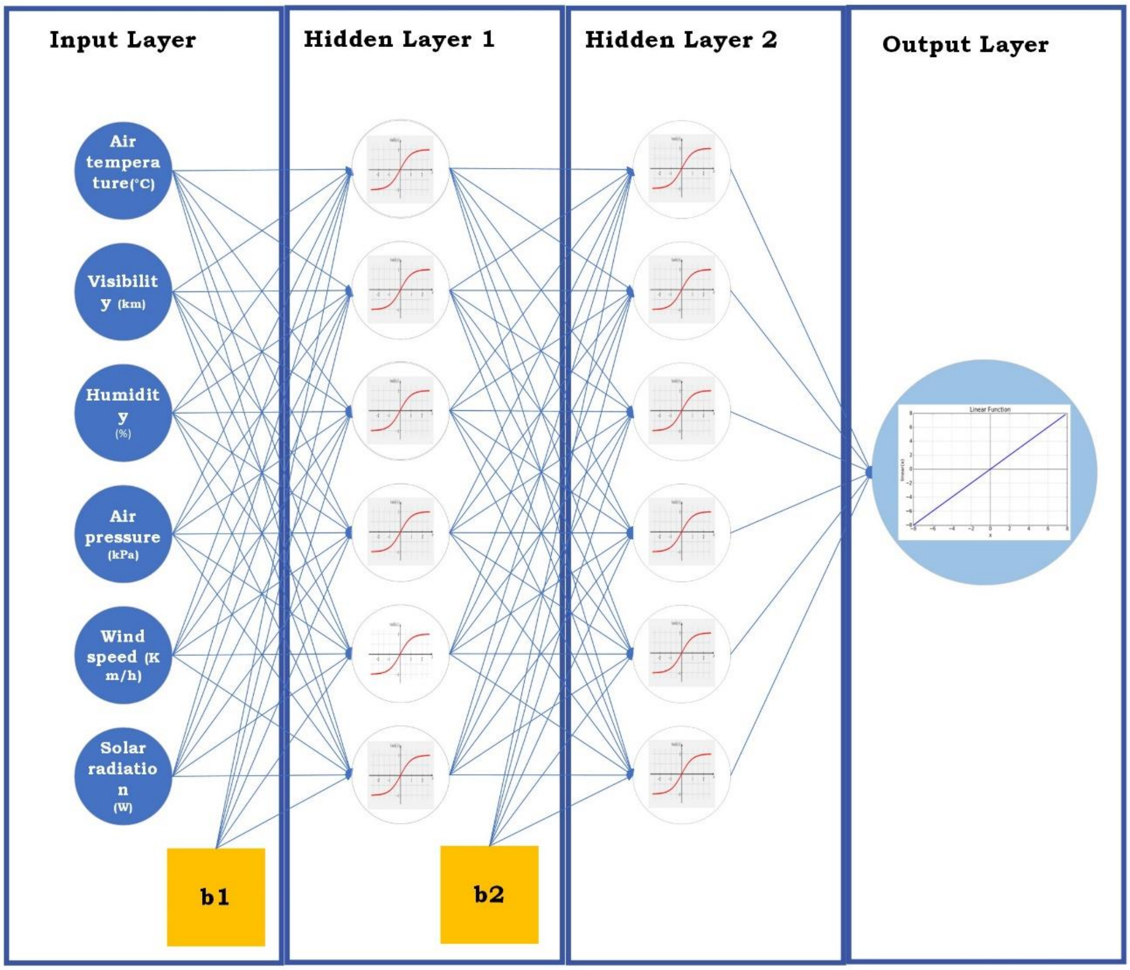

Figure 2 The PV ANN model

PEMWE basics, performance and efficiency

HyPro happens in the cells of the PEMWE. It is not only an efficient and clean method for generating H_2 from water by electrolysis but also generates O_2 as a byproduct. Proton conduction, separation of the produced gases, and electrical insulation of the electrodes occur in a zero-gap cell equipped with a solid polymer electrolyte in a stack section. From this reaction among cathode Eq.(4) and anode Eq.(3) sides and catalyst layers, H_2 and O_2 are released. The role of electricity is obvious in Eq.(5).

$$H_2O = \left(\frac{1}{2}\right)O_2 + 2H^+ + 2e^- \quad (3)$$

$$2H^+ + 2e^- = H_2 \quad (4)$$

$$\mathrm{H_2O} + \text{ electricity} = \mathrm{H_2} + \left(\frac{1}{2}\right)\mathrm{O_2} \quad (5)$$

The voltage and current of this amount of electricity depend on various parameters. Suppose the process occurs under reversible conditions, which means no exergy or enthalpy served and without losses. In that case, the potential difference at the electrodes equals 1.229 V. It is called the reversible cell voltage (V_{rev}^{0}). Without having an external heat source, the total energy for the reaction to take place would be (ΔH_R^0) that must be delivered by electrical energy. However, minimal electrical work is needed to split up water if the requisite contribution of thermal energy is present. Hence, the required voltage is higher than V_{rev}^0 and is called the thermoneutral voltage V_{th}^0 at a normal state, followed in Eq.(6). Moreover, the amount of this Higher Heating Value of Hydrogen (HHVH) is constant and at about 3.54 kWh/Nm^3 [18-20].

$$V_{th}^0 = \frac{\Delta H_R^0}{z.F} = 1.481\,V \tag{6}$$

Where z is the number of moles of electrons transferred in the reaction, the Faraday constant is F, and its value is $9.6485 \times 10^4\ (C/mol)$. The accurate cell voltage (V_{cell}) would be needed for an actual estimation. It is the division of thermoneutral voltage by cell efficiency (η_c), as shown in Eq.(7). The electrical work can be derived from Eq.(8), where η_f is faradic efficiency. This amount is about 285.8 (J/mol) or 0.08 (Wh/g).

$$V_{cell} = \frac{V_{th}^0}{\eta_c} \tag{7}$$

$$W = zF\frac{V}{\eta_f} \tag{8}$$

Generally, the representation of the electrolyzer's performance is through the polarization curve, which illustrates the current density and cell voltage relationship (Figure 3). It describes the current (I_C) and cell voltage (V_C) of the cell relation. The current directly correlates with the production rate, so the polarization curve correlates with the production rate and electric power, which is derived from Faraday's law.It can be expressed as Eq.(9), shown in Figure 3.

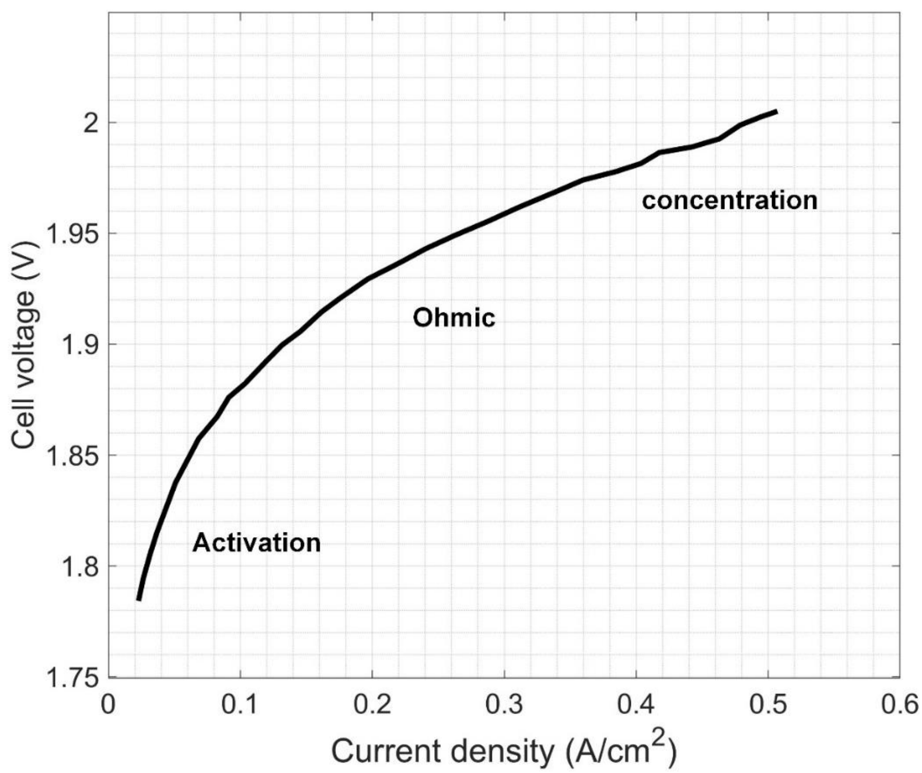

Figure 3 The PEMWE model polarization characteristics [21]

According to Figure 3, activation, ohmic, and concentration overpotentials affect the PEMWE model polarization. It is shown in Eq.(10), and each one impact different sections of this curve.

$$P_c = I_C \times V_C \tag{9}$$

$$V_C = \eta_{ac} + \eta_{oh} + \eta_{co} \tag{10}$$

Eq.(9) is written for a cell. However, a stack current and voltage depend on the system's configuration. Eq.(11) demonstrates the stack current (I_S) and voltage (V_S) relations. When an array is connected in series Eq.(12), the voltage at the stack terminals equals to the sum of voltages at the series connections. In contrast, when it is connected in parallel Eq.(12), the stack current is equal to the sum of the currents flowing through the parallel connections of the cells [22].

$$P_s = I_s \times V_s \tag{11}$$

$$P_s = I_s \times \sum_{n=1}^{N} V_c \times n \tag{12}$$

$$P_s = V_s \times \sum_{n=1}^{N} I_c \times n \tag{13}$$

Based on the relations, the dynamic amount of HyPro can be expressed by Eq.(14). In this, η_e is the dynamic amount of PEMWE efficiency derived from Eq.(15) and is related to the current density.

$$\int_0^t f_{H2}.dt = \frac{\int_0^t N \times I \times V \times \eta_e \times dt}{HHVH} \tag{14}$$

$$\eta_e = -19.5I^3 + 38.58I^2 - 43.34I + 85.02 \tag{15}$$

RESULTS AND DISCUSSION

Based on the machine learning theory and with the input variables and reference data, the trained ANN is able to anticipate the available solar energy in Trois-Rivières. With the selected features related to the solar irradiation quality and the impact of temperature on PV efficiency, the results are close to the experimental data, as shown in Figure 4.

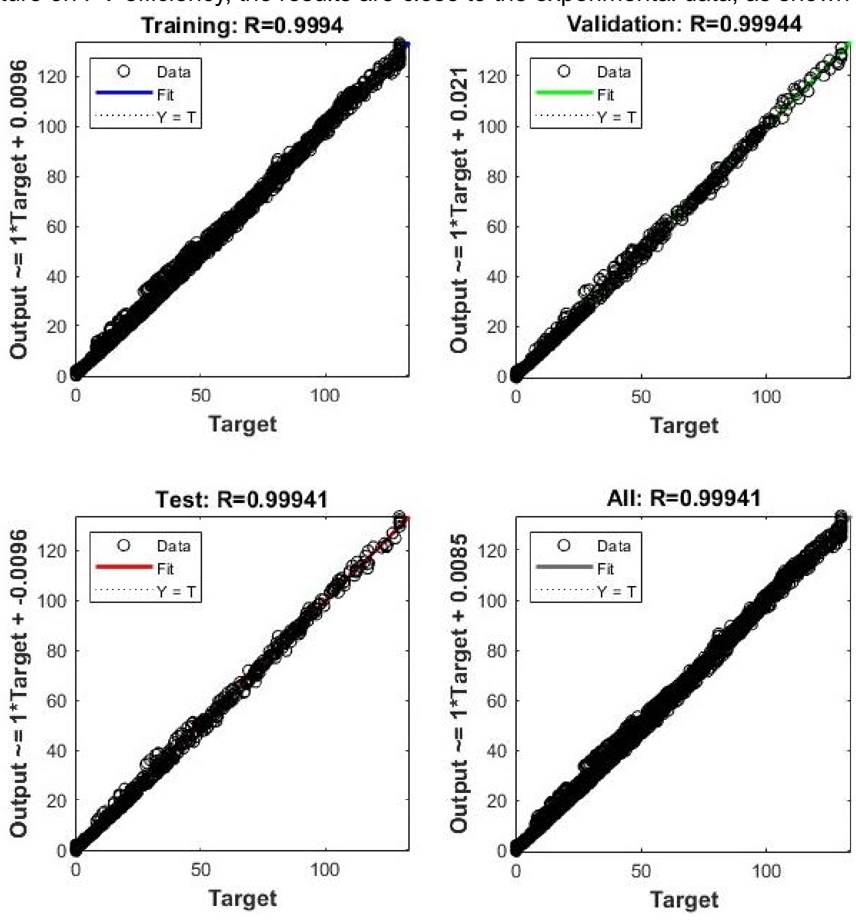

Figure 4 PEMWE ANN model regression

Based on the ANN, the available PV output power for the next year will be 171 kW. However, this amount was 168 kW in the experiments. The scaling can be done by Eq.(16) and using Eqs.(11-13). After analyzing models with PV output DC power, Eq.(17) shows that keeping the PV at the best efficiency point greatly impacts harvested energy.

$$n_p . P_{pv} . \eta_{array} \approx n_{el} . E_{el} \tag{16}$$

$$\alpha \text{HyPro}_S = \alpha PV_{max} \times \alpha \text{PEM} \times \text{CF}_{PV} \tag{17}$$

$$\text{CF}_{PV} = (\text{Output}_{\text{PV}} / \text{Output}_{\text{max}}) \tag{18}$$

According to Eq.(15), the PEMWE efficiency, which changes with current density, can be controlled by a battery or supercapacitor. In this case, by current control, the system can feed PEMWE constantly. Figure 5 illustrates the relationship between current density and PEMWE efficiency. If the control strategy adjusts the power and current in the green area, then PEMWE efficiency will be more than 0.7 each second.

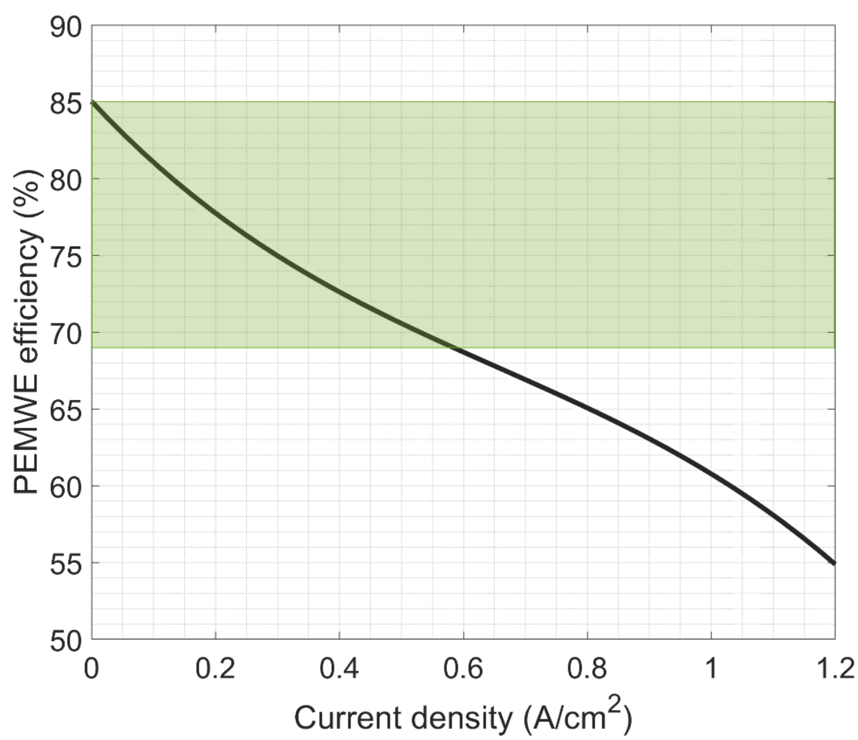

Figure 5 PEMWE model efficiency

In this regard, the HyPro is estimated for a year with direct current from the PV array and once with the control strategy to find out the differences. Figure 6 shows that using a control strategy for constant current for feeding PEMWE has a significant impact on the HyPro, and every month the amount of produced energy increases. By controlling the current in this project, 212 (m^3) hydrogen will be produced and the total amount arrives to 2746 (m^3). However, limiting the input current will ensure the PEMWE that it will not experience any overcharges.

Thus, employing a control strategy is strongly advised to increase the hydrogen production, raise the PEMWE lifespan and decrease the degradation. More studies on the increasing PEMWE efficiency using RES are required to provide a deep insight into the better arrangements for green hydrogen production.

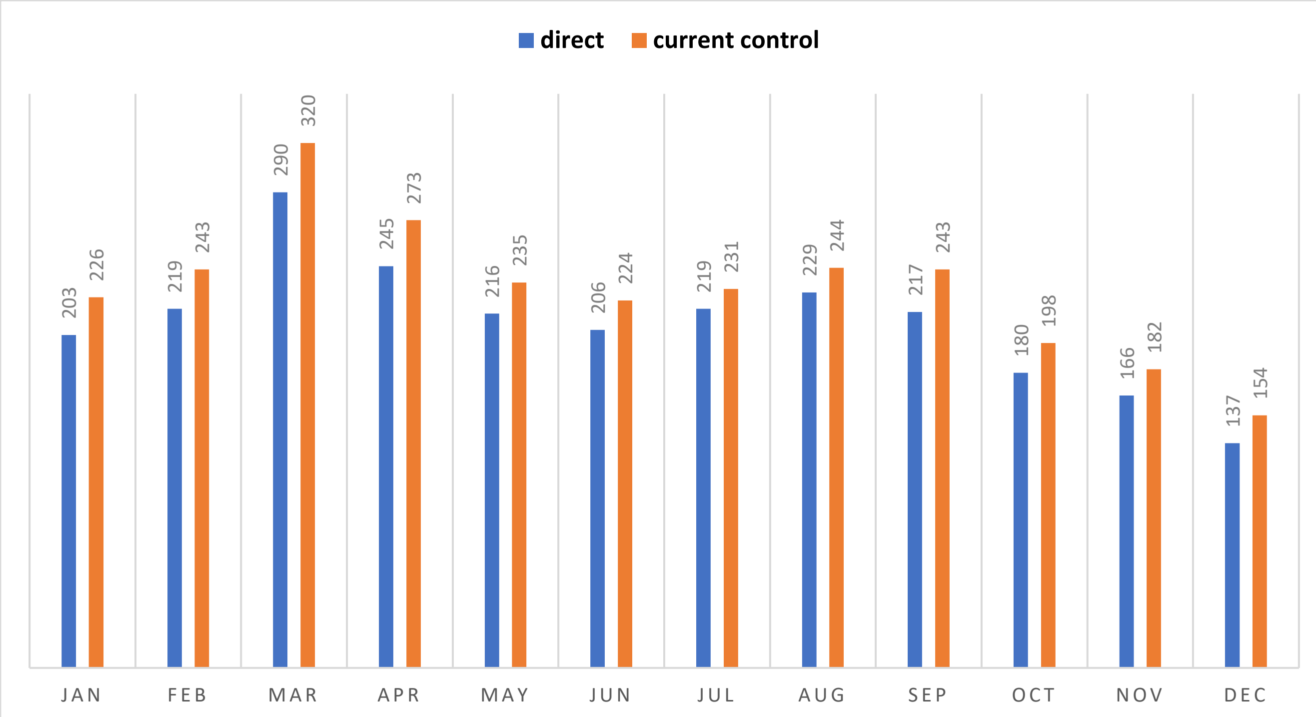

Figure 6 Hydrogen production estimation with and without control strategy

CONCLUSIONS

Renewable energies become more attractive with PEM electrolyzers because they store energy in hydrogen, which is environmentally friendly, efficient, and powerful. They also produce oxygen as a byproduct. However, RES is an intermittent source of power, and its natural behavior harms the PEMWE and decreases its efficiency and lifespan. After collecting experimental data from the PV panel, this study estimates the feasible energy by training a predictive model with machine learning. Then using an empirical model, the ability of HyPro in Trois-Rivières is investigated. Finally, the output of PEMWE is compared with and without controlling the input current. A significant increase in hydrogen production every month shows the dominant benefits of controlling input current for HyPro in by PEMWE. It is highly recommended to combine the PEMWE with an energy storage system, such as a battery or supercapacitor, to increase hydrogen production. However, it is crucial to consider the PEMWE efficiency in various scales and systems since it might change due to operating conditions. It should be noted that the design of a control strategy is also necessary to control the operation points. Furthermore, this hybrid configuration reduces electrolyzer degradation and ultimately increases its lifespan.

ACKNOWLEDGEMENT

This work was supported in part by Natural Sciences and Engineering Research Council of Canada (NSERC) [RGPIN-2018-06527]

NOMENCLATURE

RES	Renewable Energy Source
HyPro	Hydrogen Production
PEM	Proton Exchange Membrane
WE	Water Electrolyzer
FC	Fuel Cell
PV	Photovoltaic
ANN	Artificial Neural Network

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