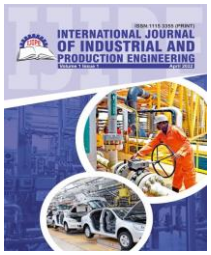

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Modelling and Simulation of Hydrogen Production Process using Proton Exchange Membrane and Alkaline Electrolysis Technologies - A review.

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Abstract
This review provides an analysis of modelling approach for hydrogen production processes employing Proton Exchange Membrane (PEM) and Alkaline Electrolysis technologies, implemented using MATLAB Simulink/Simscape. The systematic review revealed that for both technologies, emphasis is placed on intricate modelling of system components crucial for hydrogen production, transient responses, integration with renewable energy sources like photovoltaic modules, the influence of structural parameters, operating conditions, efficiency and hydrogen production rates. By comparing and contrasting these approaches, the review elucidates the strengths and limitations of each methodology and their contributions to advancements in renewable energy-based hydrogen production systems. Furthermore, the review discusses future research directions and potential areas for optimisation and innovation in hydrogen production plant modelling using MATLAB Simulink/Simscape. This review identifies gaps in current research and proposes potential avenues for future investigation, with the aim of advancing our understanding and optimisation of hydrogen production process for a sustainable energy future.

Keywords: Simulink; Electrolysers; Green Hydrogen; Clean Technology.

1. Introduction

The growing demand for sustainable energy solutions amid concerns over climate change and the depletion of conventional energy sources has spurred significant interest in hydrogen production technologies. Among these, Proton Exchange Membrane (PEM) and Alkaline Electrolysis processes stand out as promising avenues for green hydrogen production. To maximise the efficiency and performance of these hydrogen production plants, accurate modelling and simulation are essential. In recent years, MATLAB Simulink and Simscape have emerged as powerful tools for modelling and optimising the operation of such systems (Kazim & Veziroglu, 2001). This paper presents a systematic review of the modelling approaches applied to PEM and Alkaline Electrolysis hydrogen production process using MATLAB. By synthesing findings from recent literature, the paper aims to provide insights into the methodologies, challenges, and advancements in modelling these critical components of the hydrogen production process. Through a detailed examination of key studies, including those by Yigit & Selamet (2016), Niroula et al. (2023), Martinez et al. (2018), and Tijani et al. (2014),

it will elucidate the intricacies of PEM and Alkaline Electrolysis modelling, highlighting their respective strengths and limitations. Additionally, this review identifies gaps in current research and proposes potential avenues for future investigation, with the aim of advancing our understanding and optimisation of hydrogen production process for a sustainable energy future.

Hydrogen boasts an array of attractive properties as an energy carrier, notably its exceptionally high energy density surpassing that of typical solid fuels. Presently, the worldwide production of hydrogen exceeds 500 billion cubic meters annually, predominantly serving industrial applications such as fertilizers, petroleum refining, and fuel cells (Acar & Dincer, 2014). Yet, despite its vast potential, the prevalent methods of hydrogen production, particularly those reliant on fossil fuels, yield lower purity and contribute to harmful greenhouse gas emissions (Holladay et al., 2009; Rashid et al., 2015).

In the quest for a cleaner, more sustainable energy landscape, the inexorable march towards renewable energy sources gains momentum. Electrolysis of water emerges as a cornerstone in this endeavour, offering an eco-friendly pathway to high-purity hydrogen production. This shift towards water electrolysis not only aligns with global efforts to reduce carbon emissions but also underscores the imperative for innovative energy approaches that mitigate environmental impact (Sapountzi et al., 2017). The various comprehensive hydrogen production methods are shown in Figure 1.

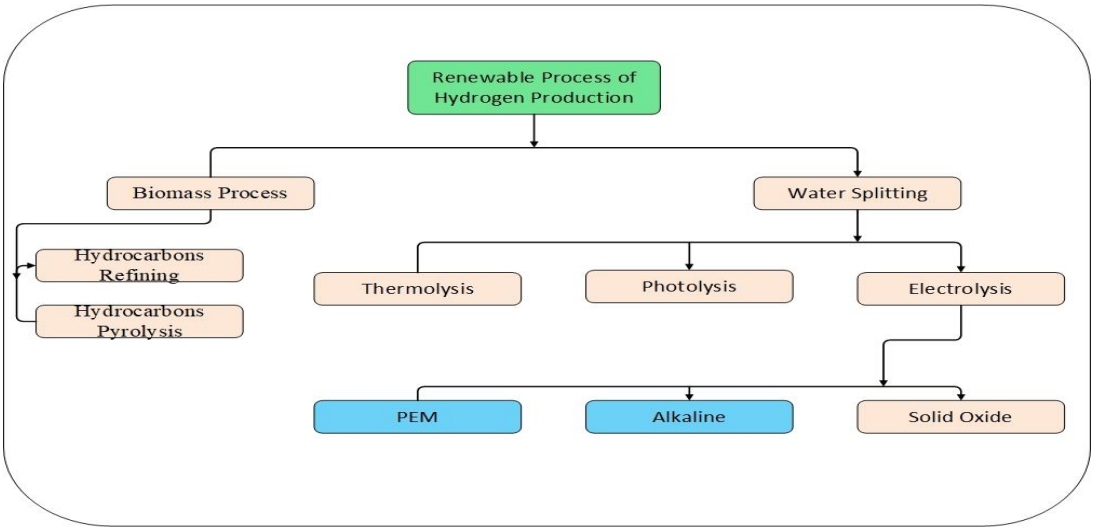

Figure 1. Hydrogen production methods

As the world gravitates towards a hydrogen-based economy, the need for robust and cost-effective production methods becomes paramount. This is where modelling and simulation becomes indispensable tools, empowering engineers and researchers to optimise the intricate processes inherent in hydrogen production processes (Olanrewaju et al., 2023). Whether through PEM electrolysis or alkaline electrolysis, these computational tools afford unparalleled precision and efficiency in the pursuit of sustainable energy solutions. The objective of this review paper is to provide a comprehensive overview of the modelling techniques employed in designing hydrogen production plants, focusing specifically on PEM and alkaline electrolysis systems. By synthesing existing literature and comparative analyses, it aims to elucidate the strengths, limitations, and emerging trends in modelling these crucial components of the hydrogen value chain. Through this endeavour, we seek to contribute to the advancement of knowledge and the informed development of sustainable hydrogen production technologies.

1.1. Fundamentals of Hydrogen Production by Water Electrolysis

Utilising electrolysis of water stands out as a highly effective technique for hydrogen production since it relies on renewable water and yields only pure oxygen as a secondary output. Furthermore, this process harnesses DC power sourced from sustainable energy outlets such as solar, wind, and biomass (Cipriani et al., 2014).

During electrolysis, the water molecule serves as the reactant, undergoing dissociation into hydrogen (H_2) and oxygen (O_2) in response to an electric current. Liquid water has the potential to break down into its basic elements, molecular hydrogen and oxygen, as demonstrated by equation 1:

$$H_2O(l) \rightarrow H_{2(g)} + \frac{1}{2}O_{2(g)} \tag{1}$$

At standard temperature (T∘ = 298 K) and pressure (P∘ = 1 bar), water exists in a liquid state while H_2 and O_2 are in a gaseous state. The standard changes in enthalpy, entropy, and free energy (Gibbs) for reaction (2.1) are given as follows (Kritharas & Watson, 2010):

$$\Delta H_d{}^o(H_2O(l)) = +285.840\ kJ\ mol^{-1}$$

$$\Delta S_d{}^o(H_2O(l)) = +163.15\ kJ\ mol^{-1}$$

$$\Delta G_d{}^o(H_2O(l)) = \Delta H_d{}^o(H_2O(l)) - T\Delta S_d{}^o\big(H_2O(l)\big) = +237.22\ kJ\ mol^{-1} \tag{2}$$

Water electrolysis can be divided into four categories depending on their electrolyte, operational circumstances, and ionic agents (OH−, H+, O2−), although the underlying principles of operation remain consistent in both scenarios. The four types of electrolysis techniques as shown in Figure 1 include (i) Proton exchange membrane (PEM) water electrolysis (Laguna-Bercero, 2012) (ii) Alkaline water electrolysis (Zeng & Zhang, 2010)(AWE) (iii)Solid oxide electrolysis (SOE) (Laguna-Bercero, 2012; Ni et al., 2008) , and (iv) Microbial electrolysis cells (MEC) (Kadier, Kalil, et al., 2016; Kadier, Simayi, et al., 2016).

1.2. PEM Water Electrolysis

Figure 2 illustrates the basic components of a PEM water electrolysis cell. Unlike traditional cells, PEM cells do not contain a liquid electrolyte; instead, only deionized water circulates within them. At the core of the cell lies a thin membrane, approximately 0.2 mm thick, composed of a proton-conducting polymer electrolyte (Abdol Rahim et al., 2016; Ju et al., 2018). These cells boast high efficiency in water splitting and are notably compact. The membrane serves a dual purpose: facilitating the movement of ionic charges (solvated protons) and acting as a barrier to prevent the spontaneous recombination of electrolysis products (hydrogen and oxygen) into water, which could result in exothermic reactions (Nikolaidis & Poullikkas, 2017). Among the various materials used for the proton-conducting membrane, a sulphonated tetrafluoroethylene-based fluoropolymer–copolymer has gained widespread popularity. Developed by E.I. DuPont Co. in the late 1960s, this material is widely recognised under its brand name, Nafion® (Kritharas & Watson, 2010).

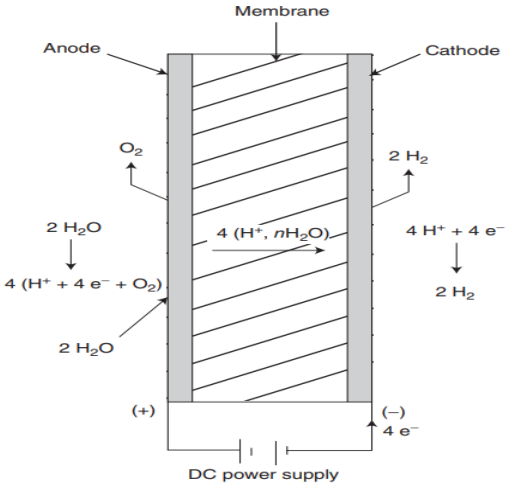

Figure 2. A PEM water electrolysis cell and its corresponding half-cell reactions. (Kritharas & Watson, 2010)

These catalytic layers are linked to an external DC power supply, which furnishes the necessary electrical energy for the reaction. Throughout the process of water electrolysis, the following half-cell reactions occur:

$$anode: H_2O(l) \rightarrow \frac{1}{2}O_{2(g)} + H^+ + 2e^- \quad (3)$$

$$Cathode: 2H^+ + +2e^- \rightarrow H_{2(g)} \quad (4)$$

$$full\ reaction: H_2O(l) \rightarrow H_{2(g)} + \frac{1}{2}O_{2(g)} \quad (5)$$

1.3.Alkaline water electrolysis

Alkaline water electrolysis has long been recognised as a viable technology for commercial hydrogen production, dating back to its initial introduction by Troostwijk and Diemann in 1789 (Trasatti, 1999; Ursua et al., 2012). In this process, at the cathode side of the electrolysis cell, two molecules of alkaline solution (typically KOH or NaOH) undergo reduction to yield one molecule of hydrogen (H_2) while generating two hydroxyl ions (OH^-) (Burnat et al., 2015). The produced H_2 is released from the cathode surface and recombines in a gaseous form, while the hydroxyl ions migrate under the influence of the electrical circuit to the anode through a porous diaphragm. At the anode, these hydroxyl ions are discharged to produce half a molecule of oxygen (O_2) and one molecule of water (H_2O). The released O_2 recombines at the electrode surface and escapes as a gas (Seetharaman et al., 2013), as depicted in Figure 3. Operating at temperatures ranging from 30 to 80°C, alkaline electrolysis employs an aqueous solution of KOH or NaOH as the electrolyte, typically with a concentration of around 20% to 30%. Asbestos diaphragms and nickel materials serve as the electrodes, with the diaphragm positioned between the cathode and anode to separate the produced gases and prevent their mixing during the electrolysis process. However, alkaline electrolysis does have limitations, including restricted current densities (below 400 mA/cm2), low operating pressures, and relatively low energy efficiency (Zeng & Zhang, 2010). A promising advancement in alkaline electrolysis involves the development of anion exchange membranes (AEM), composed of polymers with anionic conductivity, as an alternative to asbestos diaphragms. This innovative technology holds potential to enhance the efficiency and performance of alkaline water electrolysis (Sandeep et al., 2017).

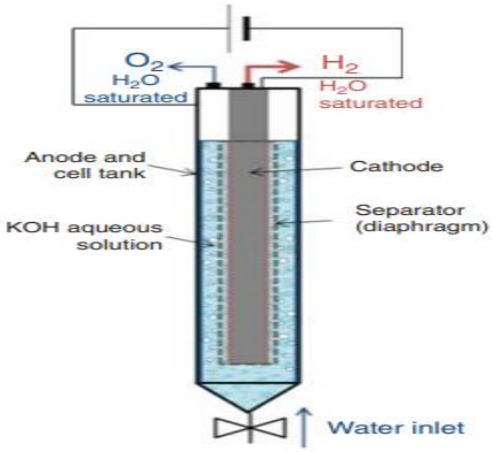

Figure 3. A Monopolar alkaline water electrolysis cell.

The hydrogen evolution reaction or HER of the Alkaline water electrolysis are:

$$\text{anode:} \quad OH^- \rightarrow O_2 + 2H_2O + 4e^- \qquad E^o = 1.23V \quad versus\ RHE \tag{6}$$

$$\text{Cathode:} \quad 4H_2O + 4e^- \rightarrow 2H_2 + 4OH^- + 4e^- \qquad E^o = 0V \quad versus\ RHE \tag{7}$$

In the Alkaline water electrolysis, two key observations should be noted:

- The two electrochemical reactions take place on the electrode's surface: specifically, at the junction between the electrolyte (comprising H_2O and OH^- ions) and the metallic electrode responsible for electron conduction.
- The volume of gas generated correlates directly with the current traversing through the electrical circuit (as per Faraday's law): for every four electrons conveyed through the power source, one oxygen molecule and two hydrogen molecules are generated simultaneously.

2. Modelling and Simulation of PEM and Alkaline Electrolysis processes.

Modelling and simulation offer several advantages which leads to better exploration and evaluation of design options including process optimisation and efficiency improvement (George et al., 2022). Models allow engineers to experiment with different designs, and operating parameters. This virtual testing facilitates quick and cost-effective evaluation of various options to identify the most efficient and optimal configuration (Thanapalan et al., 2008).

In mechanistic modelling which is employed in MATLAB Simulink/Simscape as well as other mathematical modelling software, differential and algebraic equations are derived from the underlying physics and electrochemistry governing the internal phenomena of both the cell and the stack (Hissel et al., 2008). These equations encapsulate electrochemical reactions, as well as mass and charge transfer processes. Precise water management, membrane dehydration, intricate electrode kinetics, mass transport, and the sluggish rate of oxygen reduction stand out as the most significant factors constraining fuel cell performance. Various domains are delineated to elucidate the intricate structure of fuel cells, including the gas diffusion electrode with its diffusion layer and active layer, electrolyte, and gas channel. Models of differing complexities range from simplistic single-cell one-dimensional representations to more elaborate stack or three-dimensional models. The computational demands of resolving complex models can be prohibitive, leading to the formulation of hypotheses focusing on

specific mechanisms or limiting cases. These models facilitate the quantitative description of reaction mechanisms, polarisation curves, and impedance spectra of fuel cells.

In dynamic modelling, the incorporation of mass accumulation within the mass balance equation allows for the inclusion of transient processes such as membrane hydration, water build-up, and gas transportation within the channel and gas diffusion electrode. Alongside mass accumulation, electrode capacitance plays a role in shaping transient responses. While most current dynamic models incorporate capacitance at electrode interfaces, it can also be distributed across the thickness of the active layer. Dynamic models, like their steady-state counterparts, encompass electrochemical reaction kinetics. Several multi-scale models have been developed by (Schalenbach et al., 2016) to anticipate both dynamic and steady-state behaviours within the active layer.

3. Modelling of PEM Electrolysis using Simulink

In Yigit & Selamet, (2016) MATLAB-based modelling study of PEM electrolysers, various system components crucial for hydrogen production, including the electrolyser stack, water pump, cooling fan, and control unit, among others were capture in the modelling. Particularly, the PEM electrolyser stack model stands out as the most intricate component, segmented into anode and cathode modules, membrane, and voltage calculations. The Basic diagram illustrating the PEM electrolyser system for the dynamic model is shown in Figure 4.

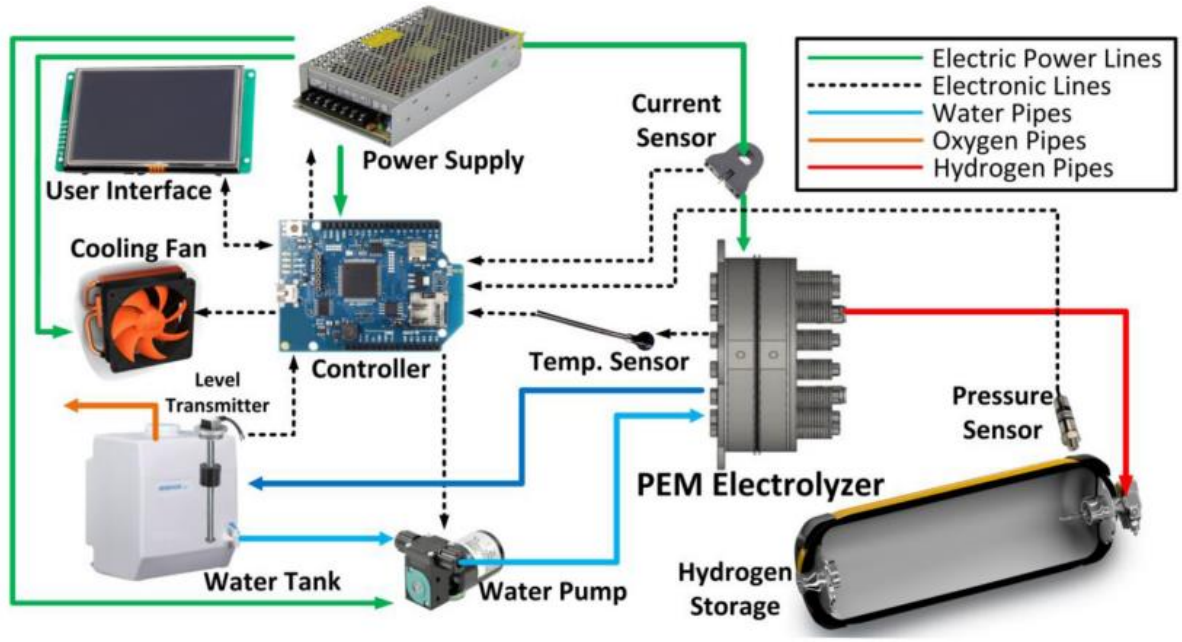

Figure 4. The PEM electrolyser system utilised for the development of the dynamic model by Yigit & Selamet, (2016).

Yigit & Selamet, (2016) model meticulously evaluates efficiency drops and voltage losses within the stack, attributing them to factors such as anode and cathode activation overpotentials, electronic and ionic ohmic resistances. Furthermore, it accounts for losses in other system components and explores dynamic changes in response to varying conditions, such as temperature and pressure. Table 1 present the system components and the corresponding model expression used by Yigit & Selamet, (2016).

Table 1. System components and the corresponding model expression by Yigit & Selamet, (2016).

S/N	System components	Model Expression
1	Anode Model	$N_{O_2} = N_{O_{2ai}} - N_{O_{2ao}} + N_{O_{2g}}$ $N_{H_2O_{an}} = N_{H_2O_{ai}} - N_{H_2O_{ao}} - N_{H_2O_{eod}} + N_{H_2O_{diff}}$ $P_{O_2} = \frac{(N_{O_2} \times R_u \times T_{el})}{v_{an}}$ $P_{H_2O_{an}} = \frac{(N_{H_2O_{an}} \times R_u \times T_{el})}{v_{an}}$ $P_{an} = P_{O_2} + P_{H_2O_{an}}$ $y_{O_2} = \frac{P_{O_2}}{P_{an}}$ $N_{O_{2g}} = \frac{n \times I}{4 \times F}$
2	Cathode Module	$\dot{N}_{H_2} = \dot{N}_{H_{2ci}} - \dot{N}_{H_{2co}} + \dot{N}_{H_{2g}}$ $\dot{N}_{H_2O_{ca}} = \dot{N}_{H_2O_{ci}} - \dot{N}_{H_2O_{co}} - \dot{N}_{H_2O_{eod}} + \dot{N}_{H_2O_{diff}}$ $P_{H_2} = \frac{(N_{H_2} \times R_u \times T_{el})}{v_{ca}}$ $P_{H_2O_{ca}} = \frac{(N_{H_2O_{ca}} \times R_u \times T_{el})}{v_{ca}}$ $P_{ca} = P_{H_2O_{ca}} + P_{H_2}$ $y_{H_2} = \frac{P_{H_2}}{P_{ca}}$ $N_{H_{2g}} = \frac{n \times I}{4 \times F}$ $P_{sat}(Pa) = -2845.4 + 411.24 - 10.554T^2 + 0.16636T^3$
3	Membrane Module	$N_{H_2O_{eod}} = \frac{(\eta_d \times i \times M_{H_2O} \times A)}{F}$ $\eta_d = 0.016T(K) - 2.89556$ $\lambda = 0.043 + 0.1781a - 39.85a^2 + 36a^3$ $\lambda_m = \frac{(\lambda_{ca} - \lambda_{an})}{2}$ $a = \frac{P}{P_{sat}}$ $N_{H_2O_{diff}} = D_w \left(\frac{C_{wc} - C_{wa}}{t_{me}}\right) \times M_{H_2O} \times A$ $D_w = D_\lambda \, exp\left[2416\left(\frac{1}{303} - \frac{1}{T}\right)\right]$ $C_w = \frac{\rho_{me}}{EW_{me}} \times \lambda_m$ $N_{H_2O_{total}} = N_{H_2O_{diff}} + N_{H_2O_{eod}}$
4	Voltage Computation Module	$V_{cell} = V_{th} + V_{act,an} + V_{act,ca} + V_{ohm,e} + V_{ohm,i} + V_{mt,an} + V_{mt,ca}$

		$$\varepsilon^{HHV} = \frac{V_{th}}{V_{cell}}$$ $$E_{th} = E_0 + \frac{R_U \times T_{el}}{2F}\left[\ln\left(\frac{P_{H_2} \times P_{O_2}^{1/2}}{P_{H_2O}}\right)\right]$$ $$V_{act,an} = \frac{R_u \times T_{an}}{\alpha_{an} F} \times arcsinh\left(\frac{i}{2i_{0,an}}\right)$$ $$V_{act,an} = \frac{R_u \times T_{ca}}{\alpha_{ca} F} \times arcsinh\left(\frac{i}{2i_{0,ca}}\right)$$ $$V_{ohm} = i \times R_{ohm,\ i}$$ $$R_{ohm,\ i} = \frac{t_{me}}{\sigma_{me}}$$ $$\sigma_{me} = (0.00514 \times \lambda_m - 0.00326) \times exp\left[1268\left(\frac{1}{303} - \frac{1}{T_{el}}\right)\right]$$ $$V_{ohm} = i \times \left(R_{ohm,\ i} + R_{ohm,\ e}\right)$$
5	The Pump and Tank Model	$$\frac{di_a(t)}{dt} = \frac{1}{L_a}[V_a(t) - R_a i_a(t) - V_b(t)]$$ $$\tau_m(t) = K_i i_a(t)$$ $$V_b(t) = K_b \frac{d\theta_m(t)}{dt} = K_b \omega_m(t)$$ $$\frac{d^2\theta_m(t)}{dt^2} = \frac{1}{J_m}\left[\tau_m(t) - \tau L(t) - B_m \frac{d\theta_m(t)}{dt}\right]$$ $$\omega_m(t) = N_{H_2O_{ai}} \times \psi_{pump}$$ $$Level_{H_2O} = Level_{initial} + (\dot{N}_{H_2O_i} - \dot{N}_{H_2O_o}) \times \left(\frac{M_{H_2O}}{A \times \rho_{H_2O}}\right)$$
6	Hydrogen Storage Tank Module	$$P_{storage} = z \times \frac{N_{H_2} \times R_u + T_{tube}}{v_{tube}} + P_{initial}$$
7	Power supply, losses, Controller and Sensors	$$P_{loss} = i^2 \times R_{ohm}$$

Where

O_{2ai}= Oxygen at the anode-in O_{2ao}= Oxygen at the anode-out H_2O_{ai} = Hydrogen at the anode-in H_2O_{ao} = Hydrogen at the anode-in H_2O_{diff}= Diffused Hydrogen N = Rates	P_{O_2}= Pressure of Oxygen $P_{H_2O_{an}}$= Pressure of Hydrogen at the anode R_u= Universal gas constant (8.3144598(48) J·mol^{-1}·K^{-1}) T_{el}= Temperature of the electrolyser v_{an}= Volume at the anode (P□$_a$□) is Saturation pressure	n= number of cells (20) I= Current F= Faraday's constant (9.64 x 10^4 C/mole) $\dot{N}_{H_2O_{ci}}$ = the flow rate of hydrogen transferred from anode to cathode $\dot{N}_{H_{2co}}$ = Hydrogen flow rate at cathode outlet $\dot{N}_{H_2O_{diff}}$ and $\dot{N}_{H_2O_{eod}}$ = diffusion and electro-

$C_{wc} and\ C_{wa}$=water concentration of the cathode and the anode respectively. t_{me}= the membrane thickness and equals to N117 thickness (0.215 mm; manufacture spec) α is charge coefficient and taken as $\alpha_{ca} = 0.5$, and $\alpha_{an} = 2$, i is the current density i_0 is the exchange current density accepted as $i_{0,an} = 2 \times 10^{-7}$ and $i_{0,ca} = 2 \times 10^{-3}$ (Dale et al., 2008). z is compressibility factor and it is approximately 1 for hydrogen	H_2O_{eod} is electro-osmotic drag associated with water i= current density M_{H_2O} = Molecular weight of the water A = Active area η_d= Electro-osmotic drag coefficient ρ_{me} is the density of the membrane EW_{me} is the equivalent weight of the membrane P_{H_2O}, P_{H_2}, and $P_{O_2}$are the partial pressure of the water, the hydrogen and oxygen, T_{el} is the absolute temperature, R is the universal gas constant. i is the current R is the resistance V is the voltage τ is the torque K is the torque constant B is the viscous friction coefficient θ is the rotor displacement J_m is the inertia of the motor ω_m is the rotor angular velocity	osmotic drag of water respectively V_{th} is the thermos-neutral voltage $V_{act,an}$ is the activation overpotentials at the anode $V_{act,ca}$ is the activation overpotentials at the cathode $V_{ohm,e} and\ V_{ohm,i}$ are the ohmic overpotentials $V_{mt,an} and\ V_{mt,ca}$ are the mass transfer overpotentials at the anode and cathode respectively $N_{H_2O_{ai}}$ is the water flow rate ψ_{pump} is constant calculated from data sheets of commercial pump

Notably, the study underscores the dominant influence of stack losses at higher current densities, highlighting its significance in overall system performance. Through simulation, the model adeptly assesses different scenarios, including constant power consumption for high-pressure operations, revealing insights such as the inverse relationship between current drawn by the stack and increasing pressure. These findings contribute valuable insights to the field of PEM electrolysis modelling and offer a comprehensive understanding of system behaviour under diverse operating conditions.

Yigit & Selamet, (2016) notable findings on the 5 cells simulations among others includes:

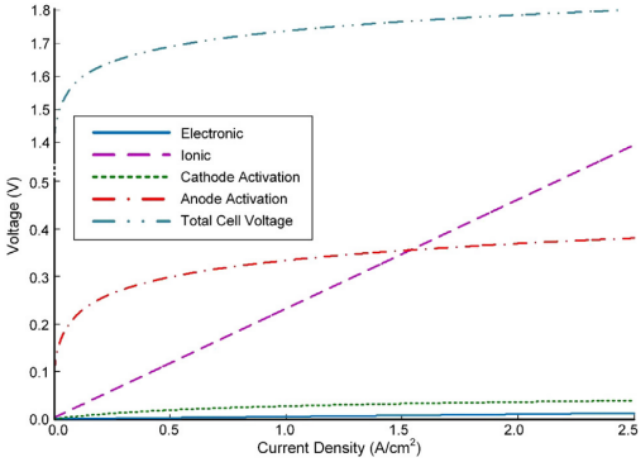

Figure 5. The impact of current density on over potentials and the performance of the PEM electrolyser stack under standard conditions of atmospheric pressure and 300 K.

Despite low current densities, anodic activation over potential significantly affects performance. Ohmic losses increase linearly with current, with ionic over potential dominating beyond 1.5 A/cm2 due to amplified ionic resistance. Despite high current density, cell potential stays below 1.8 V, ensuring over 80% efficiency.

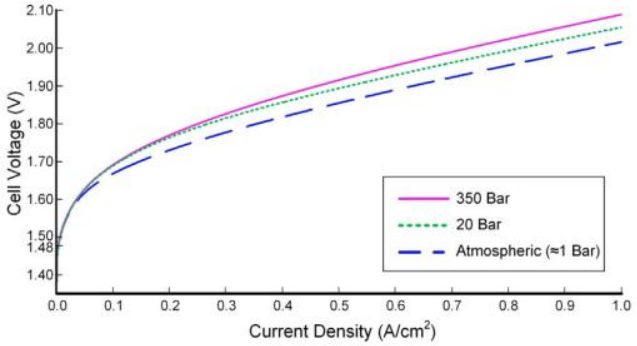

Figure 6. The impact of pressure on the performance of the PEM electrolyser at 300 K.
The stack's performance depends heavily on temperature and pressure, which also affect the thermo-neutral voltage. The model was tested at atmospheric, 20, and 350 bars. Above 1.48 V, electrolysis begins, with similar trends observed in graph paths as current density rises.

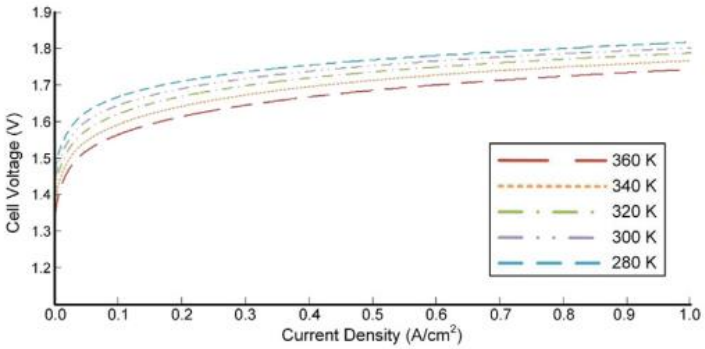

Figure 7. The impact of temperature on the performance of the PEM electrolyser stack under standard atmospheric pressure.

As temperature rises, the energy required for water splitting decreases. Efficiency approaches nearly 100% as temperature reaches around 360 K, given that PEM electrolyser efficiency calculations typically rely on thermo-neutral values.

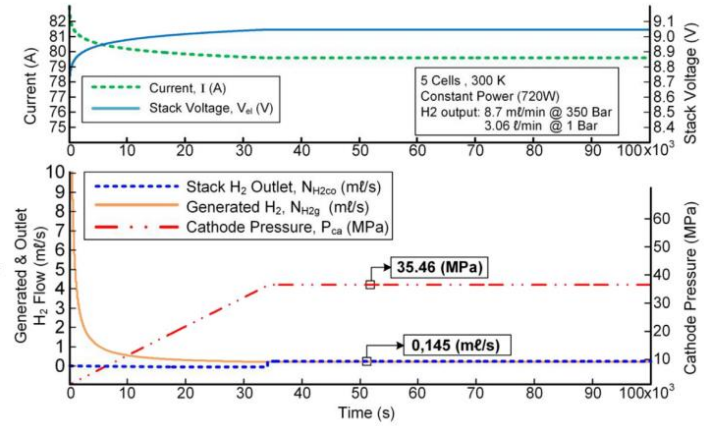

Figure 8. The model results pertain to a fixed power consumption scenario for compressing the produced gas to 350 bars. The power utilised by the stack is capped at 720 Watts.

In Figure 8, a fixed power consumption scenario is depicted for a stack consisting of 5 cells, each with a 100 cm2 active area, operating at 300 K. With constant power input, stack voltage rises with pressure, causing a drop in stack current from over 82 A to about 80 A. The hydrogen output is 8.7ml/min at 350 bar.

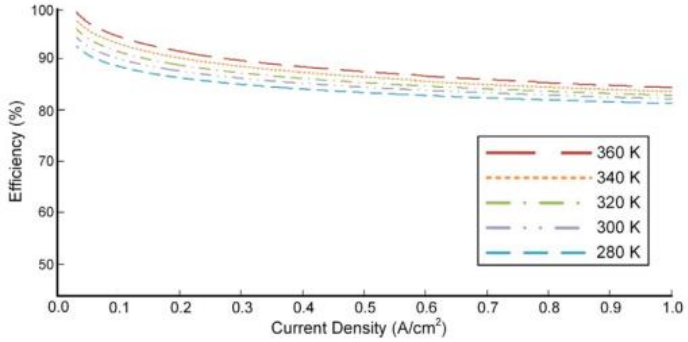

Figure 9. The impact of current density on the efficiency of the PEM electrolyser at various temperatures under standard atmospheric pressure.

As temperature approaches 360 K, the efficiency of the PEM electrolyser nearly reaches 100%. This is because PEM electrolyser efficiency calculations typically rely on the thermo-neutral voltage, which is around 1.48.

In University of Zagreb, Faculty of Mechanical Engineering and Naval Architecture's research, Brezak et al., (2023) achieved several significant milestones in modelling of PEM process using Simulink. Firstly, they developed a flexible Simulink model capable of accommodating variable operating conditions. This model was instrumental in simulating the behaviour of electrolysers under different scenarios. Additionally, their work emphasised the importance of water transfer across the membrane, acknowledging that it accounts for approximately 10% of the total incoming water. Moreover, the mathematical and Simulink models created were rigorously validated using data sourced from commercially available electrolysers, enhancing the credibility and reliability of his findings. Brezak et al., (2023) successfully implemented a balance of system approach, employing simple electronics and coding techniques to optimise the functionality of the electrolyser system. These accomplishments highlight the depth and

breadth of their contributions to the field of electrolyser research and development. Their notable all-inclusive expression was the total water transport through membrane which was given as:

$$q^{C}_{\eta_{H_2O}} = -D \cdot \frac{\left(C^{A}_{H_2O} - C^{C}_{H_2O}\right)}{\varphi_{memb}} + \eta_{drag} \cdot \frac{N_C \cdot I_{Ely}}{4 \cdot F} + \frac{K_{darcy} \cdot \rho H_2O \cdot (p_A - p_C)}{\varphi_{memb} \cdot \mu H_2O \cdot MH_2O} \left[\frac{mol}{cm^2 \cdot s}\right] \quad (8)$$

(Ismail et al., 2019) presented a mathematical model using Simulink aimed at estimating and forecasting the global solar radiation intensity in Egypt. This model underwent comparison and validation against published measurements of global solar radiation intensity. Moreover, the study introduced a hybrid system designed to generate hydrogen, consisting of a photovoltaic generator coupled with a PEM electrolyser. Modelling and simulation techniques were employed by executing a flowchart in MATLAB to minimise system losses and enhance hydrogen production. The simulation encompassed both the estimation of global solar radiation and the operation of the photovoltaic generator-PEM electrolyser system. The experiment was conducted in Suez city, Egypt. The results indicated that the global solar radiation model provided accurate predictions for estimating solar radiation intensity in Egypt. Additionally, the authors observed a notable improvement in system performance, resulting in increased hydrogen production. The entire model was simulated, and the simulation results aligned closely with experimental data. The electrolyser, powered by a PV panel, was modelled, sized, and experimentally validated as part of the study.

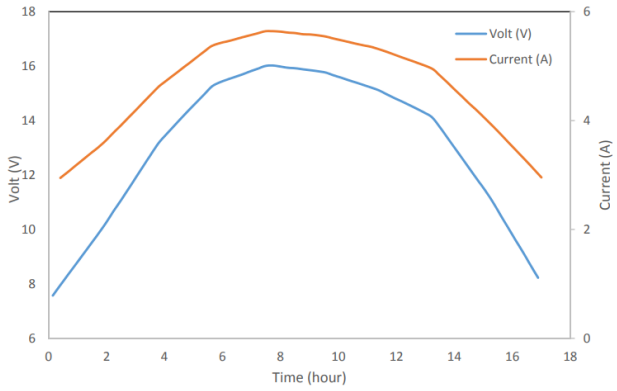

Figure 10. Variations in current and voltage as a function of time (Ismail et al., 2019).

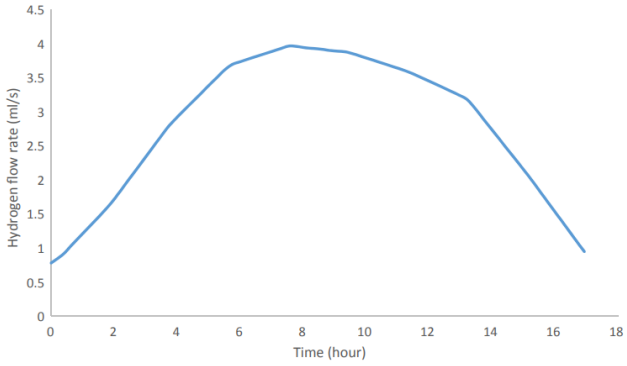

Figure 11. The power-voltage (P-V) traits across different temperatures and levels of global solar radiation intensity (Ismail et al., 2019)

The findings from Ismail et al. (2019), as depicted in Figures 10 and 11, demonstrate that variations in current, hydrogen flow, and power align closely with changes in global solar radiation. This correlation is attributed to these parameters reaching their peak values between 12:00 and 13:00 and their lowest values at 8:00 and 17:00, mirroring the pattern of the global solar radiation curve. Further examination of the differences observed in recorded and forecasted levels of global solar radiation across various cities in Egypt and Figure 10-11 reveals a robust correlation between hydrogen production and the intensity of global solar radiation. As global solar radiation increases, hydrogen production also rises, reaching its maximum level between 12:00 and 13:00 (Mohamed Albarghot et al., 2016).

The study conducted by Mohamed Albarghot et al. (2016) focused on utilising solar panels to power an electrolyser for hydrogen production. They developed an electrical equivalent circuit for a proton exchange membrane electrolyser, which was implemented in MATLAB/Simulink alongside an atmospheric hydrogen storage tank. By supplying a consistent voltage (2 volts) and current (1 ampere), they compared simulated and experimental results. Both approaches yielded a hydrogen output of approximately 7.345 ml/min.

The comparison between simulation and experimental results revealed close agreement. The maximum voltage and current from the PV panel were utilised to maximise hydrogen production, with the simulation output of 7.461 ml/min closely matching the experimental value of 7.0 ml/min, despite some discrepancy attributed to sun variability. Additionally, they observed a linear relationship between input power and hydrogen production.

The study's conclusions highlighted the development of a renewable energy hydrogen production and storage system. They emphasized the use of PV solar panels to capture solar energy, with the electrolyser converting this energy into hydrogen. A DC/DC buck converter and PID controller were incorporated to regulate and maintain current values and check error values, respectively. Both simulation and experimental trials produced corresponding results, affirming the reliability of the model. Overall, the electrolysis unit was deemed environmentally friendly due to its production of oxygen as waste.

In literature review, these findings contribute to the understanding of renewable energy-based hydrogen production systems, showcasing the efficacy of solar panels coupled with electrolysers. The integration of simulation tools like MATLAB/Simulink offers a valuable means of modelling and optimising such systems. Additionally, the study underscores the importance of experimental validation to ensure the accuracy and reliability of simulation results, paving the way for further advancements in environmentally sustainable hydrogen production technologies.

4. Modelling of Alkaline Electrolysis using Simulink/Simscape

Martinez et al., (2018) conducted a study that focused on implementing a MATLAB/Simulink/Simscape power system model of an alkaline electrolyser directly coupled to a photovoltaic module. They utilised meteorological data from Auckland, New Zealand, to simulate the system's performance over 15-hour durations during typical summer and winter days. Boundary conditions were applied to mathematical models to incorporate transient behaviour influenced by internal parameters of the photovoltaic module. Equation 9 and 10 express in equation the final set of boundary condition.

$$V = \begin{cases} V_{rev} + \dfrac{r_1 + r_2}{A} I + s \log\left(\left(t_1 + \dfrac{t_2}{T} + \dfrac{t_3}{T^2}\right)\dfrac{I}{A} + 1\right), I > -A\left(t_1 + \dfrac{t_2}{T} + \dfrac{t_3}{T^2}\right)^{-1} \\ V_{rev} + \dfrac{r_1 + r_2}{A} I, I \le -A\left(t_1 + \dfrac{t_2}{T} + \dfrac{t_3}{T^2}\right)^{-1} \\ V_{outside,}\ I = 0 \end{cases} \quad (9)$$

$$\dot{n}H_2 = \begin{cases} \left(\dfrac{\left({}^{I}/_{A}\right)^2}{f_1 + \left({}^{I}/_{A}\right)^2} f_2\right)\dfrac{I}{zF}, V > V_{rev} \\ 0, V \le V_{rev} \end{cases} \quad (10)$$

The simulation results demonstrated that the steady-state output of the proposed implementation aligned with responses observed in similar systems reported in previous studies. The electrolyser achieved an overall efficiency of 68.48% for summer and 63.32% for winter, consistent with results from referenced studies. Regarding the transient response, the voltage curve exhibited distinct zones, with steady-state operation characterized by a fully active electrolyser and transient zones indicating start up or shut down phases. Further analysis revealed that the voltage variation in the transient zone was influenced by low-level irradiance input insufficient to generate current, resulting in voltage proportional to irradiance and the internal parallel resistance of the photovoltaic module. The study also calculated the amount of electrical energy input to the system and determined the corresponding hydrogen production for both summer and winter days. The calculated electrolyser efficiencies fell within the reported range in literature. Conclusively, the study successfully implemented a direct coupling of an alkaline electrolyser cell and a PV module using MATLAB/Simulink/Simscape power systems. The model's steady-state outputs aligned with previous studies, while transient responses were influenced by the PV module's internal parallel resistance. Further research is recommended to incorporate thermal response, storage alternatives, and additional elements of the Simulink/Simscape family for a comprehensive multi-physical domain simulation. These findings contribute to the understanding of renewable energy-based hydrogen production systems and provide insights for future developments in this field.

(Niroula et al., 2023) conducted a study focusing on the parametric modelling and optimisation of an alkaline electrolyser for the production of green hydrogen. Electrolysis, the process of decomposing a liquid containing ions by passing electricity through it, is facilitated by an electrolyser. Specifically, an alkaline water electrolyser utilizes electrical energy to break the chemical bond between hydrogen and oxygen in an alkaline electrolytic medium. The performance of the electrolyser hinges on several parameters, including temperature, pressure, ohmic overpotential, and activation overpotential. In their study, Niroula et al. identified and integrated various parameters affecting the electrolyser's performance using fundamental thermodynamics and electrochemical equations. They developed a mathematical model in MATLAB/Simulink to analyse the voltage vs. current density plot of the electrolyser and attempted to optimise its performance through parameter variation. Their observations indicated that increasing operating temperature and decreasing operating pressure favoured the electrolysis process. Furthermore, they found that a 30 wt% KOH solution as electrolyte exhibited the optimal cell voltage compared to 20 and 40 wt% solutions. In conclusion, they developed a mathematical model based on thermodynamic, electrochemical, and empirical equations in MATLAB/Simulink. They generated a polarization curve using this model and validated it with previously published experimental data. The model enabled predictions regarding the behaviour of polarization under varying input parameters. Their findings suggested that adjusting operational temperature and pressure could reduce the cell voltage of the electrolysis process, with a 30 wt% KOH solution showing optimal performance. The developed model holds potential for further investigations into the effects of parameters such as electrode and membrane thickness, electrode roughness, porosity, and tortuosity on electrolyser performance. Future research could utilise the model to assess and compare the impact of these parameters on electrolyser efficiency and gas flow rate.

Hammoudi et al., (2012) introduced a novel multi-physics model for the design and diagnosis of alkaline electrolysers. Their approach allows for precise selection of design parameters, predicting energy consumption, efficiency, and hydrogen production rate under various operating conditions. Unlike conventional models that require weeks of experimental data collection, their method characterizes the electrolyser based on structural parameters within a short time frame, typically a few minutes. This approach offers flexibility by describing a range

of alkaline electrolysers, in contrast to semi-empirical models limited to specific electrolyser types. Their multi-physics model considers variations in structural parameters (such as geometry and materials) and operational parameters (temperature, pressure, concentration, etc.), while conventional models typically only incorporate temperature variations. The model was implemented using MATLAB Simulink®, and a simulation tool for alkaline electrolysers was developed and validated using industrial electrolysers (Stuart and Phoebus) with different structures and power rates. The simulation results closely matched experimental data with high accuracy, validating the effectiveness of their approach. Additionally, their simulation tool enabled a comparison of energy efficiency between two hydrogen production systems: an atmospheric electrolyser with a compressor for hydrogen storage and a barometric electrolyser under pressure with auxiliary devices. The analysis demonstrated that the latter mode of hydrogen production was more efficient, corroborating findings from literature based solely on thermodynamic approaches. In summary, Hammoudi et al.'s work represents a significant advancement in the modelling and design of alkaline electrolysers, offering a rapid and comprehensive approach for predicting performance under diverse operating conditions. Their findings contribute to the understanding of hydrogen production systems and provide insights for optimising energy efficiency in electrolyser designs.

Tijani et al., (2014) investigated the mathematical modelling and simulation analysis of an advanced alkaline electrolyser system for hydrogen production in response to escalating global energy demands and the depletion of conventional energy sources. They emphasized the significance of renewable energy technologies, particularly hydrogen production via electrolysis coupled with solar-PV or wind energy, for future sustainable energy needs. The study focused on understanding the I-V characteristics of the electrolyser and examining key parameters such as ohmic overpotential and activation overpotentials at the anode and cathode, which influence electrolyser performance. Employing fundamental thermodynamics and electrochemical reaction equations, they developed a MATLAB model to explore these parameters. Their findings underscored the substantial impact of activation overpotential, which was observed to be significantly higher, approximately 80% more, than ohmic overpotential at equivalent current densities. This research contributes to advancing the understanding of advanced alkaline electrolyser systems and provides insights that can inform the design and optimisation of such systems for efficient hydrogen production, thereby facilitating progress towards sustainable energy solutions.

5 Comparison of Modelling Approach

A comparison between modelling approaches of PEM (Proton Exchange Membrane) and Alkaline Electrolysis using MATLAB reveals distinct methodologies and focuses within each research domain. In studies by Yigit & Selamet (2016) and Brezak et al. (2023) on PEM electrolysis, the modelling intricately captures system components crucial for hydrogen production, including the electrolyser stack, pump, cooling fan, and control unit. Yigit & Selamet's model evaluates efficiency drops and voltage losses within the stack, emphasizing factors like activation overpotentials and ohmic resistances, while Brezak et al. utilize Simulink to simulate transient responses influenced by internal parameters of the photovoltaic module. Ismail et al. (2019) integrates a PEM electrolyser with a photovoltaic generator using MATLAB, showcasing a hybrid system's enhanced hydrogen production. Conversely, studies on Alkaline Electrolysis, such as Niroula et al. (2023) and Hammoudi et al. (2012), focus on structural parameters and operating conditions' influence on efficiency and hydrogen production rate. Niroula et al.'s model, developed in MATLAB, explores parameters like temperature and pressure, optimising electrolyser performance, while Hammoudi et al.'s multi-physics approach facilitates precise design parameter selection and predicts energy

consumption. These comparisons highlight PEM electrolysis models' emphasis on system components and transient responses, whereas Alkaline Electrolysis models focus on structural parameters and operational conditions' influence, both contributing to advancements in renewable energy-based hydrogen production systems.

5.1 Challenges

The modelling approaches for PEM and Alkaline Electrolysis hydrogen production process using MATLAB face several challenges, each specific to the respective electrolysis process.

For PEM electrolysis, one of the primary challenges lies in accurately capturing the complex electrochemical reactions and transport phenomena occurring within the membrane-electrode assembly (MEA). This includes accounting for phenomena such as water management, mass transport limitations, and membrane degradation, which significantly influence the performance and durability of PEM electrolysers (Kadier, Kalil, et al., 2016). Additionally, the sensitivity of PEM electrolysis to operating conditions, such as temperature and pressure, necessitates robust modelling techniques capable of accurately predicting system behavior under varying scenarios.

On the other hand, Alkaline Electrolysis modelling encounters challenges related to the dynamic nature of the electrolyte and electrode materials. The presence of alkaline solutions introduces additional complexities, such as electrolyte conductivity changes over time and electrode degradation due to corrosion. Modelling the interplay between these factors while maintaining computational efficiency poses a significant challenge (Martinez et al., 2018; Sandeep et al., 2017). Furthermore, accurately predicting performance under non-ideal operating conditions, such as fluctuations in input power or electrolyte composition, remains an ongoing challenge in Alkaline Electrolysis modelling.

Overall, both PEM and Alkaline Electrolysis modelling approaches must address these challenges to provide reliable predictions of system performance and facilitate the design and optimisation of efficient hydrogen production plants.

6 Conclusion

In conclusion, this review has provided an in-depth examination of modelling methodologies for hydrogen production plants employing both Proton Exchange Membrane (PEM) and Alkaline Electrolysis technologies, utilizing MATLAB Simulink/Simscape. Through synthesing recent literature, we have highlighted the unique characteristics and focal points of modelling studies within each domain. The review underscores the significance of PEM electrolysis modelling in capturing system dynamics, transient responses, and the integration with renewable energy sources. On the other hand, studies on Alkaline Electrolysis have emphasized the impact of structural parameters and operating conditions on efficiency and hydrogen production rates. By comparing and contrasting these approaches, we have elucidated their respective strengths and limitations, providing valuable insights into the advancements in renewable energy-based hydrogen production systems. Furthermore, this review has identified potential avenues for future research, including optimisation strategies, integration of additional system components, and exploration of innovative modelling techniques. Overall, the findings presented in this review contribute to a deeper understanding of hydrogen production plant modelling and offer valuable guidance for future research and development in this critical field of sustainable energy production.

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