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MATHEMATICAL MODELLING AND VALIDATION OF PEM ELECTROLYZER INTEGRATED WITH A STORAGE SYSTEM

Summary

This study explores the potential of PEM electrolyzers for green hydrogen production, emphasizing their advantages in renewable energy scenarios. It details the development of a mathematical model using Simulink to simulate the electrolyzer's performance, focusing on electrochemical, electrical, and flow calculations. The model's validation will involve testing with a laboratory-built prototype under various conditions. Future work includes integrating the electrolyzer with a photovoltaic system and energy storage to optimize performance. The combination aims to enhance the efficiency and sustainability of hydrogen production.

Keywords: Electrochemical, energy storage, hydrogen, mathematical model, PEM electrolyzer

1. Introduction

In the last years, hydrogen (H_2) has emerged as an important element in the global energy transition, recognized for its potential to considerably reduce carbon emissions and support energy systems. Governments and industries worldwide have increasingly invested in H_2 technologies, seeing it as a key enabler for decarbonizing sectors such as transportation, industry, and power generation. Depending on the production method, hydrogen can be classified in different categories. Blue H_2 is derived from natural gas, but with carbon capture and storage (CCS) technology to reduce CO_2 emissions. Gray hydrogen is also produced from natural gas but without any CCS, resulting in significant carbon emissions. Brown or black hydrogen is generated from coal, with brown referring to lignite coal and black to bituminous coal, both of which have high carbon footprints. Green hydrogen, on the other hand, is produced through electrolysis powered by renewable energy sources, making it the most environmentally friendly option and the type that will be taken into consideration in this work (Mehmood et.al, 2025).

In view of that, the use of surplus renewable energy (e.g. wind, solar or hydropower) to produce green hydrogen is more important than ever and the most common way to do that is through electrolysis. Hydrogen production through electrolysis is a process that uses electrical energy to split water molecules into hydrogen and oxygen gases, being considered a key technology for producing green hydrogen. The device used to perform the electrolysis is called electrolyzer and the most common types are the proton exchange membrane (PEM), alkaline and solid oxide electrolyzers.

The PEM electrolyzers have several advantages in comparison with the alkaline types, especially in renewable-energy scenarios. They have a fast response to power fluctuations and produce hydrogen with higher purity, which is essential for applications like fuel cells vehicles. Moreover, they present a compact design being able to operate at higher current densities, making them suitable for smaller, decentralized hydrogen production units. PEM electrolyzers typically operate at lower temperatures compared to alkaline electrolyzers, reducing thermal stress and improving system longevity (Stojić, et.al, 2008). Due to these benefits, PEM electrolyzers are favoured for producing high-purity hydrogen and for applications that demand dynamic operation. Consequently, this study will focus on further investigating their potential and the combination of them with renewable energy sources.

2. Methods and Methodology

The PEM electrolyzer uses a solid polymer electrolyte to conduct protons from the anode to the cathode, while separating the gases produced in the system as can be observed in Figure 1. The chemical reactions that define the anode and the cathode conversions are the following:

Anode: $2H_2O \rightarrow O_2 + 4H+ + 4e-$

Cathode: $4H+ + 4e- \rightarrow 2H_2$

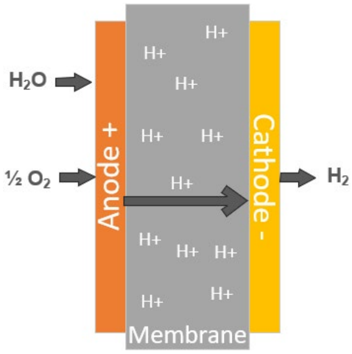

Figure 1: PEM electrolyzer principle

Here, the water introduced to the anode side is decomposed into oxygen gas, protons, and electrons. The protons traverse the proton-conductive membrane to reach the cathode side. Simultaneously, the electrons leave the electrolyzer cell via an external circuit, which provides the necessary driving force (i.e., cell potential) for the reaction. At the cathode side, the protons and electrons from the external circuit recombine to produce hydrogen gas. During the electrochemical reaction, water must be continuously supplied to the membrane-electrode interface, while hydrogen and oxygen need to be removed.

This work was divided into three phases. The first step was the development of a mathematical model of the PEM electrolyzer, which will be further described in the following section. The second and third phases are the validation of the model and the combination of it with a renewable energy source and a storage system.

3. Mathematical model

In order to clearly quantify the dynamic interactions in the calculations, the modelling of the PEM electrolyzer is divided into four ancillaries, anode, cathode, membrane and voltage ancillary which are all interconnected as can be observed in Figure 2. The model is based on electrochemical, electrical and flow calculations and was implemented using Simulink (The Mathworks, 2024), following the practice introduced by Görgün (Görgün, 2005). In the model here presented, the hydrogen production rate depending on the current density is calculated. Also, the electro-osmotic drag, the diffusion of water and the water flow at the anode inlet and outlet are calculated dynamically in real time (Abdin et al, 2015).

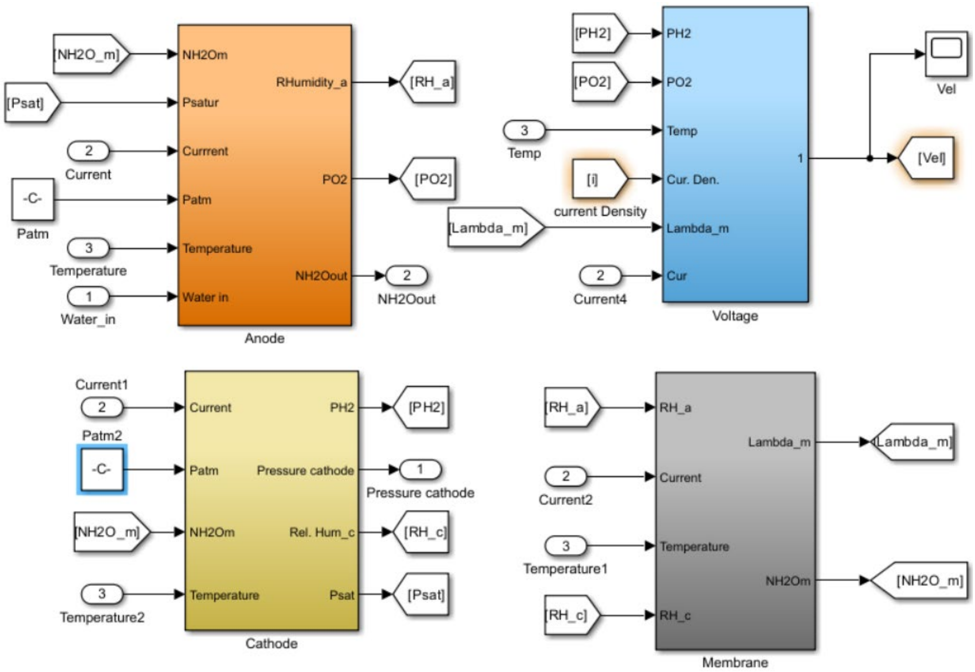

Figure 2: Simulink view of the electrolyzer model

In the anode ancillary dynamic calculations of oxygen and water flow along with their partial pressures take place. Equivalently, the cathode computes hydrogen and water partial pressures and their flows. The membrane ancillary calculates the water diffusion and conductivity of the membrane, the electro-osmotic drag and the water content. In the voltage ancillary the activation and ohmic polarizations are calculated and the Nerst Equation is used to calculate the electrolyzer applied voltage level.

A detailed description of all the chemical and physical equations and principles used to define each of the electrolyzer ancillaries will be provided in the paper. It will also include comprehensive explanations of the mechanisms and interactions involved in the electrolyzer's operation.

4. Further developments

In the upcoming phases of this project, the mathematical model will undergo validation using a laboratory-built prototype. This process will involve testing the model under various input temperatures and voltage conditions to ensure its accuracy and reliability. Moreover, the electrolyzer model will be combined with a storage system and a photovoltaic system that will work as an electrical source. The combination of electrolyzer, photovoltaic and storage will also be optimized in order to find the most efficient performance parameters.

5. References

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