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Model-based Operability and Safety Optimization for PEM Water Electrolysis

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ABSTRACT

In this paper, we present a systematic approach to quantify the safe operating window of a proton exchange membrane water electrolysis (PEMWE) system considering energy intermittency and varying hydrogen demand. The PEMWE model has been developed based on first principles, with the polarization curve validated against a lab-scale experimental setup. The impact of key operational variables is investigated which include voltage, inlet temperature, and water flowrate (utilized for both feed and system cooling). Emphasis is given on operating temperature, a safety-critical variable, as its elevation can pose significant hydrogen safety risks within both the electrolyzer cells and the storage system. The impact of temperature on process safety is quantified via a risk index considering the fault probability and consequence severity. Process operability analysis is employed to assess the achievability of a safe and feasible region for design and operations. This analysis provides a comprehensive framework to optimize PEMWE systems for enhanced operational flexibility and robust performance with application to modular hydrogen production using renewable energy sources.

Keywords: Operability Analysis, Risk Assessment, Water Electrolysis, Sustainable Hydrogen Production

1. INTRODUCTION

In recent years, the transition of the energy grid to hydropower, wind, and solar photovoltaics has gained significant attention. Renewable sources are at the core of energy transition and remain among the most critical factors in the process of industrial decarbonization. However, their output is intermittent with daily and seasonal variability, which may lead to fluctuations in energy supply [1, 2]. Advancements in electrolysis technologies, such as proton exchange membrane water electrolysis (PEMWE) systems, are critical in addressing the challenges of integrating renewable energy sources for hydrogen production [3, 4]. PEMWE stands out among other technologies (e.g., solid oxide electrolyzers and alkaline electrolyzers) due to its simplicity, reversible operation, higher current densities supported, and ability to supply highly pure hydrogen. These attributes make PEMWE a promising option for coupling with intermittent renewable energy sources, contributing to the decarbonization of various sectors such as transportation, industry, and power generation [5, 6]. Despite these advancements, significant research gaps remain in how to effectively characterize the operability of a PEMWE system. These include: (i) the lack of integrated performance analysis (and metrics) for PEMWE accounting for operability, safety, productivity, etc.; and (ii) the lack of a systematic approach to quantify the safe PEMWE operating window under conditions of energy intermittency and varying hydrogen demand.

To address these challenges, this work presents a systematic approach that integrates operability and safety analysis to quantify the safe operating window of a PEMWE system while ensuring high-efficiency hydrogen production. Section 2 provides a detailed PEMWE process description to motivate the research developments. Section 3 outlines the methods in terms of operability and risk assessment. Section 4 presents a case

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study demonstrating the practical application and effectiveness of the methodology framework in enhancing PEMWE system safety and operability.

2. PEMWE CASE STUDY

2.1 Process Description

In this work, we consider the PEMWE system as conceptualized in Figure 1a. The PEMWE design and operations are based on the reference experimental setup given in Figure 1b [6, 7]. Specifically, water is supplied to the anode at a controlled temperature and flow rate, serving a dual purpose as both a reactant and a coolant. Within the anode, water moves through the diffusion layer to reach the catalyst site, where the anodic electrochemical reaction occurs as described in Eq. (1). During this reaction, water interacts electrochemically with electrons from the current to produce oxygen and hydrogen ions. The oxygen ions at the anode combine to form oxygen molecules, while the hydrogen ions diffuse through the membrane to the cathode, where pairs of H^+ ions combine to form hydrogen molecules as described in the cathodic reaction in Eq. (2). The oxygen and hydrogen molecules generated then exit the catalyst layer via the diffusion layer. The overall reaction is presented in Eq. (3).

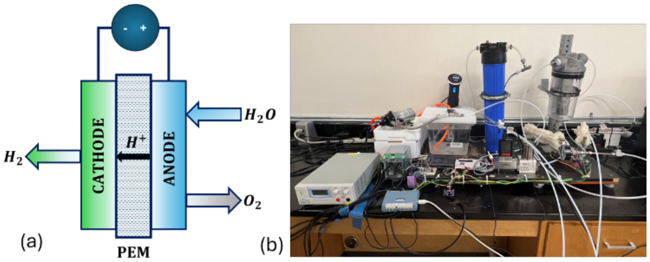

Figure 1: PEMWE system. (a) Schematic representation. (b) Experimental setup.

$$\text{Anode: } \mathrm{H_2O} \longrightarrow \tfrac{1}{2}\mathrm{O_2} + 2\mathrm{H^+} + 2\mathrm{e^-} \qquad (1)$$

$$\text{Cathode: } 2\mathrm{H^+} + 2\mathrm{e^-} \longrightarrow \mathrm{H_2} \qquad (2)$$

$$\text{Overall Reaction: } \mathrm{H_2O} \longrightarrow \tfrac{1}{2}\mathrm{O_2} + \mathrm{H_2} \qquad (3)$$

2.2 Research Objectives

The manipulated variables for this PEMWE system are considered as: (i) makeup water flowrate – which is used for both feed inlet and system cooling, and (ii) voltage – reflecting the varying electricity availability considering the scenario of electrolyzer powered by renewable energy sources. Disturbance exists at the makeup water inlet temperature. To assess the PEMWE performance, the output variables are selected as H_2 production flowrate and power consumption. Temperature is the safety-critical variable to be further correlated with the process risk calculation. Temperature elevation can pose significant hydrogen safety risks within both the electrolyzer cells and the storage system.

Key research objectives of this work include:

- Model-based analysis to characterize the entire PEMWE safe and feasible operating region for input and output variables.
- Systematic identification of the optimal input operating region under disturbances, based on the desired level of outputs (maximum hydrogen production rates).

3. AN INTEGRATED OPERABILITY AND SAFETY OPTIMIZATION APPROACH

A methodology framework has been developed in our prior work to incorporate risk considerations into steady-state operability-based process design [8]. This section provides a brief overview on the key methods (i.e., process operability analysis and risk assessment), before applying the framework to study the PEMWE system in Section 4.

3.1 Process Operability Analysis

Process operability analysis is employed to quantify the achievability of a safe and feasible operating region at the early design stage. Several approaches have been proposed to tackle the challenges of feasibility and flexibility, including evaluating and integrating these factors within process design optimization and operations [9] and employing probabilistic identification of the design space [10]. The steady-state operability framework used in this study accounts for the impact of process design variables and varying operating conditions on the outputs to address the complexities of chemical processes [11, 12]. Figure 2 illustrates a schematic for performing a generalized steady-state operability analysis. This process starts by defining the input variables' upper and lower bounds, which define the Available Input Set (AIS). The process model, represented by M, is then applied to the AIS to determine the resulting output variables, which constitute the Achievable Output Set (AOS). Next, the Desired Output Set (DOS) is specified to include the target output values for the system. Through inverse mapping (M^{-1}), the input requirements needed to achieve the entire DOS region, if possible, are identified and referred to as the Desired Input Set (DIS). Additionally, by incorporating the Expected Disturbance Set (EDS), the AOS is adjusted to account for shifts across the specified range of disturbances, reflecting how these disturbances impact the achievable outputs. The feasible regions within DIS and DOS are labeled as DIS* and DOS*, respectively.

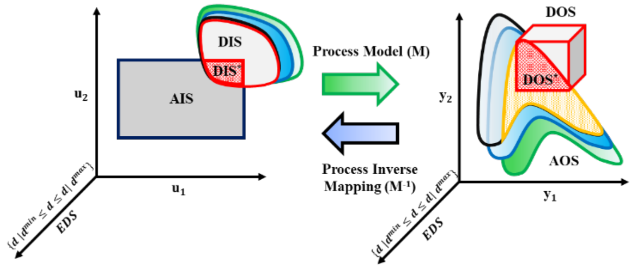

Figure 2: Schematic of the process operability concepts at steady-state.

3.2 Risk Assessment

The risk model can be established as a function of safety-critical variables in the process, inspired by the methodology described in [13]. Here, let x represent these safety-critical variables, such as states. The risk index, RI, is defined in terms of the deviation of x from the standard design or operating conditions, denoted by μ. Eq. (4) specifies RI as the product of the fault probability, $P(x)$, and the consequence severity, $S(x)$. Additional insights into using RI for real-time risk monitoring and management are provided in [14].

$$RI = P(x) \times S(x) \tag{4}$$

Fault Probability: The fault probability is determined using Eq. (5) for the case when $x \geq \mu$. The formulation incorporates a probability density function based on the mean (μ) and standard deviation (σ) of the safety-critical variables (x). This approach leverages the three-sigma rule ($\mu \pm 3\sigma$), meaning that roughly 99.7% of values are expected to lie within three standard deviations from the mean.

$$P(x) = \phi\left[\frac{x-(\mu+3\sigma)}{\sigma}\right] = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{[t-(\mu+3\sigma)]^2}{2\sigma^2}} dt, \quad \text{when } x \geq \mu \tag{5}$$

Consequence Severity: Eq. (6) is applied to measure consequence severity, which intensifies notably as the deviation of x from three-sigma region increases.

$$S(x) = 100^{\frac{x-(\mu+\mu\sigma)}{x-\mu}}, \text{ when } x \geq \mu \tag{6}$$

4. PEMWE CASE STUDY: RESULTS AND DISCUSSIONS

This section presents the stepwise procedure to analyze the operability and safety of the PEMWE system.

4.1 First-Principles Process Modeling

The first-principles electrolyzer model provided in AVEVA™ Process Simulation is used in this case study. Modifications to the model are made to better align with the parameters of the experimental system (Fig. 1b). The polarization curve is a fundamental starting point in the study of PEMWE system, providing insights into the electrochemical performance of the cell under varying operating conditions. Table 1 provides the core electrochemical equations governing the PEMWE system, covering the open circuit voltage, activation overpotential, and ohmic overpotential.

In estimating the polarization curve, parameters with high impact on the stack's electrochemical behavior are carefully calibrated using experimental data. To ensure robustness, we conducted a sensitivity analysis to identify which parameters significantly affect the model's output and are well-represented by the experimental data. These include the exchange current densities for the anode ($i_{o,an}$) and cathode ($i_{o,ca}$). Table 2 presents both the design specifications and the estimated parameters for the PEMWE system. Table 3 presents the electrochemistry parameters. The optimal exchange current density values are determined to be $i_{o,an} = 3.62 \times 10^{-6}\, A \cdot cm^{-2}$ for the anode and $i_{o,ca} = 8.20 \times 10^{-6}\, A \cdot cm^{-2}$ for the cathode. Constants α_{an} and α_{ca}, which represent the charge transfer coefficients for the anode and cathode, respectively, are adopted from literature values of 2 and 0.5. Figure 3 presents the polarization curve results, showing great agreement with experimental data.

4.2 Risk Modeling

Although the reaction is endothermic, heat is generated due to the Joule heating effect [6]. As a result, effective thermal management becomes crucial for safe PEMWE operation, as excessive heat buildup can lead to equipment failure and hazardous conditions. Applying high current densities increases electrolysis and heat generation, which risks damaging critical components like the membrane and electrodes or leads to a thermal runaway condition. Additionally, hydrogen is highly flammable. The leaks or improper handling can lead to explosive atmospheres.

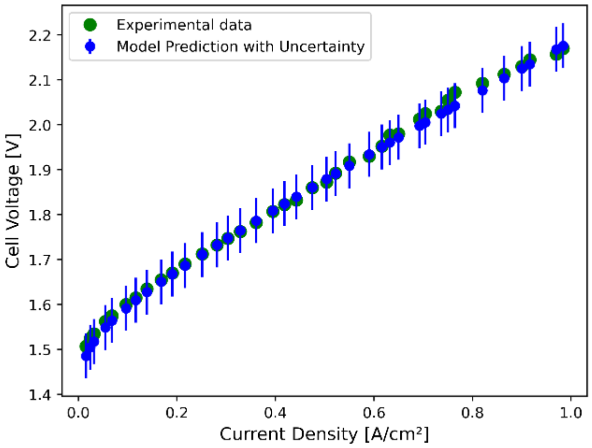

Figure 3: Parameter estimation results of the polarization curve.

Table 1: Electrochemistry equations of the PEMWE System.

Electrochemistry	
Open circuit voltage	$V = E_{oc} + V_{act} + V_{ohm}$
	$E_{oc} = E_o + \frac{RT}{2F} \ln \frac{p_{H_2} p_{O_2}^{0.5}}{p_{H_2O}}$
	$E_o = 1.229 - E_T(T - 298)$
Activation overpotential	$V_{act} = \frac{RT}{\alpha_{an} F} \sinh \frac{i}{2 i_{o,an}} + \frac{RT}{\alpha_{ca} F} \sinh \frac{i}{2 i_{o,ca}}$
Ohmic overpotential	$V_{ohm} = \tau_m \frac{i}{\sigma_m}$
	$\sigma_m = (M_a \lambda_m - M_b) \exp\left[M_c \left(\frac{1}{303} - \frac{1}{T}\right)\right]$

Table 2: Design and Estimated Parameters of the PEMWE System.

Variable	Unit	Value
$\boldsymbol{P}$	Bar	1.2
$\mathbf{T_{in}}$	℃	20
$\boldsymbol{\tau_m}$	μm	254
$\boldsymbol{A}$	cm^2	50
$\boldsymbol{N_c}$	$-$	4
$\boldsymbol{\lambda_m}$	$-$	10.5
$\boldsymbol{\alpha_{an}}$	$-$	2
$\boldsymbol{\alpha_{ca}}$	$-$	0.5
$\boldsymbol{i_{o,an}}$	A/cm^2	3.62×10^{-6}
$\boldsymbol{i_{o,ca}}$	A/cm^2	8.20×10^{-6}

Table 3: Electrochemistry Parameters of the PEMWE System [13].

Variable	Unit	Value
$\boldsymbol{E_T}$	$-$	0.0009
$\boldsymbol{M_a}$	$-$	0.005114
$\boldsymbol{M_b}$	$-$	0.00326
$\boldsymbol{M_c}$	$-$	1268

In this study, the operating temperature is selected as the safety-critical variable, as its increase can pose significant risks to both the electrolyzer cells and the hydrogen storage system. The impact of temperature is quantified using the risk index previously presented, incorporating both fault probability and consequence severity to comprehensively assess safety risks. Figure 4 illustrates the risk quantification, with a mean temperature (μ) of $318.15\ K$ and a standard deviation (σ) of 5 K, defining the three-sigma range ($\mu + 3\sigma$) up to $333.15\ K$. Given a high-risk threshold temperature within this value, the calculated risk index of 0.5 underscores the need for urgent risk management.

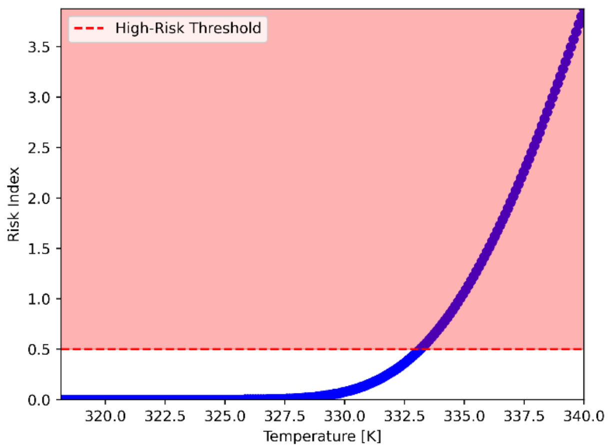

Figure 4: Risk evaluation

4.3 Operability and Safety Analysis – Forward Mapping

Forward mapping calculates the possible output space based on a given set of inputs (see Table 4). This analysis aims to provide valuable insights into how the system performs under varying conditions, such as fluctuations in renewable energy supply and demand-driven operations. The variables selected in this framework are designed to characterize these conditions. For example, makeup water is included as a manipulated variable as it serves as the raw material for hydrogen production and a key component of the system's cooling resources. Voltage is selected as the other manipulated variable to capture the impact of renewable energy source intermittency on system performance. The feed inlet temperature is considered as disturbance due to its potential variability, which may result from changes in ambient temperature or fluctuations in the cooling system.

Table 4: PEMWE System Input Variables.

Input/Disturbance Variables	Physical Description	Available Range	Unit
$\boldsymbol{Q}$	Makeup water	$0.01 - 1.2$	L/min
$\boldsymbol{T_{in}}$	Voltage	$1.4 - 2.2$	V
$\boldsymbol{V}$	Feed inlet temperature	$293.15 - 333.15$	K

Figure 5a illustrates the space discretization employed based on the available input ranges. Figure 5b shows the corresponding outputs, which include hydrogen flow, outlet temperature, the ratio of hydrogen power (the power required by the electrolyzer per unit of hydrogen produced), and the risk index, as indicated in the

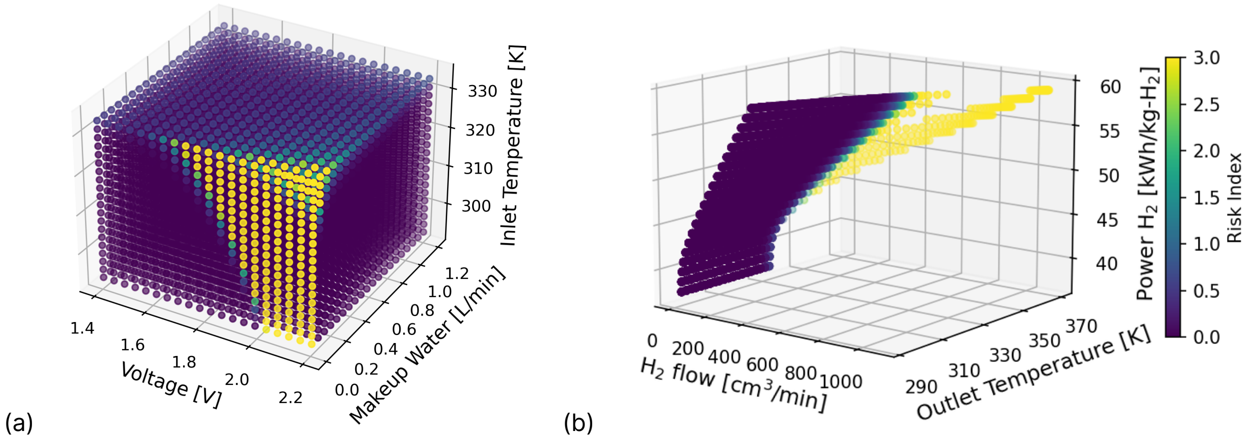

Figure 5: Forward mapping assessment for the PEMWE System. (a) Available input set (AIS). (b) Achievable output set (AOS).

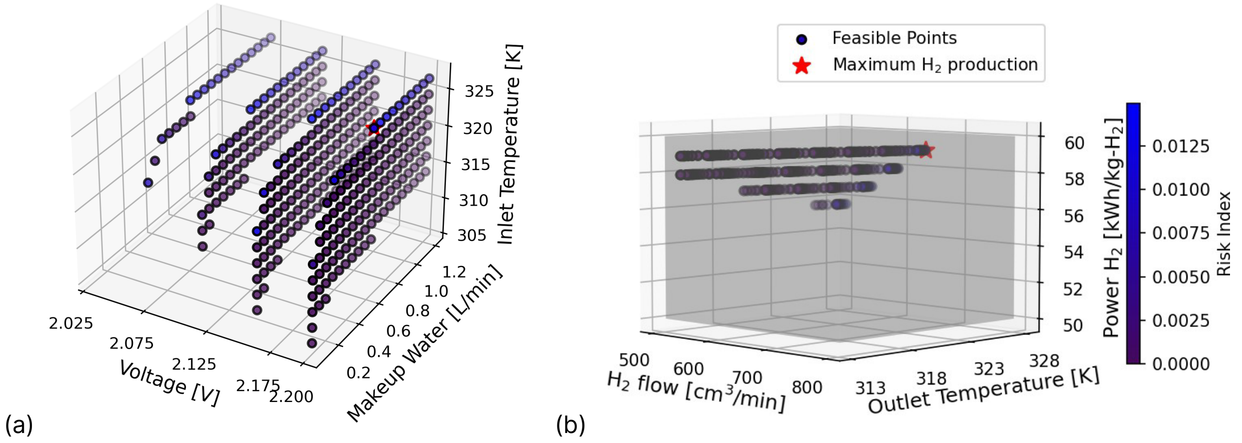

Figure 6: Inverse mapping assessment for the PEMWE System. (a) Feasible input set. (b) Feasible output set.

colormap. The high-risk region ($RI \geq 0.5$) results from a combination of inefficient cooling and elevated voltages in response to higher temperature disturbances, as depicted by the green-yellow regions in the colormap. This map enables to identify all possible configurations for the given high-risk scenarios, providing valuable insights for selecting set points in closed-loop operations. Notably, the achievability of these configurations is independent of the specific control law employed.

4.4 Operability and Safety Optimization – Inverse Mapping

Based on the entire operational space of the PEMWE system obtained via forward mapping, we further perform inverse mapping to evaluate whether the system can operate within a desired region. We identify the specific input conditions required to achieve the targeted hydrogen productivity while maintaining safety. Table 5 summarizes the target region for electrolyzer operation, derived from previous knowledge of the forward mapping results.

Table 5: PEMWE System Desired Output Set (DOS).

Output Variables	Physical Description	Desired Range	Unit
$\boldsymbol{T_{out}}$	Outlet temperature	$313.15 - 328.15$	K
$\boldsymbol{H_2\ Flow}$	Hydrogen production	$500 - 800$	cm^3/min
$\boldsymbol{Power\ H_2}$	Power H_2	$50 - 60$	$kWh/kg - H_2$

Figures 6a and 6b illustrate the feasible region from the input and output perspectives, respectively. Notably, within the feasible box, multiple points can be selected to achieve the desired target. The optimum point for maximizing hydrogen production is identified as $T_{out} = 328.1\,K$, $H_2\,Flow = 650\,cm^3/min$, and $Power\,H_2 = 58.96\,kWh/kg - H_2$, with inputs of $Q = 0.63632\,l/min$, $V = 2.2\,V$ and $T_{in} = 326.83\,K$, which corresponds to a risk index of 0.01495. This design not only achieves the highest hydrogen production but also adheres to the specified safety constraint ($RI < 0.5$).

5. CONCLUDING REMARKS

This work introduces a framework that integrates both forward and inverse mapping to optimize the operability and safety of PEMWE systems. Ongoing research is focused on implementing a multi-parametric model predictive controller (mp-MPC) to further enhance real-time control and safety performance based on the obtained regions from operability analyses.

6. ACKNOWLEDGEMENTS

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