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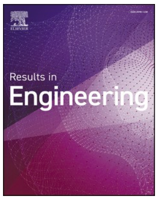

Research paper

Techno-economic analysis of design and transport parameters in PEMWEs

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ABSTRACT

Green hydrogen has emerged as a promising pathway toward decarbonization of future energy systems, with proton exchange membrane water electrolyzers (PEMWEs) attracting increasing attention due to their high efficiency, compact design, and compatibility with renewable energy sources. This study extends prior multi-physics investigations of proton exchange membrane water electrolyzers (PEMWEs) by translating performance-driven design insights into techno-economic implications for green hydrogen production. Building upon previously developed numerical models that examined the effects of membrane thickness, membrane conductivity, and operating temperature, as well as porosity distributions within porous transport layers and the influence of gas crossover under varying outlet pressures, the present work establishes a direct link between electrochemical behaviour and hydrogen production cost. Simulation-derived polarization characteristics are integrated into a simplified techno-economic framework to quantify variations in energy consummption, hydrogen yield, and levelized cost of hydrogen (LCOH) under different design and operational configurations. Unlike conventional assessments relying on assumed efficiencies or generic performance data, this study employs physics-based simulation outputs as the primary input for economic evaluation, enabling a more faithful representation of design-dependent cost behaviour. The proposed framework further enables direct assessment of how membrane properties, transport characteristics, and structural configurations influence techno-economic performance. The results reveal how subtle changes in transport and structural parameters propagate into measurable economic consequences, highlighting critical trade-offs between efficiency enhancement and cost escalation. Specifically, the investigated design and transport variations resulted in specific energy consumption values ranging from ~35–55 kWh kg^{-1} H_2, stack electrical efficiencies of ~0.5–0.9, and LCOH values of ~2.3–5 USD kg^{-1} H_2, demonstrating that relatively small transport-induced performance changes can propagate into measurable economic consequences, particularly at moderate-to-high operating current densities. The findings provide design-oriented economic insights that support informed decision-making for cost-sensitive optimization of PEMWE systems, bridging the gap between electrochemical modelling and real-world deployment considerations.

1. Introduction

Growing global efforts toward energy decarbonization have positioned green hydrogen as a key energy carrier for achieving deep emissions reductions in hard-to-abate sectors such as heavy transport, steelmaking, ammonia production, and chemical processing [1–3]. Over recent decades, water electrolysis technologies have evolved from conventional alkaline systems toward more compact and dynamically responsive electrolyzer architectures, among which PEMWEs are particularly suited to renewable-energy-driven operation [4]. Among emerging hydrogen production technologies, proton exchange membrane water electrolyzers (PEMWEs) have attracted significant attention due to their high current density capability, rapid transient response, compact design, and compatibility with intermittent renewable energy sources such as wind and solar power [4–6]. Despite these technical advantages, the large-scale deployment of PEMWE remains constrained by high capital expenditure and substantial electricity consumption, which together dominate the LCOH and hinder economic competitiveness, particularly when compared with mature alkaline systems [3,7,8].

Recent literature has emphasized that economic feasibility is strongly governed by the materials and structural composition of PEMWE stacks. A comprehensive review by García-Salaberri et al. [9]

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Nomenclature

A	Active area of cell [m^2]
C_{cap}	Total installed capital cost [USD]
$C_{cap,ann}$	Annualized capital cost [USD yr^{-1}]
C_{elec}	Electricity cost per unit of hydrogen [USD $kg^{-1}H_2$]
C_{el}	Electricity price [USD kWh^{-1}]
$C_{O\&M,ann}$	Annual operation and maintenance cost [USD yr^{-1}]
C_F	Capacity factor [—]
E_{spec}	Specific electrical energy consumption [kWh kg^{-1} H_2]
F	Faraday's constant, 96,485.3 [C/mol]
i	Current density [A/m^2]
I	Total cell current [A]
i_0	Reference exchange current densities [A/m^2]
i_m	Proton current density in the membrane [A/m^2]
i_e	Electron current density in the electrodes [A/m^2]
LCOH	Levelized cost of hydrogen
LHV_{H2}	Lower heating value of hydrogen
$\dot{m}_{H_2,ann}$	Annual hydrogen production
N	System lifetime
P	Electrical power input
r	Discount rate
T	Temperature [°C or K]
V	cell voltage [V]
V_{cell}	Simulated cell voltage [V]

Greek Symbols

α	Transfer coefficient
δ_m	Membrane thickness [μm]
δ_{aPTL}	Anode porous transport layer thickness [μm]
δ_{cPTL}	Cathode porous transport layer thickness [μm]
δ_{aCL}	Anode catalyst layer thickness [μm]
δ_{cCL}	Cathode catalyst layer thickness [μm]
ε	Porosity
η_{Stack}	Stack electrical efficiency (LHV-based)
η_F	Faradaic efficiency
σ_m	Electrical conductivity [S/m]

Subscript and superscript

a	Anode
c	Cathode
aCL, cCL	Anode/Cathode catalyst layer
aPTL, cPTL	Anode/Cathode porous transport layer
ann	Annualized
el	Electricity
m	Membrane
PEMWE	Proton Exchange Membrane Water Electrolyzer
MEA	Membrane Electrode Assembly
PTL	Porous Transport Layer
CL	Catalyst Layer

reports that the stack alone accounts for approximately 40% of the total PEMWE system cost, with the remainder attributed to power supplies (29%) and balance-of-plant components (31%). Within the stack, the catalyst-coated membrane (CCM) contributes nearly 32% of the stack cost due to the high price of Nafion-like membranes and noble metal catalysts such as iridium, while bipolar plates and anode porous transport layers each contribute over 20% of the total stack cost, primarily driven by the use of titanium and precious metal coatings. The authors highlight that meaningful cost reduction will require design-driven optimization strategies that preserve performance and durability while reducing reliance on expensive materials, rather than reliance on system-level economic assumptions alone [9]. These observations suggest that cost reduction in PEMWEs is not solely dependent on material substitution but also on design-informed optimization strategies that directly couple transport behavior with economic performance.

Parallel to materials development, extensive experimental and numerical investigations have examined the influence of operational and structural parameters on PEMWE electrochemical performance. These studies have demonstrated that membrane thickness, membrane conductivity, and operating temperature significantly affect ohmic losses and polarization behavior, thereby strongly influencing energy efficiency [10,11]. In addition, the magnitude and spatial distribution of porosity within porous transport layers have been shown to affect mass transport resistance, reactant accessibility, and local current density distribution, with direct implications for cell performance stability [12]. More recently, gas crossover and differential pressure operations have been identified as critical factors influencing efficiency, safety, and operational reliability, particularly under high current density or pressurized conditions [13]. Although these studies have significantly improved understanding of individual transport mechanisms, their coupled implications for system-level techno-economic performance remain insufficiently established. Recent investigations have also extended PEMWE research toward integrated energy-system configurations and coupled renewable-hydrogen applications, further emphasizing the importance of understanding transport–performance interactions across multiple operational scales. Integrated renewable-energy systems have increasingly demonstrated the importance of coupling hydrogen production with broader performance, sustainability, and economic indicators to achieve efficient and cost-effective energy solutions [14] More broadly, advances in renewable-energy technologies have highlighted the growing role of material engineering and nanotechnology-based approaches in enhancing system efficiency, sustainability, and energy conversion performance across emerging green-energy platforms [15,16].

In the author's previous studies, a progressive sequence of numerical investigations has systematically addressed performance-determining mechanisms in PEMWE. These studies include comprehensive parametric analyses of membrane thickness, conductivity, and operating temperature effects [10], comparative evaluation of porosity distribution strategies within porous transport layers [12], and explicit modelling of gas crossover and outlet pressure effects on electrochemical behaviour [11]. While these investigations provided detailed insight into performance trends and transport behavior, they primarily focused on electrochemical and transport characteristics without explicitly quantifying how such physics-based variations propagate into hydrogen production cost and system-level techno-economic performance. Although several techno-economic analyses of hydrogen production systems have been published in recent years, most existing frameworks treat PEMWE as black-box components, relying on assumed efficiency ranges or averaged performance data [3,7,8]. Consequently, the direct influence of design-resolved structural and transport parameters on hydrogen production cost remains insufficiently explored. This disconnect limits the ability of current economic models to inform engineering-level decisions where performance, durability, and cost are intrinsically coupled. Existing studies therefore provide limited capability for evaluating how transport-driven electrochemical behavior can be translated into practical design decisions for economically optimized PEMWE systems.

Motivated by this gap, the present study aims to bridge electrochemical performance and economic feasibility by translating physics-based simulation outputs into a techno-economic framework. Polarization characteristics derived from validated multi-physics models are integrated into a cost analysis formulation to evaluate how variations in membrane properties, porosity distributions, and gas crossover

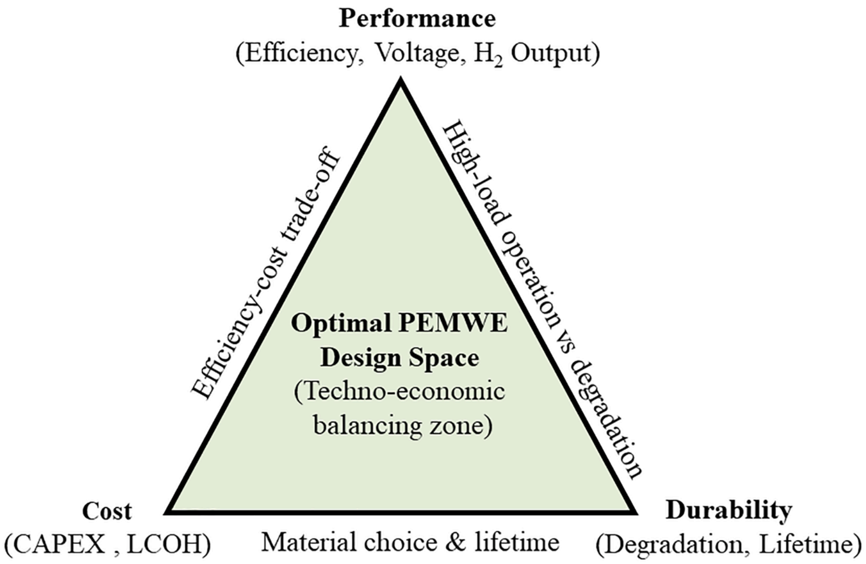

Fig. 1. Conceptual triangular framework illustrating the trade-off space between performance, cost, and durability in PEMWE design. The shaded central region represents the optimal PEMWE design space (techno-economic balancing zone), where electrochemical efficiency, hydrogen production output, economic constraints, and durability considerations converge to define system-level optimization pathways.

behaviour propagate into specific energy consumption, hydrogen production rate, and LCOH. Unlike previous studies that frequently rely on assumed efficiency values or generalized electrolyzer representations, the present work establishes a direct physics-to-cost relationship by integrating validated electrochemical simulation outputs into a design-oriented techno-economic framework. By grounding the economic assessment in simulation-derived performance data rather than generic assumptions, this work provides a more realistic representation of cost–performance coupling in PEMWE systems and delivers design-oriented insight for cost-sensitive optimization.

The remainder of this paper is structured as follows. Section 2 presents the materials, numerical modelling framework, and techno-economic methodology used to link simulation outputs with economic indicators. Section 3 discusses the results and analyzes the cost–performance relationships associated with membrane properties, porous structure, and crossover phenomena. Section 4 concludes the study and highlights key implications for PEMWE design and future research directions.

2. Modelling framework and techno-economic methodology

This section establishes the methodological foundation used to translate physics-based PEMWE performance into economically meaningful indicators. It integrates the previously validated numerical modelling framework with a techno-economic assessment strategy to quantify how design-driven variations in voltage behaviour propagate into energy consumption and hydrogen production cost. The section first introduces the baseline PEMWE architecture and operating context adopted for all simulations, followed by a concise description of the governing electrochemical and transport physics. Subsequently, the procedure for extracting performance metrics from the numerical model and embedding them within the techno-economic formulation is detailed, culminating in the definition of the investigated parametric cases.

To contextualize this methodology within a system-level decision framework, Fig. 1 illustrates the conceptual triangular relationship between cost, performance, and durability in PEMWE design. These three dimensions represent the dominant and often competing objectives in PEMWE optimization, a fact widely recognized in recent literature [17–19]. Improvements in electrochemical performance or system efficiency may lead to increased capital cost or accelerated material degradation, while durability-oriented strategies may impose performance penalties or higher upfront expenses. The “cost–activity trade-off and limited durability” challenge has been identified as one of the primary obstacles to large-scale PEMWE deployment. This triadic structure, therefore, defines the principal trade-off space governing PEMWE development and serves as a guiding lens through which the subsequent techno-economic analysis is interpreted.

2.1. PEMWE model configuration and operating conditions

The PEMWE model employed in this study is based on a three-dimensional, steady-state representation of a single repeating cell comprising a seven-layer membrane electrode assembly (MEA) structure. The computational domain consists of, from anode to cathode, an anode bipolar plate, an anode porous transport layer (aPTL), an anode catalyst layer (aCL), the proton exchange membrane, a cathode catalyst layer (cCL), a cathode porous transport layer (cPTL), and a cathode bipolar plate. Each layer is assumed to be homogeneous and isotropic, with effective transport properties assigned according to the selected design parameters and literature-supported values.

The model adopts a single-phase, isothermal framework in which liquid water is treated as the sole fluid phase within the porous media and channels, while gas generation effects are implicitly accounted for through electrochemical source terms in the charge and species balances. This single-phase formulation is intentionally adopted to isolate the techno-economic impact of voltage variations arising from structural and transport parameters, while avoiding additional uncertainty associated with explicit two-phase flow dynamics. The governing physics incorporates electrochemical reaction kinetics, ionic and electronic conduction, and porous media transport, following a validated modelling architecture reported in the literature [10]. All simulations are conducted under steady-state operating conditions, with the cell temperature maintained at a fixed value, and outlet pressure conditions applied consistently across all investigated cases. A range of current densities is imposed to generate polarization behavior, enabling systematic evaluation of cell voltage response under varying design configurations. Baseline operating conditions are selected to reflect typical PEMWE operational regimes reported in the literature and the authors’ previously validated studies.

The investigated design parameters within this study include membrane thickness, membrane proton conductivity, porosity magnitude

Table 1
Baseline operating conditions, geometrical parameters, material properties, and techno-economic constants used in the PEMWE model.

Category	Parameter	Symbol	Value	Unit	Source/Note
Operating conditions	Cell temperature	T	60	°C	Baseline operating condition
	Operating Pressure	p	1	atm	Uniform outlet pressure
	Current density range	i	0.5–3	A cm^{-2}	Used for polarization curves
	Cell voltage range	V_{cell}	1–3	V	Simulation output
Geometry	Membrane Thickness	δ_m	183	μm	Nafion-type membrane
	Anode CL thickness	δ_{aCL}	20	μm	Fixed
	Cathode CL thickness	δ_{cCL}	20	μm	Fixed
	Anode PTL thickness	δ_{aPTL}	500	μm	Fixed
	Cathode PTL thickness	δ_{cPTL}	500	μm	Fixed
Material/transport Properties	Membrane proton conductivity	σ_m	1–10	S m^{-1}	Parametric range
	PTL porosity (baseline)	ε_{PTL}	0.4	—	Baseline value
	CL porosity (baseline)	ε_{CL}	0.4	—	Baseline value
Electrochemical parameters	Exchange current density (anode)	i_o,a	2.5E-7	A cm^{-2}	Literature-based
	Exchange current density (cathode)	i_o,c	5E-3	A cm^{-2}	Literature-based
	Charge transfer coefficient	α	0.5	—	Assumed
Techno-economic constants	Electricity price	C_{elec}	See Section 2.4	\$kWh^{-1}	Scenario-dependent
	Stack lifetime	t_{life}	See Section 2.4	h	Assumed
	Hydrogen LHV	LHV_{H2}	120	MJ kg^{-1}	Standard value
	Discount rate	r	See Section 2.4	—	Assumed
	Capacity factor	CF	See Section 2.4	—	Assumed
	System lifetime	N	See Section 2.4	years	Assumed
	Annual O&M cost	COM	See Section 2.4	—	Assumed

*Note: The operating conditions, geometrical dimensions, material properties, and electrochemical parameters listed in Table 1 are selected based on commonly adopted PEMWE modelling and experimental studies reported in the literature [9–12,17,19–22].

and distribution within porous transport layers, and gas crossover-related effects under controlled pressure conditions. These parameters were selected because they directly influence the dominant voltage-loss mechanisms and represent practical design variables commonly targeted in PEMWE optimization studies. These parameters are varied independently to isolate their respective influence on electrochemical performance, forming the foundation for subsequent techno-economic evaluation.

A summary of the baseline operating conditions, geometrical specifications, material properties, and techno-economic constants adopted in the simulations is provided in Table 1, which serves as the reference configuration for all parametric studies unless otherwise stated. The numerical framework adopted in this study is based on previously validated PEMWE models developed and reported in the authors' previous studies and benchmarked against published experimental and numerical investigations, thereby ensuring consistency, predictive reliability, and physical credibility of the performance outputs used for subsequent techno-economic assessment [10–12]. The use of previously validated numerical models minimizes uncertainty associated with model formulation and improves confidence in the derived techno-economic trends.

2.2. Governing electrochemical and transport physics

The numerical framework resolves the key electrochemical and transport processes governing voltage behavior in PEMWE under steady-state operation. The purpose of this section is to briefly summarize the physical mechanisms represented in the model and to highlight the parameters most relevant to the subsequent techno-economic analysis, without reproducing full mathematical formulations. Similar modelling philosophies have been widely adopted in recent PEMWE studies to balance physical fidelity and computational tractability [17–19].

The governing relationships introduced in this section are directly associated with the physical mechanisms responsible for voltage generation and loss within PEMWEs. Parameters such as membrane thickness, proton conductivity, porosity distribution, and crossover transport terms are explicitly emphasized because they represent the principal design variables investigated in the present study and form the basis for subsequent techno-economic performance evaluation [2,4,23].

Charge conservation is enforced in both the ionic and electronic conducting phases. Proton transport through the membrane is governed by Ohmic conduction, such that membrane thickness (δ_m) and proton conductivity (σ_m) directly control the magnitude of resistive voltage losses. Ohmic losses scale with the ratio δ_m/σ_m, directly linking membrane properties to voltage behavior. Consequently, reductions in membrane resistance directly influence power consumption and hydrogen production cost through their impact on cell voltage and system efficiency. These membrane-related losses are widely recognized as a dominant contributor to PEMWE cell voltage and energy consumption, particularly at moderate to high current densities [9,17].

Electrochemical reactions within the aCL and cCL are described using the Butler–Volmer kinetics, linking local current density to activation overpotentials through exchange current density and charge transfer coefficients. This formulation captures activation losses and polarization behaviour under practical operating conditions and is commonly adopted in PEMWE modelling studies [10,12]. Variations in activation behavior influence the polarization response and therefore affect the energy demand associated with hydrogen production, creating an indirect link between electrochemical kinetics and techno-economic indicators.

Transport within the porous transport layers (PTL) is treated using a single-phase porous media formulation, where liquid water is assumed to be the continuous phase. The porosity (ε) of these layers influences effective transport properties, reactant accessibility, and local current density distribution, thereby affecting mass transport resistance and overall voltage response. Changes in porosity characteristics can therefore alter energy consumption and operational efficiency, making PTL structural design an important contributor to cost-sensitive PEMWE optimization. Both experimental and numerical investigations have demonstrated that porosity magnitude and spatial distribution play a critical role in PEMWE performance and stability [9,11,18].

Gas crossover effects are represented through effective transport terms across the membrane driven by concentration gradients and pressure differentials. Although explicit two-phase flow is not resolved, this treatment enables the influence of crossover flux on polarization behavior, efficiency, and hydrogen purity to be quantified within a simplified framework. Recent studies have highlighted that hydrogen crossover can introduce non-negligible voltage penalties and operational concerns, particularly under high current density or pressurized conditions [13]. From a techno-economic perspective, crossover-related

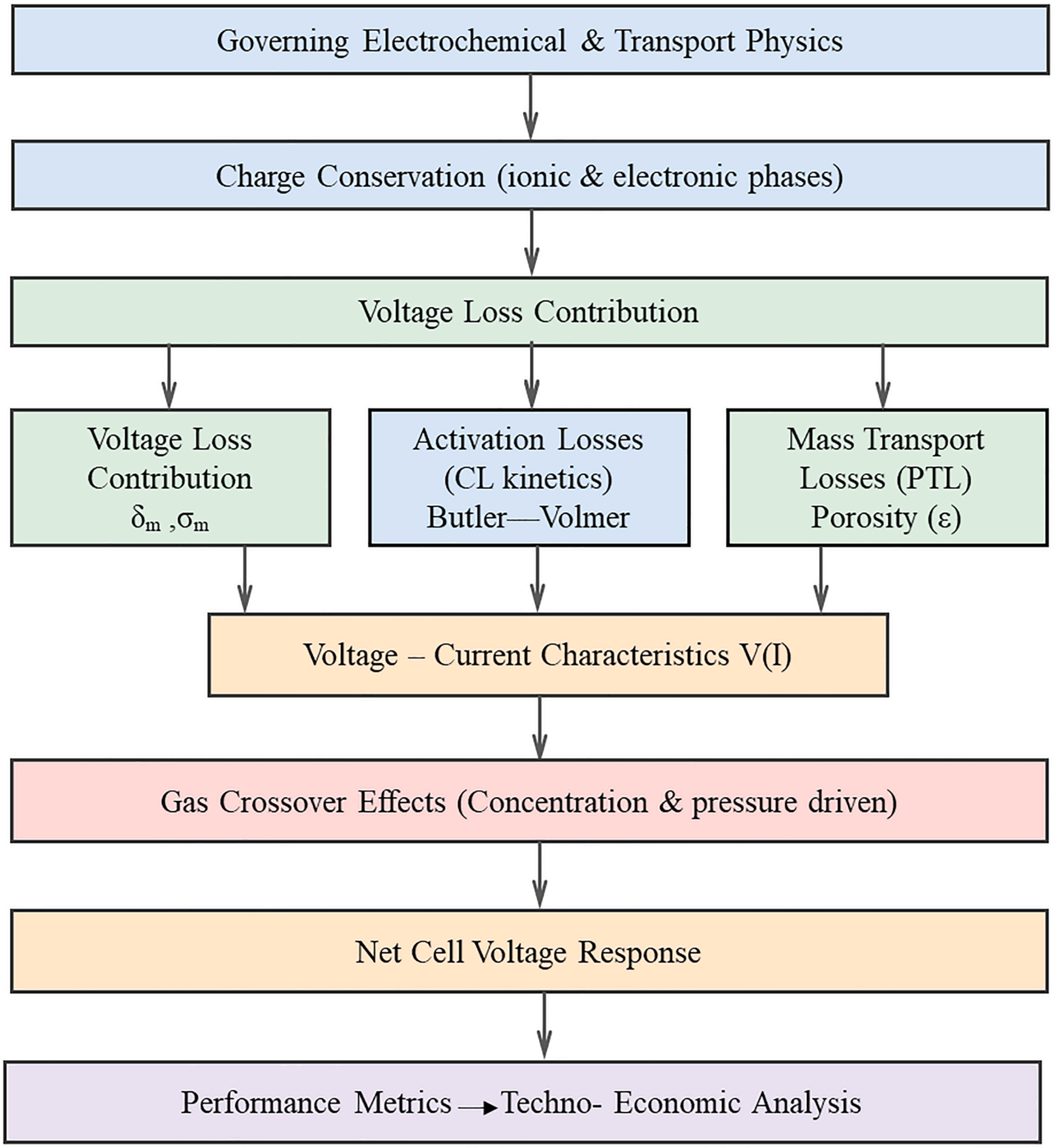

Fig. 2. Schematic overview of the governing electrochemical and transport physics resolved in the PEMWE model. Charge conservation in the ionic and electronic phases, activation losses described by Butler–Volmer kinetics, membrane ohmic losses governed by thickness and proton conductivity, and mass-transport limitations associated with PTL porosity collectively determine the voltage–current characteristics. Gas crossover effects driven by concentration and pressure gradients are incorporated to capture their impact on polarization behavior. The resulting voltage response forms the basis for performance metrics used in the subsequent techno-economic analysis.

losses may increase energy requirements and reduce effective hydrogen utilization, thereby contributing to increased hydrogen production cost.

Overall, the governing physics is employed to generate voltage–current characteristics that capture the influence of membrane properties, porous structure, and crossover phenomena. These polarization outputs form the basis for the performance metrics used in the techno-economic analysis, enabling direct translation of transport- and structure-induced voltage variations into specific energy consumption and levelized cost of hydrogen, as commonly adopted in physics-informed techno-economic assessments [2,4,23]. Fig. 2 schematically summarizes the logical coupling between the governing electrochemical and transport processes described in this section, illustrating how charge conservation, voltage loss mechanisms, and gas crossover collectively shape the polarization response and feed into the subsequent techno-economic analysis.

2.3. *Generation of performance data from simulations*

The primary role of the numerical simulations in this study is to generate physically consistent performance data that can be directly translated into techno-economic indicators. The generated performance outputs are derived from a validated modelling framework and therefore preserve physically meaningful relationships between transport behavior, voltage response, and system performance indicators. In particular, the simulated voltage–current characteristics provide the quantitative link between electrochemical transport phenomena and system-level energy consumption, forming the foundation for subsequent cost analysis.

2.3.1. *Extraction of polarization characteristics*

For each investigated design configuration, steady-state simulations are performed over a prescribed range of applied current densities. At each operating point, the numerical model resolves the coupled electrochemical and transport equations described in Section 2.2, yielding the corresponding cell voltage. This procedure produces a polarization curve, V(i), which encapsulates the combined effects of activation losses, ohmic resistance, mass-transport limitations, and gas crossover–related penalties. The resulting polarization response therefore serves as an integrated representation of the coupled electrochemical and transport processes considered in the model.

The resulting polarization behaviour reflects the sensitivity of cell voltage to membrane properties, porous transport characteristics, and crossover effects, enabling direct comparison across parametric cases under otherwise identical operating conditions. Voltage values at selected current densities are subsequently extracted from these curves to support quantitative performance evaluation and economic assessment, consistent with standard practice in PEMWE modelling studies [2,4,10]. The use of identical operating conditions across all parametric cases ensures that observed differences in voltage response and derived techno-economic metrics are attributable exclusively to the investigated design variables.

2.3.2. *Electrical power requirement*

The instantaneous electrical power input to the PEMWE is calculated directly from the simulated cell voltage and operating current. For a given operating point, the electrical power is calculated using Eq. (1):

$$P = VI \tag{1}$$

where V is the simulated cell voltage (V) and I is the total cell current (A), obtained from the imposed current density and the active electrode area. The active electrode area is maintained constant for all investigated cases to ensure that variations in electrical power demand arise solely from changes in electrochemical and transport behavior. This formulation ensures that any voltage variation arising from changes in transport resistance, membrane properties, or crossover effects is directly reflected in the electrical power demand. Accordingly, the electrical power requirement serves as an intermediate link between electrochemical performance and the subsequent calculation of energy consumption and hydrogen production cost.

2.3.3. *Specific energy consumption*

To enable techno-economic comparison, the electrical power requirement is converted into a specific electrical energy consumption per unit of mass of hydrogen produced. Under steady-state operation and assuming unity of Faradaic efficiency within the single-phase modelling framework adopted here, the hydrogen production rate is proportional to the operating current according to Faraday's law.

The specific electrical energy consumption, E_{spec}, is calculated using Eq. (2):

$$E_{spec} = \frac{VnF}{\eta_F M_{H_2}} \tag{2}$$

where n = 2 is the number of electrons transferred per hydrogen molecule, F = 96,485 C mol^{-1} is Faraday's constant, $M_{H2} = 2.016 \times 10^{-3}$ kg mol^{-1} is the molar mass of hydrogen, and $\eta_F = 1$ is the Faradaic efficiency, taken as unity unless otherwise stated. The selected parameter values and assumptions are consistent with commonly adopted PEMWE formulations and ensure that differences in calculated energy consumption arise from design- and transport-induced voltage variations rather than changes in electrochemical stoichiometry. The assumption of unity Faradaic efficiency is adopted to isolate the influence of design and transport parameters on energy consumption while avoiding additional complexity associated with side reactions and parasitic losses. When expressed in practical units, the specific energy consumption is reported in kWh kg^{-1} H_2, enabling direct comparison with literature values and techno-economic benchmarks [4,23]. This formulation highlights the central role of cell voltage in governing energy efficiency: any increase in voltage due to membrane resistance, transport limitations, or gas crossover effects translates linearly into higher specific energy consumption and, consequently, increased hydrogen production cost.

2.3.4. *Role in techno-economic assessment*

The voltage–current characteristics and derived energy consumption metrics obtained from the numerical simulations constitute the primary performance inputs to the techno-economic model developed in the subsequent section. By maintaining a consistent operating current density across parametric cases, differences in specific energy consumption can be attributed directly to physics-based design variations rather than operational assumptions. This approach enables a transparent and physically grounded translation of microscale transport phenomena into system-level economic indicators, as commonly adopted in physics-informed techno-economic assessments of PEMWE [2,4,23]. This framework further enables quantitative assessment of the relationship between electrochemical performance metrics and hydrogen production economics.

2.4. *Techno-economic modelling framework*

This section presents the techno-economic framework employed to translate simulation-derived electrochemical performance into hydrogen production cost indicators. The framework is deliberately structured to preserve transparency and to isolate the economic consequences of performance variations induced by design and transport parameters. Unlike conventional assessments that rely on assumed efficiencies or generic electrolyzer performance data, the present approach adopts voltage–current characteristics obtained directly from numerical simulations as the primary input to the economic analysis. The adopted framework therefore establishes a direct pathway through which physics-based variations in electrochemical performance propagate into energy consumption, annualized cost components, and ultimately hydrogen production economics.

Under current and near-term cost structures, electricity consumption is widely recognized as the dominant contributor to the LCOH for PEMWE, often accounting for 60–80% of the total hydrogen production cost [3,23]. Consequently, a physics-informed representation of cell voltage behavior is essential for accurately capturing cost–performance coupling.

2.4.1. *Definition of economic performance indicators*

The principal economic indicator evaluated in this study is the LCOH, expressed in USD kg^{-1} H_2. LCOH represents the average cost of producing one kilogram of hydrogen over the operational lifetime of the electrolyzer system and is commonly employed to enable consistent comparison across hydrogen production technologies and system configurations [2,18]. LCOH is adopted in the present study because it

Table 2

Key techno-economic variables used in the simulation-to-cost framework.

Symbol	Description	Unit
V	Cell voltage obtained from numerical simulations	V
i	Applied current density	A cm^{-2}
I	Total cell current	A
P	Electrical power input	W
E_{spec}	Specific electrical energy consumption	kWh kg^{-1} H_2
C_{el}	Electricity price	USD kWh^{-1}
C_{elec}	Electricity cost per unit of hydrogen	USD kg^{-1} H_2
C_{cap}	Total installed capital cost	USD
$C_{cap,ann}$	Annualized capital cost	USD yr^{-1}
$C_{O\&M,ann}$	Annual operation and maintenance cost	USD yr^{-1}
$\dot{m}_{H_2,ann}$	Annual hydrogen production	kg yr^{-1}
$LCOH$	Levelized cost of hydrogen	USD kg^{-1} H_2
η_{Stack}	Stack electrical efficiency (LHV-based)	—

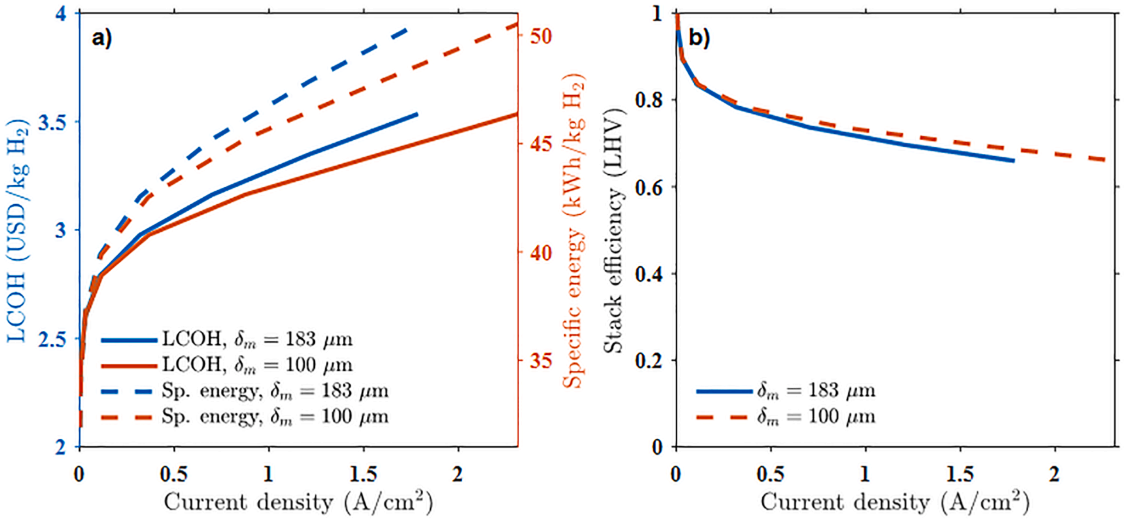

Fig. 3. Effect of membrane thickness on the energy efficiency and techno-economic performance of the PEMWE under identical operating conditions. **(a)** Combined influence on specific energy consumption (right axis) and the corresponding LCOH (left axis) as functions of current density, illustrating how voltage penalties associated with increased membrane thickness simultaneously increase energy demand and electricity-dominated hydrogen production cost. **(b)** Stack electrical efficiency (LHV-based) versus current density, highlighting the inverse relationship between specific energy consumption and efficiency.

integrates both performance-dependent operating costs and long-term economic considerations within a single metric, thereby enabling direct comparison across different design configurations.

To maintain a transparent connection between electrochemical performance and economic outcomes, intermediate performance indicators are also defined. These include the specific electrical energy consumption, E_{spec} (kWh kg^{-1} H$_2$), and the associated electrical energy input derived from the simulated polarization behavior. These indicators form the direct interface between the numerical model and the techno-economic formulation.

In addition to specific energy consumption, the stack electrical efficiency, η_{Stack}, can be defined for completeness as the ratio of the lower heating value of hydrogen to the electrical energy input, expressed using Eq. (3):

$$\eta_{Stack} = \frac{LHV_{H_2}}{E_{spec}} \tag{3}$$

Here LHV_{H_2} is the lower heating value of hydrogen. While stack efficiency is not used explicitly in the subsequent cost calculations, this definition provides an intuitive efficiency-based interpretation of voltage-driven energy penalties.

2.4.2. Electricity consumption and energy cost

Electricity consumption constitutes the primary operating cost for PEMWE. Based on the specific electrical energy consumption obtained from the numerical simulations (Section 2.3), the electricity cost per unit mass of hydrogen, C_{elec}, is calculated using Eq. (4):

$$C_{elec} = E_{spec}\ C_{el} \tag{4}$$

where C_{el} is the electricity price (USD kWh^{-1}). This formulation explicitly links voltage penalties arising from membrane resistance, transport limitations, or gas crossover effects to hydrogen production cost.

Given the strong dominance of electricity cost in PEMWE economics, even modest increases in cell voltage can translate into substantial economic penalties at the system level [2,3,6]. This relationship further emphasizes that design-induced reductions in voltage losses can provide measurable economic benefits through reduced electricity expenditure over the system lifetime.

2.4.3. Capital cost annualization

To account for capital expenditure, the total installed cost of the electrolyzer system is annualized over its operational lifetime using the capital recovery factor (CRF). The CRF is defined using Eq. (5):

$$CRF = \frac{r(1+r)^N}{(1+r)^N - 1} \tag{5}$$

where r is the discount rate and N is the system lifetime in years. The selected discount rate and lifetime assumptions are maintained consistently across all investigated cases to ensure that observed cost variations originate exclusively from design- and performance-related changes rather than economic scenario adjustments. The annualized capital cost, $C_{cap,ann}$, is then calculated using Eq. (6):

$$C_{cap,ann} = C_{cap}\ CRF \tag{6}$$

where C_{cap} denotes the total installed capital cost of the electrolyzer system. This formulation is consistent with established PEMWE techno-economic analyses and cost projection studies [3,6]. The annualization approach enables the initial capital investment to be distributed across the expected operating lifetime of the system, thereby providing a more realistic representation of long-term economic performance than direct upfront cost comparison.

2.4.4. Levelized cost of hydrogen formulation

The levelized cost of hydrogen is calculated by summing annualized capital and operating costs and dividing by the annual hydrogen production, as expressed in Eq. (7):

$$LCOH = \frac{C_{cap,ann} + C_{O\&M,ann} + C_{elec,ann}}{\dot{m}_{H_2,ann}} \tag{7}$$

where $C_{O\&M,ann}$ represents annual operation and maintenance costs, $C_{elec,ann}$ denotes annual electricity expenditure, and $\dot{m}_{H_2,ann}$ is the annual hydrogen production (kg yr^{-1}). Annual hydrogen production is calculated from the simulated hydrogen generation rate and the system capacity factor, ensuring consistent treatment across all investigated cases. Maintaining identical economic assumptions and operating conditions across all investigated cases ensures that changes in LCOH reflect only the influence of design- and transport-induced performance variations.

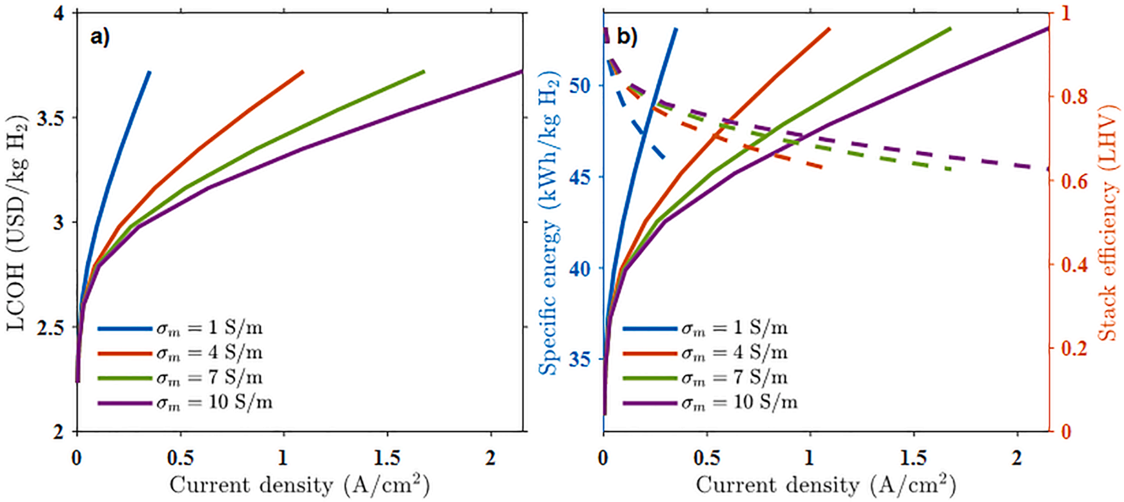

Fig. 4. Effect of intrinsic membrane proton conductivity on the energy efficiency and techno-economic performance of the PEMWE under identical operating conditions. (a) Variation in the LCOH with current density for membrane proton conductivities of σ_m=1–10 S/m, highlighting the propagation of conductivity-driven electrical losses into electricity-dominated hydrogen production cost. (b) Combined response of specific energy consumption (solid lines, left axis) and stack electrical efficiency (LHV-based; dashed lines, right axis) as functions of current density, illustrating the improvement in energetic performance with increasing membrane proton conductivity.

2.4.5. *Simulation-to-cost conversion logic*

The techno-economic framework follows a direct and transparent conversion pathway, as illustrated in Eq. (8):

$$V(i) \rightarrow P \rightarrow E_{spec} \rightarrow C_{elec} \rightarrow LCOH \tag{8}$$

This structure ensures that any performance variation resolved by the numerical simulations propagates explicitly into energy consumption and hydrogen production cost. The direct propagation pathway also minimizes reliance on empirical correction factors and preserves the physical relationships between design modifications and economic outcomes. By maintaining identical economic assumptions across all parametric cases, differences in LCOH can be attributed solely to physics-based variations in electrochemical and transport behaviour rather than external economic parameters.

This physics-informed techno-economic approach enables systematic evaluation of design-driven cost–performance trade-offs and supports engineering-level decision-making for PEMWE optimization, as advocated in recent techno-economic and system-level assessment studies [2,3,6,18,23].

For clarity and reference, Table 2 summarizes the principal techno-economic variables and performance indicators employed throughout the simulation-to-cost framework together with their corresponding definitions and units, providing a concise reference for the equations and calculations presented in this section.

2.5. *Definition of investigated cases*

To systematically assess how design and transport parameters influence both electrochemical performance and hydrogen production cost, a set of parametric cases is defined. Each case isolates a single class of parameters while all other operating conditions, geometric features, and economic assumptions are held constant. This approach ensures that differences in performance and techno-economic indicators can be attributed directly to the investigated parameter rather than to confounding effects.

The investigated cases are structured to align with previously reported numerical investigations of PEMWE [10,12,21] and to enable direct translation of established performance trends into economic implications. The selected cases further represent key design variables frequently targeted in PEMWE optimization studies because of their direct influence on voltage losses, transport behavior, and overall system efficiency.

i. Case A: Membrane Thickness Variation:

In Case A, the effect of membrane thickness on PEMWE performance and cost is examined. Membrane thickness directly influences ionic resistance and ohmic voltage losses, thereby affecting cell voltage and specific energy consumption. A range of membrane thickness values is considered while maintaining constant membrane conductivity, operating temperature, and porous layer properties. This case evaluates the trade-off between reduced ohmic losses and potential material-related cost implications. Variations in membrane thickness are also relevant from a practical design perspective because excessive membrane thinning may improve performance while introducing potential durability and crossover-related concerns.

ii. Case B: Membrane Conductivity Variation:

Case B focuses on the influence of membrane proton conductivity on electrochemical performance and techno-economic outcomes. Proton conductivity governs the magnitude of membrane-related ohmic losses and is affected by material selection, hydration state, and operating conditions. In this case, membrane conductivity varies independently while membrane thickness and all other model parameters are held fixed, allowing isolation of conductivity-driven effects on polarization behaviour and hydrogen production cost. Conductivity enhancement strategies are of practical interest because they provide a potential pathway for improving performance without requiring significant geometric modifications to the membrane structure.

iii. Case C: Porosity Distribution Strategies:

Case C investigates the role of porosity magnitude and spatial distribution within the porous transport layers. Different porosity configurations are examined to assess their impact on mass transport resistance, reactant accessibility, and local current density distribution. By comparing uniform and non-uniform porosity distributions under identical operating conditions, this case evaluates how porous structure design influences both electrochemical performance and cost-relevant energy consumption. Porosity distribution strategies are particularly important because localized transport behavior within PTLs can substantially influence current density uniformity and associated voltage losses under practical operating conditions.

iv. Case D: Gas Crossover and Pressure Effects:

Case D examines the influence of gas crossover and outlet pressure conditions on PEMWE performance and techno-economic metrics. Gas crossover is represented through effective transport terms across the membrane driven by concentration gradients and pressure differentials. By varying pressure conditions while maintaining consistent structural and material parameters, this case quantifies the performance penalties and associated cost implications arising from crossover phenomena. Crossover effects are particularly relevant under practical PEMWE operating conditions because they can influence efficiency, hydrogen purity, and operational reliability while introducing hidden economic penalties. Collectively, these investigated cases provide a structured framework for evaluating how individual design modifications propagate through electrochemical performance and ultimately influence system-level techno-economic outcomes.

3. Results and discussion

This section presents the techno-economic implications of design and transport parameter variations in PEM water electrolyzers, based on the simulation-to-cost framework described in Section 2. The results are organized according to the parametric cases investigated in Section 2.5, enabling systematic assessment of how electrochemical performance variations propagate into energy consumption and hydrogen production cost.

For each case, cell voltage response, specific energy consumption, and LCOH are evaluated under otherwise identical operating and economic assumptions. This structure allows direct attribution of techno-economic trends to the underlying physics-based design parameters rather than external cost or operational factors.

3.1. Case A: effect of membrane thickness

In this case, the influence of membrane thickness on PEMWE performance and techno-economic metrics is examined by comparing two representative membrane configurations. A membrane thickness of 183 μm is adopted as the baseline case, corresponding to the widely used Nafion® 117 membrane and commonly reported reference values in the literature [13]. In contrast, a thinner membrane with a thickness of 100 μm is considered to represent advanced or reduced-thickness membrane designs that have been investigated to mitigate ohmic losses and enhance efficiency [10]. These two thickness values are selected to capture both conventional and performance-oriented membrane configurations while maintaining consistency with experimentally and numerically validated studies.

3.1.1. Impact on electrochemical performance

Membrane thickness governs PEMWE performance primarily through its effect on ionic transport resistance within the membrane phase. As membrane thickness increases, proton conduction pathways lengthen, leading to higher membrane ohmic resistance and increased cell voltage under identical operating conditions. This behaviour has been well documented in both experimental and numerical studies and is consistent with the polarization characteristics reported in the authors' previous parametric investigations [10].

At low current densities, voltage differences associated with membrane thickness variation remain relatively small, as activation losses dominate the overall polarization behavior. However, as current density increases, membrane-related ohmic losses become progressively more significant, amplifying the voltage penalty associated with thicker membranes. This behaviour is consistent with prior studies identifying membrane ohmic losses as a dominant contributor to PEMWE cell voltage at moderate to high current densities [10,17].

3.1.2. Effect on specific energy consumption

The voltage penalties induced by increased membrane thickness translate directly into higher specific electrical energy consumption. For a given operating current density, thinner membranes operate at lower cell voltage and therefore require less electrical energy per unit mass of hydrogen produced, whereas thicker membranes demand greater electrical input to sustain the same hydrogen production rate [20].

Table 3
Comparative assessment of membrane thickness reduction and proton conductivity enhancement strategies in PEM water electrolyzers.

Design aspect	Membrane thickness reduction	Membrane conductivity enhancement	Ref
Primary physical mechanism	Shorter proton path; reduced membrane resistance	Higher ionic mobility; reduced effective resistance	[9, 10, 17]
Impact on cell voltage	Strong reduction at moderate–high current densities	Moderate–strong reduction depending on σ_m	[10, 17, 19]
Effect on specific energy consumption	Noticeable decrease via voltage reduction	Comparable decrease via improved transport	[10, 18, 24]
Effect on LCOH	Lower cost driven by reduced electricity demand	Lower cost driven by reduced electrical losses	[1,6, 17, 18]
Impact on stack electrical efficiency	High efficiency gains at elevated currents	Comparable gains with enhanced transport	[10, 17]
Durability implications	Higher crossover risk; mechanical stress	Hydration, ageing, and chemical stability issues	[9, 13, 17]
Manufacturing considerations	Handling and robustness challenges	Advanced polymer or composite membrane required	[9, 19, 25]
Design flexibility	Limited by crossover and integrity constraints	Higher flexibility; geometry unchanged	[17, 24]
Scalability challenges	Lifetime and crossover at industrial loads	Material cost and long-term stability	[6,9, 17]
Recommended application regime	Performance-driven designs with durability trade-offs	Balanced performance–durability optimization	[9, 17, 18]

Because specific energy consumption scales linearly with cell voltage, even moderate increases in membrane thickness result in noticeable increases in E_{spec}, particularly at higher current densities where ohmic losses dominate. At a representative operating current density in the moderate-to-high operating range (≈1.7–1.8 A cm^{-2}), increasing membrane thickness from 100 μm to 183 μm increased the specific energy consumption by approximately 5–7%, accompanied by an increase in the LCOH of approximately 4–6%. These results indicate that relatively modest membrane-induced voltage penalties can propagate into measurable techno-economic consequences. This trend is illustrated in Fig. 3(a), where the specific energy consumption (right axis) exhibits an increasing separation between thin and thick membrane configurations as current density increases, accompanied by a corresponding increase in LCOH (left axis), highlighting the strong sensitivity of PEMWE energy efficiency and hydrogen production cost to membrane geometric design.

3.1.3. Implications for LCOH

The increase in specific energy consumption associated with thicker membranes propagates directly into higher hydrogen production cost through elevated electricity expenditure. Given that electricity consumption represents the dominant contributor to the LCOH in PEMWE, membrane thickness emerges as a critical design parameter governing economic performance.

As shown in Fig. 3(a) (left axis), thicker membranes systematically increase LCOH across the entire operating current density range, with the cost penalty becoming increasingly pronounced at higher current densities. The stronger cost sensitivity observed at elevated current densities reflects the increasing contribution of membrane-related ohmic losses to the overall voltage response. Consequently, the economic impact of membrane thickness becomes progressively amplified under operating conditions relevant to industrial hydrogen production. While thinner membranes offer clear techno-economic advantages in

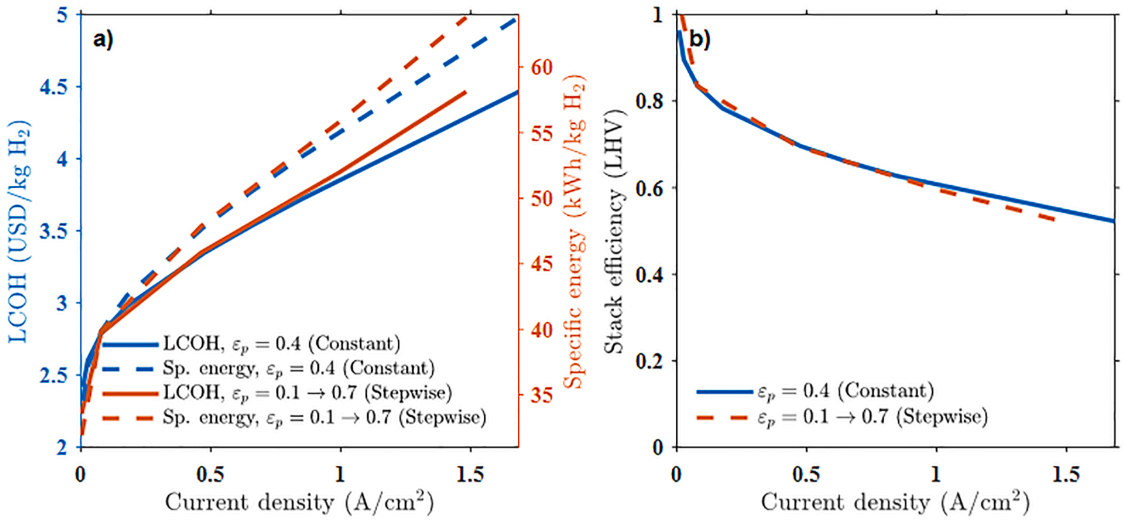

Fig. 5. Effect of porous transport layer (PTL) porosity distribution on the energy efficiency and techno-economic performance of the PEMWE under identical operating conditions. **(a)** Combined variation of the LCOH (left axis) and specific energy consumption (right axis) with current density for constant porosity (εp=0.4) and stepwise porosity (εp=0.1→0.7) in the anode PTL. **(b)** Stack electrical efficiency (LHV-based) versus current density, illustrating efficiency gains enabled by tailored porosity distributions at moderate to high operating currents.

terms of reduced energy consumption and lower LCOH, practical considerations such as mechanical robustness, gas crossover mitigation, and long-term durability constrain the minimum viable membrane thickness in real systems. Consequently, membrane thickness optimization must balance performance gains against material and operational limitations.

3.1.4. *Effect on stack electrical efficiency*

The influence of membrane thickness on energy consumption is also reflected in the overall stack of electrical efficiency. Thinner membranes, by reducing membrane ohmic losses and operating voltage, enable more efficient conversion of electrical energy into chemical energy on an LHV basis.

This behaviour is illustrated in Fig. 3(b), which shows higher stack electrical efficiency for thinner membranes across the investigated current density range, with efficiency gains becoming more pronounced at moderate to high operating currents. These results confirm that membrane thickness affects not only absolute energy and cost metrics but also the fundamental energetic performance of the PEMWE system.

3.1.5. *Summary of Case A*

Overall, Case A demonstrates that membrane thickness variations exert a strong and systematic influence on PEMWE performance and hydrogen production cost through their impact on membrane ohmic losses. Thinner membranes consistently reduce specific energy consumption, lower LCOH, and improve stack electrical efficiency, with benefits becoming increasingly significant at moderate to high current densities. However, these techno-economic advantages must be balanced against durability and operational constraints, reinforcing the necessity of integrated performance–cost assessment in membrane design for practical PEMWE deployment. These findings suggest that aggressive membrane thinning alone is unlikely to provide a universally optimal solution, particularly when long-term operation and system reliability are considered.

3.2. *Case B: effect of membrane proton conductivity*

To complement the geometric optimization explored in Case A, this

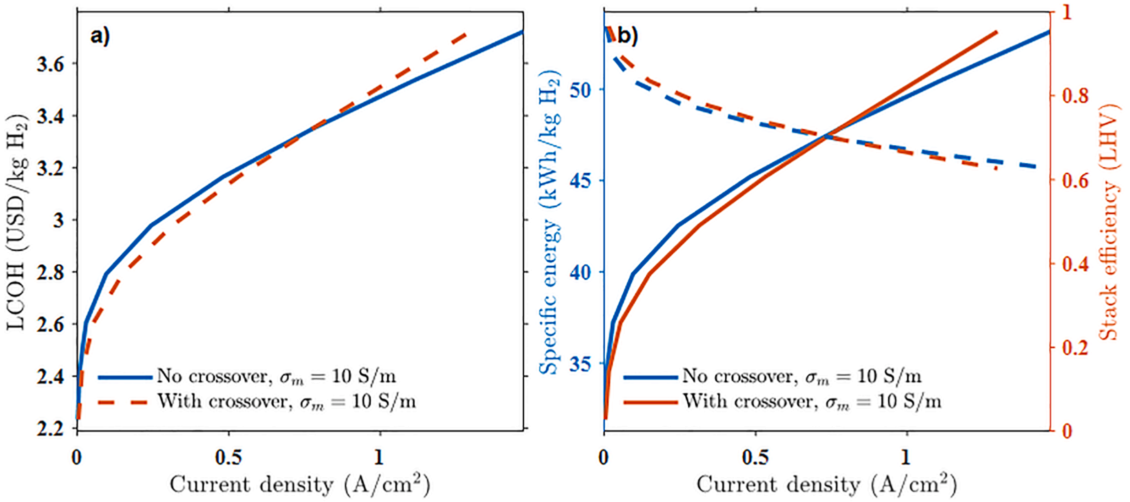

Fig. 6. Effect of gas crossover on the energy efficiency and techno-economic performance of the PEM water electrolyzer for a fixed membrane proton conductivity of σ_m=10 S/m. (a) Variation of the LCOH with current density for cases with and without gas crossover. (b) Combined response of specific energy consumption (left axis) and stack electrical efficiency (LHV-based; right axis) as functions of current density, illustrating the crossover-induced increase in energy demand and corresponding reduction in efficiency at moderate to high operating currents. (Solid lines: specific energy; dashed lines: stack efficiency).

case investigates the influence of intrinsic membrane proton conductivity on PEMWE performance and techno-economic metrics while maintaining a fixed membrane thickness. Four representative conductivity values, σ_m=1, 4, 7, and 10 S/m, are examined. These values span the range from relatively low-conductivity membranes to highly conductive, optimized membrane states and are selected based on previously validated numerical and experimental investigations reported by the authors [10]. This range enables a systematic assessment of how conductivity enhancement alone, independent of membrane thickness, affects electrochemical behavior, energy efficiency, and hydrogen production cost.

3.2.1. *Impact on electrochemical performance*

Membrane proton conductivity directly governs ionic transport resistance within the membrane and therefore plays a central role in determining PEMWE voltage response and overall electrochemical performance. For a fixed membrane thickness, increasing σ_m reduces the effective membrane resistance, resulting in lower cell voltage under otherwise identical operating conditions. At low current densities, variations in membrane conductivity lead to relatively modest voltage differences, as activation losses dominate the electrochemical response. As current density increases, membrane-related ohmic losses become increasingly significant, amplifying conductivity-driven voltage differences. This behaviour highlights the growing importance of membrane transport properties under practical operating regimes and is consistent with prior studies identifying proton conductivity as a key determinant of PEMWE voltage efficiency at moderate to high current densities [10, 21].

3.2.2. *Effect on specific energy consumption*

The reduction in cell voltage associated with increased membrane proton conductivity translates directly into lower specific electrical energy consumption. For a given operating current density, membranes with higher σ_m require less electrical energy per unit mass of hydrogen produced due to reduced membrane-related ohmic losses. Consistent with the linear dependence of specific energy consumption on cell voltage, increasing membrane conductivity yields a systematic decrease in energy demand across the investigated operating range. At representative moderate-to-high operating current densities, increasing membrane proton conductivity from σ_m = 1 to 10 S m^{-1} reduced the specific energy consumption by approximately 8–12%, accompanied by a reduction in LCOH of approximately 7–10%. These results demonstrate that conductivity enhancement can translate efficiently into measurable techno-economic gains through mitigation of membrane-related ohmic losses. This trend is illustrated in Fig. 4(b), where higher membrane conductivity results in lower specific energy consumption, with the separation between conductivity cases becoming more pronounced at elevated current densities where ohmic losses dominate.

3.2.3. *Implications for LCOH*

The decrease in specific energy consumption achieved through enhanced membrane proton conductivity propagates directly into lower hydrogen production cost via reduced electricity expenditure. Consequently, membrane conductivity emerges as a critical material-level parameter governing economic performance.

As shown in Fig. 4(a), increasing σ_m systematically reduces the LCOH across the investigated current density range, with cost reductions becoming increasingly pronounced at higher operating currents. These results demonstrate that conductivity-driven reductions in electrical losses translate efficiently and directly into techno-economic benefits for PEMWE operation. The observed economic benefits further suggest that conductivity enhancement strategies may offer a more flexible optimization pathway than aggressive membrane thinning, since performance improvements can be achieved without substantial modifications to membrane geometry.

3.2.4. *Effect on stack electrical efficiency*

The conductivity-driven reduction in energy consumption is also reflected in the overall stack electrical efficiency. As membrane proton conductivity increases, the lower voltage requirement per unit current enables more efficient conversion of electrical energy into chemical energy on an LHV basis. This behaviour is illustrated in Fig. 4(b), where stack electrical efficiency (right axis) increases systematically with membrane proton conductivity across the investigated operating range, with efficiency gains becoming more pronounced at moderate to high current densities. These results confirm that enhancing intrinsic membrane conductivity improves not only absolute energy and cost metrics but also the fundamental energetic performance of the PEMWE system.

3.2.5. *Summary of Case B*

Overall, Case B demonstrates that increasing intrinsic membrane proton conductivity significantly enhances PEMWE performance and reduces hydrogen production cost by mitigating membrane-related ohmic losses. Higher conductivity membranes consistently lower specific energy consumption, reduce LCOH, and improve stack electrical efficiency, with benefits becoming increasingly pronounced at moderate to high current densities. The results further indicate that conductivity enhancement produces increasingly pronounced benefits at moderate-to-high operating current densities, where membrane-related ohmic losses become dominant and directly influence electricity-dominated hydrogen production cost. However, these advantages must be balanced against material feasibility, durability, and manufacturing considerations, underscoring the importance of conductivity optimization within an integrated performance–cost framework for PEMWE membrane design.

3.3. *Comparative assessment of membrane design strategies*

Cases A and B demonstrate that membrane thickness reduction and intrinsic proton conductivity enhancement constitute two complementary design strategies for mitigating membrane-related ohmic losses in proton exchange membrane water electrolyzers. Reducing membrane thickness shortens the proton transport pathway, whereas enhancing proton conductivity improves the efficiency of ionic transport within the membrane material. Although both approaches effectively lower cell voltage and associated energy consumption, particularly at moderate to high current densities, their underlying mechanisms, feasibility, and practical limitations differ, as also discussed in recent comprehensive reviews of PEMWE membrane design and system-level trade-offs [24].

To facilitate a structured comparison of these two membrane optimization strategies, their primary electrochemical, techno-economic, durability, and scalability implications are summarized in Table 3, based on the present results and recent literature [9,10,13,17–19,22,24, 25].

From an electrochemical and techno-economic perspective, both strategies yield comparable qualitative benefits, including reduced specific energy consumption and lower electricity-dominated LCOH. However, membrane thickness reduction provides a more direct reduction in ohmic resistance and can lead to pronounced voltage improvements. This approach, however, is constrained by increased susceptibility to hydrogen crossover, mechanical stress, and long-term durability concerns. These limitations have been increasingly emphasized in recent studies that explicitly consider the coupled effects of efficiency enhancement and gas permeation in thin membranes [13,22].

In contrast, improving membrane proton conductivity can partially offset the performance penalties of thicker membranes without altering cell geometry, thereby offering greater flexibility in membrane selection and cell design. Nevertheless, achieving high proton conductivity often relies on advanced polymer chemistry, hydration management, or operating condition optimization, which may introduce additional material complexity, cost, or stability challenges at scale [9,10,19].

From a practical design standpoint, neither thickness reduction nor conductivity enhancement alone represents a universally optimal solution. Consequently, the results of this study suggest that robust membrane designs are most likely to emerge from integrated optimization strategies that combine moderate thickness reduction with targeted conductivity enhancement. Such balanced approaches enable meaningful improvements in electrochemical efficiency and hydrogen production cost while mitigating durability and manufacturability risks. This conclusion aligns with recent material engineering and component-level analyses that advocate co-optimization of membrane geometry and transport properties to support scalable, high-performance, and economically viable PEMWE operation [9,18,25].

3.4. Case C: effect of porosity magnitude and distribution in porous transport layers

While membrane thickness and proton conductivity primarily govern membrane-related ohmic losses, transport phenomena within the PTL play a critical role in determining mass transport resistance, reactant accessibility, and local current density distribution in PEMWE. Case C therefore extends the present analysis beyond membrane-focused optimization by examining how porosity magnitude and spatial distribution within the PTL influence system-level energy efficiency and techno-economic performance.

PTL porosity directly affects effective transport properties such as permeability, tortuosity, and effective diffusivity, thereby regulating liquid water supply, gas evacuation pathways, and reactant access to the catalyst layers. Insufficient porosity can lead to increased mass transport resistance and local reactant starvation, while excessively high porosity may compromise mechanical integrity and electrical contact. As a result, PTL porosity represents a key structural design parameter that interacts strongly with membrane-level optimization strategies.

Rather than introducing additional simulations, this case builds on the authors' previously published numerical investigation of porosity distribution strategies in PEMWE, in which constant and stepwise porosity profiles in the anode PTL were systematically evaluated under otherwise identical operating conditions [12]. That study demonstrated that non-uniform porosity distributions, particularly stepwise configurations, can significantly alleviate mass transport limitations near the catalyst layer, leading to reduced operating voltage and improved electrochemical performance at moderate to high current densities.

The techno-economic implications of PTL porosity optimization are shown in Fig. 5(a), which presents the combined variation of specific energy consumption and the LCOH with current density for constant and stepwise porosity configurations. By reducing mass transport losses and associated voltage penalties, the stepwise porosity profile yields lower specific energy consumption and correspondingly reduced electricity-dominated hydrogen production cost, with benefits becoming increasingly pronounced at higher operating currents where mass transport limitations dominate. At moderate-to-high current densities, the stepwise porosity configuration reduced the specific energy consumption and LCOH by approximately 3–6% relative to the constant porosity case, demonstrating that relatively small structural modifications within the PTL can propagate into measurable system-level economic benefits.

The corresponding impact on energetic performance is shown in Fig. 5(b), where the stack electrical efficiency is plotted as a function of current density. The stepwise porosity configuration consistently exhibits higher efficiency relative to the constant porosity case, particularly in the moderate-to-high current density regime, confirming that tailored porosity distributions enable more effective conversion of electrical energy into chemical energy. These results indicate that optimization of PTL microstructural characteristics can complement membrane-level improvements by reducing transport bottlenecks that otherwise limit the translation of electrochemical gains into system-level performance benefits.

The results of Case C reinforce a key insight of this study: membrane optimization alone is insufficient to guarantee minimal energy consumption and cost-effective operation across all operating regimes. Even with optimized membrane thickness and proton conductivity, poorly designed PTL porosity can introduce mass transport bottlenecks that offset membrane-level performance gains. Conversely, appropriately tailored porosity distributions enable membrane improvements to translate more effectively into system-level energy and cost benefits.

In the context of integrated PEMWE design, PTL porosity optimization should therefore be viewed as a structural counterpart to membrane optimization. When combined with moderate membrane thickness reduction and targeted conductivity enhancement, tailored porosity distributions offer a pathway to simultaneously improve electrochemical performance, energy efficiency, and techno-economic viability, without excessive reliance on extreme membrane designs. These conclusions are consistent with recent studies advocating co-optimization of membrane properties and porous electrode structures to support scalable, high-performance, and economically viable PEMWE operation [9,12,18].

3.5. Case D: gas crossover and pressure effects

Gas crossover constitutes an intrinsic membrane transport phenomenon in PEMWE that becomes increasingly relevant at elevated current densities and under pressurized operating conditions. Unlike the design parameters examined in Cases A–C, which primarily influence ohmic and mass-transport losses, gas crossover introduces parasitic species transport across the membrane that directly affects voltage response, hydrogen utilization, and techno-economic performance. In this case, the impact of crossover effects is assessed within the present modelling framework by comparing operating scenarios with and without crossover for a fixed membrane proton conductivity of σ_m=10 S/m, based on the authors' previously published crossover-aware modelling studies.

3.5.1. Physical origin of gas crossover

Gas crossover in PEMWE arise from the diffusion of hydrogen and oxygen species across the polymer electrolyte membrane, driven by concentration gradients and pressure differentials between the cathode and anode compartments. Hydrogen crossover is typically dominant due to its higher diffusivity and smaller molecular size in hydrated polymer membranes. These transport processes are strongly influenced by membrane thickness, hydration state, and operating pressure, and therefore interact directly with the membrane optimization strategies examined in Cases A and B. Recent experimental and numerical studies have demonstrated that gas crossover cannot be neglected at high current densities or elevated operating pressures, as it introduces parasitic losses that alter local reaction equilibria and increase the effective voltage required to sustain a given hydrogen production rate [26–28]. The authors' prior modelling work further indicates that measurable crossover-induced voltage penalties can arise even within simplified single-phase frameworks when effective transport terms are incorporated [29].

3.5.2. Impact on energy consumption and hydrogen production cost

The techno-economic consequences of gas crossover are illustrated in Fig. 6(a), which presents the variation of the LCOH with current density for operating cases with and without crossover. The inclusion of crossover effects systematically increases LCOH across the investigated operating range, with the cost penalty becoming increasingly pronounced at higher current densities. At moderate-to-high operating current densities, inclusion of crossover effects increased the LCOH by approximately 4–8%, accompanied by an increase in specific energy consumption of approximately 5–9% relative to the crossover-free case. These results demonstrate that parasitic membrane transport can introduce economically meaningful penalties even when all other design and operating conditions remain unchanged.

This behaviour reflects the direct coupling between crossover-induced voltage penalties and electricity-dominated hydrogen production cost. As parasitic hydrogen transport reduces effective faradaic efficiency and modifies local electrochemical conditions, additional electrical energy input is required to maintain the same hydrogen production rate. Consequently, crossover effects propagate efficiently into higher electricity expenditure per unit mass of hydrogen produced, elevating LCOH even when all other techno-economic parameters are held constant [26–28].

3.5.3. *Effect on energy efficiency and stack performance*

The energetic implications of gas crossover are further quantified in Fig. 6(b), which shows the combined variation of specific energy consumption and stack electrical efficiency as functions of current density. In the absence of crossover, the system exhibits lower specific energy demand and higher stack efficiency across the operating range. When crossover effects are included, specific energy consumption increases systematically, accompanied by a corresponding reduction in stack efficiency.

These crossover-induced efficiency losses become increasingly significant at moderate to high current densities, where concentration-driven transport across the membrane intensifies. The results confirm that gas crossover constitutes an additional loss mechanism beyond conventional activation and ohmic contributions, reducing the effectiveness with which electrical energy is converted into chemical energy on an LHV basis [28,30].

3.5.4. *Interaction with membrane design strategies*

The findings of Case D highlight a strong coupling between crossover phenomena and the membrane design strategies explored in Cases A and B. While reducing membrane thickness is an effective approach for mitigating ohmic losses, it inherently increases susceptibility to gas crossover by shortening diffusion pathways. Conversely, enhancing intrinsic membrane proton conductivity enables efficiency improvements without reducing membrane thickness, thereby offering a pathway to partially mitigate crossover-related penalties while preserving mechanical robustness and durability [26–28].

These interactions demonstrate that membrane optimization strategies focused solely on minimizing ohmic resistance may inadvertently exacerbate crossover-induced inefficiencies if parasitic transport phenomena are not simultaneously considered. This observation highlights the importance of avoiding isolated optimization strategies, since improvements in one transport mechanism may unintentionally introduce competing penalties that offset the expected techno-economic benefits. As a result, membrane design decisions must be evaluated within an integrated framework that accounts for both efficiency gains and crossover-related losses [26,27,29].

3.5.5. *Summary of Case D*

Overall, Case D demonstrates that gas crossover constitutes a critical determinant of PEMWE energy efficiency and hydrogen production cost. Crossover effects introduce additional voltage penalties that increase specific energy consumption and elevate LCOH, particularly at high current densities relevant to industrial operation. The results emphasize that robust PEMWE design requires coordinated optimization of membrane conductivity, thickness, and operating conditions to ensure that electrochemical performance improvements translate reliably into techno-economic gains. These findings reinforce the importance of incorporating crossover-aware transport modelling when evaluating advanced PEMWE design strategies for large-scale and pressurized hydrogen production [26–30].

Collectively, the investigated cases demonstrate that PEMWE techno-economic performance is governed by strongly coupled interactions between membrane properties, porous transport characteristics, and parasitic transport phenomena. While individual design modifications can yield measurable improvements in energy efficiency and hydrogen production cost, the results consistently indicate that balanced optimization strategies provide more robust pathways toward economically viable PEMWE operation than isolated parameter adjustments.

4. Conclusions

This study presents a physics-informed techno-economic assessment of key design and transport parameters governing the performance and hydrogen production cost of proton exchange membrane water electrolyzers. By systematically investigating membrane thickness, intrinsic membrane proton conductivity, PTL porosity strategies, and gas crossover phenomena, direct relationships between electrochemical transport behaviour, voltage response, and system-level techno-economic performance were established.

The results demonstrate that membrane thickness and proton conductivity are dominant factors controlling membrane-related ohmic losses and therefore strongly influence specific energy consumption, stack efficiency, and LCOH. Moderate membrane thinning reduced specific energy consumption by approximately **5–7%** and LCOH by **4–6%**, although thinner membranes increase susceptibility to durability limitations and gas crossover. In contrast, increasing membrane proton conductivity reduced specific energy consumption by approximately **8–12%** and lowered LCOH by **7–10%** while preserving structural integrity. These findings suggest that neither membrane thinning nor conductivity enhancement alone provides a universally optimal solution; instead, balanced membrane optimization strategies combining moderate thickness reduction with targeted conductivity enhancement are more likely to achieve practical performance gains.

Beyond membrane properties, PTL porosity magnitude and spatial distribution were found to significantly influence mass transport behaviour and local current density distributions. Stepwise porosity configurations reduced transport-induced voltage penalties and lowered specific energy consumption and LCOH by approximately **3–6%** relative to constant porosity cases, highlighting PTL structural design as an important complement to membrane optimization.

The inclusion of gas crossover effects further demonstrated that parasitic membrane transport represents an economically important loss mechanism. Crossover-induced voltage penalties increased specific energy consumption by approximately **5–9%** and elevated LCOH by **4–8%**, particularly at moderate-to-high current densities. These findings emphasize that membrane optimization strategies should be evaluated within a crossover-aware framework to ensure that electrochemical improvements translate into reliable techno-economic benefits.

Overall, this work provides a unified physics-informed framework linking electrochemical transport behaviour to energy efficiency and hydrogen production cost. The findings demonstrate that effective PEMWE optimization requires coordinated consideration of electrochemical transport, material properties, porous structure design, and operating conditions rather than isolated parameter tuning. Future work will extend the present framework toward fully coupled two-phase transport modelling, durability-aware lifetime analysis, sensitivity-based uncertainty quantification, and system-level integration studies.

Data availability

Data supporting the findings of this study are included within the article and its supplementary information. Additional simulation data and model outputs are available from the corresponding author upon reasonable request.

Ethics approval and consent to participate

Not applicable. This study is based on numerical simulations and techno-economic modelling and does not involve human participants, animals, or clinical data.

Consent for publication

All authors have reviewed the manuscript and consent to its publication.

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Declaration of AI use

AI tools were used exclusively for grammar checking and language refinement during manuscript preparation. No AI tools were used for data analysis, scientific reasoning, interpretation, or generating research content. All scientific results, analyses, and conclusions are entirely the work of the authors, who take full responsibility for the accuracy and integrity of the manuscript.

CRediT authorship contribution statement

Ali Bayat: Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis. **Prodip K. Das:** Writing – review & editing, Supervision. **David Eager:** Writing – review & editing, Supervision. **Suvash C. Saha:** Writing – review & editing, Supervision, Project administration, Conceptualization.

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.

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