

OPTIMAL DESIGN, SCHEDULING, AND CONTROL OF ELECTROLYSIS-BASED HYDROGEN PRODUCTION PLANTS

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Abstract

Hydrogen has long been utilized as an energy carrier, from its early applications in internal combustion engines, balloons, and airships over 200 years ago to its modern role in oil refining and industrial processes. Amid growing climate change concerns, global demand for low-carbon hydrogen has increased significantly, positioning green hydrogen—produced via water electrolysis powered by renewable or other low-carbon electricity sources—as a key pathway toward energy decarbonization. However, most low-carbon hydrogen technologies remain economically uncompetitive with fossil-fuel-based alternatives. Among commercial electrolysis technologies, alkaline electrolyzers (AE) and proton exchange membrane electrolyzers (PEME) are mature solutions, while solid oxide electrolyzer cells (SOEC) are still under development. PEME technology is particularly promising due to its compact design, high current density, high efficiency, fast dynamic response, and capability to produce ultra-pure hydrogen, but its reliance on noble metals results in high capital costs and elevated levelized cost of hydrogen (LCOH). Therefore, optimal integration and operation of electrolysis hydrogen production plants (EHPPs), particularly PEME-based systems, within power grids is essential to improve economic viability and enhance grid resilience. This dissertation develops a comprehensive modeling and optimization framework for EHPP design, configuration, and operation. Detailed electrochemical models for AE and PEME technologies are formulated and embedded into novel optimization problems that simulta-

neously determine plant sizing, equipment ratings, internal electrolyzer parameters, configuration options (with or without battery energy storage systems), and hourly operational scheduling. The proposed formulations aim to minimize LCOH while extending PEME safe operating ranges, improving efficiency at partial loading, and enhancing integration with renewable energy sources. Furthermore, a comprehensive framework is developed to optimize EHPP participation in grid ancillary services—including capacity auction markets, operating reserves, and renewable power smoothing—under various electricity pricing schemes, while meeting hydrogen demand across multiple sectors and pressure requirements. Finally, a coordinated dynamic control and scheduling strategy is introduced to optimally regulate PEME cathodic pressure and operating temperature, thereby improving efficiency across all loading conditions and further reducing hydrogen production costs. The proposed methodologies contribute toward economically viable hydrogen production and improved power system flexibility in low-carbon energy systems.

Dedication

To the souls of more than 72,000 innocent Palestinians who have lost their lives, and to the over 172,000 who have been injured in Gaza between 2023 and 2025.

To all Palestinians who continue to endure hardship with resilience and who persist in their struggle for their land, dignity, and future.

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Acronyms

H_2	Hydrogen.
C_{Deg}	Degradation Cost.
AE	Alkaline Electrolyzer.
AE-HPP	Alkaline Electrolyzer based Hydrogen Production Plant.
ATR	Auto Thermal Reforming.
BESS	Battery Energy Storage System.
CA	Capacity Auction.
CAPEX	Capital Expenditure.
CCUS	Carbon Capture, Usage and Storage.
cdf	Cumulative Density Function.
CEH	Carbon Emissions per kg of Hydrogen.
CI	Carbon Intensity.
DR	Demand Response.
EHPP	Electrolysis Hydrogen Production Plant.
FC	Fuel Cell.
FCEV	Fuel Cell Electric Vehicle.
GOF	Grid Operation Fees.
HOEP	Hourly Ontario Energy Price.
HS	Hydrogen Storage.
IESO	Independent Electricity System Operator.
ITC	Investment Tax Credit.

LCOH	Levelized Cost of Hydrogen.
LHV	Lower Heating Value.
MCS	Monte Carlo Scenarios.
Mt	million tonnes.
OPEX	Operational Expenditure.
OR	Operating Reserve.
pdf	Probability Density Function.
PEME	Proton Exchange Membrane Electrolyzer.
PEME-HPP	Proton Exchange Membrane Electrolyzer based Hydrogen Production Plant.
POX	Partial Oxidation.
PPA	Power Purchase Agreement.
PTC	Production Tax Credit.
RES	Renewable Energy Sources.
RS	Renewable Power Smoothing.
SAF	Sustainable Aviation Fuel.
SCM	Separately Controlled Module.
SMR	steam Methane Reforming.
SoC	State of Charge.
SOEC	Solid Oxide Electrolyzer Cell.
SoH	State of Hydrogen.
SQP	Sequential Quadratic Programming.

Nomenclature

Constants

F	Faraday's constant
R	Universal gas constant

AE Parameters and Variables

α_{an}^{AE}	Anodic charge-transfer coefficient of the AE
α_{cat}^{AE}	Cathodic charge-transfer coefficient of the AE
β_{an}	Width of anodic bubble area in the AE
β_{cat}	Width of cathodic bubble area in the AE
$\Delta\pi$	Pressure difference across the AE separator
δ_s	Separator thickness of the AE
δ_{an}	Thickness of the anodic electrode in the AE
δ_{cat}	Thickness of the cathodic electrode in the AE
ϵ_s	Separator porosity of the AE
ϵ_{an}	Porosity of the anodic electrode in the AE
ϵ_{cat}	Porosity of the cathodic electrode in the AE
η_{AE}	AE total efficiency
η_F^{AE}	AE Faraday's efficiency
η_p^{AE}	AE production efficiency
ω_s	Separator wettability factor of the AE

Π^{AE}	Total pressure at the anodic or cathodic compartments of the AE
$\pi_{H_2}^{AE}$	Hydrogen partial pressure at the AE cathodic compartment (i.e., cathodic pressure)
$\pi_{O_2}^{AE}$	Oxygen partial pressure at the AE anodic compartment (i.e., anodic pressure)
$\Psi_{H_2}^{AE}$	Hydrogen-in-oxygen percentage in the AE
$\rho_{eff,an}$	Effective resistivity of the anodic electrode in the AE
$\rho_{eff,cat}$	Effective resistivity of the cathodic electrode in the AE
$\rho_{el,bz}$	Effective resistivity of the electrolyte in the bubble zone in the AE
ρ_{el}	Resistivity of the bubble-free electrolyte in the AE
ρ_o^{an}	Resistivity of the anodic electrode material at the reference temperature T_{ref} in the AE
ρ_o^{cat}	Resistivity of the cathodic electrode material at the reference temperature T_{ref} in the AE
τ_s	Separator tortuosity of the AE
ϑ	Fractional bubble coverage on the AE electrode
ζ	Viscosity of the solvent in the AE
A_{cell}^{AE}	Cell area (effective electrode area) of the AE
D_{eff}	Effective diffusion coefficient of the AE
I^{AE}	AE operating current
J^{AE}	Operating current density of the AE
J_{loss}^{AE}	Equivalent lost current density due to gas crossover in the AE
$J_{0,an}^{AE}$	Anodic exchange current density of the AE
$J_{0,cat}^{AE}$	Cathodic exchange current density of the AE
k_{an}	Temperature coefficient of anodic electrode resistivity in the AE
k_{cat}	Temperature coefficient of cathodic electrode resistivity in the AE
k_{el}	Temperature coefficient of the electrolyte resistivity in the AE

l_{an}	Anode electrode–separator gap in the AE
l_{cat}	Cathode electrode–separator gap the AE
M	Electrolyte concentration of the AE
$N_{H_2}^{AE}$	Hydrogen production flow rate of the AE
$N_{O_2}^{AE}$	Oxygen production flow rate of the AE
$n_{conv}^{H_2}$	Hydrogen convection crossover flow in the AE
$n_{diff}^{H_2}$	Hydrogen diffusion crossover flow in the AE
$n_{diff}^{O_2}$	Oxygen diffusion crossover flow in the AE
$n_{el}^{H_2}$	Hydrogen crossover flow due to electrolyte mixing in the AE
$n_{el}^{O_2}$	Oxygen crossover molar flow due to electrolyte mixing in the AE
n_{H_2}	Total hydrogen crossover flow in the AE
n_{O_2}	Total oxygen crossover flow in the AE
$Pr_{H_2}^{AE}$	AE separator permeability to hydrogen
R_{el}^{AE}	Electrolyte resistance of the AE
R_e^{AE}	Total electrode resistance of the AE
R_s^{AE}	Separator resistance of the AE
$S_{H_2}(M)$	Hydrogen solubility at electrolyte concentration M in the AE
$S_{O_2}(M)$	Oxygen solubility at electrolyte concentration M in the AE
T_{cell}^{AE}	AE cell temperature
V_{act}^{AE}	AE activation overpotential
V_{cell}^{AE}	AE cell voltage
V_{res}^{AE}	AE resistive overpotential
V_{oc}^{AE}	Nernst voltage (open-circuit electrochemical voltage) of the AE

PEME Parameters and Variables

α^{PEM}	PEME charge-transfer coefficient
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δ_m^{PEM}	PEME membrane thickness
η^{PEM}	PEME total efficiency
η_F^{PEM}	PEME Faraday's efficiency
η_p^{PEM}	PEME production efficiency
$\mathcal{M}_{ct}^{H_2}$	Amount of hydrogen in the PEME cathodic compartment and hydrogen separator
$\mathcal{V}_{ct}$	Volume of the PEME cathodic compartment and the associated hydrogen separator
$\mathfrak{M}$	Mathematical constant defined as $\mathfrak{M} = \frac{E_m}{R}$
$\mathfrak{s}_m^{PEM}$	PEME membrane swelling factor
Φ_{th}	Thermal flow rate used for temperature control
$\pi_{H_2}^{PEM}$	Hydrogen partial pressure in the cathodic compartment of the PEME (i.e., cathodic pressure)
$\pi_{O_2}^{PEM}$	Oxygen partial pressure in the anodic compartment of the PEME (i.e., anodic pressure)
$\pi_{H_2}^*$	Cathodic pressure (i.e., Hydrogen pressure) setpoint
$\pi_{H_2}^{PEM, max}$	Maximum PEME cathodic pressure
$\pi_{H_2}^{PEM, min}$	Minimum PEME cathodic pressure
$\Psi_{H_2}^{PEM}$	Hydrogen-in-oxygen percentage in the PEME
$\Psi_{H_2}^{PEM, safe}$	Maximum safe limit for hydrogen in oxygen percentage in PEME
σ_m	PEME membrane ionic conductivity
ξ_L	Lower threshold ratio of the hysteresis relay
ξ_U	Upper threshold ratio of the hysteresis relay
A, B, C	Mathematical constants used to simplify the activation overpotential expression
$A_{cell}^{PEM, max}$	Maximum PEME effective cell area
$A_{cell}^{PEM, min}$	Minimum PEME effective cell area

A_{cell}^{PEM}	Effective cell area of PEME
a_x	Current-density impact coefficient on gas permeation in PEME
A_{srv}	Modular PEME cell in-service area
C_a	Activation capacitance of a PEME cell
E	Input voltage applied to the PEME
E_m	Activation energy
I^{PEM}	PEME operating current
I_{min}^{PEM}	Minimum PEME operating current (i.e. Minimum Loading)
i_1	Dynamic current through the activation capacitance of a PEME cell
i_2	Dynamic current through the activation resistance of a PEME cell
i_{PEM}	PEME dynamic current
J^{PEM}	Operating current density of the PEME
J_o^{PEM}	PEME Exchange current density
J_{loss,H_2}^{PEM}	Hydrogen crossover equivalent current density in the PEME
J_{loss,O_2}^{PEM}	Oxygen crossover equivalent current density in the PEME
J_{loss}^{PEM}	Gas crossover equivalent current density in the PEME
J_{max}^{PEM}	PEME maximum current density
$J_{o,ref}^{PEM}$	Reference exchange current density at the reference cell temperature
k	Gain of the PEME feedforward power correction
L_d	Coupling inductance between the PEME converter and the electric grid
N	Number of modules in the modular PEME
n	Number of in-service modules in the modular PEME
$N_{H_2O}^{PEM}$	Steam flow rate in the PEME
$N_{H_2}^{PEM}$	Hydrogen production flow rate of the PEME
$N_{O_2}^{PEM}$	Oxygen production flow rate of the PEME

N_c	Number of cells per PEME stack
N_s	Number of stacks in the PEME
$P_{FF}(t)$	PEME feedforward power correction at time t
$P_{FF}(t^-)$	Previous value of the PEME feedforward power correction
P_{PEM}^*	Active power setpoint of the PEME
P_{PEM}^{rate}	PEME rated power
$P_{H_2}^{PEM}$	Hydrogen permeability coefficient of the PEME membrane
$Q_{H_2}^{in}$	Hydrogen dynamic inlet flow rate to the cathodic compartment and hydrogen separator in a PEME system
$Q_{H_2}^{out}$	Hydrogen dynamic outlet flow rate through the control valve of the hydrogen separator in a PEME system
$Q_{H_2}^{per}$	Hydrogen permeation dynamic flow rate to the anodic compartment of the PEME
R_a	Activation resistance of a PEME cell
R_m	Membrane ohmic resistance of a PEME cell
T_{cell}^{PEM}	PEME cell temperature
T_{ref}^{PEM}	Reference cell temperature
T_{cell}^*	PEME cell temperature setpoint
V_{act}^{PEM}	PEME activation overpotential
V_{cell}^{PEM}	PEME cell voltage
V_{heat}^{PEM}	Equivalent voltage corresponding to external heat input to the PEME
V_{load}^{PEM}	PEME vapor loading equivalent voltage
V_{oc}^{PEM}	Nernst voltage (open-circuit electrochemical voltage) of the PEME
V_{res}^{PEM}	PEME resistive overpotential
V_{ther}^{PEM}	PEME thermoneutral voltage
V_a	PEME dynamic activation voltage

V_{PEM}^{rate} PEME rated voltage

EHPP Parameters and Variables

$\Delta H_{LHV}^{H_2}$ Lower heating value of hydrogen

ΔH_{vap} Vaporization enthalpy of water

η_{BESS} Charging/discharging efficiency of the BESS

η_{Comp} Compressor efficiency

η_{Conv} Power converter efficiency

η_{mc} Mechanical compression effect on EHPP efficiency

η_T Total hydrogen production efficiency of the EHPP

γ Slack variable

γ_{BESS} Self-dissipation factor of the BESS

γ_{HS} HS dissipation rate

$\mathcal{V}_{HS}$ HS tank volume

π_{HS} Hydrogen storage pressure

π_{HS}^{max} Maximum HS pressure

π_{out} Output pressure of hydrogen (i.e. the pressure needed by the hydrogen application)

$\rho_{ElecPrice}^{mc}$ Probability of the electricity price scenario mc

ρ_{OR}^{mc} Probability of OR payment scenario mc

Υ Clean hydrogen subsidy

a_{H_2O} Water activity

Acc^t BESS achievable cycle count

C_* Specific capital cost of the equipment per unit capacity

C_{Inv} Total grid services payment

CA_{Inv} Payment from CA service participation

CA_{prc}^S	CA payment price during summer obligation period
CA_{prc}^W	CA payment price during winter obligation period
E_{BESS}	Energy capacity of the BESS
E_{H_2}	Amount of hydrogen stored in the HS
E_{HS}	Maximum HS capacity
I_{FC}	FC current
k	Polytropic coefficient of the compressor
N_{loss}^{Elz}	Hydrogen flow lost due to gas crossover applies to both AE and PEME
$N_{H_2}^{FC}$	Hydrogen flow consumption of the FC
N_{day}	Number of days in the obligation period
O_*	Specific hourly operational cost of the equipment per unit of power or hydrogen production
OR_{Inv}	Payment from OR service participation
$OR_{prc}^{t,mc}$	OR payment price at time t for Monte Carlo Scenarios (MCS) mc
P_{BESS}^{rate}	BESS rated power
P_{BESS}^t	Charging/discharging power of the BESS at time t
P_{Cmp}	Power consumption of the hydrogen compressor
P_{Cmp}^{rate}	Compressor rated power
P_{Conv}^{rate}	Power converter rated power
$P_{EHPP,CA}^{t,Act}$	EHPP power during CA activation window at time t
$P_{EHPP,CA}^{t,Av}$	EHPP power during CA availability window (i.e., deactivated) at time t
$P_{EHPP,OR}^t$	EHPP power consumption during OR participation at time t
P_{EHPP}^t	Baseline EHPP power without grid service participation at time t
P_{Elz}	Electrolyzer power consumption applies to both AE and PEME

P_{FC}	FC electrical power output
Pc_{CA}^S	Agreed CA participation power during summer obligation period
Pc_{CA}^t	Agreed CA power participation at time t
Pc_{CA}^W	Agreed CA power participation during winter obligation period
$Pc_{OR,Elz}^t$	Electrolyzer contribution to OR service at time t
$Pc_{RS}^{t_s}$	Average EHPP participation in RS at time step t
$Pc_{RS}^{t_s}$	EHPP participation in RS at time step t_s
$Price_{elec}^t$	Electricity price at time t
Q_d	Hydrogen demand flow rate
Q_{H_2}	Total hydrogen production from the EHPP over the simulation period $\mathbb{T}$
Q_{HS}	Hydrogen flow into the HS
r	The yearly discount rate
RR_{Elz}	Electrolyzer ramp rate limit
RS_{BESS}	BESS residual value
RS_{Inv}	Payment from RS service participation
RS_{prc}	RS payment price
SoC^{max}	Maximum state of charge of the BESS
SoC^{min}	Minimum state of charge of the BESS
SoC^t	State of charge of the BESS at time t
SoH^{max}	Maximum state of hydrogen in the HS
SoH^{min}	Minimum state of hydrogen in the HS
SoH^t	State of hydrogen storage at time t
T_{HS}	Temperature of the HS
T_{HS}^{min}	Minimum HS temperature

V_{act}^{FC}	Activation voltage drop in the FC
V_{con}^{FC}	Concentration voltage drop in the FC
V_{oc}^{FC}	Open-circuit voltage of the FC
V_{res}^{FC}	Voltage drop due to membrane resistance in the FC
$V_{LHV}^{H_2}$	Equivalent voltage corresponding to the hydrogen Lower Heating Value (LHV)
V_{FC}	Output voltage of the FC
Y	EHPP lifetime in years
Z	Hydrogen compressibility factor

Electric Grid Parameters and Variables

$\delta_b^{s,t}$	Voltage phase angle at bus b for state s at time t
$\mathbb{B}$	Boolean variable indicating whether pure green hydrogen production is enforced
$\mathbb{T}^S$	Set of time corresponding to CA summer obligation period
$\mathbb{T}^W$	Set of time corresponding to CA winter obligation period
$\mathbb{Y}_{b,q}$	Magnitude of the admittance between buses b and q
$\mathfrak{R}$	A sufficiently large constant
$\rho(SI^{i,t})$	Probability of solar irradiation state i at time t
$\rho(W S^{j,t})$	Probability of wind speed state j at time t
$\rho^{s,t}$	Probability of combined renewable state s at time t
$\theta_{b,q}$	Admittance phase angle between buses b and q
B	Total number of buses
b^*	Bus to which the EHPP is connected
CA_{Act}	Set of time corresponding to CA activation window
CA_{Av}	Set of time corresponding to CA availability window
f_b	Beta probability density function

f_r	Rayleigh probability density function
G	Total number of photovoltaic power plants connected to the grid
h	Number of discretized states for solar irradiation and wind speed
M	Total number of wind power plants connected to the grid
OR_{Act}	Set of time corresponding to OR activation
$P_{b,d}^{s,t}$	Active power demand at bus b for state s at time t
$P_{b,g}^{s,t}$	Active power generated at bus b for state s at time t
$P_{b^*,max}^t$	Maximum available power at bus b^* at time t
$P_{b^*}^{s,t}$	Maximum available power at bus b^* for state s at time t
P_{grid}^t	EHPP power consumption from the electric grid at time t
$P_{PV,g}^{s,t}$	Power generated by photovoltaic plant g for state s at time t
$P_{W,m}^{s,t}$	Power generated by wind plant m for state s at time t
$Q_{b,d}^{s,t}$	Reactive power demand at bus b for state s at time t
$Q_{b,g}^{s,t}$	Reactive power generated at bus b for state s at time t
s	Index of the combined renewable generation state
$S_{b,q}^{max}$	Maximum apparent power flow limit between buses b and q
$S_{b,q}^{s,t}$	Apparent power flow between buses b and q for state s at time t
$SI^{i,t}$	Solar irradiation state i at time t
V_b^{max}	Maximum allowable voltage magnitude at bus b
V_b^{min}	Minimum allowable voltage magnitude at bus b
$V_b^{s,t}$	Voltage magnitude at bus b for state s at time t
$WS^{j,t}$	Wind speed state j at time t

Chapter 1

Introduction

1.1 Background

Hydrogen has a long history as an energy source. It was utilized to run the first internal combustion engines and to lift balloons and airships 200 years ago. Later, hydrogen became a part of the energy industry and oil refining [1]. Under the pressure of climate change, the global demand for hydrogen has significantly increased. In this context, low-carbon hydrogen emerges as a reliable energy carrier and a clean fuel [2]. However, the majority of low-carbon hydrogen production technologies are still in their infancy. Additionally, the production of low-carbon hydrogen encounters big challenges in terms of competing with the prices of conventional fossil fuels. This chapter provides a background review of hydrogen utilization, production technologies, and its opportunities to replace conventional fuel.

1.1.1 Hydrogen Utilization

As compared to 2020, the global hydrogen demand reached approximately 94 Mt in 2021 with a 5% rise million tonnes (Mt). Most of that increase was due to conventional hydrogen applications such as refining and industry. However, some new applications for hydrogen utilization have also experienced a rapid increase. New steel projects in which

pure hydrogen is directly used for iron reduction have also increased. In the transportation sector, the global stock of Fuel Cell Electric Vehicle (FCEV) increased from 33000 in 2020 to 51000 by the end of 2022. Although, the majority of FCEVs are passenger cars, China led the production of 800 fuel cell trucks in 2021. Further, Germany started the operation of the first hydrogen fuel cell train. Also, more than 100 pilot projects have announced to use hydrogen or its derivatives in shipping. In the power sector, about 3.5 GW are announced to use hydrogen and ammonia by the end of 2030 [3].

The hydrogen demand around the globe is estimated to approach 130 Mt by 2030 to meet the climate commitments already announced by the governments around the world. However, to meet net-zero emissions by 2050, the global hydrogen demand has to reach 200 Mt in 2030 [3]. Fig. 1.1 shows the annual variation in hydrogen demand for different applications from 2019 to 2021. It also shows the projected demand by the end of 2030.

Oil refineries are industrial plants that transform crude oil into other petroleum products like gasoline, diesel, aviation fuel, and naphtha. In this process, hydrogen is used to remove impurities such as sulphur and also in converting heavy oil into lighter products [4]. The use of hydrogen in refining approached 40 Mt in 2018 and then dropped sharply to reach 38 Mt, due to the pandemic, in 2020 before restoring to the 40 Mt level by the end of 2021. In 2021, the majority of hydrogen utilized in refining is produced from fossil fuel, leading to the release of over 200 Mt of CO_2 [3].

The hydrogen usage in refineries is not limited to refining, some new application associated to these processes are expected to rise in the short term including upgrade of biofuels and high-temperature heating. In Canada, the Varennes Carbon Recycling project would annually convert more than 200,000 tonnes of non-recyclable waste into 125 million litres of biofuels. The project deploys a 90 MW electrolyzer for clean hydrogen production, and is expected to start the commissioning phase in 2025 [5]. The first pure hydrogen operated furnace is deployed in Essar's Stanlow refinery in UK. The furnace operation would initially be based on natural gas and will be operated by hydrogen later in 2026 when the HyNet North West project for clean hydrogen production begins [6].

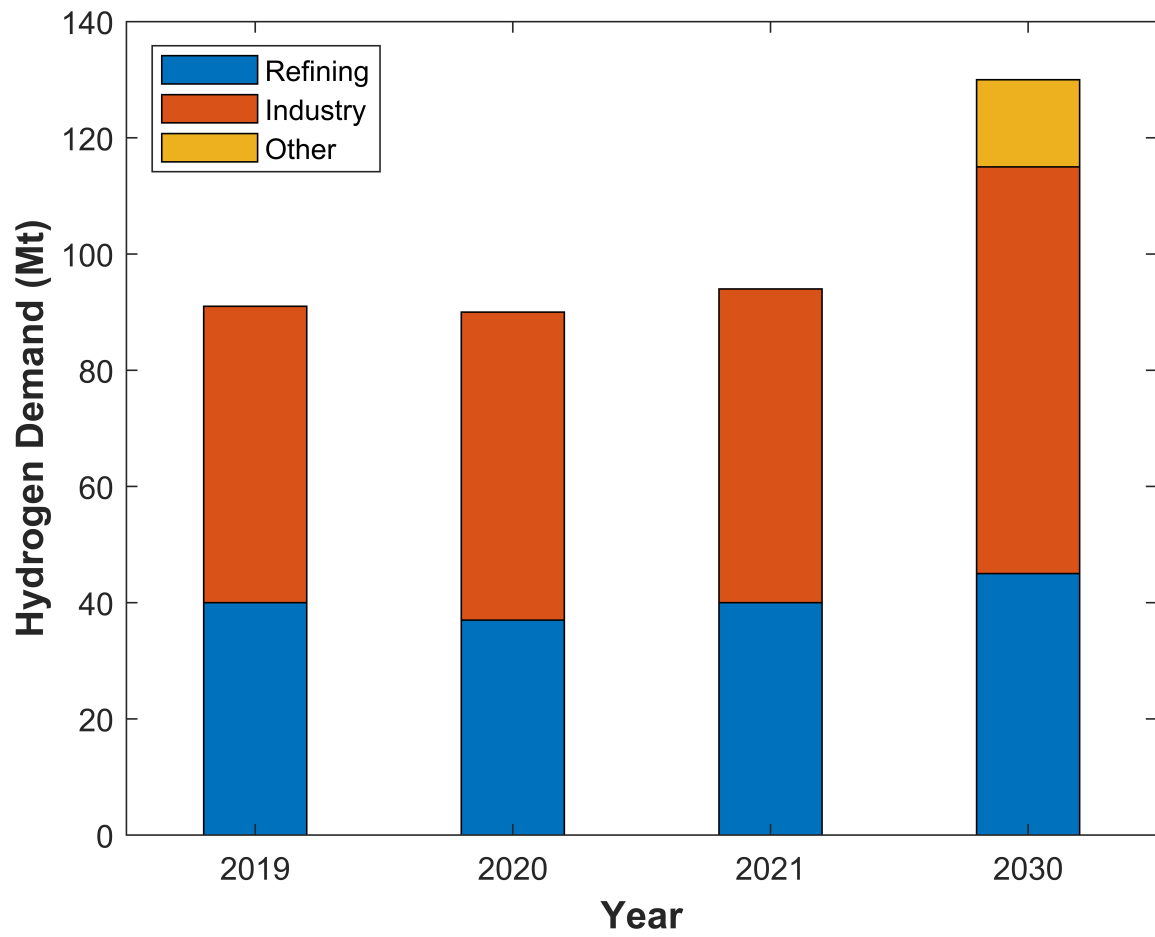


Figure 1.1: Annual hydrogen demand for different applications

Currently, the primary uses of hydrogen in industry are ammonia production, methanol production, and steel industry that annually accounts for 34, 15, and 5 Mt of hydrogen market, respectively. Other applications such as glassmaking, electronics, and chemical industries account to relatively a small volume of hydrogen [3].

In 2021, almost all hydrogen utilized within the industry sector is produced from fossil fuels (natural gas, and coal), resulting in 630 Mt of CO_2 that accounts for 7% of industrial emissions. Due to the economic expansion, hydrogen derived products are expected to rise in the medium term, which, in turn, will increase the industrial demand for hydrogen. Therefore, the industrial hydrogen demand is expected to reach 65 Mt in 2030. To achieve the climate goals of different governments around the globe, low-emission new hydrogen production technologies are projected to account for 13 Mt of industrial hydrogen production by the end of 2030 [3].

In the transportation sector, hydrogen demand exceeded 30 kilotonnes in 2021, marking 60% growth as compared to 2020. However hydrogen accounts for only 0.003% of the total energy used in transportation. Among the various modes of transportation, road vehicles, particularly trucks and buses, are the primary driver for hydrogen demand because of its high annual mileage and heavy weight [3]. Additionally, hydrogen presents a viable solution for decarbonizing diesel-based rail lines, especially when the electrification is not feasible and the distance exceeds the electric batteries capabilities. In August 2022, Germany succeeded to deploy the first fuel cell train fleet in Lower Saxony [7].

The maritime and aviation sectors also witnessed a growing interest for utilizing hydrogen and synthetic fuels derived from hydrogen. It is worth noting that the technologies for utilizing hydrogen in these sectors are not mature yet. However, there is a considerable number of ongoing pilot projects: approximately 45 focus on utilizing hydrogen, 40 pertain to ammonia, and 25 are exploring the use of methanol in shipping. Most of the hydrogen projects concentrate on smaller vessels, while the ammonia projects focus on larger vessels. The methanol projects are distributed between both small and large vessels. In the aviation sector, there are two key development areas: the manufacturing of a hydrogen based

Sustainable Aviation Fuel (SAF), and the hydrogen powered aircraft for flights covering short to medium distances. The progress of hydrogen based SAF is more mature, with cost emerging as the primary obstacle to implementation. On the other hand, the realization of hydrogen powered aviation faces greater challenges, as the associated technologies are still in the initial phase of development [3].

The contribution of hydrogen in satisfying the energy demand in the buildings sector is still negligible. The use of natural gas in cooking and heating is about 25% of the energy demand in the buildings sector. Given the current energy crisis and the global drive to attain net zero emissions, a number of countries prohibited the utilization of fossil fuels in new constructions. For instance, France has enforced such a ban since 2022. The existing reliance on fossil fuels for generating energy for buildings is expected to transfer to environmentally-friendly alternatives like electricity, district heating, and decentralized renewable sources, prior to adopting hydrogen technologies. Hydrogen technologies in buildings suffers from low efficiency as compared to other viable solutions due to the energy losses during hydrogen conversion, transportation, and utilization [3].

Yet, there are some opportunities for hydrogen utilization in buildings particularly in cases where there's existing natural gas infrastructure and challenges in decarbonization. This could be especially relevant in scenarios involving cold climates, historical city centers, and structures with inadequate insulation. Hydrogen demand in the buildings sector could increase up to 2 Mt by 2030, accounting for only 0.2% of the buildings' total energy demand [3].

In the power sector, hydrogen has a much reduced 0.2% share of the electricity generation around the globe. The majority of this generation uses a mix of gases with high hydrogen content. Hydrogen based electricity generators are commercially available and have many forms such as reciprocating gas engines, fuel cells and gas turbines. Many forthcoming projects that involves natural gas-fired power generation, take into consideration either partially blended hydrogen or transition to using hydrogen exclusively at a later stage. The electrical efficiency of fuel cells is around 50-60% even when operating at partial load,

making it attractive for flexible operation with the electricity system. During the year 2021, a global total of 348 megawatts of stationary fuel cell capacity was introduced [3].

1.1.2 Hydrogen Types

Hydrogen production techniques differs in terms of energy source, feedstock, technology, production cost, and the level of carbon emissions. In literature, a color spectrum is often used to illustrate mature hydrogen production techniques. Fig. 1.2 shows the different hydrogen colors and the corresponding energy source, production technology, and the type of emissions.

Brown hydrogen is the hydrogen produced from coal gasification process. Brown hydrogen accounts for more than 22% of the the current global hydrogen production [8], as coal represents the greatest reserve of fossil fuel around the world. Coal gasification is a main hydrogen production method in China, where large coal reserves exist [9]. The coal gasification is a mature technology and its efficiency ranges from 74% to 85%. However, brown hydrogen results in the highest level of carbon emissions compared to other hydrogen production techniques.

In the gasifier unit, dry coal is inserted and reacted with oxygen and steam under high temperature to produce CO_2 and H_2 . This reaction is divided into two stages [9]. In the first stage, air oxidizes a part of the coal to produce CO_2 while storing the heat in the fuel layer as illustrated in the following equation.



Then in the second stage, steam is injected instead of air to react with coal, resulting in CO_2 and H_2 as below.



Another major hydrogen production technique is the grey hydrogen, which refers to the hydrogen produced from natural gas through steam Methane Reforming (SMR). The

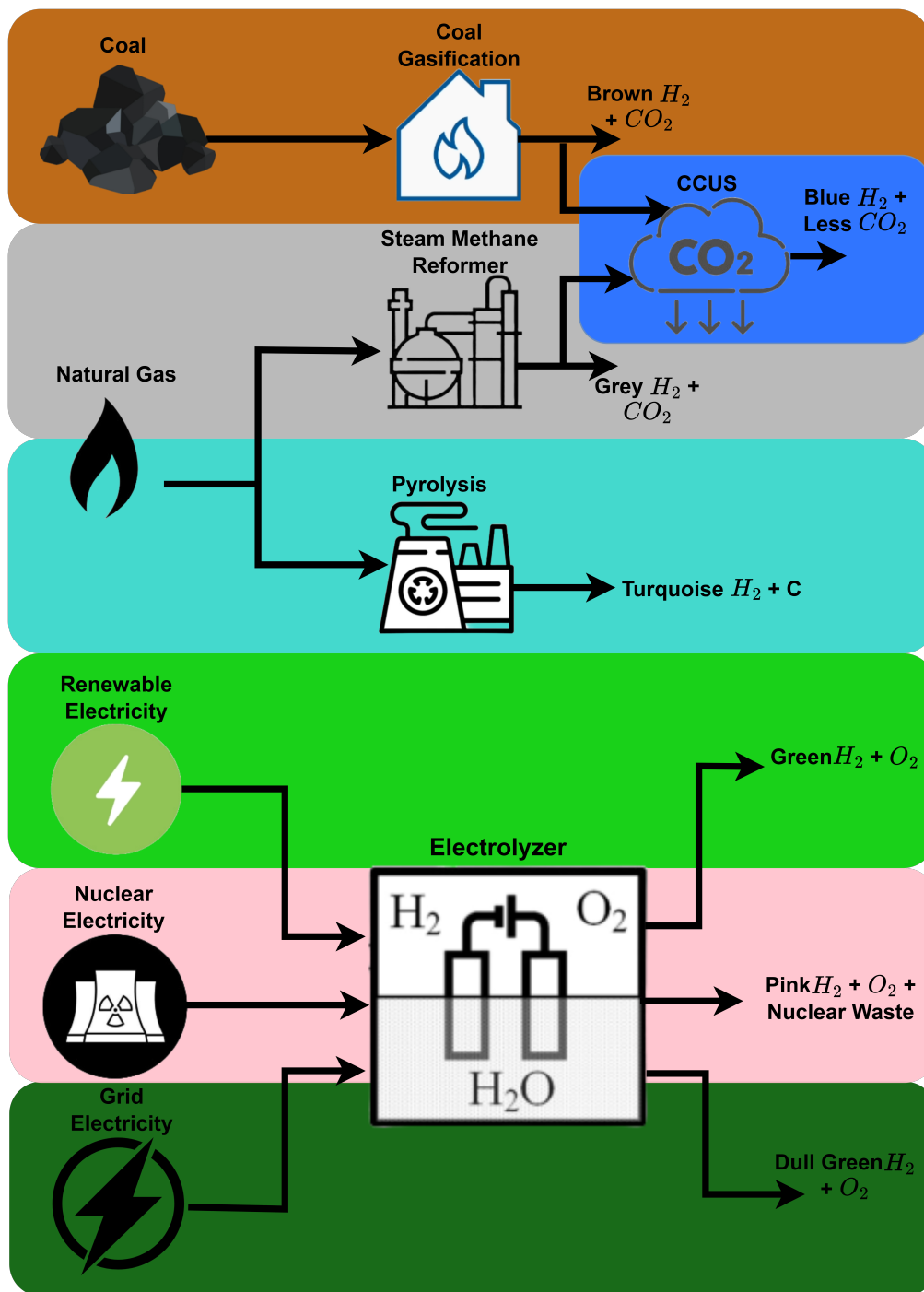


Figure 1.2: Hydrogen Colors

grey hydrogen is usually produced as a by-product of some chemical processes [10], and it represents about 73% of the global hydrogen production [8]. Yet, grey hydrogen is the second technology in terms of the high level of carbon emissions. The level of CO_2 emissions of both brown and grey hydrogen technologies approaches 830 Mt per year [11].

The SMR process starts with natural gas treatment. Then, methane is fragmented within the reformer using steam ($700^\circ C - 1000^\circ C$), resulting in syngas consists of carbon monoxide, CO, and Hydrogen (H_2) as depicted in (1.3).



This syngas is then transformed through the water gas shift reaction, leading to the production of CO_2 and hydrogen H_2 as follows.



Finally, CO_2 is separated, and the hydrogen is purified for storage or usage. The SMR technology has a relatively high efficiency (60% – 85%). Other hydrocarbon reforming technologies such as Auto Thermal Reforming (ATR), and Partial Oxidation (POX) of methane and oil products are also considered within the category of grey hydrogen [9].

Blue hydrogen is the brown or the grey hydrogen production plant but equipped with Carbon Capture, Usage and Storage (CCUS) [11]. The level of carbon capturing is not defined, however, the capture rate is reported to reach up to 90% [11]. Blue hydrogen is an intermediate step towards producing clean hydrogen. Yet, the environmental impact of CCUS technology is still questionable. Authors in [12] show that CCUS doesn't consider and underestimates the upstream emissions of hydrocarbons' production and transportation. Thus, blue hydrogen, in its optimistic view, is limited to halving the emissions of brown and grey hydrogen even when the CCUS is supplied by renewable energy [13]. The use of CCUS with SMR reduces the efficiency of hydrogen production in the range of 5% to 14% [14]. Another challenge is the suitable storage needed for non-utilized CO_2 . In certain situations, particularly when carbon is stored underground, higher initial investments might

be necessary [14]. Additionally, a reliable transportation technique (ex. pipeline) is needed if the blue hydrogen facility is not co-located with the carbon storage.

In the process of generating 1 kilogram of hydrogen from coal and gas with CCUS, approximately 22 kilograms and 8 kilograms of CO_2 , respectively, need to be captured, transported and stored. Therefore, hydrogen production using coal gasification with CCUS requires higher capital investment as compared to using SMR with CCUS. Further, the cost of producing hydrogen from coal with CCUS is more susceptible to variations in CO_2 transport and storage expenses as compared to gas-based production [8].

Turquoise hydrogen is the hydrogen produced from methane pyrolysis, which is an evolving technology for hydrogen production employs high temperature heat to break down methane molecules into their elemental constituents (1.5), generating solid carbon as a by-product [15]. As carbon is sequestered in the solid form, and unlike the blue hydrogen, turquoise hydrogen production does not need to be co-located near CO_2 storage or high capital investment to build a CO_2 pipeline. The produced carbon is solid and takes the form of filamentous carbon or carbon nanotubes [16]. This carbon can be used in further manufacturing processes, stored, or sold at varying prices, ranging from 150 to 1 million EUR per metric ton of carbon depending on its type [17]. The solid carbon is chemically stable and can be utilized as a raw material in many industries such as rubber, plastics, or used in printers.

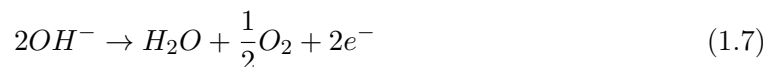


There are two main pyrolysis techniques: thermal and plasma pyrolysis. In thermal pyrolysis, heat derived from natural gas is employed to disassemble methane molecules. However, some of the methane remains unreacted, and hence it is recollected and used as a fuel for the process. This behaviour decreases the conversion efficiency and results in higher CO_2 emissions. In Plasma pyrolysis, a high-temperature plasma is generated by means of an electric arc. Till now, Pyrolysis is not commercialized as a hydrogen production technique [14].

Green hydrogen refers to the hydrogen produced from water using an electrolyzer powered by RES. Green hydrogen technologies offer the lowest carbon intensity alternatives

for hydrogen production. Electrolysis technology employs direct current electricity to split water molecules into hydrogen and oxygen. Approximately 9 liters of freshwater are necessary for each 1 kilogram of hydrogen and 8 kilograms of oxygen generated. The produced hydrogen is of high purity and can be utilized directly in transportation and other applications without the need for additional treatment. The oxygen produced as a by-product can be discharged in air or utilized for medical or industrial purposes [15].

Currently, there are three main electrolyzer technologies named: AE, PEME, and Solid Oxide Electrolyzer Cell (SOEC). AE is the most well-established technology that have been used over a century and accounts for approximately 70% of the market share [18]. AE technology offers the lowest capital cost and relatively long lifespan. However, AE necessitates continuous operation to prevent damage, making it unsuitable for relying solely on the intermittent RES [14]. Further, AE systems face challenges in operating at high current densities and handling corrosive conditions [19]. The chemical reactions at the AE cathode and anode electrodes are given in (1.6) and (1.7) respectively.



PEME relies on the same technology used in the PEM fuel cell. The PEME technology is in operation since the mid of the previous century and it offers higher power density, better efficiency, and faster response compared to AE. Thus, PEME is more suitable for urban areas, and for coupling with RES [19]. Further, PEME can produce hydrogen at high pressure, which may avoid the use of mechanical compressor. Nevertheless, the PEME technology necessitates initial investment costs due to costly electrode catalysts and membrane materials [20]. The PEME's cathodic and anodic reactions are shown in (1.8) and (1.9) respectively.



Table 1.1: Comparison between electrolyzer technologies

Characteristics	AE	PEME	SOEC
Cell temperature (°C)	60–90	50–80	700–900
Load flexibility (% of nominal load)	20–100	0–100	-100/+100
Cold start-up time	1–2 h	5–10 min	hours
Warm start-up time	1–5 min	<10 s	15 min
Nominal system efficiency (LHV)	51–60%	46–60%	76–81%
Specific energy consumption (kWh/Nm ³)	5.0–5.9	5.0–6.5	3.7–3.9
Max. nominal power per stack (MW)	6	2	<0.01
Cell area (m ²)	<3.6	<0.13	<0.06
Investment costs (\$/kW)	950–1750	1650–2500	(>2400)
Maintenance costs (% of investment costs per year)	2–3	3–5	n.a.

The SOEC technology is projected to offer lower capital costs and higher efficiency as compared to other electrolyzer technologies [21]. The operating temperatures of SOEC range from 700 to 1000 °C which is advantageous in terms of electricity conservation due to improved thermodynamic conditions for the reaction, and the possibility of introducing heat into the process [22]. Yet, SOEC suffers from electrode’s delamination, instability, and some safety concerns [21], and is still in the commercializing phase [15] (i.e., SOEC is in technology readiness level (TRL) 7 [23]). The cathodic and anodic chemical reactions of SOEC are shown in (1.10) and (1.11) respectively. Table 1.1 summarizes the main technical differences between the three pre-mentioned electrolyzer technologies [24, 25].



When an electrolyzer system is powered from a nuclear power source the produced hydrogen is named pink hydrogen. Incorporating a hydrogen production plant could potentially alleviate the curtailment of nuclear power plants [26], while presenting an additional avenue

for energy storage, particularly when the need for seasonal storage arises. Pink hydrogen is also considered a low carbon intensity hydrogen. Large reactors could be employed to operate with centralized hydrogen plants, while small reactors would be useful for distributed hydrogen generation. Another advantage, SOEC, which requires high operating temperatures, could utilize the steam generated by the nuclear reactors. This utilization would enhance the efficiency of hydrogen production and make use of the wasted heat in nuclear reactors [15].

When a water electrolyzer is integrated with the electric grid, the level of carbon emissions within the grid would determine the environmental cleanliness of the generated hydrogen. Some research works in the literature have classified hydrogen produced from grid-connected electrolyzers as yellow hydrogen. However, the term yellow hydrogen has also been applied to hydrogen produced through an electrolyzer powered by solar energy. To resolve this ambiguity, this study introduces the term dull green hydrogen to describe hydrogen generated from a grid-connected electrolyzer. It is worthy to note that the carbon intensity of the electric grid is extremely critical, as it can lead to the production of dull green hydrogen with carbon emissions exceeding those of grey or even brown hydrogen.

The work in [8] indicates that when the carbon intensity of the electric grid exceeds 165 kg CO_2 /MWh, the carbon emissions associated with dull green hydrogen potentially exceed the emissions level of grey hydrogen produced through SMR.

There are different hydrogen production techniques that utilize biomass as feedstock. The most mature techniques are the thermochemical ones, such as biomass gasification. In the biomass gasification process, biomass is converted to hydrogen and other products [27]. The increase of biomass reduces the amount of CO_2 in the atmosphere, and hence the net carbon emissions of biomass-based hydrogen production are low. Additionally, coupling biomass gasification with CCUS will not only decrease emissions of hydrogen production, but also reduces carbon emissions of other sectors, due to the carbon negativity of the process. Another biomass-based hydrogen production technology is the microbial biomass, in which microorganisms break down biomass to generate hydrogen. Over the medium to

long term, it is anticipated that microbial biomass will be produced on a commercial scale. Further hydrogen production technologies are in the research and development phases, such as solar thermochemical, photoelectrochemical water splitting, and photobiological [27]. However, most of these hydrogen production techniques are not categorized yet, as it is still uncertain whether these techniques should be classified under green hydrogen [11].

1.1.3 Economy of Hydrogen

Energy transition to hydrogen is controlled by three main aspects: cost of hydrogen production, level of carbon emissions, and the capability of hydrogen to be utilized in different applications. This section compares different hydrogen production technologies in terms of the cost of production and the level of carbon emissions. It also discusses the opportunity of utilizing hydrogen in various applications.

In the foreseeable future, the economic advantage of fossil fuels is expected to persist in most regions. Hydrogen derived from natural gas without CCUS is projected to cost approximately USD 1–2 per kilogram of hydrogen depending on local gas prices. The most substantial component of hydrogen production cost is the fuel prices, except for the case of coal-based hydrogen, as illustrated in Fig. 1.3. Further, the factors which affects fuel cost, such as operating efficiency, will also dominate the cost of hydrogen production [1]. The capital cost of renewable-powered electrolyzers (green hydrogen plants) is higher than that of grid-operated electrolyzers (dull green hydrogen plants), as the renewable-powered electrolyzers run at partial load for long periods.

The production cost is not the only factor that determines the opportunity of certain hydrogen production technologies. The level of carbon emissions is also a key factor in this regard. As depicted in Fig. 1.4, the carbon footprint of grey hydrogen (produced from natural gas), is approximately half that of brown hydrogen (produced from coal) [1]. The use of CCUS significantly reduces the level of carbon emissions. Yet, the green hydrogen technology is superior with zero carbon emissions. As discussed before the dull green hydrogen could results in carbon emissions more than those of grey and brown hydrogen

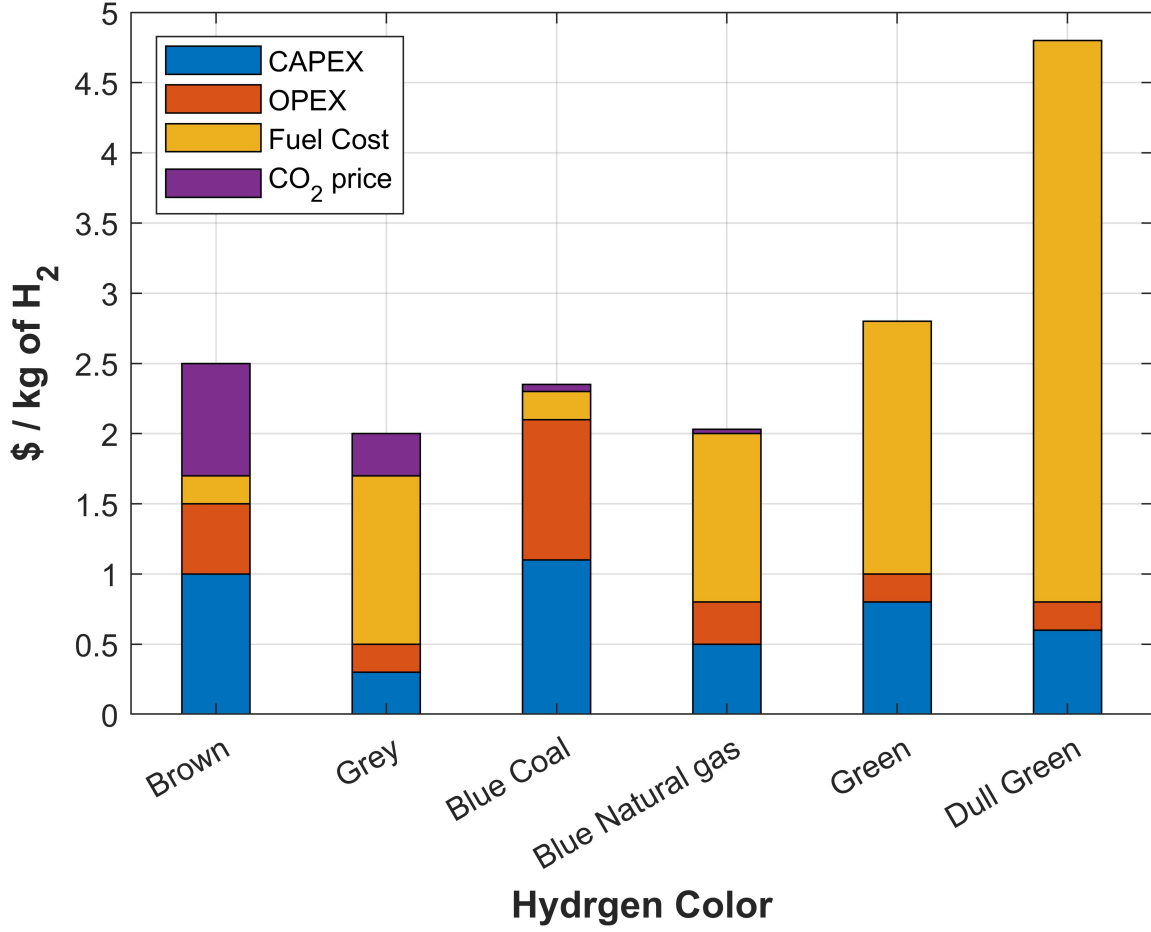


Figure 1.3: Price of different hydrogen colors.

based on the carbon intensity of the electric grid. Fig. 1.4 considers the current global average grid carbon intensity which resulted in carbon emissions level exceeding the level of the grey hydrogen.

Although hydrogen can be theoretically utilized in many applications as discussed in section 1.1.1, hydrogen couldn't be economically used for everything. Clean hydrogen has to find its economical pathway among different applications. For each application, we may find hydrogen alternatives that are cheaper, simpler, safer or more convenient. Therefore, hydrogen ladder [28] given in Fig. 1.5 classifies hydrogen applications from A

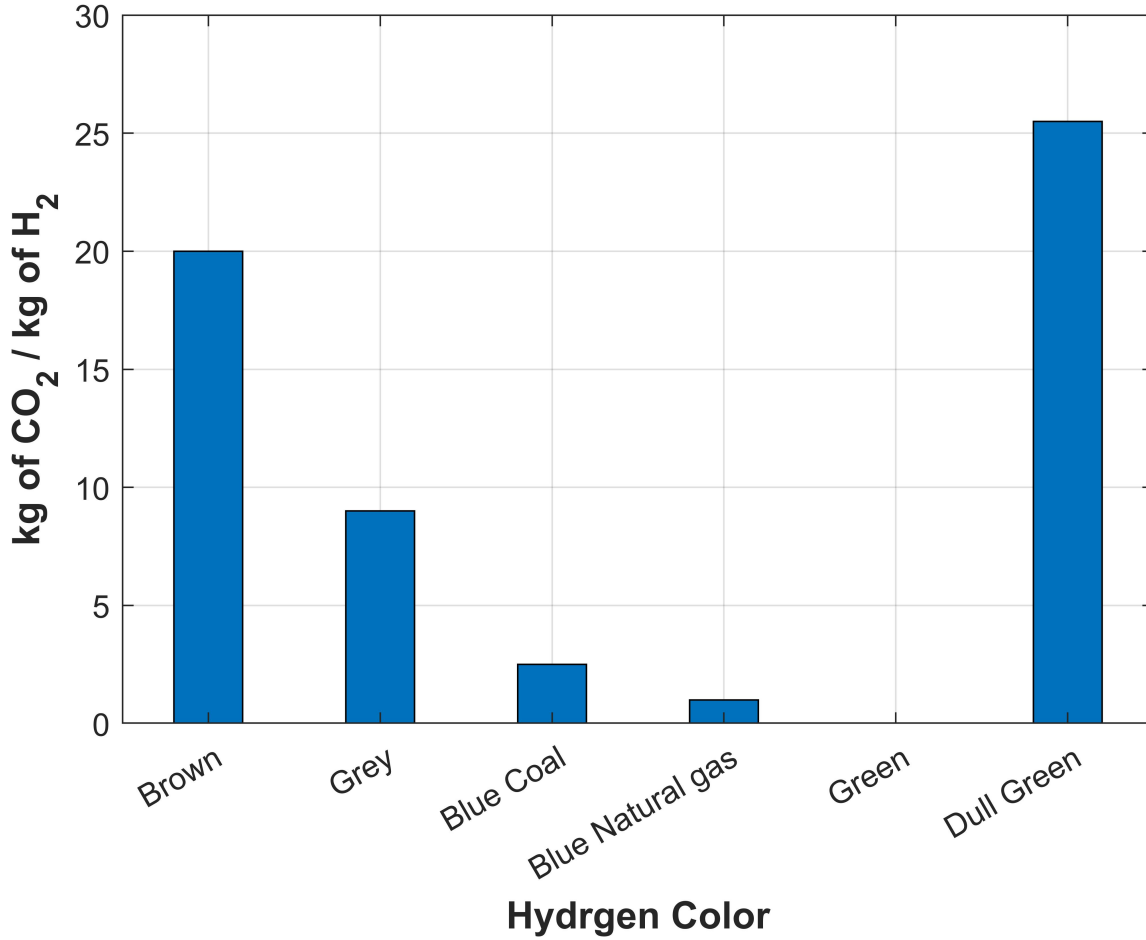


Figure 1.4: Carbon emissions of different hydrogen production technologies

to G, where class A presents the most unavoidable applications in which hydrogen has the highest potential compared to other alternatives. Class G contains the applications for which hydrogen is not an economical competitor.

Classes A and B mainly consider the current hydrogen applications for which there are almost no alternatives, thus these applications can't avoid hydrogen utilization. Most of these applications are chemicals and industrial processes. Hydrogen also has significant potential in some transportation sectors, especially shipping and long-haul aviation. However, light aviation, metro and rural trains are not that suitable as hydrogen applications and

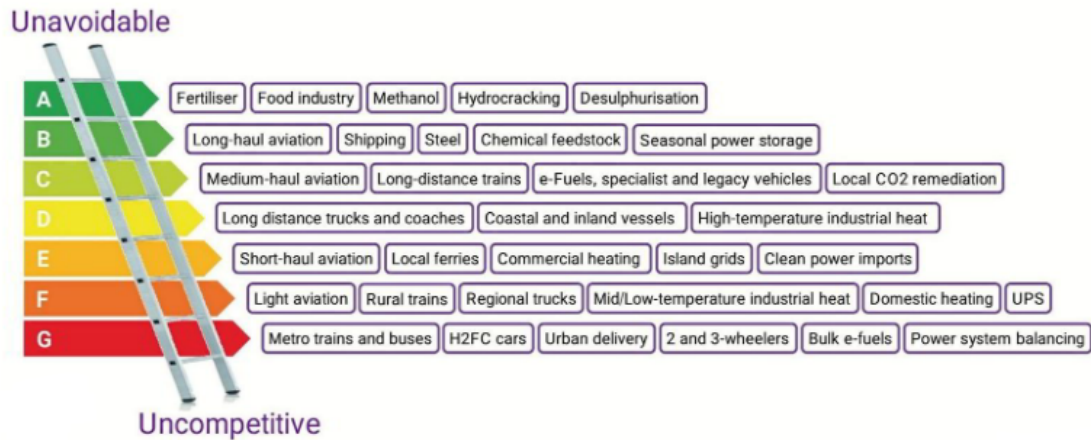


Figure 1.5: Ladder of hydrogen utilization. Reprinted from M. Liebreich. The clean hydrogen ladder [now updated to v4.1]. [Online]. Available: <https://www.linkedin.com/pulse/clean-hydrogen-ladder-v40-michael-liebreich/>

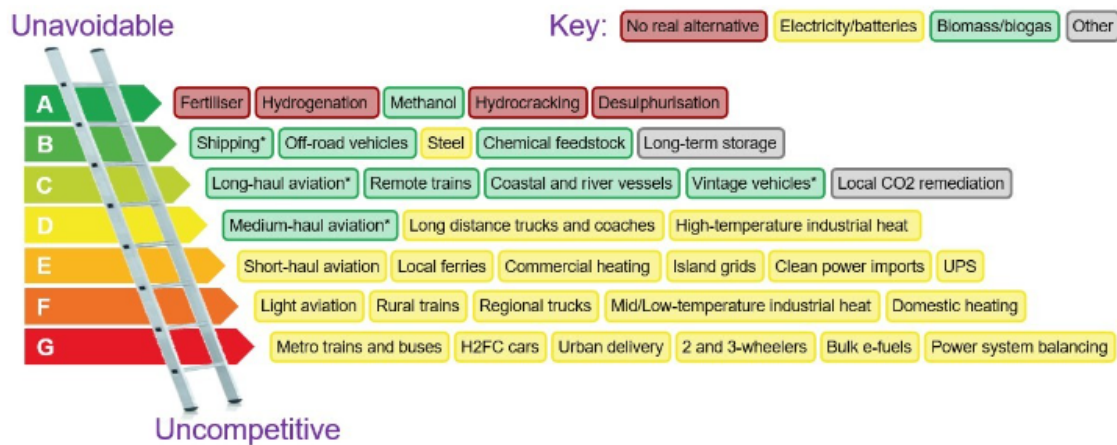


Figure 1.6: Ladder of hydrogen utilization with the opportunity of other alternatives. Reprinted from M. Liebreich. The clean hydrogen ladder [now updated to v4.1]. [Online]. Available: <https://www.linkedin.com/pulse/clean-hydrogen-ladder-v40-michael-liebreich/>

comes in classes F and G where other alternatives such as renewable electricity or electric batteries would be more appropriate.

Power systems applications are distributed among classes, seasonal storage is considered among applications with the highest hydrogen potential, but short term storage and power

balancing applications comes in class F and G as batteries would be a superior alternative. Yet, hydrogen has a good potential for stand alone or island grids.

Heating seems to be a perfect application for hydrogen, in which hydrogen will just replace natural gas using almost the same infrastructure. Nevertheless, electric heat pumps driven by RES are much more efficient, and hence most of the heating applications come in the middle classes.

Alternatives that compete hydrogen vary from a specific application to another. Fig. 1.6 shows the hydrogen's ladder comprising potential alternatives for each application. Most of class A applications doesn't have a real alternative. Classes B and C are mainly competed by biomass fuels, while electric battery is the main alternative for other classes from D to G.

1.2 Dissertation Objectives

This dissertation aims to facilitate the integration of EHPP into power grids and enhance their performance to reduce hydrogen production costs while improving the resilience of the power grid. The EHPP configuration can highly impact its operation, hence the hydrogen production cost and participation in power grid resiliency. Further, the electrolyzer itself is a complex device whose performance varies widely according to its technology, internal design, and operating conditions. As such, the consideration of EHPP configuration, electrolyzer technology, electrolyzer internal design, and electrolyzer operating conditions in both sizing and scheduling problems of such hydrogen plants is a must. Based on the previous discussion, this dissertation has the following objectives:

- O1) Development of a comprehensive EHPP model and detailed electrochemical models for the two commercialized electrolyzer technologies (i.e., AE, PEME).
- O2) Development of a novel formulation, incorporating the detailed electrochemical electrolyzer models, to optimize the grid-connected EHPP configuration (i.e., with and

without BESS), operation (i.e., hourly power consumption and hydrogen production flow) and design (i.e., ratings of the EHPP equipment including Power Converter, electrolyzer, compressor, local HS, and optional BESS) as well as the electrolyzer internal parameters (cell area, membrane thickness, cathodic pressure), aiming at minimizing the LCOH.

- O3) Development of an optimization formulation to minimize the cost of hydrogen production and enhance PEME-HPP integration with RESs by extending the PEME safe operating range and improving its efficiency at low loading conditions. Such formulation shall optimize the number of PEME modules (stacks) along with the ratings of the EHPP equipment (Power Converter, PEME, and Compressor) and the electrolyzer internal parameters (cell area, membrane thickness, cathodic pressure).
- O4) Development of a comprehensive framework for optimizing EHPP design and operation for the provision of grid ancillary services (CA, OR, RS) under different electricity pricing schemes (variable hourly pricing, fixed pricing, and fixed pricing through a Power Purchase Agreement (PPA)) while supplying hydrogen to various applications (sectors). The framework would determine the suitable electrolyzer technology (i.e., AE and PEME) for the provision of each ancillary service while supplying hydrogen to various applications that consume hydrogen at different pressures.
- O5) Development of a novel scheduling formulation and coordinated dynamic controller to hourly optimize and control PEME cathodic pressure and operating temperature, aiming at enhancing PEME efficiency at all loading levels and hence minimizing hydrogen production costs.

1.3 Dissertation Outline

The remainder of this thesis is organized into the following chapters:

- **Chapter 1** provides a background of hydrogen applications, production technologies,

and its economic opportunities for energy transition. It also provides dissertation objectives and chapter outlines.

- **Chapter 2** reviews the existing research work on configuration, modeling, design, scheduling, and control of EHPPs and summarizes the current research gaps.
- **Chapter 3** presents a detailed mathematical modeling of the EHPP components, including the steady-state and dynamic models of various electrolyzers, the FC, compressor, HS, and the BESS. These models form the basis for the optimization formulations and analyses conducted in the subsequent chapters.
- **Chapter 4** presents a detailed electrochemical model of a PEME-HPP and introduces a novel mathematical formulation aimed at minimizing the LCOH. This is achieved by optimizing both the design and operation of the PEME-HPP, with an optional BESS, while also incorporating the optimization of internal electrolysis parameters.
- **Chapter 5** introduces a modular configuration for PEME-HPP in which the PEME is divided into multiple SCM to extend the safe operating range and enhance the efficiency at low loading levels of the EHPP. It develops a formulation aimed at minimizing the LCOH for a PEME-HPP powered by RES, through the joint optimization of the number of SCM, the internal parameters of the PEME, and the equipment ratings of the EHPP.
- **Chapter 6** starts by the models developed in chapter 4 and then converts it into a comprehensive framework that determines the electrolysis technology suitability and proper internal design for the provision of multiple ancillary grid services while supplying the produced hydrogen to a range of applications requiring different levels of hydrogen pressure. Additionally, the developed framework considers different electricity pricing schemes and their impact on the suitability of the determined electrolysis technology and internal design.
- **Chapter 7** presents an optimal sizing and scheduling formulation for a PEME-HPP. This formulation simultaneously optimizes the PEME loading, cathodic pressure, and

operating temperature on an hourly basis, with the goal of enhancing the PEME efficiency and minimizing the LCOH. Additionally, a coordinated control strategy is developed to effectively manage the simultaneous variations in these operating parameters without exceeding the safe operational limits of the PEME.

- **Chapter 8** summarizes the conclusion of this dissertation, identifies the contributions, and draws directions for possible future work.

Chapter 2

Literature Review

Several megawatt-scale green hydrogen projects have recently been deployed or announced for commissioning worldwide [29–31]. With ongoing advancements in electrolysis technologies, particularly in terms of size and stackability, EHPPs are expected to scale up rapidly to gigawatt-scale facilities capable of producing tons of hydrogen per day [32]. However, EHPPs are still considered complex and high-cost systems. Therefore, their large-scale deployment and integration into electricity systems require the development of advanced modeling tools for techno-economic analysis, optimal operation, and optimal design [33,34]. Driven by the goal of reducing the LCOH, several studies—such as those in [35–37]—have proposed techno-economic frameworks to optimize the sizing and operation of EHPPs. This chapter presents a comprehensive literature review on the planning, modeling, scheduling, and control of EHPPs, and highlights the current research gaps in the field.

2.1 Configuration of EHPP

The typical EHPP, shown in Fig. 2.1, consists of four main components: power converter, electrolyzer, mechanical compressor, and hydrogen storage. Power converters are controlled rectifiers that produce DC current to supply the electrolyzer. Usually these power rectifiers

are equipped with current controllers, which in turn control the flow of produced hydrogen. The electrolyzer is responsible for splitting water into oxygen and hydrogen. As this study focuses on applications of hydrogen generated from EHPP, we always assume that oxygen is released in air and no storage or compression is considered for the oxygen produced. Hydrogen is usually produced at a pressure lower than the one required for storage or other applications. Therefore, a mechanical compressor is needed to increase the pressure of the produced hydrogen. A local hydrogen storage unit is mandatory in hydrogen plants especially when these plants are not connected to a hydrogen pipeline system. This basic configuration has been introduced in many studies as in [38–41]. Yet, EHPP is not limited to these components, it can be also equipped with a Fuel Cell and/or BESS to reduce the LCOH by providing grid ancillary services, increasing the plant capacity factor, and avoiding high electricity tariffs. The work in [42, 43] incorporates the EHPP with a fuel cell to allow utilization of the energy stored in the form of hydrogen to support an islanded electric-hydrogen system. In [44], authors proposed employing a fuel cell and BESS in a hydrogen-based microgrid operated by RES. Similarly, authors of [45] introduce an energy integrating model in the forms of hydrogen and electricity. The integrated system considers utilizing a fuel cell with the EHPP and employing an off-site BESS. The work in [46] optimally designs a regional multi-energy system considering different penetration levels of RES. The multi energy system includes RES, EHPP with fuel cells, electric boilers, and BESS. The EHPP may also contain multiple auxiliary systems such as a heat ex-changer, gas separator, and gas dryer [47]. However, these auxiliaries do not significantly affect the behavior or cost of the whole plant.

2.2 EHPP Coupling with The Electrical System

2.2.1 EHPP Coupling Modes

Integrating EHPP with electrical systems primarily involves four distinct coupling modes. In the first mode, hydrogen is produced from RES at the source side and then it is utilized

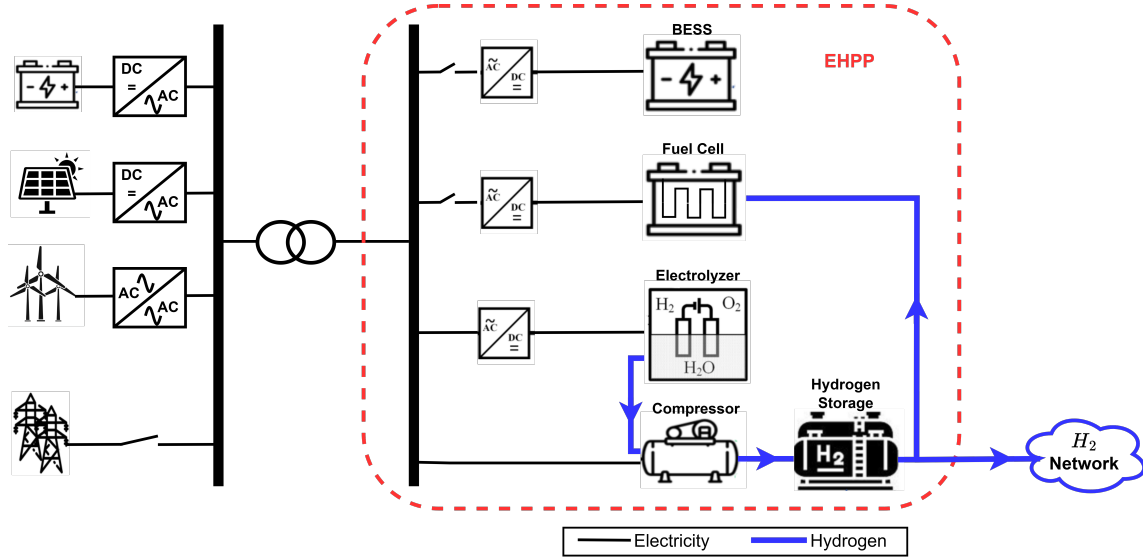


Figure 2.1: Typical electrolyzer hydrogen production plant

locally serving purposes such as supplying chemical plants or powering fuel cell vehicles. As there is no need to transport electricity or hydrogen over a long distance, this mode has one of the lowest energy losses and LCOH. However, the success of this approach hinges heavily on the local demand for hydrogen. In cases where demand falls short, surplus hydrogen will be transported to other regions. Thus, in regions with abundant renewable energy, hydrogen-based industries should be planned [48]. In the second mode, hydrogen is produced from RES at the source side and then conveyed over long distances through pipelines to the area where it is needed. This mode allows producing hydrogen away from the demand centers without stressing the power grid to transmit the renewable power over long distances. Another advantage of this mode is that hydrogen exhibits greater resilience to fluctuations as it does not require instantaneous balance between its supply and demand. Furthermore, hydrogen pipelines can also function as a form of storage. Yet, this coupling mode suffers from the high cost of establishing new hydrogen pipelines with a substantial cost estimated at approximately one million dollars per kilometer [48]. A more cost-effective alternative approach is to blend hydrogen with natural gas in existing pipelines, but the

blending is limited to a maximum of 15% hydrogen [49]. Multiple studies addressed these two modes of coupling at the RES source side. The works in [38, 39, 50] address the direct coupling of EHPPs with the RES and compare different combinations of RES. Efforts presented in [39, 50] optimize the design of EHPP aiming at maximizing the plant capacity factor and minimizing the cost of hydrogen production. In [51], authors propose a wind-hydrogen storage system to address the wind power curtailment and transmit the produced hydrogen to the market. In [52], authors introduce an economic feasibility analysis to evaluate different scenarios for establishing hydrogen pipelines system. The study showed that modifying the existing natural gas pipelines to hydrogen pipelines provides a lower cost solution, however, it raises significant safety issues.

The third mode considers coupling the EHPP at the load side and providing hydrogen locally. The RES are installed in areas rich with renewable energy and then transferred through electrical transmission lines to the EHPPs located near hydrogen demand centers. This coupling at the load side allows to flexibly place the EHPP near hydrogen demand centers without being restricted by the locations of the RES usually placed away from cities. Further, it avoids the safety issues of transporting hydrogen over long distances. The works in [53] showed that the cost per unit of power transmission is approximately one-fifth to one-fourth of the cost for transporting hydrogen. Consequently, energy transfer through electrical transmission lines is more economically efficient compared to utilizing hydrogen pipelines. Yet, the relatively smaller initial capital investment in power transmission lines doesn't necessarily result in a lower total cost for energy transmission. This is because of the significant fluctuations in RES, which necessitate combining them with other power resources to create a more stable and consistent power supply [48]. Therefore, the fourth mode considers coupling EHPP near the load side and then transports the hydrogen through pipelines to the demand center. This mode could have more potential as an intermediate stage that utilizes a combination of the existing power network and natural gas pipeline system till establishing the required hydrogen infrastructure. Further, it introduces a balance between minimizing the capital cost needed to transfer the energy and providing a pipeline system that increases the flexibility of balancing hydrogen supply and demand and

acts as a hydrogen storage system. The studies in [54, 55] optimize the design of EHPP coupled at the load side in addition to minimizing the investment, operational, and grid costs. The work in [56–58] addressed the economic feasibility of producing green hydrogen from EHPP to meet the regional hydrogen demand and make use of RES curtailment in conventional and distributed power networks. In [59], authors have introduced the concept of using dynamic pricing for hydrogen generated from an EHPP that is coupled at the load side to meet the local hydrogen demand. The research conducted in [60, 61] explored the fourth mode of coupling the EHPPs and proposed optimizing the coordination between the electrical grid and the hydrogen pipeline system. The findings revealed that this coordination could potentially enhance the RES generation by 13-56% and reduce the total cost by 7–16%.

The configuration and ownership of EHPP can undergo significant changes depending on the coupling mode. In cases of source side coupling, where EHPP is co-located alongside RES, there’s a greater likelihood that private investors would own the RES as well as the hydrogen plant. This joint ownership aims to reduce electricity costs. Additionally, within EHPP configuration, there’s consideration for incorporating BESS or fuel cells to address the intermittent nature of RES. Conversely, with load side coupling, it primarily depends on utility-scale RES, typically owned by other investors or the utility. Furthermore, since load side coupling may be at a considerable distance from the RES, there is a higher probability of receiving a relatively smooth power profile, reducing the necessity for employing BESS [48].

2.2.2 Electrolyzer Power Converters

There are multiple configurations for electrolyzer power converters. However, a common thing between these different configurations is the rectifier stage. This section provides a brief overview of the common configurations presented in the literature.

Single Stage – Uncontrolled Rectifier: The uncontrolled rectifier is the simplest converter that can drive an electrolyzer. There are different diode-based topologies for uncontrolled rectifiers. Yet, these topologies can not even control the current supplied to

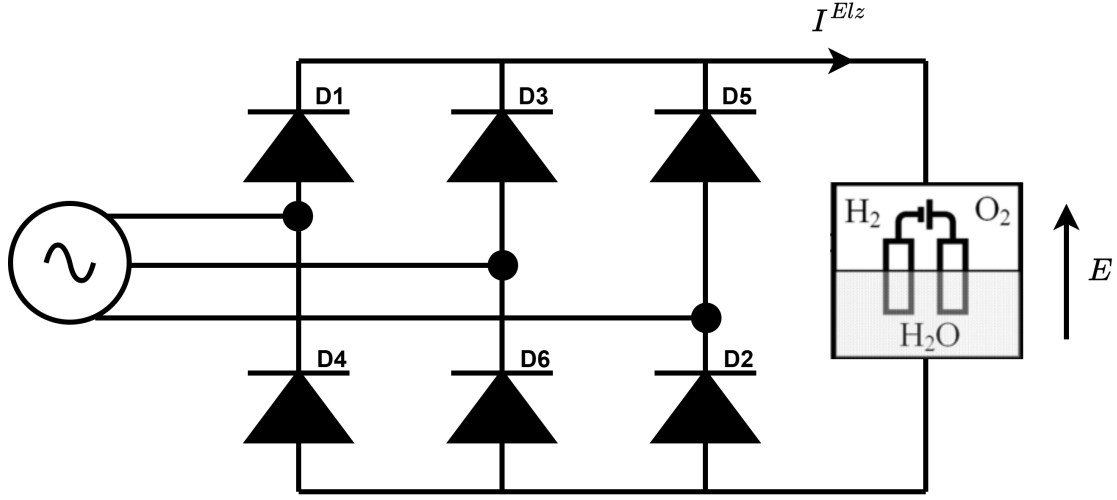


Figure 2.2: Schematic diagram of a six-diode uncontrolled rectifier

the electrolyzer. Hence, such converters are limited to running the electrolyzer at constant voltage and current, making them unsuitable for coupling with RES or providing ancillary services to the electrical grid. Uncontrolled rectifiers have low cost, relatively high efficiency, and can guarantee good power quality for the AC power supply [62]. Fig. 2.2 shows the basic configuration of an uncontrolled rectifier that consists of six diodes.

Single Stage – Controlled Rectifier: Unlike uncontrolled rectifiers, which are diode-based, controlled rectifiers are thyristor-based converters. The use of thyristors allows controlling the electrolyzer voltage or current, which in turn controls the output hydrogen flow. This also allows the coupling with RES where the controlled rectifier can manage electrolyzer loading and operating efficiency. The firing angle control increases current harmonics and reduces the power factor [63], making it challenging to improve the power quality of thyristor-based converters. Further, thyristor-based rectifiers suffer from high current ripples that have a ripple factor ranging from 14% and 71%. These ripples reduce the converter's efficiency and even the quality of produced hydrogen [64]. One of the common techniques used to handle such ripples is the use of passive filters between the converter and the electrolyzer unit [65]. Fig. 2.3 shows a basic configuration for a thyristor-

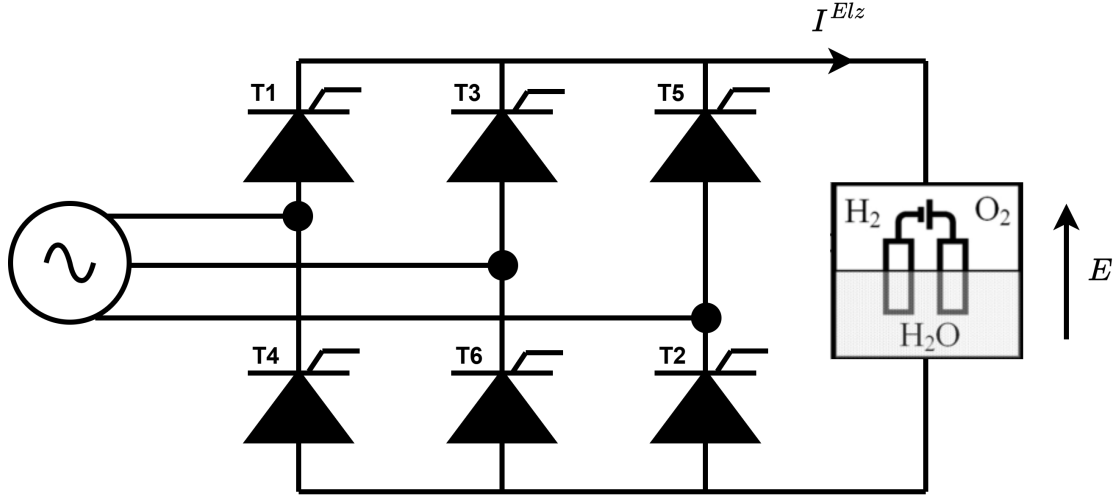


Figure 2.3: Schematic diagram of a six thyristors controlled rectifier

based controlled rectifier. Changing the firing angle of the converter's thyristors controls the electrolyzer voltage as expressed below:

$$E = \frac{3\sqrt{3}V_{max}}{\pi} \cos\alpha \quad (2.1)$$

Two Stages (Rectifier + Buck Converter): The two-stage AC/DC converters combine an uncontrolled rectifier with a high-frequency chopper. Such a combination allows for improving the power factor without needing bulky passive filters, which might reduce the converter's cost. Fig. 2.4 shows a typical two-stage rectifier in which a 6-diode uncontrolled rectifier provides fixed DC for the second stage, a three-phase interleaved buck converter. The second stage is responsible for electrolyzer current control, which, in turn, controls the hydrogen production flow rate. The switching frequency of these converters is much higher than the line frequency, and hence they offer faster dynamics and require smaller reactive elements. The decision to use three phases represents a trade-off between minimizing output current ripple, reducing volume, improving energy efficiency, and ensuring reliability in the event of power switch failures. The output voltage of the DC step-down stage can be

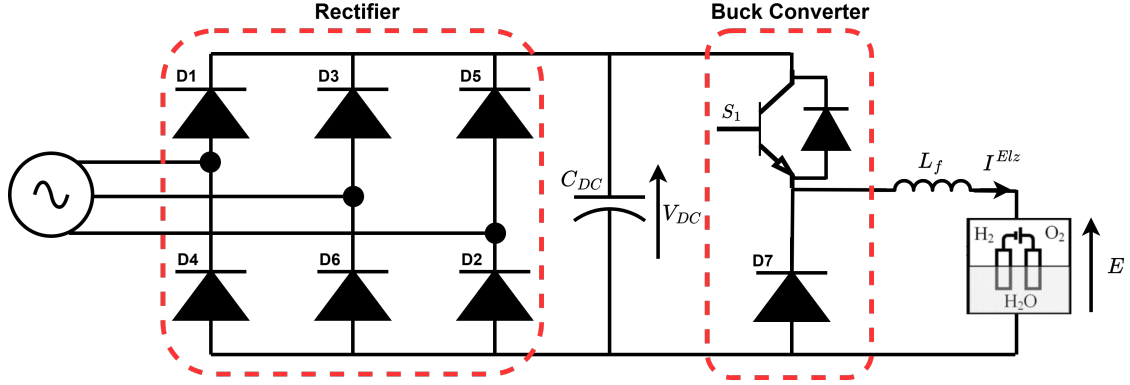


Figure 2.4: Schematic diagram of a six-diode uncontrolled rectifier

expressed as follows:

$$E = DV_{DC}. \quad (2.2)$$

The output current ripples are also a function of duty cycles as given hereunder:

$$\Delta I^{Elz} = \frac{ED(1-3D)}{L_{fs}}, \quad 0 < D < \frac{1}{3}, \quad (2.3)$$

$$\Delta I^{Elz} = \frac{E(3D-1)(2-3D)}{3L_{fs}}, \quad \frac{1}{3} < D < \frac{2}{3}, \quad (2.4)$$

$$\text{and } \Delta I^{Elz} = \frac{ED(3D-2)}{L_{fs}}, \quad \frac{2}{3} < D < 1. \quad (2.5)$$

For specific duty cycles (1/3 and 2/3) the output current ripple can be eliminated. Such a 2-stage converter is suitable for high-power applications due to the distribution of the input current among the phases [66]. It's important to note that the higher the duty cycle, the lower is the energy efficiency.

2.3 Electrolyzer Modeling

Electrolyzer modeling approaches can be categorized into four distinct types: linear, empirical, semi-empirical, and multiphysics models, as shown in Fig. 2.5. These modeling

approaches can be applied to both AE and PEME. In linear models, the electrical portion of the AE is represented as a constant voltage source with series resistance, while a fixed conversion factor in kg/kW is employed to estimate the produced hydrogen. Such linear models can not properly describe the electrolyzer characteristics, and hence their application is limited to rough estimation and preliminary studies [67]. Therefore, empirical models are introduced to more precisely depict the AE characteristics. These empirical models are estimated based on fitting experimental measurements without utilizing any theoretical models. Empirical models can reveal the electrochemical reactions and other AE characteristics. However, the empirical model doesn't provide any physical meaning or define the real parameters of the AE [68]. To address these issues, semi-empirical models are developed to combine theoretical modeling with experimental data. A theoretical model is developed based on thermodynamics, heat transfer, and electrochemical fundamentals. Then, the key parameters within the theoretical model are determined using experimental data. The semi-empirical models are the most commonly used models for both static and dynamic studies. The static models are particularly effective at simulating AE performance, including electrical characteristics, hydrogen production model, efficiency, and hydrogen purity under different temperature and pressure conditions [69–71]. Authors in [72] present a semi-empirical dynamic model for the electrical part of an AE cell. The developed model is validated by comparing the dynamic time response of the developed model with a lab experimental setup. The work in [73] develops a semi-empirical static and dynamic model for a commercial lab scale AE and evaluates its performance with wind and solar power profiles, showing that the developed model is very close to the experimental results. However, these dynamic models are limited to only one specific aspect of AE dynamics (i.e., electrical aspect). In contrast, other studies, such as [74, 75], provide more comprehensive dynamic models of AE, encompassing dynamics of voltage, current, temperature, hydrogen purity, liquid level, pressure, and other parameters during the startup and variation in current or power reference values. Yet, semi-empirical models can't be easily adapted to other AE. To address these challenges, multi-physics models are introduced, taking into account the variations in all structural and operational parameters of the elec-

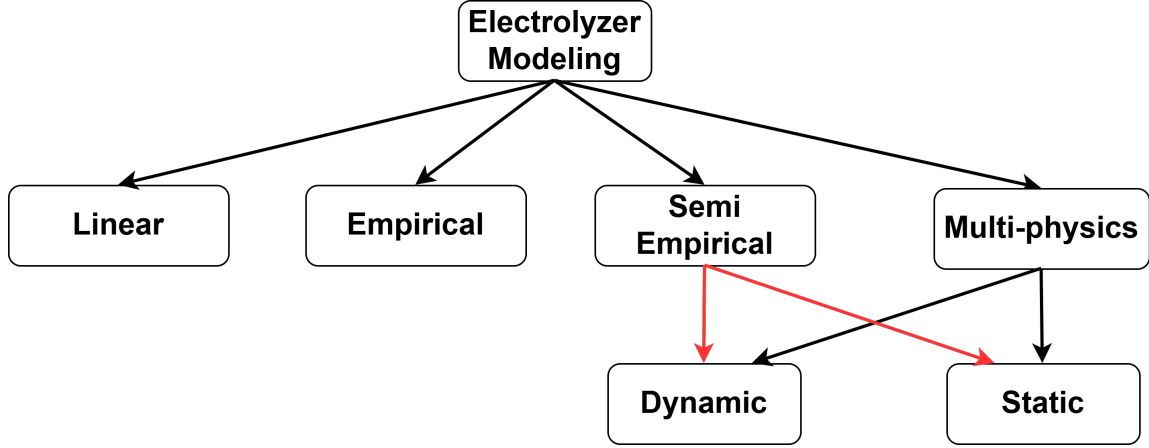


Figure 2.5: Electrolyzer modeling types

trolyzer [76]. Few studies propose other multi-physics AE models to universally describe the AE characteristics [77, 78].

In the literature, some studies have classified PEME models into thermal, electrochemical, and mass transfer models as in [79, 80]. However, this classification is challenging to apply because most studies necessitate a comprehensive model that integrates multiple aspects. Therefore, a classification approach similar to that of AE is introduced as in [81]. Similar to AE, linear models of PEME only assume linear electrical characteristics and/or define a fixed conversion rate in kg/kW as in [82]. Also, the PEME empirical models are derived directly from experimental data to capture the static characteristics of PEME [83, 84]. Additionally, the static and dynamic PEME models can be distinguished when a semi-empirical or multi-physics approach is employed. In terms of the PEME static modeling, the theoretical model is still being developed based on theories of thermodynamics, heat transfer, and electrochemistry. Yet, the PEME studies differ from AE ones in analyzing the impact of operating and structural parameters, with a greater focus on the effect of various temperatures on the exchange current and charge transfer coefficients [85, 86]. The work in [87] introduces a PEME steady-state model that considers its safety constraints. However, it employs an empirical Faraday’s efficiency formula, which limits the model’s

comprehensiveness.

In terms of the PEME dynamic modeling, there are two scales of modeling named stack and plant scales. The works in [88, 89] introduce an empirical dynamic model for the electrical part as well as a formula for its efficiency. Similarly, the models in [90, 91] evaluate the dynamic performance of various PEME parameters, including electrolyzer voltage, current, energy efficiency, energy consumption, and temperature. While the studies in [90, 91] focus on the electrical and thermal aspects of PEME dynamics, the work in [92] specifically addresses the coupled dynamics between mass transfer and thermal domains. Yet, the previously mentioned models are linear time invariant, which may not accurately model the complex PEME dynamics, especially at different input currents. To address this issue, the work in [93] proposes an adaptive dynamic model that allows the model's parameters to be independently adjusted under varying input current conditions. In [94], a dynamic model of a PEME-HPP, comprising a PEME and a hydrogen storage tank, is developed using Simulink to evaluate the overall efficiency of the plant.

2.4 Design of EHPP

Improving the design of EHPP is covered at multiple levels in the literature. The main objective behind such improvements is to enhance the efficiency of hydrogen production and minimize the LCOH. As the electrolyzer is the core and most expensive component in the EHPP, there are numerous efforts reported in literature that focus on improving different electrolyzer technologies. The authors in [95] introduced a zero electrode gap design for AE in which the gap between the electrode and diaphragm is reduced to zero compared to the 2 mm gap used in the conventional design. The zero gap design reduces the ohmic resistance by 30% and hence increases the AE efficiency, especially at high current density. In [96], the authors presented a novel design for the flow-plate used in zero gap AE to avoid machining cost. The novel design resulted in achieving 84% efficiency with the electrolyzer cost around 140 \$/kW. Similarly, many studies addressed enhancing the design of PEME. Authors of [97] reported integrated electrode architectures consisting of plat-

inum nano wires on ultra-thin titanium gas diffusion layers. The integrated design reduced the cell voltage, thereby enhancing efficiency. Additionally, the work in [98] developed ionomer-free integrated electrodes using molybdenum sulfide nano sheets, demonstrating outstanding performance with an extremely low overpotential. In terms of cost reduction, the work in [99] reported noble metal-free graphene-encapsulated Nickel-Molybdenum alloy that provided highly stable electrochemical performance in a single cell PEME. Further studies on the design of AE and PEME are reviewed in [100], showing performance enhancement. However, the studies in [95–99] focus on improving the electrolysis technology without considering its integration with other equipment in the EHPP. Furthermore, the findings of such lab-scale studies have yet to be verified for real-world applications at the MW-scale and GW-scale EHPP.

Authors of [101] optimize the AE’s temperature and diaphragm thickness to increase the electrolyzer efficiency, showing that a diaphragm of 0.1 mm at a temperature of 100°C significantly enhances the electrolyzer efficiency. However, such a configuration increases the hydrogen crossover, and hence requires limiting the pressure lower than 8 bar. The work in [102] proposes a machine learning-based algorithm to optimize the designs of both small-scale and commercial-scale PEME. The algorithm estimates the following design parameters: anode type, cathode type, membrane type, cathode catalyst, anode catalyst, anolyte, catholyte, power, water flow rate, cell temperature, and number of cells, to maximize the hydrogen production. Yet, the work in [101, 102] doesn’t consider the effect of varying the operating point on the electrolyzer efficiency. The study in [103] enhances PEME’s efficiency over the entire current density range by optimizing its cathodic pressure. The work in [104] shows that optimizing the PEME’s cathodic pressure and temperature over the entire current density range yields a significant improvement of the overall system efficiency. However, the work in [103, 104] does not discuss the dynamics of varying the cathodic pressure and temperature. These dynamics are quite slow, and hence the fast response time of the PEME could be wiped out, and thus, the integration with RES will be negatively impacted.

Yet, these efforts in [101–104] optimize the electrolyzer’s internal parameters without

considering the specific operating conditions and limitations imposed on the EHPP when it is connected to the source of electricity. There are several considerations, such as the RES generation profile, electricity tariff, electrical grid constraints, and hydrogen demand, that might affect the operating range of the electrolyzer. This could, in turn, lead to a violation of the electrolyzer safety constraints at low current densities, and/or (ii) operating the plant at relatively low efficiency [105]. Further, none of these studies provides the economic analysis or the techno-economic planning tools needed for the mass deployment of EHPP.

Authors in [38] aim to obtain the optimal combination of solar and wind power that minimizes the non-utilized RES power supplied to an AE in a standalone EHPP. The work in [39] compares the solar and wind power solutions to supply a standalone MW-scale EHPP. The proposed formulation obtains the optimal size of the AE that achieves the minimum LCOH and the maximum hydrogen production. However, the work in [38, 39] doesn't address the sizing of other components in the EHPP. Authors in [40] plan and study the capacity of the battery storage required for realizing hydrogen production from a 20 MW AE-HPP operated by RES in an islanded medium voltage DC network. Reference [106] proposes a 2-layer optimization for the planning and operation of an EHPP driven by wind power. The proposed configuration assumes that the wind plant is a part of the EHPP and aims to maximize the net profit value. The proposed formulation yields the optimal sizes of the wind plant, AE, mechanical compressor, power converter, and hydrogen storage capacity. Yet, [38–40, 106] utilize simplified AE models and don't consider the effect of the variations in AE efficiency with different loading levels.

For PEME based EHPP, the authors in [41] introduce an evolutionary algorithm to optimize the size of a PEME interconnected with an onsite wind turbine to supply hydrogen refueling stations, considering real refueling behavior data. Reference [107] applies a novel hybrid optimization algorithm to increase the sizing accuracy of an isolated solar-wind EHPP using weather forecasting data. In [108], the authors optimize the PEME size for a PV-powered EHPP in various regions of Turkey to assess its economic viability and project the future LCOH. In [109], the authors simultaneously optimize the size and operation of a solar-hydropower-wind EHPP, considering the safe loading range constraints for the PEME.

Yet, the efforts in [38–41, 106–109] don’t consider the effect of the electrical grid operational constraints or the advantages of providing ancillary services to the power grid. In [82], a centralized EHPP with liquid organic hydrogen carrier is optimally sized to supply the transportation sector and provide ancillary services to the power grid, where solar and wind power resources are connected to different locations in the grid. In [110], authors optimally allocate RES, BESS, pumped hydro-power storage, and hydrogen storage systems (PEME, hydrogen tank, and fuel cell). The authors show that the most economical solution for capacity expansion of the studied power grid requires deploying hydrogen storage systems in all considered case studies. However, the works in [82, 110] use simplified models of the PEME and assume a constant conversion rate of kg/kWh of hydrogen under all operating conditions and don’t consider the impacts of the hydrogen downstream system on the integration with the gas and heating networks.

The study in [111] proposes multistage co-planning of a distribution network with high RES penetration and the hydrogen energy system. The co-planning reduced the total planning cost and enhanced the utilization of RES. In [112], the power system and the PEME based hydrogen supply chain are co-planned to minimize the investment and operation costs of both the power system and the hydrogen supply chain and to mitigate the seasonal limitation of RES power generation. In [113], the authors optimize the size of a PV-PEME system to produce hydrogen for a textile industry facility, where the hydrogen is combined with natural gas and used in the heat supply section. Another co-planning study is provided in [55], where the electric system is co-planned with the heating system to obtain the optimal capacities of the RES, AE based EHPP, heat pumps, BESS, gas turbines, and hydrogen storage systems. In [114], the authors proposed a model for planning an integrated electricity, hydrogen, and transportation system aiming at reducing equipment cost, energy consumption cost, travel time cost, and carbon emissions. The study in [115] proposes a novel design for a solar-powered multi-energy system and optimizes its operation to meet the heat, hydrogen, methane, and electricity demands for a large steel industry, aiming to minimize the electricity purchase cost. Yet, the works in [55, 111, 114, 115] still employ simplified models of electrolyzer and assume a constant conversion rate of hydrogen

in kg/kWh under all operating conditions, while [112, 113] utilizes a simplified empirical model. Such an assumption may lead to inaccurate sizing of the EHPP and the integrated energy systems. It is also noted that these studies [38–41, 55, 82, 106–115] have common shortfalls in terms of ignoring the optimal design of electrolyzer parameters, and/or the electrolyzer safety constraints. In [116], the authors propose an optimization formulation aimed at maximizing the efficiency of the PEME system, considering a detailed PEME model. However, the work in [116] overlooks optimizing the internal design of the PEME and is limited to optimizing two operational variables (inlet water flow and temperature). Additionally, it doesn’t address the economic aspects related to the initial capital cost of the PEME and the electricity tariff, nor does it optimize the sizing of other components within the EHPP, which could significantly influence the optimal design and operation of the PEME.

2.5 Scheduling and Operation of EHPP

The work in [36] develops an energy management system to minimize the cost of hydrogen produced from an EHPP equipped with an on-site photovoltaic system and BESS. In [35], the authors propose an optimal scheduling algorithm of a PEME connected to the power grid, where additional power grid services are considered to maximize the net profit of the privately owned EHPP. A techno-economic study is introduced in [37] to assess the LCOH when PEME is optimally scheduled concurrently with renewable-based virtual power plants while considering multiple grid ancillary services. In [82], the authors optimize the operation of a centralized EHPP that uses a liquid organic hydrogen carrier to supply hydrogen fueling stations and provide Demand Response (DR) and reactive power grid services to the power grid. The work in [117] optimizes the operation of hydrogen fueling stations while providing frequency grid services to enhance grid stability. The study in [118] introduces a novel scheduling algorithm for gaseous-liquid hydrogen plants and considers enhancing operational revenue by participating in the DR grid service.

To enhance the EHPP capabilities in providing ancillary services and improving its

operational flexibility, the studies in [119–125] equipped the hydrogen plant with a fuel cell. In [119], an energy management strategy is developed for a hybrid energy storage system comprising a hydrogen storage system (AE, hydrogen tank, and fuel cell) and a BESS. The management strategy aims to avoid the blackout of a standalone renewable-based power system when available wind power is inadequate to supply the existing load. The study in [120] proposes a quite similar configuration for a hybrid charging station that consists of PEME, hydrogen tank, fuel cell, DC chargers, BESS, and PV system. A model predictive control-based energy management system is developed to minimize the utilization cost and the energy absorbed from the grid by controlling the energy flow among different power sources. The authors in [121] present a supervisory scheduling model for hydrogen fueling stations comprising a PEME, hydrogen storage tank, and fuel cell. The system is designed to serve the transportation sector while also participating in OR grid services. The objective of the model is to enhance the economic viability of hydrogen fueling stations. In [122], a multi-energy framework is proposed for an EHPP that includes a PEME, hydrogen storage tank, fuel cell, and BESS. The system is designed to harvest power from RESs, supply hydrogen to fueling stations, and provide OR grid services. Participation in these grid services is intended to increase the revenue of the EHPP and enhance the operational flexibility of the power grid. The work in [123] proposes a unified optimization model for planning and operating an EHPP (comprising a PEME, a hydrogen storage tank, and a fuel cell), considering participation in the energy, hydrogen, and grid service markets. It also highlights the benefits of considering hybrid hydrogen demand, where the produced hydrogen is supplied to multiple sectors. In [124], a PEME and fuel cell with supercapacitors are used as an energy storage system to enhance power quality and improve voltage ride-through capability of wind turbines, thereby facilitating the integration of converter-less wind turbines into the electrical grid. In [125], the authors aim to increase the flexibility of wind farm connections and mitigate the limitations of using BESS when wind fluctuations exceed the limit for a long time. Authors propose a hybrid energy storage system that consists of a hydrogen storage system and a BESS to minimize power fluctuations, energy loss, and maximize the lifetime of the battery system. However, these efforts don't consider

the limitations imposed on the operation of the EHPP due to the integration with other energy systems.

Authors in [126] propose the integration of electricity, heat, and hydrogen storage systems to increase the flexibility of a power grid with high renewable power penetration. The proposed integration represents a more cost-efficient alternative for BESS. The work in [127] minimizes the operational cost of hydrogen generation, transportation, and storage, considering the power systems constraints in an integrated electricity-hydrogen energy system. In [128], authors develop a strategy for optimal operation and unit commitment of AE units operated by wind turbines within an integrated energy system (electricity-heat-gas network). Authors demonstrate that increasing the hydrogen injection fraction enhances the reliability of both gas and heat networks, while also reducing the total operational cost.

Yet, all of these works in [35–37, 82, 117–128] utilize a simplified electrolyzer models without paying attention to the different operating conditions of the EHPP such as the electrolyzer temperature and the cathodic pressure and how these operating conditions could be chosen to enhance the EHPP efficiency. Moreover, none of these studies investigate the dynamic (e.g., hourly) adjustment of these operating conditions. Furthermore, the optimal operation and scheduling studies that consider EHPP participation in grid service provision, such as those presented in [35, 37, 82, 117–125], share several common shortcomings. These include: i) neglect of safety constraints and their influence on electrolyzer performance across different grid services; and ii) failure to determine the most suitable electrolyzer technology for each service. Moreover, none of the previously mentioned studies address the electrolyzer dynamics and their impacts on the operation of the EHPP. These dynamics can be particularly significant when accounting for the intermittency of RESs and/or the provision of the grid ancillary services that require fast response times.

2.6 Dynamic Control of EHPP

A fractional-order PID controller is introduced in [129] to control the frequency response of a hybrid power system comprising RES, a FC, and an electrolyzer. The electrolyzer is modeled as a first-order dynamic model. The work in [130] proposes the use of AE as a fast response system to support the grid frequency of a wind-dominated power system and studies the effect of such contribution on the net profit value. The work in [131] provides a compensation strategy for the intermittency of a PV system using a PEME based hydrogen storage system, supercapacitor, and BESS. The hydrogen storage system is used to mitigate slow fluctuations, while the supercapacitors and battery system are dedicated to compensating for fast fluctuations. The PEME is represented as an electrical dynamic empirical model. The study in [132] develops an adaptive electrical dynamic model for PEME and uses it to enhance grid frequency, demonstrating that PEME can respond faster than conventional synchronous generators. However, these studies [129–132] don't take into account the EHPP downstream operational constraints and neglect the impact of providing grid services on the electrolyzer efficiency and hydrogen production efficacy.

The authors in [133] deploy a large-scale wind-operated EHPP to provide secondary frequency regulation by responding to automatic generation control signals. The case studies show an increase in the EHPP's full load hours and a reduction in hydrogen production costs. The work in [133] employs an empirical AE model and considers the downstream hydrogen buffer constraints. In [134], an electrical empirical dynamic utility scale PEME model is utilized to provide fast frequency support to a power grid with 50% renewable power penetration. The model considers the stack, converter, and hydrogen downstream operational constraints. The authors in [135] compare the deployment of AE and PEME to support the frequency of the power grid for frequency support and show that the PEME is more convenient due to its fast dynamic response. Further, authors propose a virtual synchronous machine control approach to provide a similar behavior to that of the BESS. The AE is more suitable for frequency regulation. The work in [135] represents the electrolyzer using a dynamic electrical empirical model and distinguishes the AE model from

the PEME one by adding a series inductance to mimic its slow dynamic response. Yet, all of these efforts provided in [129–131, 133–135] are limited to the empirical electrical model and don’t explain how the electrolyzer parameters may affect its dynamics. Furthermore, they overlook the impact of gas production and thermal dynamics, which may limit EHPP capabilities to provide grid services.

The work in [136] designs a PID controller to for AE temperature. The developed controller is capable of handling the time delay associated with heat exchanger. Authors also show that the temperature feedback should be taken before the stack for small scale AE and after the stack for large scale systems to achieve the highest economic benefits. To expand the loading range of AE, authors of [137] introduced a model predictive controller to control the electrolyzer pressure to achieve a minimum of 10% loading. The paper provides a multi-physics dynamic model for the gas production portion of the AE. Authors of [138] used a mix of static and dynamic multi-physics models where the electrical portion of the PEME is represented using a static model while the thermal portion is considered as a dynamic model. The proposed PEME model is employed to develop a model predictive control energy management strategy that regulates the frequency of the microgrid. The work in [139] introduces an adaptive feedforward temperature control for a PEME. This work employs a multi-physics based thermal dynamic model of a real 100 kW PEME and compares the developed controller with the conventional temperature PID controller under different solar and wind power profiles. Yet, the multi-physics dynamic models and the developed controllers provided in [136–139] falls short to: i) analyze how the electrolyzer dynamics vary with its parameters and operating conditions, and; ii) develop a coordinated control strategy that tracks the defined loading set point and operating conditions while taking into consideration the EHPP safety and operation constrains.

2.7 Research Gaps

Based on the provided literature, there are several research gaps in terms of design, scheduling, and control of EHPP as explained hereunder.

- G1) Few efforts in the literature have considered optimizing the internal parameters, such as cathodic pressure, membrane thickness, temperature, and cell area of a large-scale electrolyzer. However, none of these studies addressed optimizing these parameters as a part of the EHPP sizing problem, or considered the effect of optimizing these parameters on the size of other equipment in the EHPP or on the LCOH. Further, the impact of the electrical power profile, the hydrogen demand profile, and the electricity tariff on choosing these parameters has never been considered.
- G2) Previous work that considered integrating the electrolyzer with a BESS did not address the sizing of BESS as a part of the EHPP or reviewed the effect of the BESS on the size, operating range, and internal parameters of the cooperated electrolyzer.
- G3) The structure of the electrolyzer unit consists of a number of modules (stacks). Yet, the optimal number of modules and the effect of this number on the performance of the EHPP, particularly when integrated with intermittent RESs, are not explored.
- G4) Many studies in the literature studied the sizing of EHPPs considering different electrolyzer technologies and their provision of grid services. However, these studies employ simple generic electrolyzer models that can not adequately assess the suitability of the electrolyzer technology or determine the proper electrolyzer internal design to provide various grid services. Further, none of the previous studies considered how hydrogen application may impact the EHPP capability to participate in grid services.
- G5) The literature has never addressed varying the electrolyzer operating parameters, such as cathodic pressure and operating temperature, with its loading level to enhance the operating efficiency or avoid violating the safety constraints on the hydrogen in oxygen percentage.
- G6) Operating the PEME with variable cathodic pressure and/or temperature can be beneficial in terms of improving operating efficiency and extending the operating range. However, the dynamics associated with varying these parameters, and their impact

on the fast response capability of the PEME, which may in turn affect its ability to integrate with intermittent renewable energy sources, require further investigation. Additionally, the coordination of pressure and temperature controllers with the loading conditions (i.e., operating current density) has not yet been adequately addressed in the literature.

Chapter 3

Modeling of EHPP

This chapter builds on the EHPP configuration presented in Section 2.1 and Fig. 2.1, and develops the mathematical models of its key components, which are used throughout the subsequent chapters. These components include various types of electrolyzers (AE, PEME), the FC, compressor, HS, and the BESS. It is important to note that AE technology is generally characterized by slow dynamic response; therefore, only its steady-state model is considered. In contrast, PEME is used in both steady-state and dynamic analyses, and accordingly, both its dynamic and steady-state models are presented.

3.1 AE Modeling

The AE is a multi-nature device that couples electrical and chemical processes. Accordingly, its steady-state model accounts for these interacting natures and is represented by two main components: i) an electrical model describing the voltage–current characteristics, and ii) an electrochemical gas crossover model. These components are subsequently combined to formulate the hydrogen production efficiency of the electrolyzer.

3.1.1 Electrical Model

The voltage across the AE cell, V_{cell}^{AE} , consists of three components: the open circuit electrochemical voltage required to split water, known as the Nernst voltage V_{oc} , activation overpotential V_{act}^{AE} , and resistive overpotential V_{res}^{AE} as given in (3.1).

$$V_{cell}^{AE} = V_{oc}^{AE} + V_{act}^{AE} + V_{res}^{AE} \quad (3.1)$$

The open circuit voltage is obtained using Nernst equation and varies with cell temperature, T_{cell}^{AE} , and the gas pressures (i.e., the cathodic and anodic pressures), denoted by $\pi^{AE}H_2$ and $\pi^{AE}O_2$, respectively, as shown below [103]:

$$\begin{aligned} V_{oc}^{AE} &= V_{rev}^{AE} + \frac{RT_{cell}^{AE}}{2F} \ln \left(\sqrt{\frac{\pi_{O_2}^{AE}}{\pi_o}} \frac{\pi_{H_2}^{AE}}{\pi_o} \right) \\ &= 1.229 - 0.9 \times 10^{-3} (T_{cell}^{AE} - 298) + \frac{RT_{cell}^{AE}}{2F} \ln \left(\sqrt{\frac{\pi_{O_2}^{AE}}{\pi_o}} \frac{\pi_{H_2}^{AE}}{\pi_o} \right), \end{aligned} \quad (3.2)$$

where R and F are the universal gas constant and Faraday's constant, respectively.

The electrode kinetics and charge transfer between the electrodes and electrolyte solution is expressed with the activation overpotential [140] as follows:

$$V_{act}^{AE} = \frac{RT_{cell}^{AE}}{\alpha_{an}^{AE} F} \ln \left(\frac{J^{AE}}{J_{o,an}^{AE} (1 - \vartheta_{an})} \right) + \frac{RT_{cell}^{AE}}{\alpha_{cat}^{AE} F} \ln \left(\frac{J^{AE}}{J_{o,cat}^{AE} (1 - \vartheta_{cat})} \right) \quad (3.3)$$

where J^{AE} is the operating current density of the AE, while $J_{0,an}^{AE}$ and $J_{0,cat}^{AE}$ are the anodic and cathodic exchange current densities of the AE, respectively. These exchange current densities are calculated as functions of the electrode roughness using empirical reference exchange current densities [140]. α_{cat}^{AE} and α_{an}^{AE} are the anodic and cathodic charge transfer coefficients, respectively. ϑ is the fractional bubble coverage on the electrode surface of the AE and is calculated through the following empirical formula as explained in [140]:

$$\vartheta = \left(-97.25 + 182 \frac{T_{cell}^{AE}}{T_{ref}} - 84 \left(\frac{T_{cell}^{AE}}{T_{ref}} \right)^2 \right) \left(\frac{J^{AE}}{J_{lim}} \right)^{0.3} \left(\frac{\Pi^{AE}}{\pi^{AE}} \right), \quad (3.4)$$

here, J_{lim} is the limiting current density at 100% bubble coverage. Π^{AE} and π^{AE} denote the total and corresponding gas partial pressures of the AE, respectively, referring to the anode or cathode depending on whether ϑ_{an} or ϑ_{cat} is calculated.

The AE equivalent resistance is determined by the combined resistances of the electrodes (R_e^{AE}), electrolyte (R_{el}^{AE}), and separator (R_s^{AE}). Therefore, the resistive overpotential is calculated as follows:

$$V_{res}^{AE} = I^{AE} (R_e^{AE} + R_{el}^{AE} + R_s^{AE}). \quad (3.5)$$

Electrodes, electrolyte, and separator resistances are expressed as given in (3.6), (3.7), and (3.8), respectively [140].

The anodic and cathodic electrode resistances are calculated using the corresponding effective electrode resistivities, $\rho_{eff,an}$ and $\rho_{eff,cat}$, the physical dimensions of the electrodes, and the cell temperature. The effective electrode resistivity depends on the electrode material resistivity, where ρ_o^{an} and ρ_o^{cat} denote the anodic and cathodic material resistivities at the reference temperature T_{ref} , respectively. The total electrodes' resistance is then obtained as follows:

$$R_e^{AE} = \underbrace{\frac{\rho_{o,an}}{(1 - \epsilon_{an})^{3/2}}}_{\rho_{eff,an}} \frac{\delta_{an}}{A_{cell}^{AE}} (1 + k_{an}(T_{cell}^{AE} - T_{ref})) + \underbrace{\frac{\rho_o^{cat}}{(1 - \epsilon_{cat})^{3/2}}}_{\rho_{eff,cat}} \frac{\delta_{cat}}{A_{cell}^{AE}} (1 + k_{cat}(T_{cell}^{AE} - T_{ref})), \quad (3.6)$$

where δ_{an} and δ_{cat} denote the anodic and cathodic electrode thicknesses, respectively; ϵ_{an} and ϵ_{cat} represent the anodic and cathodic electrode porosities; k_{an} and k_{cat} are the temperature coefficients of the anodic and cathodic electrode resistivities; and A_{cell}^{AE} is the cell area, which is equal to the effective electrode area.

In a similar manner, the electrolyte resistance is calculated using the effective resistivities of the bubble-free and bubble-zone electrolytes. Here, ρ_{el} denotes the resistivity of the bubble-free electrolyte, from which the resistivity of the bubble-zone electrolyte is determined as $\rho_{el,bz} = \frac{\rho_{el} \beta}{(1 - \vartheta)^{3/2}}$. By combining the resistances of the anodic and cathodic

compartments for both the bubble-free and bubble-zone regions, the total electrolyte resistance is calculated as follows [140]:

$$R_{el}^{AE} = \underbrace{\frac{\rho_{o,el}(M)}{(1 + k_{el}(T_{cell}^{AE} - T_{ref}))}}_{\rho_{el}} \left(\underbrace{\underbrace{l_{an} - \beta_{an}}_{\text{bubble-free}} + \underbrace{\frac{\beta_{an}}{(1 - \vartheta_{an})^{3/2}}}_{\text{bubble-zone}}}_{\text{Anode}} + \underbrace{\underbrace{l_{cat} - \beta_{cat}}_{\text{bubble-free}} + \underbrace{\frac{\beta_{cat}}{(1 - \vartheta_{cat})^{3/2}}}_{\text{bubble-zone}}}_{\text{Cathode}} \right) A_{cell}^{-1}, \quad (3.7)$$

where l_{an} and l_{cat} are the anode and cathode electrode-separator gaps, respectively, while β_{an} and β_{cat} denote the anodic and cathodic bubble area widths. Additionally, k_{el} is the temperature coefficient of the electrolyte resistivity, and M represents the electrolyte concentration.

The separator resistance is a function of the separator wettability factor ω_s , tortuosity τ_s , porosity ϵ_s , and thickness δ_s , and is calculated as follows [141]:

$$R_s^{AE} = \rho_{el}(M) \frac{\tau_s^2 \delta_s}{\omega_s \epsilon_s A_{cell}^{AE}}. \quad (3.8)$$

3.1.2 Gas Crossover Model

The hydrogen production using AE suffers from production losses widely known as hydrogen crossover that consists of three components [137]: diffusion ($n_{diff}^{H_2}$), convection ($n_{conv}^{H_2}$), and electrolyte mixing ($n_{el}^{H_2}$). The total hydrogen crossover molar flow, n_{H_2} , is determined by summing these three components as below:

$$n_{H_2}^{AE} = n_{diff}^{H_2} + n_{conv}^{H_2} + n_{el}^{H_2}. \quad (3.9)$$

The hydrogen diffusion and convection fluxes through the separator are described by Fick's law and Darcy's law, respectively, as given in (3.10) and (3.11) below [137]:

$$n_{diff}^{H_2} = \frac{D_{eff} \pi_{H_2}^{AE} S_{H_2}(M)}{\delta_s}, \quad (3.10)$$

$$n_{conv}^{H_2} = \frac{Pr_{H_2}^{AE} \Delta\pi S_{H_2}(M) \pi_{H_2}^{AE}}{\zeta \delta_s}, \quad (3.11)$$

where D_{eff} is the effective diffusion coefficient, $S_{H_2}(M)$ is the hydrogen solubility at electrolyte concentration M , $Pr_{H_2}^{AE}$ is the separator permeability, $\Delta\pi$ is the pressure difference across the separator, and ζ is the viscosity of the solvent.

The hydrogen crossover flow due to electrolyte mixing is proportional to hydrogen solubility, the recirculated electrolyte flow rate (v_{el}), and cathodic pressure [137], as in (3.12). Yet, when a separate electrolyte cycle is considered, this component, $n_{el}^{H_2}$, can be omitted.

$$n_{el}^{H_2} = \frac{S_{H_2}(M) \pi_{H_2}^{AE} v_{el}}{4} \quad (3.12)$$

Similarly, the oxygen crossover molar flow, n_{O_2} , can be obtained. However, the convection component can be neglected considering that the cathodic pressure (i.e., hydrogen pressure) is higher than the anodic pressure (i.e., oxygen pressure). The total oxygen crossover is determined as follows [141]:

$$n_{O_2}^{AE} = n_{diff}^{O_2} + n_{el}^{O_2} = \frac{D_{eff} \pi_{O_2}^{AE} S_{O_2}(M)}{\delta_s} + \frac{S_{O_2}(M) \pi_{O_2}^{AE} v_{el}}{4} \quad (3.13)$$

where $n_{diff}^{O_2}$ and $n_{el}^{O_2}$ represent the oxygen diffusion crossover flux and the electrolyte-induced crossover flux, respectively, and $S_{O_2}(M)$ is the oxygen solubility at electrolyte concentration M .

Gas crossover may lead to the formation of an explosive mixture within the electrolyzer compartments, particularly at low loads [140]. Hydrogen crossover is typically higher than oxygen crossover due to the smaller molecular size and higher diffusivity of hydrogen [103]. Consequently, the hydrogen-in-oxygen percentage in the anodic compartment is more critical than the oxygen-in-hydrogen percentage in the cathodic compartment. Therefore, the hydrogen-in-oxygen percentage, $\Psi_{H_2}^{AE}$, must be continuously monitored and maintained within safe limits. The hydrogen-in-oxygen percentage is defined as the ratio of the hydrogen crossover molar flow to the sum of the produced oxygen molar flow, $N_{O_2}^{AE}$, and the

hydrogen crossover molar flow, as expressed below [137]:

$$\Psi_{H_2}^{AE} = \frac{n_{H_2}^{AE}}{N_{O_2}^{AE} + n_{H_2}^{AE}}, \quad (3.14)$$

where $N_{O_2}^{AE}$ is determined according to Faraday's law as $N_{O_2}^{AE} = \frac{J^{AE}}{4F}$.

3.1.3 AE Efficiency Model

The efficiency of AE consists of two components: production efficiency and Faraday efficiency [141]. The production efficiency is defined as the ratio between the power of the produced hydrogen and the input electrical power. The output power is calculated as the product of the hydrogen molar production flow, $N_{H_2}^{AE}$, and the heating value of hydrogen. The heating value used in this work corresponds to the LHV, assuming that the heat released during condensation is not recovered. The LHV of hydrogen is $\Delta H_{LHV}^{H_2} = 241 \text{ kJ mol}^{-1}$, which corresponds to an equivalent voltage of approximately $V_{LHV}^{H_2} = \frac{\Delta H_{LHV}^{H_2}}{2F} = 1.25 \text{ V}$. Accordingly, the production efficiency is calculated as follows [103]:

$$\eta_p^{AE} = \frac{V_{LHV}^{H_2} I^{AE}}{V_{cell}^{AE} I^{AE}} = \frac{V_{LHV}^{H_2}}{V_{cell}^{AE}}. \quad (3.15)$$

Faraday's efficiency mainly depends on the amount of gas crossover. The equivalent lost current density, J_{loss}^{AE} , is obtained using Faraday's law as in (3.16), while Faraday's efficiency is calculated as given in (3.17) [141].

$$J_{loss}^{AE} = 2F n_{H_2} + 4F n_{O_2} \quad (3.16)$$

$$\eta_F^{AE} = 1 - \frac{J_{loss}^{AE}}{J^{AE}} \quad (3.17)$$

The total AE efficiency is the multiplication of these two components as below [141]:

$$\eta_{AE} = \eta_p^{AE} \eta_F^{AE}. \quad (3.18)$$

3.2 PEME Modeling

Unlike AE, PEME is characterized by its fast response [24, 25]. Consequently, it is particularly suitable for applications that require rapid dynamic behavior. In this work, for such fast-response applications, we account for the dynamic characteristics of PEME. Accordingly, this subsection first develops the steady-state model of PEME, followed by the development of its dynamic model.

3.2.1 PEME Steady-State Modeling

The PEME steady-state modeling comprises multiple submodels, including the electrical model and the electrochemical gas crossover model, similar to the AE. However, when integrated with RESs, the PEME may operate at low loading levels. Under such conditions, the cell voltage may fall below the thermoneutral voltage (i.e., the threshold required for self-sustained hydrogen production). Consequently, an external heat input may be required [103]. Therefore, an additional submodel, namely a thermal model, is incorporated to fully represent the steady-state behavior of the PEME.

3.2.1.1 Electrical Model

Similar to the AE, the voltage across the PEME cell, V_{cell}^{PEM} , consists of three components: the open-circuit electrochemical voltage required to split water, referred to as the Nernst voltage V_{oc}^{PEM} ; the activation overpotential, V_{act}^{PEM} ; and the resistive overpotential, V_{res}^{PEM} , as given in (3.19) below:

$$V_{cell}^{PEM} = V_{oc}^{PEM} + V_{act}^{PEM} + V_{res}^{PEM}. \quad (3.19)$$

The open circuit voltage, V_{oc}^{PEM} , is also determined using the Nernst equation, as in the case of the AE, and is expressed as follows [103]:

$$\begin{aligned} V_{oc}^{PEM} &= V_{rev}^{PEM} + \frac{RT_{cell}^{PEM}}{2F} \ln \left(\sqrt{\frac{\pi_{O_2}^{PEM}}{\pi_o}} \frac{\pi_{H_2}^{PEM}}{\pi_o} \right) \\ &= 1.229 - 0.9 \times 10^{-3} (T_{cell}^{PEM} - 298) + \frac{RT_{cell}^{PEM}}{2F} \ln \left(\sqrt{\frac{\pi_{O_2}^{PEM}}{\pi_o}} \frac{\pi_{H_2}^{PEM}}{\pi_o} \right). \end{aligned} \quad (3.20)$$

where $\pi_{H_2}^{PEM}$ and $\pi_{O_2}^{PEM}$ are the cathodic and anodic pressures, respectively, and T_{cell}^{PEM} is the cell temperature.

The activation overpotential, V_{act}^{PEM} , can be approximated using the Tafel equation, as given in (3.21), under the assumption that the PEME operating current density, J^{PEM} , is significantly higher than the exchange current density, J_o^{PEM} . The charge-transfer coefficient, α^{PEM} , and the exchange current density, J_o^{PEM} , are estimated experimentally [103].

$$V_{act}^{PEM} = \frac{RT_{cell}^{PEM}}{\alpha^{PEM} z F} \ln \left(\frac{J^{PEM}}{J_o^{PEM}} \right) \quad (3.21)$$

where z is the number of transferred electrons. The membrane plays a crucial role in the PEME, as it separates the electrolyzer into two half-cells, namely the anode and cathode compartments. Perfluorosulfonic acid polymer membranes, such as Nafion, Fumapem, Flemion, and Aciplex, are commonly used due to their high mechanical strength, efficiency, proton conductivity, oxidative stability, and durability [142]. Among these, Nafion exhibits superior durability and proton conductivity, along with good mechanical stability, enabling operation at higher current densities [142,143]. Therefore, without loss of generality, Nafion is considered as the membrane material in all subsequent modeling and analyses. As shown in (3.22), the resistive voltage of the PEME depends on the membrane thickness, swelling, and conductivity, and increases with the operating current density. The conductivity of Nafion is a function of the water activity and the cell temperature.

$$V_{res}^{PEM} = \left(R_o^{PEM} + \frac{\mathfrak{s}_m^{PEM} \delta_m^{PEM}}{\sigma_m(T_{cell}^{PEM}, a_{H_2O})} \right) J^{PEM} \quad (3.22)$$

where δ_m^{PEM} and $\mathfrak{s}_m^{PEM}$ denote the membrane thickness and swelling factor, respectively; σ_m represents the membrane conductivity, and a_{H_2O} denotes the water activity.

3.2.1.2 Thermal Model

Under low loading conditions, the PEME may operate at cell voltages lower than the thermoneutral voltage, V_{ther}^{PEM} , which represents the minimum voltage required for the electrochemical reaction, or operate at voltages lower than the sum of the thermoneutral voltage and the vapor loading voltage, V_{load}^{PEM} [142, 143]. In such cases, an external heat input may be required. This heat contribution can be expressed as an equivalent voltage, V_{heat}^{PEM} , defined as the difference between the sum of the thermoneutral voltage and the vapor loading voltage, and the cell voltage [142, 143]. The heat equivalent voltage, V_{heat}^{PEM} , is expressed as follows:

$$V_{heat}^{PEM} = V_{ther}^{PEM} + V_{load}^{PEM} - V_{cell}^{PEM}. \quad (3.23)$$

The equation (3.23) indicates that when the argument of V_{heat}^{PEM} is positive, external heating is required to maintain thermal equilibrium. Conversely, a negative argument implies that cooling is necessary to sustain a constant T_{cell}^{PEM} . However, for negative values, V_{heat}^{PEM} can be set to zero, as effective cooling is inherently provided by the high water circulation rates within the cell, supplemented by passive heat dissipation to the surroundings. In this case, the energy consumption associated with pumping and cooling is considered negligible [144].

The thermoneutral voltage of the PEME, V_{ther}^{PEM} , is derived from the enthalpy of liquid water splitting under standard conditions ($T = 298$ K, $\pi = 1.013$ bar, $\text{pH} = 7$). The corresponding reaction enthalpy, $\Delta H = 286$ kJ/mol, is converted into its electrical equivalent, resulting in a thermoneutral voltage of 1.48 V [103, 143]. To calculate the vapor loading voltage, V_{load}^{PEM} , assuming ideal gas behavior, the molar steam flow rate is first determined using (3.24). Then the voltage equivalent of the loading vaporization energy is obtained by multiplying the calculated steam molar flow rate by the vaporization enthalpy, ΔH_{vap} , and expressing the molar flow rate in terms of electric current through Faraday's law, leading to the formulation given in (3.25) [103, 143].

$$N_{H_2O}^{PEM} = \frac{N_{H_2}^{PEM} \pi_{H_2O}^{PEM}}{\pi_{H_2}^{PEM}} + \frac{N_{O_2}^{PEM} \pi_{H_2O}^{PEM}}{\pi_{O_2}^{PEM}} \quad (3.24)$$

$$V_{load}^{PEM} = \frac{\pi_{H_2O}^{PEM}}{2F} \left(\frac{1}{\pi_{H_2}^{PEM}} + \frac{1}{2\pi_{O_2}^{PEM}} \right) \Delta H_{vap} \quad (3.25)$$

where $N_{H_2O}^{PEM}$ denotes the steam molar flow rate, while $N_{H_2}^{PEM}$ and $N_{O_2}^{PEM}$ represent the molar flow rates of the produced hydrogen and oxygen, respectively.

3.2.1.3 Gas Crossover Model

Produced gases can permeate across the membrane, where the hydrogen crossover equivalent current density J_{loss,H_2}^{PEM} is a function of the operating current density J^{PEM} and cathodic pressure $\pi_{H_2}^{PEM}$.

$$J_{loss,H_2}^{PEM} = 2F Pr_{H_2}^{PEM} \frac{\pi_{H_2}^{PEM}}{\mathfrak{s}_m^{PEM} \delta_m^{PEM}} + \frac{a_x}{\mathfrak{s}_m^{PEM} \delta_m^{PEM}} J^{PEM} \quad (3.26)$$

The total gases crossover equivalent current density is the sum of the hydrogen and oxygen crossover. For the Nafion membrane, the oxygen permeation factor is about twice the hydrogen [103] and, thus, the total crossover equivalent current density can be obtained as follows [145]:

$$J_{loss}^{PEM} = J_{loss,H_2}^{PEM} + J_{loss,O_2}^{PEM} = 2 \left(F Pr_{H_2}^{PEM} \frac{\pi_{H_2}^{PEM} + \pi_{O_2}^{PEM}}{\mathfrak{s}_m^{PEM} \delta_m^{PEM}} + \frac{a_x}{\mathfrak{s}_m^{PEM} \delta_m^{PEM}} J^{PEM} \right) \quad (3.27)$$

where a_x is the current density impact on permeation.

For safety purposes, the concentration of hydrogen in oxygen percentage, $\Psi_{H_2}^{PEM}$, has to be monitored continuously and maintained within the safe limits. The percentage of hydrogen in oxygen is calculated as below [143]:

$$\Psi_{H_2}^{PEM} = \frac{J_{loss,H_2}^{PEM}}{J_{loss,H_2}^{PEM} + 0.5 J^{PEM}} \quad (3.28)$$

3.2.1.4 PEME Efficiency Model

Similar AE efficiency calculations, the efficiency of PEME consists of two components: production efficiency η_p^{PEM} and Faraday's efficiency η_F^{PEM} , which represent the electrical-heat losses and permeation losses expressed in (3.29) and (3.30), respectively [103, 143].

Then, the product of the two efficiencies yields the total PEME efficiency as expressed in (3.31) [103, 143].

$$\eta_p^{PEM} = \frac{V_{LHV}^{H_2}}{V_{heat}^{PEM} + V_{cell}^{PEM}} \quad (3.29)$$

$$\eta_F^{PEM} = 1 - \frac{J_{loss}^{PEM}}{J^{PEM}} \quad (3.30)$$

$$\eta_{PEM} = \eta_p^{PEM} \eta_F^{PEM} \quad (3.31)$$

3.2.2 PEME Dynamic Modeling

As a multiphysics device, the PEME dynamic model comprises three domains: the electrical domain, the mass transfer domain, and the thermal domain. Fig. 3.1 shows the three domains of PEME. As shown in the figure, the electrical domain is represented by its equivalent circuit that is connected through a coupling inductor, L_d , to the AC grid via a power converter. The power converter is responsible for controlling the electrical power flow to the PEME and, hence, determines its loading. The mass transfer domain includes the flow of the feeding water through PEME before being split into hydrogen and oxygen, which then transfer to the hydrogen and oxygen separators, respectively. In the separators, gases are separated from the water, with oxygen released into the atmosphere. The hydrogen outlet flow is regulated by a control valve, which determines the cathodic pressure ($\pi_{H_2}^{PEM}$) in both the cathodic compartment and the hydrogen separator. The thermal domain represents the heat flow in the PEME. PEME experiences electrical losses, which increase its temperature; hence, a heat exchanger is used to control the temperature of the PEME water feed to regulate its operating temperature by controlling the water flow in the second water loop via a control valve. It is worth noting that heat exchange is primarily used to cool the PEME. However, in rare cases under light loading conditions, it may be used to heat the PEME to sustain the electrochemical reaction.

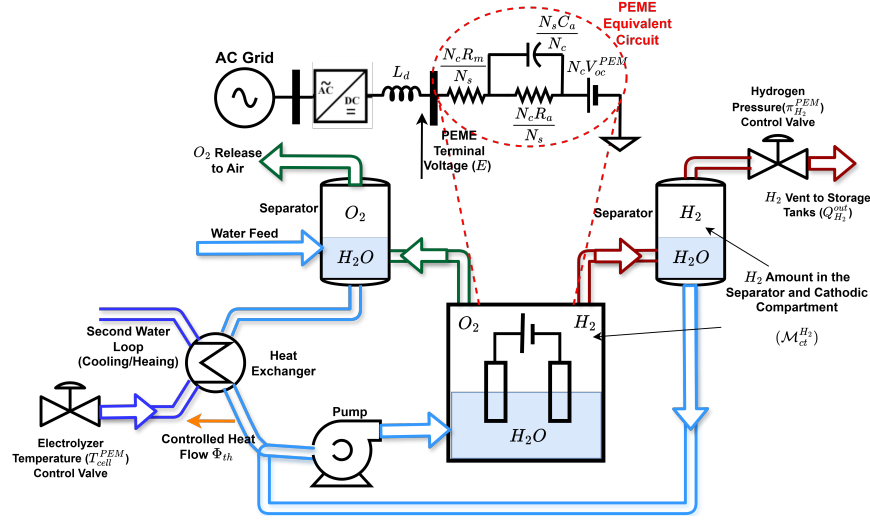


Figure 3.1: The multiphysics PEME schematic.

3.2.2.1 Electrical Domain Modeling

The electrical model of a PEME cell is represented by a voltage source representing the cell open circuit voltage V_{oc}^{PEM} , a series resistance R_m representing the ohmic resistance of the cell membrane and electrodes, and a parallel RC branch (R_a , C_a) representing the build-up of the cell activation voltage [135]. A large-scale PEME can be built from N_s stacks each of N_c cells as in Fig. 3.2 (a). Assuming identical cells within each stack, the currents through C_a and R_a of all series cells in the stack are i_1 and i_2 , respectively. Thus, a stack model can consider all C_a are in series (have the same current i_1) and similarly all the R_a (have the same current i_1), ending up with the equivalent circuit in Fig. 3.2 (b). A similar concept can be applied to the N_s stacks; the voltage across the resistance $N_c R_m$ of any stack is identical (Note: all cells are identical, and hence all stacks are identical). As such, all $N_c R_m$ of all stacks are in parallel connection. Similarly, all RC branches ($N_c R_a$, $N_c C_a$) of all stacks are in parallel connection. Then, the PEME equivalent circuit is obtained as shown in Fig. 3.2 (c). By applying the circuit laws considering the capacitor voltage (V_a) and coupling inductor current (i_{PEM}) as the states, and the voltage across PEME E is the

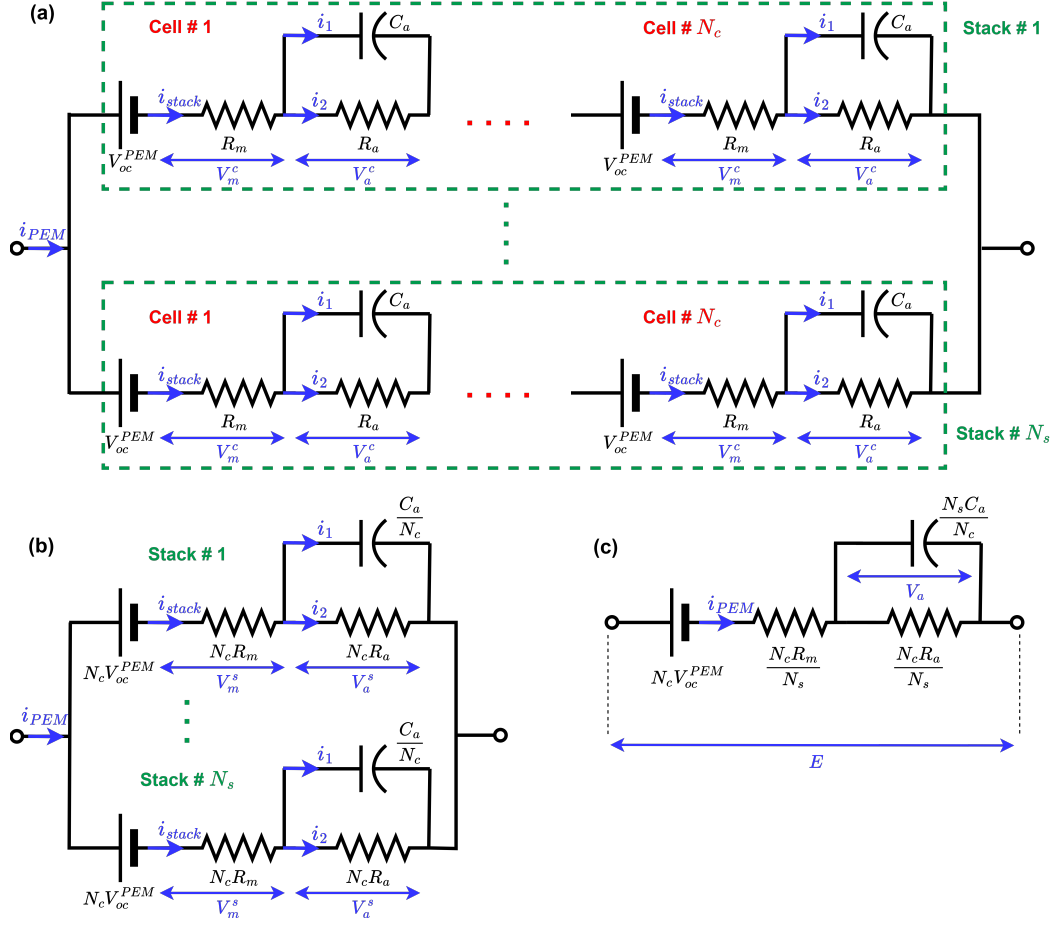


Figure 3.2: Electrical model of a large-scale PEME with N_c cells per stack and N_s stacks. (a) basic model with $N_c N_s$ cell circuits, (b) reduced model to N_s stack circuits, and (c) reduced model of one circuit for the whole PEME.

input, the dynamic model of the electrical domain can be represented by the following state space model:

$$\begin{bmatrix} \dot{V}_a \\ i_{PEM} \end{bmatrix} = \begin{bmatrix} \frac{-1}{R_a C_a} & \frac{N_c}{N_s C_a} \\ \frac{-1}{L_d} & -\frac{N_c R_m}{N_s L_d} \end{bmatrix} \begin{bmatrix} V_a \\ i_{PEM} \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{1}{L_d} \end{bmatrix} E + \begin{bmatrix} 0 \\ -\frac{N_c V_{oc}^{PEM} (T_{cell}^{PEM}, \pi_{H_2}^{PEM})}{L_d} \end{bmatrix}. \quad (3.32)$$

3.2.2.2 Mass Transfer Domain Modeling

The mass transfer domain focuses on the cathodic side, i.e., related to hydrogen production, assuming the produced oxygen is released into the air. The cathodic compartment and hydrogen separator can be treated as a tank of volume $\mathcal{V}_{ct}$ with inlet $Q_{H_2}^{in}$ flow obtained as (3.33a) and two discharges [146]: i) the hydrogen outlet flow, $Q_{H_2}^{out}$, through the control valve, and ii) the hydrogen permeation to the anodic compartment denoted as $Q_{H_2}^{per}$ and calculated as in (3.33b).

$$Q_{H_2}^{in} = \frac{i_{PEM}}{2F} \quad (3.33a)$$

$$Q_{H_2}^{per} = \frac{(A_{cell}^{PEM} N_c N_s Pr_{H_2}^{PEM} \pi_{H_2}^{PEM} + a_x i_{PEM})}{\mathfrak{s}_m^{PEM} \delta_m^{PEM}} \quad (3.33b)$$

Considering the amount of hydrogen in the cathodic compartment, $\mathcal{M}_{ct}^{H_2}$, as a state variable and Q_{H_2} as the input, and substituting $\pi_{H_2}^{PEM}$ with its equivalent expression derived from the ideal gas law as given in (3.34), the mass transfer domain can be modeled according to (3.35) as follows [146]:

$$\pi_{H_2}^{PEM} = \frac{R \mathcal{M}_{ct}^{H_2} T_{cell}^{PEM}}{\mathcal{V}_{ct}} \quad (3.34)$$

$$\dot{\mathcal{M}}_{ct}^{H_2} = \left(\frac{-a_x}{\mathfrak{s}_m^{PEM} \delta_m^{PEM}} + \frac{1}{2F} \right) i_{PEM} - \frac{A_{cell}^{PEM} N_c N_s Pr_{H_2}^{PEM} R}{\mathfrak{s}_m^{PEM} \delta_m^{PEM} \mathcal{V}_{ct}} \mathcal{M}_{ct}^{H_2} T_{cell}^{PEM} - Q_{H_2}^{out} \quad (3.35)$$

3.2.2.3 Thermal Domain Modeling

The thermal domain represents the dynamics of heat flow in the PEME. The main source of heating in PEME is the electrical losses that are the difference between the PEME input power $E i_{PEM}$ and the thermoneutral power $V_{ther}^{PEM} i_{PEM}$ [91, 139]. As the PEME cell temperature T_{cell}^{PEM} increases, the heat dissipation through the PEME surface to the ambient through a thermal resistance $\mathcal{R}_{th}$ increases. Further, additional controlled cooling/heating flow Φ_{th} could be needed to maintain the cell temperature at the determined value. Assuming that the cell temperature T_{cell}^{PEM} is uniform across all PEME cells, and considering T_{cell}^{PEM} as a state variable and Φ_{th} as the input, the thermal domain can be

modeled as follows:

$$\dot{T}_{cell}^{PEM} = (E - V_{ther}^{PEM})i_{PEM} - \frac{T_{cell}^{PEM}}{\mathcal{R}_{th}} + \frac{T_{amb}}{\mathcal{R}_{th}} + \Phi_{th}, \quad (3.36)$$

where C_{th} is the PEME thermal capacitance and T_{amb} is the ambient temperature.

By combining the electrical, mass transfer, and thermal domains of the PEME (i.e., (3.32), (3.35), and (3.36)), the complete dynamic model of the PEME is obtained as follows:

$$\begin{bmatrix} \dot{V}_a \\ \dot{i}_{PEM} \\ \dot{\mathcal{M}}_{ct}^{H_2} \\ \dot{T}_{cell}^{PEM} \end{bmatrix} = \begin{bmatrix} \frac{-1}{R_a C_a} V_a + \frac{N_c}{N_s C_a} i_{PEM} \\ \frac{-1}{L_d} V_a - \frac{N_c R_m}{N_s L_d} i_{PEM} + \frac{E}{L_d} - \frac{N_c V_{oc}(T_{cell}^{PEM}, \pi_{H_2}^{PEM})}{L_d} \\ \left(\frac{-a_x}{s_m^{PEM} \delta_m^{PEM}} + \frac{1}{2F} \right) i_{PEM} \frac{A_{cell}^{PEM} N_c N_s P r_{H_2}^{PEM} R}{s_m^{PEM} \delta_m^{PEM} \mathcal{V}_{ct}} \mathcal{M}_{ct}^{H_2} T_{cell}^{PEM} - Q_{H_2}^{out} \\ (E - V_{ther}^{PEM}) i_{PEM} - \frac{T_{cell}^{PEM}}{\mathcal{R}_{th}} + \frac{T_{amb}}{\mathcal{R}_{th}} + \Phi_{th} \end{bmatrix}. \quad (3.37)$$

3.3 FC Modeling

The output voltage of the FC, V_{FC} , consists of four components as follows [147]:

$$V_{FC} = V_{oc}^{FC} - V_{act}^{FC} - V_{res}^{FC} - V_{con}^{FC}, \quad (3.38)$$

where V_{oc}^{FC} is the open circuit voltage of the FC obtained using the Nernst equation, V_{act}^{FC} is the activation voltage drop that is a function of oxygen concentration in the cathode catalytic interface, V_{res}^{FC} is the voltage drop across membrane resistance, and V_{con}^{FC} is the concentration voltage drop that is driven by the gas mass transport which changes hydrogen and oxygen concentrations. The detailed calculation of these four voltage components are provided in [147]. The relation between the FC current, I_{FC} , and its hourly hydrogen flow consumption is represented by Faraday's law as in (3.39a) [148]. As such, the FC power generation, P_{FC} , is obtained as a function of the FC hydrogen flow consumption, $N_{H_2}^{FC}$, as provided in (3.39b) [147].

$$I_{FC} = 2F N_{H_2}^{FC} \quad (3.39a)$$

$$P_{FC} = V_{FC} I_{FC} = 2F V_{FC} N_{H_2}^{FC} \quad (3.39b)$$

3.4 Compressor Modeling

The produced hydrogen from the electrolyzer at pressure π_{H_2} can be less than the pressure required for hydrogen utilization. Hence, a mechanical compressor may be needed to pressurize the produced hydrogen from the electrolyzer cathodic pressure (i.e., hydrogen pressure), $\pi_{H_2}^{Elz}$, to the hydrogen storage pressure π_{HS} . The subscript/superscript *Elz* generically denotes either PEM or AE, enabling a unified representation of both cases.

The power consumption of the compressor, P_{Cmp} , can be calculated as a function of the electrolyzer cathodic pressure, hydrogen storage pressure, and electrolyzer hydrogen production flow $N_{H_2}^{Elz}$ as follows [143]:

$$P_{Cmp} = \frac{2RT_{cell}^{Elz} k N_{H_2}^{Elz}}{(k-1)\eta_{Cmp}} \left(\left(\frac{\pi_{HS}}{\pi_{H_2}^{Elz}} \right)^{\frac{k-1}{k}} - 1 \right), \quad (3.40)$$

where k and η_{Cmp} are the polytropic coefficient and compressor efficiency, respectively. The hourly electrolyzer hydrogen flow is a function of its power consumption P_{Elz} and efficiency η_{Elz} given by (3.18) and (3.31), which is calculated as below [143]:

$$N_{H_2}^{Elz} = \frac{P_{Elz}\eta_{Elz}}{\Delta H_{LHV}}, \quad (3.41)$$

where ΔH_{LHV} is the lower heating value and equal to $241 kJ/mole$. Then, the compression effect, η_{mc} , on hydrogen production efficiency, η_T , is expressed as follows [103]:

$$\eta_{mc} = 1 - \frac{P_{Cmp}}{(N_{H_2}^{Elz} - N_{loss}^{Elz})\Delta H_{LHV}^{H_2}}, \quad (3.42)$$

here $N_{H_2}^{Elz}$ and N_{loss}^{Elz} represent the hydrogen production flow and the hydrogen flow lost due to the gases crossover phenomenon, respectively.

3.5 HS Modeling

The excess hydrogen production is stored in the local HS. The relation between hydrogen pressure and temperature inside the HS can be modeled using the gas state equation [149].

As the hydrogen starts behaving non-ideally at high-pressure levels, the gas state equation follows the real gas form by including the gas compressibility factor, Z , as follows [150]:

$$\pi_{HS} = \frac{Z E_{H_2} R T_{HS}}{\mathcal{V}_{HS}}, \quad (3.43)$$

where π_{HS} , T_{HS} , and E_{H_2} are the hydrogen pressure, temperature, and amount of substance in HS, respectively. Z is the hydrogen compressibility factor as defined in [151] and [152]. The amount of hydrogen inside the HS, E_{H_2} , is the sum of the HS hourly hydrogen flow, Q_{HS} , as given below:

$$E_{H_2} = \sum_{q=1}^{q=t-1} (1 - \gamma_{HS}) Q_{HS}^q + Q_{HS}^t, \quad (3.44)$$

where γ_{HS} is the HS dissipation rate. The SoH in the HS at hour t is the ratio between the hydrogen amount in the HS at that hour, $E_{H_2}^t$, and the HS capacity in kg of hydrogen, E_{HS} , as follows [143]:

$$SoH^t = \frac{E_{H_2}^t}{E_{HS}}. \quad (3.45)$$

E_{HS} is calculated using the gas state equation, with π_{HS} at its maximum value (i.e., $\pi_{HS}^{\max}$) and T_{HS} at its minimum value (i.e., $T_{HS}^{\min}$). Hence, it is obtained as follows:

$$E_{HS} = \frac{\pi_{HS}^{\max} \mathcal{V}_{HS}}{Z R T_{HS}^{\min}}. \quad (3.46)$$

3.6 BESS Modeling

The associated BESS is modeled according to its SoC at each time instant as a function of its charging and discharging powers, and efficiencies as given hereunder:

$$SoC^t = \begin{cases} (1 - \gamma_{BESS}) SoC^{t-1} + \frac{\eta_{BESS} P_{BESS}^t}{E_{BESS}}, & P_{BESS} \geq 0 \\ (1 - \gamma_{BESS}) SoC^{t-1} + \frac{P_{BESS}^t}{\eta_{BESS} E_{BESS}}, & P_{BESS} < 0 \end{cases}, \quad (3.47)$$

where γ_{BESS} is the BESS dissipation factor and P_{BESS} is positive while charging and negative during the discharge time. The charging and discharging efficiencies are the same and denoted by η_{BESS} .

3.7 Summary

This chapter presents a comprehensive mathematical model of the EHPP, including the steady-state models of the AE and PEME, the dynamic model of the PEME, and the models of the FC, compressor, HS, and BESS. This complete mathematical framework serves as the foundation for the subsequent chapters, which employ these models in the optimal design and scheduling problems.

Chapter 4

Optimal Design of PEME-HPP

Prior studies on the design of PEME-HPPs—such as [82, 110–112, 114]—share common limitations. These include the use of simplified PEME models, the lack of optimization for internal design parameters, and the omission of hydrogen crossover safety constraints. Moreover, these studies do not enforce the requirement for PEME-HPPs to produce green hydrogen, i.e., by consuming electricity solely from RES. They also fail to assess the economic feasibility of integrating on-site BESS or to account for the impact of clean hydrogen subsidies recently introduced by various governments.

To address these research gaps, this chapter introduces a novel mathematical formulation to optimally design grid-connected PEME-HPPs. The findings and methodology presented in this chapter have been published by the researcher in [143, 153]. The objective of the formulated optimization model is to minimize the LCOH for the PEME-HPP shown in Fig. 4.1 to meet a pre-specified hydrogen demand profile. The proposed formulation aims at determining i) the optimal ratings of the main components in the PEME-HPP (PEME, compressor, and power converter), ii) the internal parameters of the PEME (membrane thickness, cell area, and cathodic pressure), and iii) the capacities of the local HS and an optional on-site BESS. In order to consider the source of electricity used to produce hydrogen, six color codes are introduced, as shown in Fig. 4.1. When the PEME-HPP is

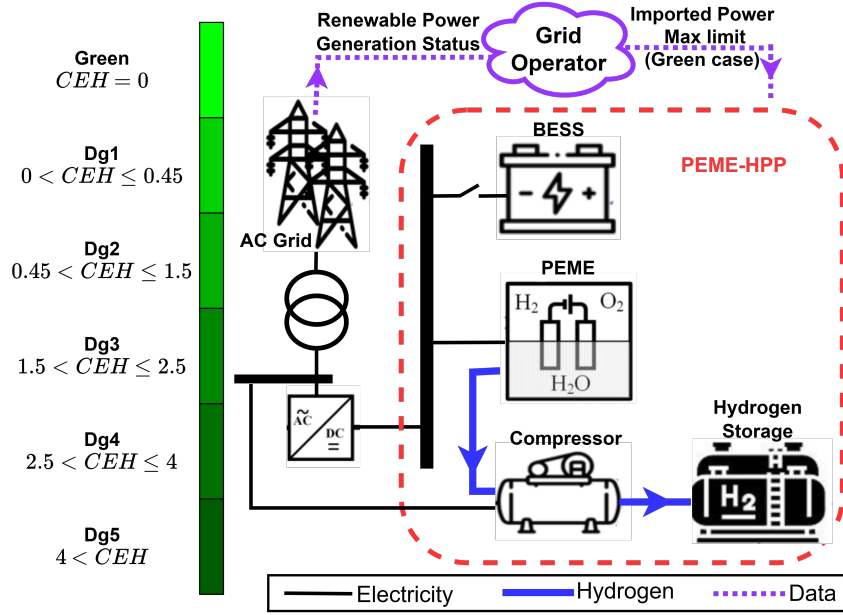


Figure 4.1: Layout of a grid-connected PEME-HPP with BESS.

supplied by 100% renewable power, the produced hydrogen is labelled as green. However, when a mix of renewable and conventional electrical sources is used to supply the PEME-HPP, five levels of dull green color defined as Dg1 to Dg5 are assumed based on the Carbon Emissions per kg of Hydrogen (CEH), where higher numbers refer to higher CEH. For green hydrogen production, this work considers a long-term fixed price PPA between the hydrogen producer and the renewable power generators. Based on the PPA and the grid constraints, the power system operator determines the maximum available renewable power to be consumed by the PEME-HPP. Table 4.1 summarizes the key features of the proposed optimal design of EHPPs compared to previous works. As shown in the table, the following are the main contributions of the proposed model:

- The proposed optimization model incorporates a detailed electrochemical modeling of PEME and defines the internal parameters of its stacks (membrane thickness, cell area, cathodic pressure) as design variables to optimize these parameters in conjunction with the sizing of the PEME-HPP components. This consideration would, in

turn, guide PEME manufacturers to customize the design of their stacks based on the specified application case.

- The model takes into consideration the PEME safety constraints, i.e., permissible amount of hydrogen in oxygen, and their variations with the operating current density, membrane thickness, and cathodic pressure. The inclusion of the PEME safety constraints guarantees that the hydrogen in oxygen percentage would remain within the permissible safe limits for all loading levels.
- An on-site BESS is included in the proposed model as an optional component in the design of the PEME-HPP, where its economic viability, optimal sizing, and effect on the PEME parameters are determined and analyzed. The deployment of on-site BESS could provide a significant reduction in the LCOH and/or cause changes in the required/optimized internal parameters of PEME.
- The model takes into account the clean hydrogen subsidies recently announced by different governments, and analyzes the impact of different subsidies on the LCOH, design of the PEME-HPP, and the PEME parameters. These subsidies have recently announced to propel the hydrogen economy; thus, their impacts on the design of PEME-HPPs should be taken into consideration.

Other features also have various implications on the design of the PEME-HPP and its PEME as follows: i) coupling hydrogen plants with the power grid imposes limitations on the PEME-HPP design and operation such as the available power generation profile (e.g., from RES), electricity tariff, and electrical grid operation constraints (e.g., lines capacity, voltage limits, etc.), ii) enforcing the hydrogen plant to produce green hydrogen from renewable energy resources imposes limitations on the available power supplied to the plant, which forces the PEME-HPP to follow the variations in the produced renewable power and, thus, continuously operate under a wide range of loading levels, iii) consideration of the detailed (practical) PEME model at which the efficiency changes with the change of the loading is paramount; especially when the PEME-HPP is supplied from RES, i.e., variable

Table 4.1: Comparison of Different PEME-HPP Design Formulations

Features of the Proposed Formulation	[35]	[36]	[37]	[107]	[154]	[82]	[110, 111, 114]	[155]	This Work
Coupling with the power grid	✓	✓	✓	✗	✗	✓	✓	✓	✓
Green hydrogen production	✗	✗	✓	✓	✓	✗	✗	✗	✓
Consideration of the PEME efficiency variation with loading	✗	✓	✗	✗	✗	✗	✗	✓	✓
Design of PEME parameters	✗	✗	✗	✗	✗	✗	✗	✗	✓
PEME safety constraint	✗	✗	✗	✗	✗	✗	✗	✗	✓
Consideration of the PEME degradation cost	✗	✓	✗	✗	✗	✗	✗	✓	✓
Clean hydrogen subsidy	✗	✗	✗	✗	✗	✗	✗	✗	✓
On-site BESS	✗	✓	✗	✗	✗	✗	✗	✗	✓
Sizing of the PEME-HPP	✗	✗	✗	✓	✓	✓	✓	✗	✓
Scheduling of the PEME-HPP	✓	✓	✓	✗	✓	✓	✗	✓	✓

loading. Such detailed model is expected to impact the design of the PEME-HPP and PEME parameters (membrane thickness, cell area, and cathodic pressure) aiming at minimizing the LCOH of the plant, iv) including the PEME degradation cost in the formulated optimization model ensures the realistic design and accurate estimation of the LCOH of the hydrogen plant, v) the formulated optimization model combines both sizing and scheduling of the PEME-HPP. This combination will ensure that the optimal design of PEME-HPP components considers the dynamic changes and operational aspects.

The remainder of this chapter analyzes the impact of PEME parameters on its efficiency in Section 4.1 and introduces the proposed optimal design formulation in Section 4.2. Section 4.3 presents the case studies and simulation results. Finally, the summary is provided in Section 4.4.

4.1 Impacts of PEME Parameters on the PEME-HPP Performance

The total hydrogen production efficiency of the PEME-HPP, η_T , is calculated as the product of the PEME efficiency, the power converter efficiency, and the mechanical compression efficiency, as follows:

$$\eta_T = \eta_{PEM} \eta_{Conv} \eta_{mc}. \quad (4.1)$$

Here, the converter efficiency, η_{Conv} , is assumed to be constant as in [143] while η_{PEM} and η_{mc} are obtained as provided earlier in (3.31) and (3.42), respectively.

The effect of the PEME internal parameters, i.e., membrane thickness, cell area, and cathodic pressure, on the total hydrogen production efficiency of the PEME-HPP is investigated over the full range of current densities for a 46 kW PEME with Nafion membrane N117 and 20 bar hydrogen pressure (i.e., cathodic pressure) [103].

Fig. 4.2 (a) shows the impact of the change of different cathodic pressures (10 to 170 bar) on the PEME-HPP efficiency at cell area $A_{cell}^{PEM} = 72.5 \text{ cm}^2$ and membrane thickness $\delta_m^{PEM} = 127 \mu\text{m}$. As shown in the figure, increasing the cathodic pressure at low current

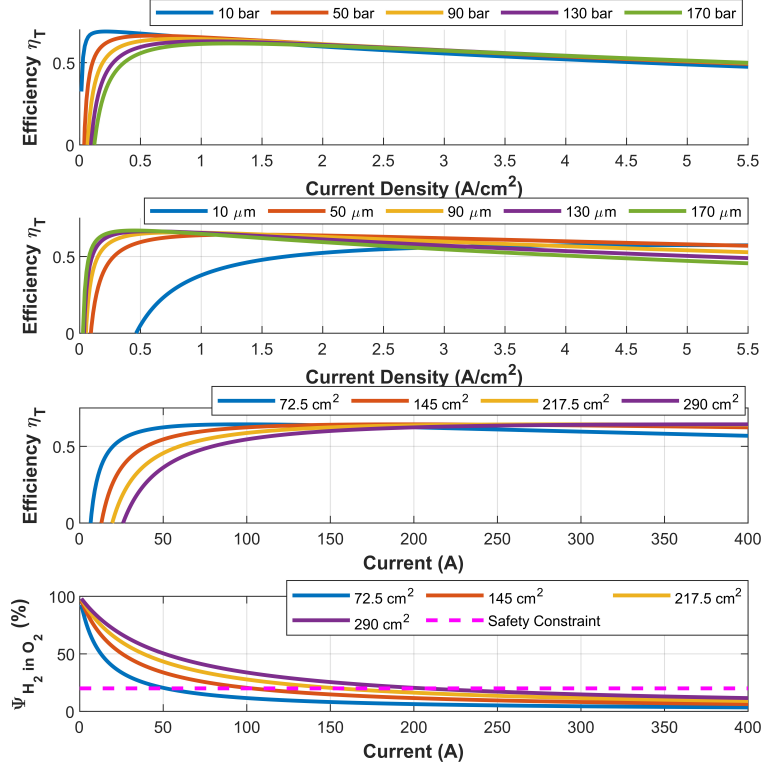


Figure 4.2: PEME-HPP total efficiency η_T at (a) different cathodic pressures, (b) different membrane thicknesses, and (c) different cell areas. (d) Hydrogen in oxygen percentage at different cell areas.

densities reduces the overall PEME-HPP efficiency while surging permeation losses due to the rise in hydrogen crossover. However, the Faraday's efficiency gradually increases, hence its effect at higher current density is no longer significant. In contrast, the compression effort becomes the dominant component at relatively high current densities, which results in slightly higher efficiency for PEME-HPP operating at higher cathodic pressure. In Fig. 4.2 (b), the efficiency characteristic of the same PEME is depicted at different membrane thicknesses, i.e., from 10 to 170 μm , where the cathodic pressure is set at 50 bar and the cell area $A_{cell}^{PEM} = 72.5 \text{ cm}^2$. As shown, unlike the impact of cathodic pressure, increasing the membrane thickness reduces the permeation losses at low current densities as it decreases the hydrogen crossover. However, at higher operating current densities, the efficiency de-

clines significantly as the use of a thicker membrane increases the electrical resistance and hence the corresponding losses.

For a PEME running at $\pi_{H_2}^{PEM} = 50 \text{ bar}$, and $\delta_m^{PEM} = 51 \mu\text{m}$, the total efficiency at different cell areas will follow the same pattern but the rating current density increases when the cell area decreases. However, the total efficiency versus PEME current presented in Fig. 4.2 (c) shows noticeably higher efficiency at low current operation when smaller cell areas are used. The obtained results are expected, since the efficiency curves for small cell areas reach their peak at lower current values, which corresponds to relatively high current density with lower permeation losses. Moreover, the hydrogen production at low current values is much higher when small cells are used, where increasing the operating current density via reducing the cell area will avoid shutting down the PEME when hydrogen in oxygen percentage exceeds the safe value, which is set at 20% [103], at relatively low current values. Fig. 4.2 (d) illustrates how hydrogen in oxygen percentage, $\Psi_{H_2}^{PEM}$, changes with the change of the actual current at different cell areas and constant cathodic pressure and membrane thickness. As shown in the figure, the percentage of hydrogen in oxygen decreases as the current increases. Further, small cell areas offer higher current density and hence lower hydrogen in oxygen percentage compared to larger cell areas. The horizontal dashed line represents the permissible safe limit of hydrogen in oxygen percentage, which shouldn't be exceeded during normal operation, i.e., the PEME would shut down whenever its hydrogen in oxygen percentage exceeds that safe limit. Therefore, the actual and safe operating range of the PEME decreases as its cell area increases. For instance, as shown in Fig. 4.2 (d), a PEME with $A_{cell}^{PEM} = 72.5 \text{ cm}^2$ has a safe operating range from 50 A to 400 A, while a PEME with $A_{cell}^{PEM} = 145 \text{ cm}^2$ has a safe operating range from 100 A to 400 A. From the above discussion, it is noted that continuous hydrogen production is more achievable at low current values for PEMEs with smaller cell areas.

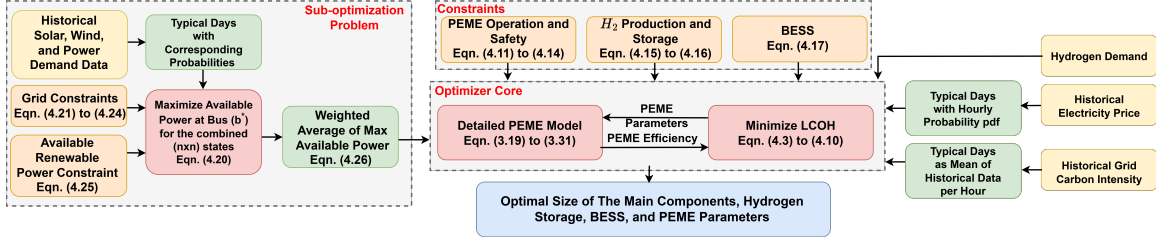


Figure 4.3: Schematic diagram of the proposed optimal design framework for a PEME-HPP.

4.2 Problem Hypothesis and Formulation

This section presents the mathematical formulation required to optimally design the components of the PEME-HPP illustrated in Fig. 4.1. Fig. 4.3 presents a schematic diagram of the proposed design framework. As illustrated in the figure, the core of the optimization problem contains two main interdependent modules (Minimization Module, and PEME model), where PEME efficiency is determined by its model based on the PEME' parameters sent by the minimization module. This data exchange is repeated in each optimization iteration.

The optimizer core is inputted by the pre-specified hydrogen demand profile and historical data for the grid Carbon Intensity (CI) and the electricity price. To account for the uncertainty of the electricity price, the historical data is used to get a normal Probability Density Function (pdf) for each hour in the time period under study. The electricity price pdf functions are discretized into multiple states and the probability of each state is calculated. Then N_{MCS} MCS are generated with their probabilities. The probability of each scenario is calculated as the average of the hourly probability of the electricity prices in that scenario given as:

$$\rho_{ElecPrice}^{mc} = \frac{1}{T} \sum_{t=1}^T \rho_{ElecPrice}^{mc,t} \quad \forall mc \in N_{MCS} \quad (4.2)$$

The optimizer core is also inputted by the maximum available power from RES and/or the grid to be converted into hydrogen at each time step, which is determined based on the

RES generation profile and the grid constraints as described later in section 4.2.3. Assuming that the PEME-HPP is connected to a power transmission system, the objective function of the PEME-HPP design optimization problem is formulated to minimize the LCOH as follows:

$$\text{Min} \left(\frac{CAPEX + \sum_{y \in Y} \left(\frac{\sum_{mc=1}^{N_{MCS}} \rho_{ElecPrice}^{mc} OPEX(mc)}{\sum_{mc=1}^{N_{MCS}} \rho_{ElecPrice}^{mc}} + C_{Deg} \right) / (1+r)^y}{\sum_{y \in Y} (\sum_{t=1}^{\mathbb{T}} Q_d^t) / (1+r)^y} - \Upsilon \right) \quad (4.3)$$

where Y is the PEME-HPP life time in years, and r is the yearly discount rate. The LCOH function given in (4.3) consists of four components: Capital Expenditure (CAPEX), weighted average of Operational Expenditure (OPEX), Degradation Cost (C_{Deg}), and clean hydrogen subsidy represented by (Υ). CAPEX is a function of the power ratings of the PEME, power converter, and compressor, as well as the BESS and HS capacities expressed as follows:

$$CAPEX = P_{PEM}^{rate} C_{PEM} + P_{BESS}^{rate} C_{BESS} + P_{Conv}^{rate} C_{Conv} + P_{Cmp}^{rate} C_{Cmp} + E_{HS} C_{HS} \quad (4.4)$$

Here, the rated power and capacities of the different equipment in the PEME-HPP are treated as decision variables.

The OPEX of each electricity price scenario is the summation of the hourly electricity and operational costs given as:

$$\begin{aligned} OPEX(mc) = & \sum_{t=1}^{\mathbb{T}} P_{grid}^t Price_{elec}^t(mc) + N_{PEM}^{H_2,t} O_w + Q_{HS}^t O_{HS} \\ & + P_{PEM}^t O_{PEM} + P_{Cmp}^t O_{Cmp} \end{aligned} \quad (4.5)$$

The electricity price, $Price_{elec}^t$, employed for hydrogen production depends on the agreement between the grid and PEME-HPP operators. In this work, the electricity price is assumed to follow a PPA when the PEME-HPP produces hydrogen from RES. Otherwise, the price is determined based on the applied electricity market rules. In both scenarios, Grid Operation Fees (GOF) such as delivery charges, are added to the costs of electricity. Hence,

the electricity price at each time step t could be expressed as follows:

$$Price_{elec}^t = \begin{cases} PPA: \text{Fixed PPA Price} + GOF \\ Grid: \text{Hourly Generation Price} + GOF \end{cases} \quad \forall t \in \mathbb{T} \quad (4.6)$$

The hourly electricity cost of the PEME-HPP depends on the total power imported from the grid (P_{grid}^t), which is the sum of power consumed by the PEME, compressor, and BESS. The total imported power can be expressed as:

$$P_{grid}^t = P_{PEM}^t + P_{Cmp}^t + P_{BESS}^t \quad \forall t \in \mathbb{T} \quad (4.7)$$

Here, in the OPEX formula, P_{PEM}^t , P_{BESS}^t , and Q_{HS}^t are the decision variables, while P_{Cmp}^t and $N_{PEM}^{H_2}$ are calculated according to (3.40) and (3.41), respectively, as described in Section 3.5.

The C_{Deg} considers both the PEME and BESS as below:

$$C_{Deg} = \sum_{t=1}^{\mathbb{T}} |P_{BESS}^t| D_{BESS}^t + P_{PEM}^t D_{PEM}, \quad (4.8)$$

The BESS degradation cost is a function of its SoC, charging and discharging frequency, BESS capital cost, C_{BESS} , and residual value, RS_{BESS} , as well as its capacity and round-trip efficiency given as [36]:

$$D_{BESS}^t = \frac{C_{BESS} - RS_{BESS}}{2(1 - SoC^t) Acc^t E_{BESS} \eta_{BESS}} \quad \forall t \in \mathbb{T} \quad (4.9)$$

where Acc^t is the achievable cycle count, which is calculated as follows:

$$Acc^t = \frac{a}{(1 - SoC^t)^b} \quad \forall t \in \mathbb{T} \quad (4.10)$$

4.2.1 PEME Operation and Safety Constraints

The operation of the PEME includes constraints on the current densities, cell area, and maximum cathodic pressure, expressed in (4.11), (4.12), and (4.13), respectively.

$$0 \leq \frac{P_{PEM}^t}{V_{PEM}^{rate} A_{cell}^{PEM}} \leq J_{max}^{PEM} \quad \forall t \in \mathbb{T} \quad (4.11)$$

$$A_{cell}^{PEM,min} \leq A_{cell}^{PEM} \leq A_{cell}^{PEM,max} \quad (4.12)$$

$$\pi_{H_2}^{PEM,min} \leq \pi_{H_2}^{PEM} \leq \pi_{H_2}^{PEM,max} \quad (4.13)$$

For safety considerations, the percentage of hydrogen in oxygen given in (3.28) is restricted by the maximum allowable limit of hydrogen in oxygen, $\Psi_{H_2}^{PEM,safe}$, as follows:

$$\Psi_{H_2}^{PEM} \leq \Psi_{H_2}^{PEM,safe} \quad (4.14)$$

4.2.2 HS and BESS Constraints

The excess of hydrogen production is stored in local HS tanks, where the SoH is constrained by the maximum and minimum allowed SoH given as follows:

$$SoH^{min} \leq SoH^t \leq SoH^{max} \quad \forall t \in \mathbb{T} \quad (4.15)$$

In addition, the hydrogen flow must satisfy the hydrogen balance equation expressed as:

$$N_{H_2}^{PEM,t} + Q_{HS}^t = Q_d^t \quad \forall t \in \mathbb{T} \quad (4.16)$$

The SoC for the BESS has to be limited between the manufacturer-prescribed minimum and maximum percentages as given hereunder:

$$SoC^{min} \leq SoC^t \leq SoC^{max} \quad \forall t \in \mathbb{T} \quad (4.17)$$

4.2.3 Power Grid Constraints

The design of a PEME-HPP connected to the power grid is constrained by the maximum available power at the point of connection, bus (b^*). The maximum available power is determined by the grid operator based on capacity assessment and power flow studies. However, when the plant is designed mainly to produce green hydrogen, the maximum available power should consider the dynamic changes of the produced power from RES. In such a case, the maximum available power to the PEME-HPP will vary based not only on the grid constraints but also the RES generation profile. For this reason, a sub-optimization

problem is formulated in this work to yield the maximum available power, $(P_{b^*,max}^t)$, at bus b^* to which the PEME-HPP is connected. Based on this approach, all grid constraints, including the production of green hydrogen from RES are represented in the PEME-HPP design problem with one constraint expressed as follows:

$$0 \leq P_{grid}^t \leq P_{b^*,max}^t \quad \forall t \in \mathbb{T} \quad (4.18)$$

The sub-optimization problem is inputted by historical wind speed and solar irradiation data, which is used to obtain typical days representing the four seasons. The pdf of each hour is calculated using Beta pdf (f_b) and Rayleigh pdf (f_r) for solar irradiation and wind speed, respectively [156]. The obtained pdf functions of each hour are discretized into n states covering the whole solar irradiation and wind speed ranges of that hour. Next, the probability of each irradiation state $\rho(SI^{i,t})$ and wind speed state $\rho(WS^{j,t})$ is calculated using Cumulative Density Function (cdf) as in [156]. Hence, the total number of the combined states at each hour equals (hxx) , where the probability of each combined state is given in (4.19) assuming no correlation exists between the renewable power generation in each hour and its adjacent ones. Also, typical days of the electrical demand are produced as the mean of historical power demand data to represent the four seasons.

$$\rho^{s,t} = \rho(SI^{i,t}) \cdot \rho(WS^{j,t}) \quad \forall t \in \mathbb{T} \wedge s = 1, \dots, hxx \wedge i, j = 1, \dots, h \quad (4.19)$$

The objective function of the sub-optimization problem at each hour is formulated as follows:

$$\text{Maximize } P_{b^*}^{s,t} \quad \forall t \in \mathbb{T} \wedge s = 1, \dots, hxx \quad (4.20)$$

where (4.20) is subject to the voltage magnitude, thermal line capacity, and active and reactive power flow constraints as given in (4.21), (4.22), (4.23), and (4.24), respectively.

$$V_b^{min} \leq V_b^{s,t} \leq V_b^{max} \quad \forall t \in \mathbb{T} \wedge s = 1, \dots, hxx \quad (4.21)$$

$$S_{b,q}^{s,t} \leq S_{b,q}^{max} \quad \forall t \in \mathbb{T} \wedge s = 1, \dots, hxx \quad (4.22)$$

$$P_{b,g}^{s,t} = P_{b,d}^{s,t} + V_b^{s,t} \sum_{q=1}^B V_q^{s,t} \mathbb{Y}_{b,q} \text{Cos}(\delta_b^{s,t} - \delta_q^{s,t} - \theta_{b,q}) \quad \forall t \in \mathbb{T} \wedge s = 1, \dots, hxx \quad (4.23)$$

$$Q_{b,g}^{s,t} = Q_{b,d}^{s,t} + V_b^{s,t} \sum_{q=1}^B V_q^{s,t} \mathbb{Y}_{b,q} \text{Sin}(\delta_b^{s,t} - \delta_q^{s,t} - \theta_{b,q}) \quad \forall t \in \mathbb{T} \wedge s = 1, \dots, hxx \quad (4.24)$$

When the produced hydrogen is specified to be fully green, the sub-optimizer objective function is constrained by the maximum available renewable power, given as:

$$P_{b^*}^{s,t} \leq \sum_{g=1}^G P_{PV,g}^{s,t} + \sum_{m=1}^M P_{W,m}^{s,t} + \Re(1 - \mathbb{B}) \quad \forall t \in \mathbb{T} \wedge s = 1, \dots, hxx \quad (4.25)$$

where $\Re$ is a very large number and $\mathbb{B}$ is a Boolean variable that activates and deactivates the renewable generation constraint in (4.25). $\mathbb{B}$ equals to one if pure green hydrogen production is mandated and zero otherwise.

It is noteworthy that the objective function in (4.20) is calculated (hxx) times at each hour to obtain the hourly maximum available power of each combined state $P_{b^*}^{s,t}$. Then, at each hour, the weighted average of the power obtained for these (hxx) states is calculated to get the hourly maximum available power $P_{b^*,max}^t$ at the selected bus b^* as follows:

$$P_{b^*,max}^t = \frac{\sum_{s=1}^{hxx} \rho^{s,t} \times P_{b^*,max}^{s,t}}{\sum_{s=1}^{hxx} \rho^{s,t}} \quad \forall t \in \mathbb{T} \quad (4.26)$$

4.3 Case Studies and Simulation Results

The IEEE 30-bus test transmission system [157] shown in Fig. 4.4 is used to validate the effectiveness of the proposed design for a PEME-HPP. Two wind power plants, sized at 600 MW each, are connected to buses 20 and 30. Also, a 500 MW solar PV plant is connected to bus 26. The PEME-HPP is to be connected to bus 18. Six case studies are carried out to validate the effectiveness of the proposed problem formulation as summarized in Table 4.2. In the first case, the PEME is modeled by a constant conversion rate in kWh/kg as utilized in [82]. The other five cases utilize the detailed steady state model provided in subsection 3.2.1. In case 2, predefined PEME internal parameters (obtained from a manufacturer's technical sheet) are utilized without considering the safety constraints. In the third case, PEME parameters are optimized concurrently with the sizing of the PEME-HPP without

Table 4.2: Summary of Case Studies

Case No.	BESS	PEME Parameters	Safety Constraints	PEME Model
1 [82]	✗	✗	✗	Constant Efficiency and kg/kWh
2	✗	✗	✗	Detailed Model Presented in 3.2.1
3	✗	✓	✗	
4	✗	✗	✓	
5	✗	✓	✓	
6	✓	✓	✓	

considering the PEME safety constraints. The fourth case considers predetermined PEME parameters, as in case 2, but takes into account its safety constraints. The fifth case considers both the optimal design of the PEME parameters and the safety constraints into account. In the sixth case study, the PEME-HPP is equipped with a BESS where the PEME parameters are optimized as in case 5 while considering the PEME safety constraints.

Five years hourly historical data for solar irradiation and wind speed in the province of Ontario, Canada [158] has been collected. The historical data is then used to generate the hourly solar irradiation and wind speed profiles of four typical days representing the four seasons of the year. Each hour is represented by five states for both solar irradiation and wind speed. Hence, there are 25 (5x5) combined states for each hour. Also, the historical electrical demand in the province of Ontario [159] is used to calculate the mean of hourly demand for four typical days of the four seasons as given in Fig. 4.5 (a). At each hour, the weighted average of maximum available power of the 25 combined states is calculated at the selected bus ($b^* = 18$) to obtain the available power for green and dull green hydrogen production as demonstrated in Fig. 4.5 (b). As shown in the figure, the available power profile to produce dull green hydrogen at bus 18 is quite different from the renewable available power to produce green hydrogen at the same bus. The latter

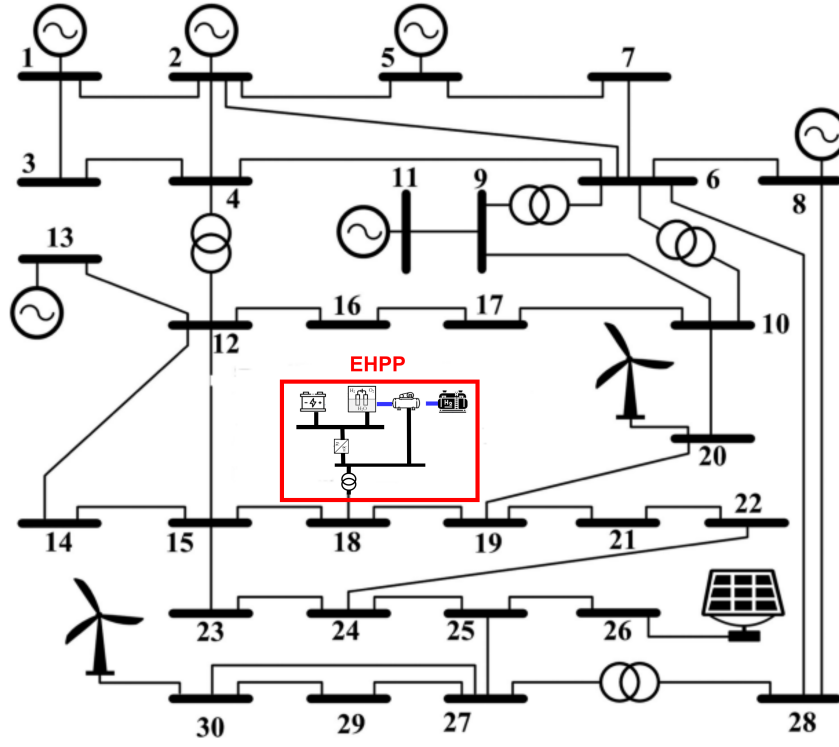


Figure 4.4: Single line diagram of the IEEE 30-bus system under study with the PEME-HPP connected to bus 18.

is capped by both grid constraints and maximum renewable generation connected to the studied network. Clearly, as depicted in Fig. 4.5 (b) renewable power generation limits the maximum renewable available power for green hydrogen production during night time while other grid constraints cap the available power during day time.

Historical data for the electricity market price given by the Independent Electricity System Operator (IESO) [159] in Ontario is used to generate 1000 scenarios, where each scenario has its own probability as given in (4.2). High power consumers are charged with multiple components that include Hourly Ontario Energy Price (HOEP) and GOFs such as regulatory services, delivery charges, and supply services. When a renewable PPA is used, the energy price is set at a fixed rate while the same GOFs are applied. In this work, it is assumed that the energy price for PPA is set at $20\$/MWh$ as given in [105] and [160]. The

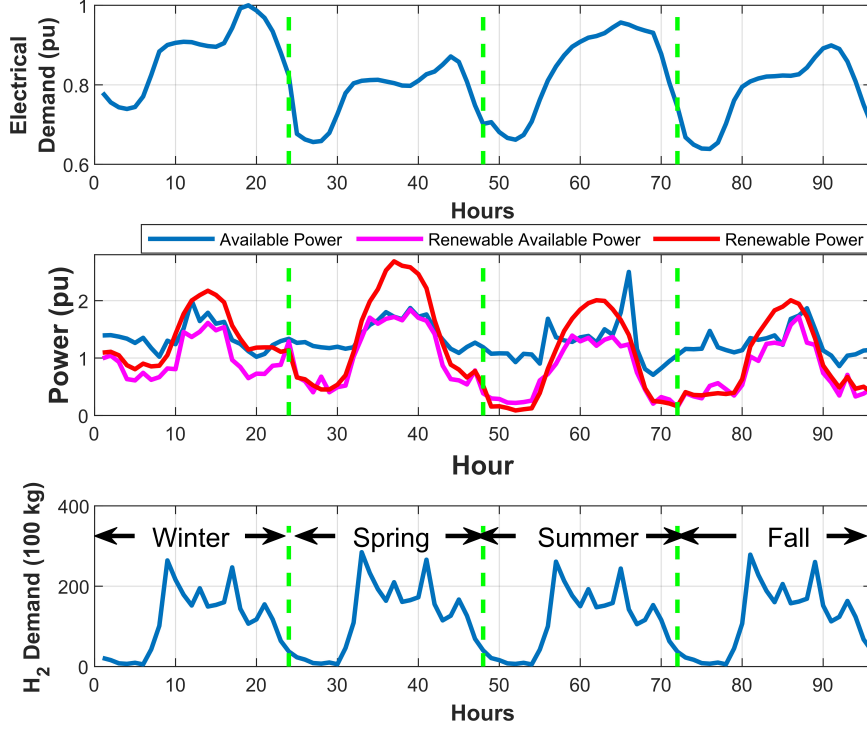


Figure 4.5: (a) Electrical demand profile, (b) Available power at bus 18, available renewable power at bus 18, and total connected renewable power, (c) Hydrogen demand profile of the four typical days.

subsidy term, represented by Υ , is assumed to be set based on the Production Tax Credit (PTC), which is modeled as a function of the CEH as given in (4.27). The subsidy values are chosen as announced by the USA federal government in [161].

$$\Upsilon = \begin{cases} 3 \$ & , 0 \leq CEH \leq 0.45 \\ 1 \$ & , 0.45 < CEH \leq 1.5 \\ 0.75 \$ & , 1.5 < CEH \leq 2.5 \\ 0.6 \$ & , 2.5 < CEH \leq 4 \\ 0 \$ & , CEH > 4 \end{cases} \quad (4.27)$$

The CEH is a function of the hourly CI and can be obtained as in (4.28). The used hourly

CI is the mean of the historical hourly CI of the Ontario electrical grid.

$$CEH = \frac{\sum_{t=1}^T CI^t P_{grid}^t}{\sum_{t=1}^T N_{H_2}^{PEM,t}} \quad \forall t \in \mathbb{T} \quad (4.28)$$

Without loss of generality, the hydrogen demand profile is derived from the aggregation of vehicles demand in several gas stations [34], assuming that internal combustion engine vehicles are replaced by hydrogen-powered cars. The aggregated demand is then used to find four typical days of hydrogen demand to represent the whole year by finding the mean of the hydrogen demand profile as shown in Fig. 4.5 (c). Other simulation parameters listed in Table 4.3 are imported from previous techno-economic studies in the literature [36], [82].

The proposed formulation explained in section 4.2 is solved using Sequential Quadratic Programming (SQP) that is available as a built-in function in MATLAB's optimization toolbox. The convergence, constraints and decision variables tolerances are set to 10^{-6} . The platform used to conduct these simulations has the following specs: Core i7-10700K, 3.8 GHz CPU, 32 GB RAM, and 64 bits system.

4.3.1 Cases 1 to 3: The Significance of Optimizing the PEME Internal Parameters

In this subsection, the results obtained for cases 1, 2, and 3 are presented and analyzed. In case 1, the PEME is modeled with a constant conversion rate in kg/kWh, i.e., without consideration of i) the detailed model provided in section 3.2.1, or ii) the design of the PEME internal parameters, and iii) safety constraints. In this case, the cathodic pressure π_{H_2} needs to be predetermined in order to facilitate the design of other components in the PEME-HPP, e.g., the mechanical compressor. Therefore, and without loss of generality, the cathodic pressure π_{H_2} is set in this case at 30 bar as given in most commercially available PEME [162]. Table 4.4 shows the obtained optimal sizes of the PEME-HPP components for pure green and dull green scenarios. As shown in the table, the rated powers of the different components in the designed dull green PEME-HPP is higher than those in pure green PEME-HPP as the dull green scenario suffers from larger variations in electricity

Table 4.3: Simulation Parameters

Parameter	Value	Parameter	Value
C_{PEM}	600 $k\$/MW$	k	1.4
C_{BESS}	100 $k\$/MW$	η_{BESS}	97.5%
C_{Cmp}	7.52 $k\$/MW$	$\gamma_{BESS}, \gamma_{HS}$	0.006%
C_{HS}	124 $\$/kg$	α^{PEM}	0.43
O_w	0.08 $\$/kg$	a_x	1.2×10^{-5}
O_{PEM}	17 $k\$/MWh$	$Pr_{H_2}^{PEM}$	$5.31 \times 10^{-16} \text{ mole/sPa}$
O_{Cmp}	1.5% C_{Cmp} $k\$/MWh$	R_o^{PEM}	$27 m\Omega cm^2$
O_{HS}	2% $C_{HS}\$/kg$	ΔH_{vap}	41572 $J/mole$
D_{PEM}	40% C_{PEM} $k\$/MWh$	$\pi_{H_2O}^{PEM}, \pi_{O_2}^{PEM}$	0.48 bar , 1 bar
C_{Conv}	120 $k\$/MVA$	$\pi_{HS}, \Psi_{H_2}^{PEM, safe}$	500 bar , 10%
V_{LHV}	1.25 V	η_{Cmp}	63%
ΔH_{LHV}	241 $kJ/mole$	$a, b, \mathfrak{s}_m^{PEM}$	2744, 1.665, 1.15

Table 4.4: Parameters of the optimally designed PEME-HPP for cases 1 to 4

Item	Parameter	Green				Dull Green (Dg3)			
		Case 1	Case 2	Case 3	Case 4	Case 1	Case 2	Case 3	Case 4
PEME	δ_m^{PEM}	–	N212	N211	N212	–	N212	N212	N212
	$\pi_{H_2}^{PEM} (bar)$	30	30	28	30	30	30	54	30
	$A_{cell}^{PEM} (m^2)$	–	2124	1888	1102	–	1877	1968	1368
	$Pr_{PEM}^{rate} (MW)$	113	121	104	63	115	107	112	78
Elec. Devices	$Pr_{Conv}^{rate} (MW)$	116	124	107	65	118	110	116	80
	$Pr_{Cmp}^{rate} (MW)$	18	21	19	11	18	18	14	13
H_2 Storage	$E_{HS} (100kg)$	224	240	228	216	247	247	247	213
Cost	$LCOH (\$/kg)$	4.88	4.5	4.3	5.9	7	6.7	6.4	7.9

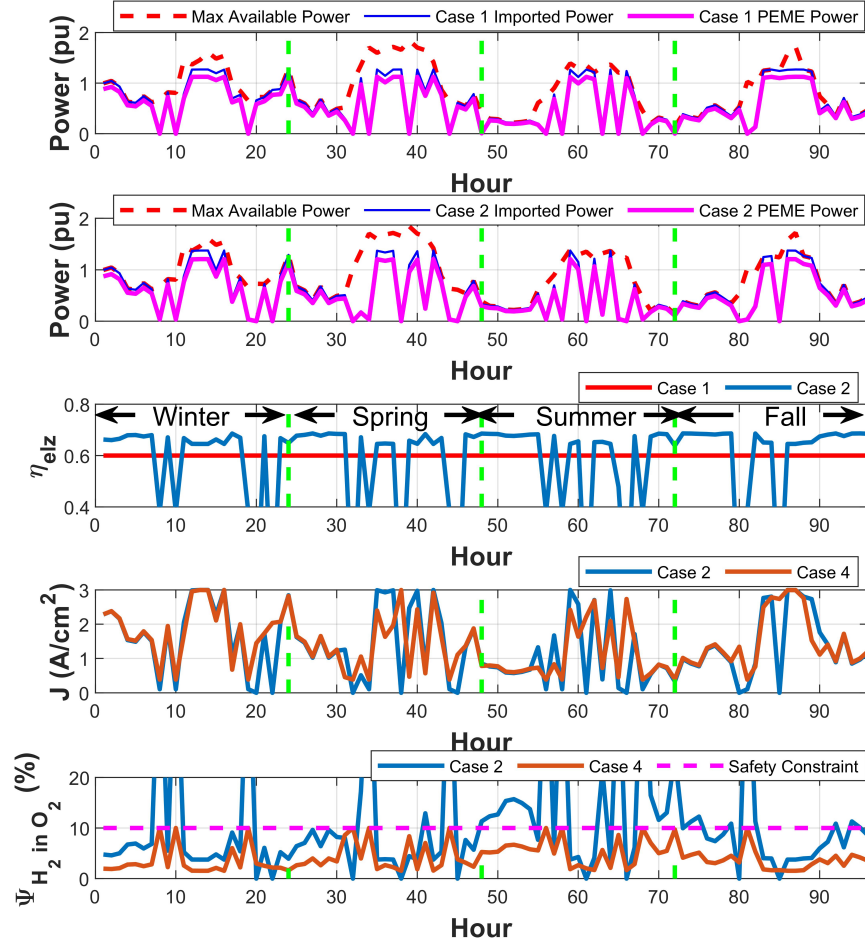


Figure 4.6: (a) Imported and PEME power of case 1, (b) Imported and PEME power of case 2, (c) PEME efficiency of case 1 and case 2, (d) PEME current density of case 2 and 4, and (e) Hydrogen in oxygen percentage of case 2 and 4

prices compared to the green scenario that obtains electricity through a PPA. Hence, higher power ratings are required to minimize/avoid the operation of the dull green PEME-HPP at high electricity prices. As depicted in the table, the LCOH in the pure green PEME-HPP scenario is 30% lower than the dull green PEME-HPP. The produced dull green hydrogen is labeled as Dg3 as the resultant CEH equals to $1.82 \text{ CO}_2\text{kg}/\text{H}_2\text{kg}$. Thus, the dull green PEME-HPP qualifies to 0.75\$ subsidy. Fig. 4.6 (a) shows the total imported power and PEME power consumption for the pure green hydrogen production of case 1. As depicted in

Fig. 4.6 (a), the total power consumption is kept within the limits of the maximum available renewable power. The corresponding PEME efficiency is given in Fig. 4.6 (c). As illustrated in the figure, the efficiency is constant over the entire time window (the four typical days) under study. Modeling the PEME with a constant conversion rate does not reflect the impacts of PEME loading (power consumption) variation on its operating efficiency. As such, the PEME efficiency doesn't change during the four typical days. Further, ignoring the detailed modeling of PEME makes it impossible to calculate the hydrogen in oxygen percentage and hence safe operation of PEME during the studied time window can not be explored and is not guaranteed.

In case 2, the PEME detailed model provided in 3.2.1 is considered. However, membrane thickness and cathodic pressure are not considered as a part of the optimization problem, i.e. these two PEME parameters are chosen as utilized in the most commercially available units instead of being optimized within the optimization problem. The Nafion membrane thickness is chosen to be N212, which is known to be one of the economic options [103]. The cathodic pressure $\pi_{H_2}^{PEM}$ is set at 30 bar as the case in most commercially available PEME [162]. The cell area is determined by the optimization algorithm as the rated power (sizing) of PEME depends on the selection of the cell area, i.e., the PEME rated power can not exceed the capability (maximum current) of the chosen cell area, and thus, the cell area can not be predefined while optimizing the PEME rating. As shown in Table 4, the utilization of the PEME model has resulted in different LCOH. Specifically, the LCOH has been decreased by 8% and 4% for pure and dull green hydrogen, respectively. Fig. 4.6 (b) depicts the total imported power and PEME power consumption for the pure green hydrogen production in case 2. Fig. 4.6 (c) shows the changes of the PEME efficiency with the change of loading. In contrast to case 1, where PEME efficiency remains constant regardless of loading, Fig. 4.6 (c) highlights that in case 2, the efficiency of PEME varies with its loading. As such, case 2 properly considers the impact of loading level on PEME efficiency and, hence, on the LCOH.

In case 3, the detailed model of PEME is considered and the PEME internal parameters are optimized in accordance with the design of the PEME-HPP. It's important to mention

that the membrane thickness is optimized among the four commercially available Nafion membrane thickness options ($N211-25.4\mu m$, $N212-51\mu m$, $N115-127\mu m$, $N117-183\mu m$). Compared with case 2, optimizing the PEME parameters decreased the LCOH by 4.4% and 4.5% for green and dull green hydrogen, respectively, as shown in Table 4.4. For the pure green hydrogen the optimal PEME design incorporates a thin membrane, N211, and a 28 bar cathodic pressure that keeps relatively high PEME efficiency at both low and high current densities to fit the large variations of the available renewable power profile. For the dull green hydrogen, the available power profile exhibits a more uniform distribution, requiring a shift of the peak of the PEME efficiency curve to a relatively high current density, and hence a thicker membrane, N212, with 54 bar cathodic pressure are employed.

For the pure PEME-HPP of case 3, Fig. 4.7 (a) shows that the total imported power fulfills the constraint of maximum available power. The SoH illustrated in Fig. 4.7 (b) varies mainly with the hydrogen demand and slightly affected by other factors such as the electricity price. Fig. 4.7 (c) shows large variations in the PEME current density that lead to corresponding fluctuations in the level of hydrogen in oxygen percentage as depicted in Fig. 4.7 (d). As case 3 ignores the PEME safety constraints, the hydrogen in oxygen percentage freely exceeds the safe limit, 10%, as shown in Fig. 4.7 (d).

4.3.2 Cases 4 and 5: The Impact of Considering the PEME Safety Constraint

In case 4, the design of the PEME-HPP employs the detailed PEME model without optimizing its internal parameters. Further, case 4 takes into account the safety constraints of the PEME. As in case 2, the Nafion membrane thickness and the cathodic pressure are chosen to be N212, and 30 bar, while the cell area is determined by the optimization algorithm. As provided in Table 4.4, the green and dull green hydrogen LCOH is, respectively, 31% and 18% higher than that of case 2. This highlights the influence of considering the PEME safety constraints on the LCOH. Additionally, the incorporation of these safety constraints restricts the PEME's operation at lower current densities, resulting in the uti-

lization of smaller PEME units when compared to the first three cases. Fig. 4.6 (d) shows the hourly variations in current densities of case 2 and case 4. As shown in the figure, PEME current density in case 2 ranges from 0.1 to $3A/cm^2$, while in case 4 it fluctuates between 0.4 and $3A/cm^2$. This reflects the avoidance of operating at very low current densities when safety constraints are employed as in case 4. Fig. 4.6 (e) shows the hydrogen in oxygen percentage for both case 2 and case 4. As depicted in the figure, case 2 does not ensure that the percentage of hydrogen in oxygen remains within the safe range. Conversely, case 4 adheres to the safety constraints applied to the hydrogen in oxygen percentage. Case 5 considers sizing the PEME-HPP components (PEME, power converters, and compressor units) while optimizing the PEME parameters. Table 4.5 provides the obtained parameters of the optimally designed PEME-HPP at the four commercially available Nafion membrane thicknesses ($N211 - 25.4\mu m$, $N212 - 51\mu m$, $N115 - 127\mu m$, $N117 - 183\mu m$) [103]. In the scenario of pure PEME-HPP, the corresponding LCOH shows that the choice of medium membrane thicknesses, i.e., N212 and N115, achieves the least LCOH. It is noted that PEME with thinner membrane, N211, suffers from high hydrogen crossover losses at low current densities and, thus, its LCOH is 8.5% higher than the N212. Also, the thicker membrane, N117, suffers from high ohmic losses when it operates at high current densities, hence wider cell area is needed to limit such losses. Nevertheless, it is noted that the LCOH would be 6.4% higher than the N212. To achieve optimal operation, the PEME cathodic pressure rises when the electrolyzer membrane becomes thicker, where increasing the thickness allows such rise in pressure while maintaining hydrogen crossover within the safe limits.

For dull green PEME-HPP, similar variations in the cathodic pressure and the cell area of the PEME can be observed with increasing the membrane thickness. Table 4.5 shows that the N212 membrane provides the lowest LCOH for dull green PEME-HPP, which is the same as in the green PEME-HPP scenario. For all membrane thicknesses, the produced hydrogen is labeled as Dg3 based on its level of CEH.

Compared to Case 4, non optimized PEME parameters, Case 5 provides 20% and 9% reduction in the LCOH for green and dull green hydrogen, respectively. The optimal cathodic

Table 4.5: Parameters of the optimally designed PEME-HPP for cases 5 and 6

	Item	Parameter	Green				Dull Green (Dg3)				
Case 5	PEME	δ_m^{PEM}	N211	N212	N115	N117	N211	N212	N115	N117	
		$\pi_{H_2}^{PEM}(bar)$	7	13	32	40	6	12	21	28	
		$A_{cell}^{PEM}(m^2)$	1513	1747	1899	2156	1640	1717	1877	2170	
		$P_{PEM}^{rate}(MW)$	82	99	119	132	89	97	117	120	
		$P_{Conv}^{rate}(MW)$	85	102	122	136	92	100	121	124	
	Elec. Devices	$P_{Cmp}^{rate}(MW)$	29	26	18	17	34	27	22	19	
		H_2 Storage	$E_{HS}(100kg)$	217	229	239	241	247	247	247	247
	Cost	$LCOH(\$/kg)$	5.1	4.7	4.8	5	7.6	7.2	7.4	7.5	
	Case 6	PEME	δ_m^{PEM}	N211	N212	N115	N117	N211	N212	N115	N117
$\pi_{H_2}^{PEM}(bar)$			22	45	38	54	26	50	33	52	
$A_{cell}^{PEM}(m^2)$			1301	1424	2098	2228	1235	1254	1842	2124	
$P_{PEM}^{rate}(MW)$			71	81	132	149	68	72	115	142	
$P_{Conv}^{rate}(MW)$			153	138	169	168	158	156	236	163	
Elec. Devices		$P_{Cmp}^{rate}(MW)$	15	11	13	15	13	9	17	10	
		$P_{BESS}^{rate}(MW)$	78	52	102	94	88	83	120	111	
		$E_{BESS}(MWh)$	312	209	406	377	350	331	480	445	
		H_2 Storage	$E_{HS}(100kg)$	195	222	186	205	226	222	221	233
		Cost	$LCOH(\$/kg)$	4.6	4.2	4.9	5.1	6.8	6.6	7.3	7.6

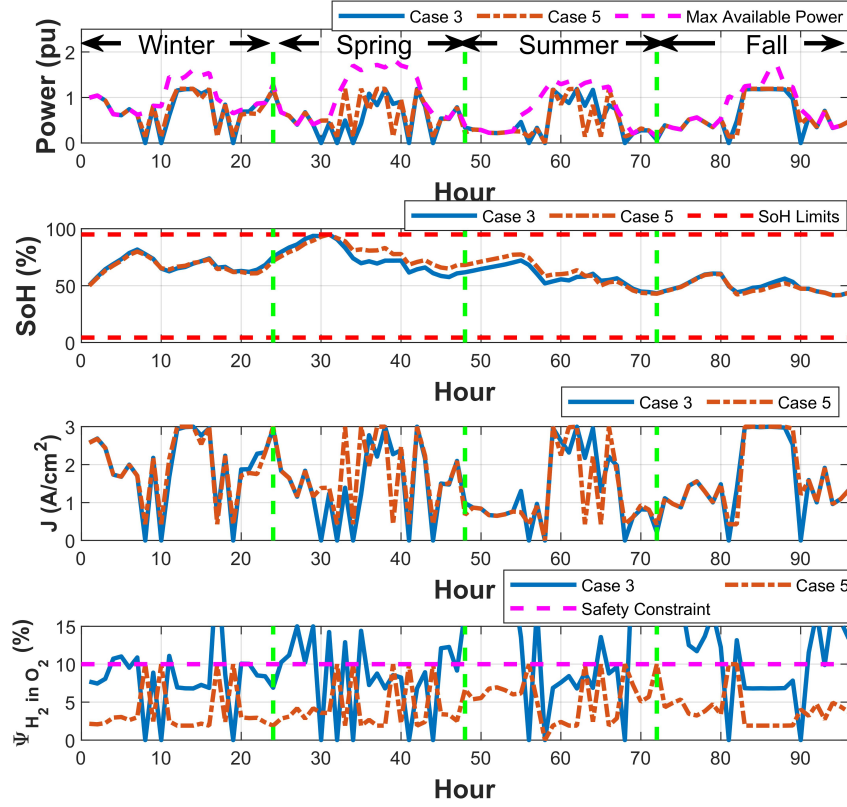


Figure 4.7: (a) Imported power, (b) SoH, (c) current density, (d) hydrogen in oxygen percentage of the optimal PEME-HPP of case 3 and 5.

pressure for both green and dull green hydrogen is much lower than that proposed in case 4. Further, the employment of that low pressure allowed utilizing wider cell area to achieve higher efficiency without violating the PEME safety constraints. When compared with case 3, Fig. 4.7 (a), shows the total imported power of the green PEME-HPP of case 5 with N212 membrane, the optimal membrane thickness. As shown in the figure, the imported power has a pattern similar to that of the green PEME-HPP in case 3. Similarly, the SoH and PEME current density are quite similar to those of case 3 as depicted in Fig. 4.7 (b) and (c). However, in case 5, the hydrogen in oxygen percentage is kept within the safe limit as illustrated in Fig. 4.7 (d). This safe limit has been achieved as case 5 utilizes lower cathodic pressure for both green and dull green hydrogen scenarios, in addition to employing

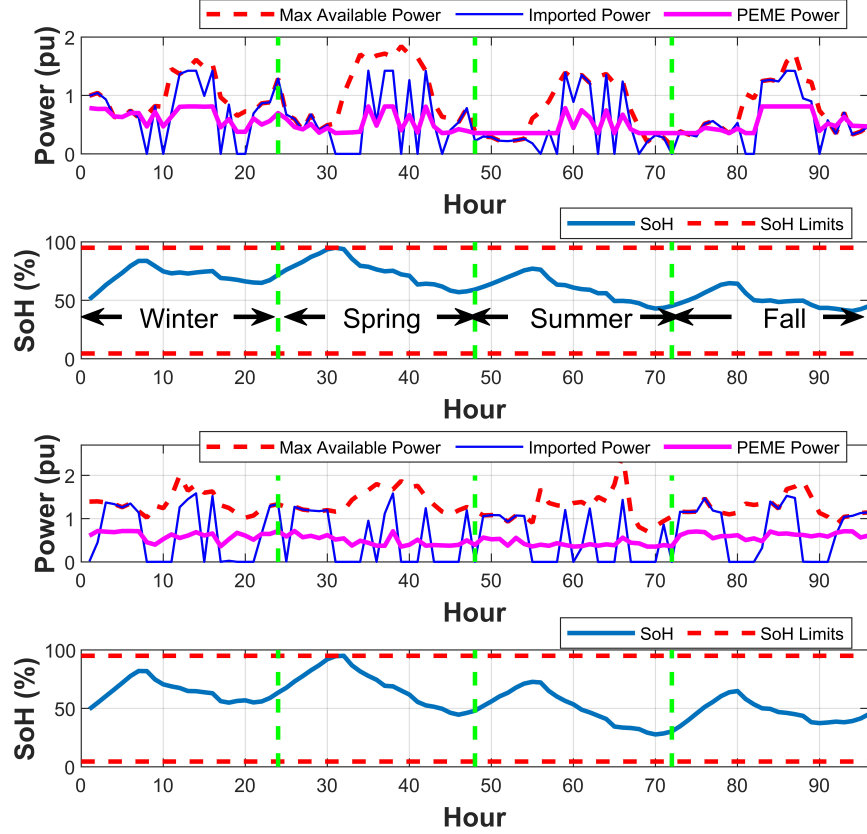


Figure 4.8: (a) Imported power, PEME power, and (b) SoH of the optimal green PEME-HPP of case 6, (c) Imported Power, PEME power, and (d) SoH of the optimal dull green PEME-HPP of case 6.

a thicker membrane for the green hydrogen scenario when compared with case 3.

4.3.3 Case 6: The Effect of BESS on The PEME Internal Parameters

Table 4.5 gives the optimal sizing parameters for the four commercially available Nafion membrane thicknesses and depicts the corresponding LCOH for both green PEME-HPP and dull green PEME-HPP. Similar to case 5, the cost of green hydrogen production is minimum for intermediate membrane thicknesses of N212 and N115. With thinner and thicker membrane thicknesses, LCOH increases by 9.5% and 21%, respectively.

As the membrane becomes thicker, the PEME tends to operate at lower current densities

to minimize the ohmic losses, which could also increase the electrolyzer cell area. Simultaneously, the cathodic pressure rises to achieve the optimal operation as the increase of membrane thickness allows such rise in the pressure without surging the hydrogen crossover. However, such described behaviour contradicts the one associated with the reduction of the operating current densities caused by increasing the cell area. It is observed that the reduction in operating current densities upsurges hydrogen crossover as explained earlier in Fig. 4.2 (d). For this reason, the cathodic pressure declines to 38 bar with N115 membrane. Compared to Case 5 (without BESS), the optimal cathodic pressure in Case 6 (with BESS) is much higher at the same membrane thickness. This is because the BESS enables the PEME to avoid low current density operation without being forced to import power from the grid at high prices.

Fig. 4.8 (a) and (b) show the imported power from the grid, PEME consumed power, and SoH for membrane N212 that yields the minimum LCOH. As shown, the imported power from the grid is kept within the envelop of the maximum available renewable power. The results show that the PEME power profile does not follow the imported power from the grid, where large fluctuations are handled by the BESS. The SoH shows a quietly repeated pattern, where it increases during night and decreases in daytime which is consistent with the hydrogen demand profile. Fig. 4.9 (a) shows the variations in the SoC of the BESS that is shaped based on the power availability. The Compressor power consumption shown in Fig. 4.9 (b) has a similar pattern to the one shown for the PEME.

Fig. 4.9 (c) and (d) shows the changes of the PEME operating current density and efficiency for both N212 and N117 membranes. As shown in the figure, the current density of N212 is around $2A/cm^2$ at most of the time and, thus, there are small variations in the efficiency. On the other hand, when membrane is employed, the current density is lower than that of N212 due to the utilization of larger cell area. It is also noted that the efficiency fluctuations in membrane N117 is more obvious because thicker membranes have higher resistances and hence the negative slope of their efficiency curve is sharper, which cause larger efficiency variations even for the same current density changes.

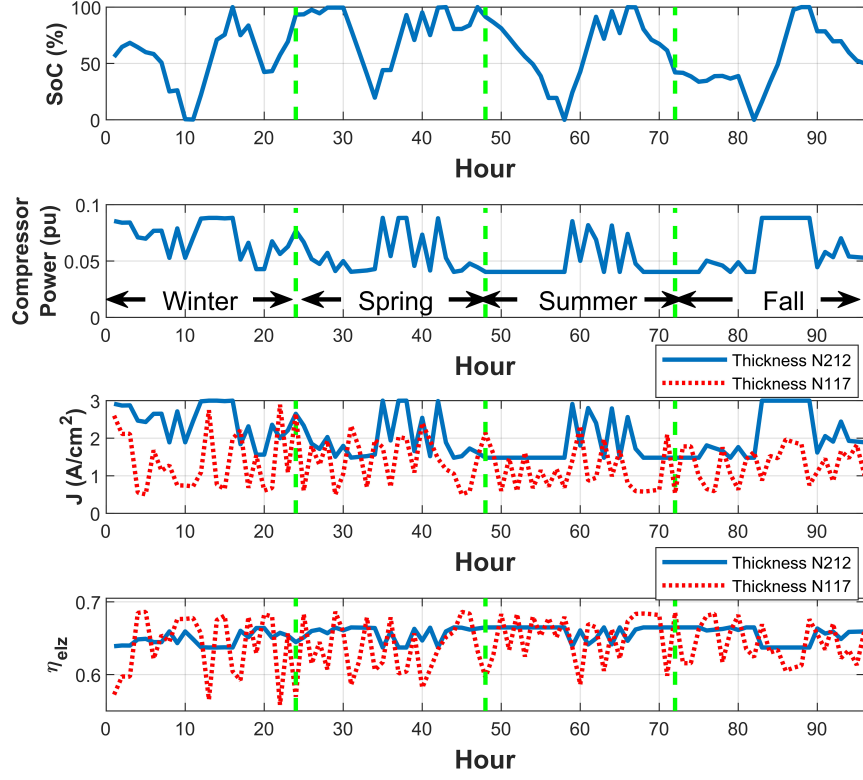


Figure 4.9: (a) SoC, and (b) compressor power of the optimal green PEME-HPP of case 6 (c) PEME current density, and (d) hydrogen in oxygen percentage of the optimal green PEME-HPP and the N117 membrane green PEME-HPP of case 6.

For dull green PEME-HPP, Table 4.5 shows that intermediate thicknesses (N212,N115) provide the minimum LCOH. The cathodic pressure shows same pattern as the green PEME-HPP scenario at different thicknesses. As in case 5, the produced dull green hydrogen is categorized as Dg3 color for all membrane thicknesses. The results show that the optimal LCOH using dull green PEME-HPP is 57% higher than green PEME-HPP. Fig. 4.8 (c) and (d) show the available power profile, imported power, PEME power, and SoH for N212 membrane that are similar to the green PEME-HPP scenario.

4.3.4 The Impact of Different Clean Hydrogen Subsidies

There are many announced governmental clean hydrogen subsidies. The way in which these subsidies affect the green PEME-HPP design and its PEME parameters differs according to the subsidy definition. As such, the clean hydrogen Investment Tax Credit (ITC) announced in [163] by the Canadian government is considered instead of the PTC of USA utilized in the previous case studies. Based on the clean hydrogen ITC of Canada, the new subsidy is formulated as follows:

$$\Upsilon = \begin{cases} 0.4 \text{ CAPEX} / \sum_{t=1}^T Q_d^t \$ & , 0 \leq CEH \leq 0.75 \\ 0.25 \text{ CAPEX} / \sum_{t=1}^T Q_d^t \$ & , 0.75 < CEH \leq 2 \\ 0.15 \text{ CAPEX} / \sum_{t=1}^T Q_d^t \$ & , 2 < CEH \leq 4 \\ 0 \$ & , CEH > 4 \end{cases} \quad (4.29)$$

The impact of employing the above mentioned subsidy compared to the base scenario which employs the USA PTC is depicted in Fig. 4.10. The figure shows the deviation in the LCOH, cell area, cathodic pressure, and BESS power rating as a percentage of the base scenario for case 5 and 6 for both green and dull green hydrogen production. Regarding the membrane thickness and compared with the base scenario, case 5 with the new subsidy utilizes a thicker membrane, N115, while case 6 employs the same membrane as of the base scenario.

The new subsidy reduces the component of the capital cost especially for the green hydrogen where the capital cost is reduced by 40%. For the dull green hydrogen production the CEH is around $1.82 \text{ CO}_2\text{kg}/\text{H}_2\text{kg}$ and hence, it qualifies for 25% reduction. This capital cost reduction increases the share of the operation cost in the LCOH which, in turn, promotes rising the cathodic pressure to decrease the power consumption of the compressor. Rising the pressure could require utilizing thicker membrane to reduce the hydrogen crossover. Yet, thicker membrane increases the ohmic losses and hence, it could employ wider cell area or and/or larger BESS to restore the efficiency. This behavior would be more clear for green hydrogen scenario as it offers higher reduction in the capital cost.

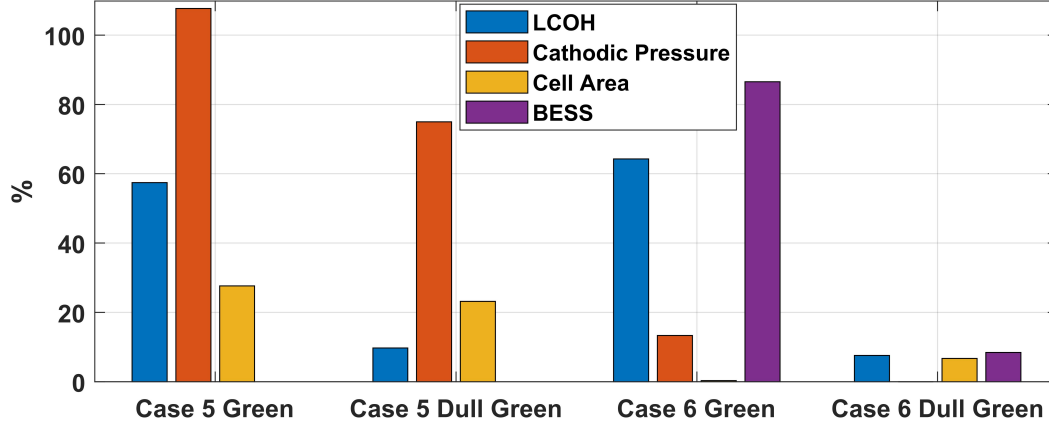


Figure 4.10: The impact of utilizing the new subsidy on the LCOH, cell area, cathodic pressure, and BESS power rating of case 5 and 6 as a percentage of the base scenario.

4.4 Summary

This chapter presents a novel mathematical model to optimize the design of grid-connected PEME-HPPs. The design aims at minimizing the LCOH by determining i) the optimal ratings of the main components in the PEME-HPP (PEME, compressor, and power converter), ii) the internal parameters of the PEME (membrane thickness, cell area, and cathodic pressure), and iii) the capacities of the local hydrogen storage and an optional on-site BESS. The proposed formulation is the first to i) incorporate the detailed modeling of PEME as a part of the PEME-HPP sizing problem, ii) consider the PEME safety constraints, iii) optimally size an optional on-site BESS and explore its economic viability, and iv) account for the clean hydrogen subsidies recently announced by different governments.

Two hydrogen production scenarios are considered in this work: pure green exclusive from RES and dull green from a mix of RES and conventional sources. Six case studies have been carried out to validate the effectiveness of the proposed model. Compared to the utilization of commercially available PEME units, optimizing the PEME parameters results in a 20% reduction in the LCOH. The presence of BESS contributes to a 9% additional reduction in the LCOH, and also impacts the choice of the PEME parameters, necessitating the use of high cathodic pressure with a moderate membrane thickness. Further, the

results show that ignoring the PEME safety constraint leads to an improper PEME design. Additionally, different clean hydrogen subsidies result in varied designs for both PEME-HPP and PEME. For instance, an optimized PEME-HPP without BESS requires a thicker membrane and double the cathodic pressure when the clean hydrogen ITC of Canada is considered instead of the PTC of the USA.

The proposed design scheme guides the manufacturers to customize the design of PEME to a specified application (specific power profile, electricity tariff, equipment cost, and clean hydrogen subsidy) while keeping the amount of hydrogen in oxygen within permissible safe limits. As such, it could be utilized by different stakeholders as an effective design, business model, and planning tool for the deployment of PEME-HPPs.

Chapter 5

Modular Configuration of PEME-HPP

Previous works in the literature, such as studies [41, 107–109, 113, 115, 116, 143, 153, 164], treated the PEME as one unit and didn’t consider the impact of dividing the PEME into several modules and controlling these modules separately. PEME is a scalable and modular technology in nature, and the selection of the number of modules forming a PEME-HPP might affect its overall performance. Adjusting the number of in-service PEME modules can change the in-service PEME’s cell area, which in turn affects the efficiency and the PEME permissible operating range. This permissible operating range is defined as the loading range in which the H_2 permeation through the PEME’s membrane is within the safety limit. Further, the power profile of the RES feeding the PEME (e.g., from solar or wind plants) as well as the optimization objectives (i.e., minimizing the LCOH, or maximizing the produced H_2) might impact the PEME performance. As such, the problem of optimal design for PEME-HPPs needs to be revisited to account for the PEME modularity, as well as the impacts of the RES power profile feeding the PEME and the optimization objectives on the PEME-HPP design, particularly on the PEME parameters design and the number of its modules.

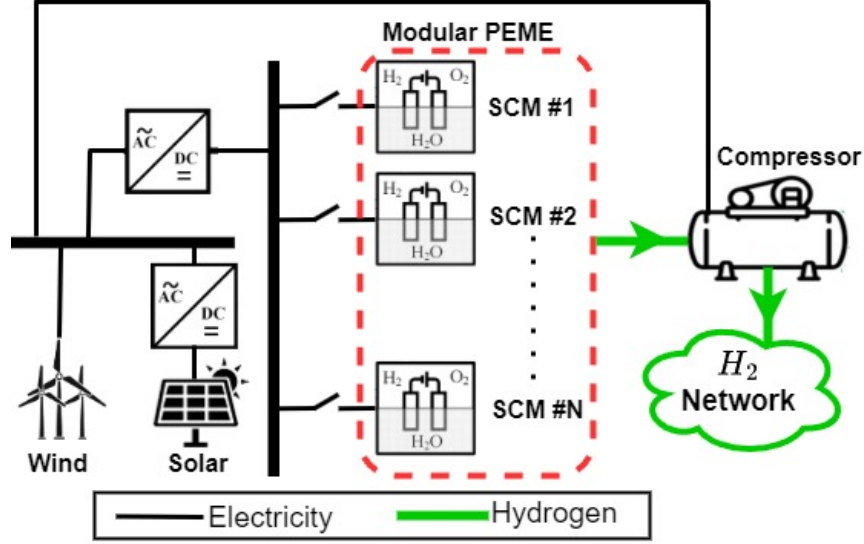


Figure 5.1: Schematic diagram of the proposed modular-based PEME-HPP.

To fill in the aforementioned research gaps, this chapter introduces a novel modular-based configuration for the design of large-scale PEME-HPPs. The researcher has published the results and formulation presented in this chapter in [165]. Fig. 5.1 shows a layout of the proposed configuration of a modular-based PEME-HPP powered by RES. As shown in the figure, the PEME-HPP consists of a modular PEME, AC/DC converter, and a compressor. The proposed design framework divides the PEME into a number of modules; named SCMs, where each module can be controlled independently. The proposed modular-based design aims to enhance PEME-HPP efficiency, extend its safe operating range, and improve its integration with intermittent RES. To this end, a new multi-objective mathematical formulation is developed to optimize the design of the modular-based PEME-HPP. The developed formulation determines the optimal i) number of PEME SCMs, ii) PEME parameters (cathodic pressure, membrane thickness, cell area), and iii) ratings of the PEME-HPP equipment (PEME, AC/DC converter, compressor), considering the effects of the RES power profile and optimization objectives on the PEME's optimal number of SCMs and parameters.

Table 5.1: The Features of the Proposed PEME-HPP Design Framework Compared to Previous Studies in the Literature

Design Feature	[41, 107], [108, 115]	[109]	[113, 164]	[116]	This Work
Green hydrogen production	✓	✓	✓	✓	✓
PEME detailed electrochemical model	✗	✗	✗	✓	✓
Optimizing PEME parameters	✗	✗	✗	✗	✓
PEME safety constraint	✗	✓	✗	✓	✓
Detailed model for the modular-based PEME	✗	✗	✗	✗	✓
Optimizing the number of PEME's SCMs	✗	✗	✗	✗	✓
Multi-objective optimization formulation	✗	✗	✗	✗	✓
Different RES power profiles feeding the PEME-HPP	✗	✗	✗	✗	✓

The optimization model aims to minimize the LCOH and maximize the produced hydrogen. Table 5.1 compares the proposed PEME-HPP design framework with prior works in the literature. As shown in the table and to the best of the authors' knowledge, this work is the first to introduce a modular-based configuration for designing PEME-HPPs powered by RES. The key contributions of this work are summarized below:

- A novel modular-based PEME configuration is introduced, accompanied by a mathematical model to investigate and analyze the impact of splitting the PEME into multiple SCMs on its efficiency and operating range.
- A new multi-objective optimization formulation is developed to optimize the proposed modular-based PEME configuration along with the PEME parameters (cathodic pres-

sure, membrane thickness, cell area), and the ratings of the PEME-HPP equipment (PEME, AC/DC converter, compressor).

- The Pareto frontiers of the developed multi-objective formulation are obtained, and the effect of changing the weights of the formulation objectives on the PEME's optimal number of SCMs and parameters is analyzed.
- The developed multi-objective formulation considers different RES power profiles as inputs to the PEME-HPP and examines their impacts on the PEME's optimal number of SCMs and parameters.

The remainder of this chapter is organized as follows. Section 5.1 presents the modeling of a modular PEME. Section 5.2 introduces the proposed multi-objective optimization formulation, while Section 5.3 presents the case studies and results. Finally, Section 5.4 provides the conclusions of this chapter.

5.1 Modeling of Modular PEME

This section builds upon the singular PEME steady-state model introduced in Section 3.2.1 and illustrates how the PEME model is further extended to represent a modular PEME consisting of N SCMs.

The modular design divides the PEME into N number of SCMs. In such a case, the in-service cell area, A_{srv} , depends on the number of in-service SCMs, n , number of SCMs, N , and total PEME cell area, A_{cell}^{PEM} , as given below:

$$A_{srv}^{PEM} = \frac{n A_{cell}^{PEM}}{N}. \quad (5.1)$$

Both the production and Faraday's efficiencies change with the current density change, which is influenced by the in-service cell area of PEME, as shown in (5.2), and consequently, by the number of in-service SCMs.

$$J^{PEM} = \frac{I^{PEM}}{A_{srv}} = \frac{I^{PEM} N}{n A_{Elz}} \quad (5.2)$$

where I^{PEM} is the PEME operating current (loading). By substituting from (5.2) into (3.21) and (3.22), it could be noted that both V_{act}^{PEM} and V_{res}^{PEM} are inversely proportional to n . As a result, the production efficiency, $\eta_p^{PEM,n}$, could be represented as a function of the number of in-service SCMs, n , as follows:

$$\eta_p^{PEM,n} = \frac{V_{LHV}^{H_2}}{V_{heat}^{PEM} + V_{oc}^{PEM} + \frac{RT_{cell}^{PEM}}{\alpha^{PEM} z F} \ln \left(\frac{I^{PEM} N}{J_o^{PEM} n A_{cell}^{PEM}} \right) + \frac{I^{PEM} N}{n A_{cell}^{PEM}} \left(R_o^{PEM} + \frac{\delta_m^{PEM} \mathfrak{s}_m^{PEM}}{\sigma_m} \right)}. \quad (5.3)$$

Equation (5.3) shows that the $\eta_p^{PEM,n}$ is improved with the increase of the in-service SCMs. The crossover equivalent current density can be represented as a function of the in-service SCMs as formulated in (5.4). Then, Faraday's efficiency is reformulated as expressed in (5.5).

$$J_{loss}^{PEM,n} = 2 \left(F Pr_{H_2}^{PEM} \frac{\pi_{H_2}^{PEM} + \pi_{O_2}^{PEM}}{\delta_m^{PEM} \mathfrak{s}_m^{PEM}} + \frac{a_x I^{PEM} N}{\delta_m^{PEM} \mathfrak{s}_m^{PEM} n A_{cell}^{PEM}} \right) \quad (5.4)$$

$$\eta_F^{PEM,n} = 1 - 2 \left(F Pr_{H_2}^{PEM} \frac{n A_{cell}^{PEM}}{I^{PEM} N} \cdot \frac{\pi_{H_2} + \pi_{O_2}}{\delta_m^{PEM} \mathfrak{s}_m^{PEM}} + \frac{a_x}{\delta_m^{PEM} \mathfrak{s}_m^{PEM}} \right) \quad (5.5)$$

As noted in (5.5), Faraday's efficiency decreases with the increase in in-service SCMs. The compression effect, η_{mc} , and converter efficiency, η_{Conv} , are independent of the cell area and thus are unaffected by the number of in-service SCMs. As such, the total efficiency of a modular PEME-HPP, η_T^n , when n SCMs are in service and equally loaded (i.e., each in-service SCM has a loading of I^{PEM}/n), is calculated in the same manner as the efficiency of a singular PEME-HPP, as follows:

$$\eta_T^n = \eta_P^{PEM,n} \eta_F^{PEM,n} \eta_{mc} \eta_{Conv}. \quad (5.6)$$

Similarly, the H_2 in O_2 ratio, $\Psi_{H_2}^{PEM,n}$, varies with n as expressed in (5.7). From (5.7), it could be observed that at no load and full load, the H_2 in O_2 ratio approaches 100% and zero%, respectively, irrespective of the value of n . At different loadings, however, the values of n significantly affect the largest term ($\frac{0.5 I^{PEM} N}{n A_{cell}^{PEM}}$) in both the numerator and denominator in $\Psi_{H_2}^{PEM,n}$, and hence the smaller n becomes the faster $\Psi_{H_2}^{PEM,n}$ decays while

loading increases.

$$\Psi_{H_2}^{PEM,n} = \frac{2F Pr_{H_2}^{PEM} \frac{\pi_{H_2}^{PEM}}{\delta_m^{PEM} \mathfrak{s}_m^{PEM}} + \frac{a_x I^{PEM} N}{\delta_m^{PEM} \mathfrak{s}_m^{PEM} n A_{cell}^{PEM}}}{2F Pr_{H_2}^{PEM} \frac{\pi_{H_2}^{PEM}}{\delta_m^{PEM} \mathfrak{s}_m^{PEM}} + \frac{a_x I^{PEM} N}{\delta_m^{PEM} \mathfrak{s}_m^{PEM} n A_{cell}^{PEM}} + \frac{0.5 I^{PEM} N}{n A_{cell}^{PEM}}} \quad (5.7)$$

The cumulative efficiency; named effective controlled efficiency, η_e , of a modular PEME-HPP with a PEME consisting of N SCMs at a certain operating current (loading), I^{PEM} , can be formulated as follows:

$$\eta_e(I^{PEM}) = \max_{n=1,\dots,N} \eta_T^n(I^{PEM}) \quad (5.8)$$

It is worth noting that when $n = N$, A_{srv} equals A_{cell}^{PEM} and the modular PEME-HPP acts as a singular one. Further, the singular PEME-HPP is a special case of the modular PEME-HPP when $n = N = 1$. As such, for singular PEME-HPP, $\Psi_{H_2}^{PEM,n=N=1} = \Psi_{H_2}^{PEM}$ and $\eta_e = \eta_T^{n=N=1} = \eta_T$.

Terminology Declaration: Throughout all subsequent analyses and discussions, the term *loading* will refer to the PEME operating current (I^{PEM}). Additionally, for all types of PEME-HPP, i.e., singular and modular, we will use the modular PEME-HPP symbols η_e and $\Psi_{H_2}^{PEM,n}$, as the singular PEME-HPP is a special case of the modular PEME-HPP, as mentioned earlier.

5.2 Proposed Optimization Model

Based on the modeling of the modular PEME presented in Section 5.1, this section presents the problem hypothesis and the mathematical formulation required to optimally design a modular-based PEME-HPP. Two different objectives are defined for the design problem: minimizing the LCOH and maximizing the produced hydrogen. The PEME-HPP designer needs to make a decision that strikes a balance between minimizing the LCOH and maximizing the amount of hydrogen produced. Without loss of generality, the proposed formulation has the following assumptions and hypotheses:

- The PEME-HPP is supplied from a co-located RES (wind and/or solar plant), where the electric power is supplied to the PEME-HPP through a PPA [160].
- The produced hydrogen is injected into a hydrogen pipeline system and, thus, there are no local storage limits on the produced hydrogen.
- The PEME-HPP is designed to adhere to a typical RES profile, considering that RES power can be curtailed and/or injected into the grid whenever it exceeds the PEME-HPP capacity.

The decision variables of the proposed optimization problem are as follows: the number of SCMs, PEME rated power and parameters (cathodic pressure, membrane thickness, cell area), ratings of the compressor and AC/DC converter, and hourly PEME power, P_{PEM}^t . In addition to the decision variables, the optimization model yields the LCOH, amount of produced H_2 , and average energy consumption per kg of H_2 .

The optimization problem's objective function is constructed to minimize the LCOH and maximize the produced H_2 as expressed in (5.9). The first objective (f_1), minimizing the LCOH, consists of three components: CAPEX, OPEX, and C_{Deg} divided by the total H_2 production, Q_{H_2} . The second objective (f_2), maximizing the produced H_2 , is defined as the total H_2 production. γ is a slack variable applied to relax an equality constraint, as discussed later in (5.20).

$$Obj = Min(f_1 - f_2 + \gamma)$$

$$\text{where, } f_1 = \left(\frac{CAPEX + \sum_{y \in Y} (OPEX + C_{Deg}) / (1 + r)^y}{\sum_{y \in Y} (Q_{H_2}) / (1 + r)^y} \right), \quad f_2 = Q_{H_2} \quad (5.9)$$

where Y is the PEME-HPP life time in years, and r is the yearly discount rate. The CAPEX is a function of the equipment (PEME, AC/DC converter, compressor) ratings and PEME cell area, A_{cell}^{PEM} , as given in (5.10). A PEME with a rated power of P_{PEM}^{rate} requires a rated cell area of $A_{cell}^{PEM, rate} = \frac{P_{PEM}^{rate}}{V_{PEM}^{rate} J_{max}^{PEM}}$, where V_{PEM}^{rate} and J_{max}^{PEM} are the rated voltage and maximum current density of the PEME, respectively. If the PEME is equipped with a larger cell area, A_{cell}^{PEM} , such that $A_{cell}^{PEM} > A_{cell}^{PEM, rate}$, it can theoretically operate

above its rated power. However, in practice, its electrical components are limited to P_{PEM}^{rate} . While a larger cell area may improve PEME efficiency, it increases the capital cost due to the additional required noble material. In this work, both the PEME rating (P_{Elz}^{rate}) and cell area (A_{cell}^{PEM}) are independent decision variables, allowing the actual cell area (A_{cell}^{PEM}) to differ from the rated cell area ($A_{cell}^{PEM, rate}$). To account for the additional cost of a larger cell area, an adjustment factor, $A_{cell}^{PEM} / A_{cell}^{PEM, rate}$, is incorporated into the PEME term in CAPEX calculation.

$$CAPEX = \frac{P_{PEM}^{rate} A_{cell}^{PEM}}{A_{cell}^{PEM, rate}} C_{PEM} + P_{Conv}^{rate} C_{Conv} + P_{Cmp}^{rate} C_{Cmp}. \quad (5.10)$$

The OPEX comprises the electricity and water consumption costs as well as the PEME and compressor operational expenses, expressed as:

$$OPEX = \sum_{t=1}^{\mathbb{T}} P_{EHPP}^t Price_{elec}^t + L_{H_2}^t O_w + P_{Elz}^t O_{Elz} + P_{Cmp}^t O_{Cmp}. \quad (5.11)$$

The PEME-HPP electricity cost at the hour t is the multiplication of its electricity price, $Price_{elec}^t$, by the corresponding plant's consumption, P_{EHPP}^t , that combines the consumption of PEME and compressor as provided hereunder:

$$P_{EHPP}^t = P_{PEM}^t + P_{Cmp}^t \quad \forall t \in \mathbb{T}, \quad (5.12)$$

where the compressor power P_{Cmp}^t can be calculated as previously defined in (3.40). However, since the compressor is directly connected to the H_2 network, the compressor outlet pressure corresponds to the H_2 network pressure π_{HN} (i.e., the delivery pressure). Additionally, the hydrogen production flow $N_{H_2}^{PEM}$ used in compressor power calculation is obtained using the effective controlled efficiency η_e of the modular PEME as follows:

$$N_{H_2}^{PEM, t} = \frac{P_{EHPP}^t \eta_e^t(N, \pi_{H_2}^{PEM}, A_{cell}^{PEM}, \delta_m^{PEM})}{\Delta H_{LHV}} \quad \forall t \in \mathbb{T}. \quad (5.13)$$

The effective efficiency, η_e , depends on the total efficiency of PEME-HPP, η_T , which, in turn, is a function of four decision variables, i.e. the number of SCMs N , and PEME's parameters (cathodic pressure $\pi_{H_2}^{PEM}$, cell area A_{cell}^{PEM} , and membrane thickness δ_m^{PEM}).

The total H_2 production, Q_{H_2} , is the sum of the hourly hydrogen production flow over the simulation period as expressed below:

$$Q_{H_2} = \sum_{t=1}^{\mathbb{T}} N_{H_2}^{PEM,t} \quad \forall t \in \mathbb{T}. \quad (5.14)$$

The PEME lifetime is defined by a specific number of operating hours; in other words, the longer the PEME operates, the more degradation it experiences [166]. Additionally, the level of degradation increases with higher current densities, which is normally proportional to PEME power consumption [167], [168]. As such, PEME degradation cost C_{Deg} depends on the operation duration and power consumption. Hence, PEME C_{Deg} can be expressed as the sum of its hourly power consumption (where the summation accounts for the operation duration, and the power reflects the loading level) multiplied by the cost of degradation per MWh, D_{Elz} , as provided below [36]:

$$C_{Deg} = \sum_{t=1}^{\mathbb{T}} P_{PEM}^t D_{PEM} \quad (5.15)$$

The objective function provided in (5.9) is subject to the design, safety, and operational constraints of the PEME, as well as the power balance constraints. For PEME's design, the cell area and cathodic pressure are constrained by minimum and maximum limits as expressed in (5.16), and (5.17), respectively.

$$A_{cell}^{PEM,min} \leq A_{cell}^{PEM} \leq A_{cell}^{PEM,max} \quad (5.16)$$

$$\pi_{H_2}^{PEM,min} \leq \pi_{H_2}^{PEM} \leq \pi_{H_2}^{PEM,max} \quad (5.17)$$

The optimization of membrane thickness is limited to the market-available thicknesses $\{25.4 \mu m, 51 \mu m, 127 \mu m, 183 \mu m\}$ [103], and hence the membrane thickness is constrained as follows:

$$\delta_m^{PEM} \in \{25.4 \mu m, 51 \mu m, 127 \mu m, 183 \mu m\} \quad (5.18)$$

To avoid the forcefully PEME turnoff, the H_2 in O_2 amount, $\Psi_{H_2}^{PEM,n}$, must be kept less than its safety limit, $\Psi_{H_2}^{PEM,safe}$, as expressed below:

$$\Psi_{H_2}^{PEM,n} \leq \Psi_{H_2}^{PEM,safe} \quad (5.19)$$

The previous constraint ensures keeping $\Psi_{H_2}^{PEM,n}$ within the safety bound at different levels of loading. However, it doesn't impose a lower limit, which might lead to a PEME design that unnecessarily expands the PEME safe operating range beyond the minimum PEME loading (I_{min}^{PEM}). To avoid this unnecessary expansion and confine the PEME safe operating range to cover only up to the minimum PEME loading (I_{min}^{PEM}), the H_2 in O_2 ratio at the minimum PEME loading, $\Psi_{H_2}^{PEM,n}(I_{min}^{PEM})$, is subject to the following equality constraint:

$$\begin{aligned} \Psi_{H_2}^{PEM,n}(I_{min}^{PEM}) &= \Psi_{H_2}^{PEM,safe} - \gamma \\ \text{where, } \gamma &\in [0, \Psi_{H_2}^{PEM,safe}] \end{aligned} \quad (5.20)$$

The equality constraint in (5.20) is relaxed using the slack variable γ , as the decision variables include integer and discrete variables, i.e. N and δ_m^{PEM} , which may lead to violations of the strict equality constraints. In terms of PEME operation, the PEME's current density, $J^{PEM,t} = \frac{P_{PEM}^t}{V_{PEM}^{rate} A_{cell}^{PEM}}$, has to be limited by its maximum current density, J_{max}^{PEM} , as follows:

$$0 \leq J^{PEM,t} = \frac{P_{PEM}^t}{V_{PEM}^{rate} A_{cell}^{PEM}} \leq J_{max}^{PEM} \quad (5.21)$$

Additionally, the hourly power consumptions of PEME and compressor are limited by their rated power as provided in (5.27) and (5.23).

$$P_{PEM}^t \leq P_{PEM}^{rate} \quad (5.22)$$

$$P_{Cmp}^t \leq P_{Cmp}^{rate} \quad (5.23)$$

The total PEME-HPP power consumption, P_{EHPP}^t , must adhere to the power balance constraint as shown in equation (5.24). Specifically, P_{EHPP}^t should match the provided RES power profile, P_{RES}^t , as long as it does not exceed the PEME-HPP rated power, P_{EHPP}^{rate} .

$$P_{EHPP}^t = \min(P_{EHPP}^{rate}, P_{RES}^t) \quad (5.24)$$

The RES power profile, P_{RES}^t , is a typical-days power profile that constitutes a simulation period of $\mathbb{T}$ hours to represent the four seasons. This RES power profile, P_{RES}^t , is obtained from the solar irradiation and wind speed historical data of Windsor, Ontario,

Canada [158]. For each hour t in the simulation period $\mathbb{T}$, solar irradiation and wind speed are represented considering two pdf (i.e., Beta f_b and Rayleigh f_r) [143]. Each pdf function is divided into h discrete states, ending with a total of $h \times h$ combined states. Given that there is no correlation between the RES power at the hour t and the adjacent one, the probability of each combined state is calculated as follows:

$$\rho^{s,t} = \rho(SI^{i,t}) \cdot \rho(W S^{j,t}) \quad \forall t \in \mathbb{T} \wedge s = 1, \dots, h \times h \wedge i, j = 1, \dots, h \quad (5.25)$$

where $\rho(SI^{i,t})$ and $\rho(W S^{j,t})$ are, respectively, the probability of the solar and wind power at the state i and hour t . The hourly weighted average of the $P_{PV}^{s,t}$ and $P_W^{s,t}$ is determined for the $(h \times h)$ states to obtain the unified RES profile, P_{RES}^t , as follows:

$$P_{RES}^t = \frac{\sum_{s=1}^{h \times h} \rho^{s,t} (P_{PV}^{s,t} + P_W^{s,t})}{\sum_{s=1}^{h \times h} \rho^{s,t}} \quad \forall t \in \mathbb{T} \wedge s = 1, \dots, h \times h \quad (5.26)$$

5.3 Results and Discussion

This section numerically validates the proposed PEME configurations and optimization models. Subsection 5.3.1 validates the modular PEME configuration presented in section 5.1 and investigates the impact of changing the number of in-service SCMs in PEME on its efficiency. Further, it provides an example of a modular PEME-HPP consisting of four SCMs, demonstrating its efficiency improvements and expanded operating range compared to a singular PEME-HPP of the same capacity. Subsections 5.3.2 and 5.3.3 apply the optimization model proposed in section 5.2 to both singular and modular PEME-HPPs, showing the impact of optimal modularization on the performance of PEME-HPP and the effect of different optimization objectives on PEME internal design. Six case studies are conducted, divided as follows: three for the singular PEME-HPP configuration, each with a different optimization objective (i.e., minimizing the LCOH, minimizing the LCOH while maximizing hydrogen production with equal weight for each objective, and maximizing hydrogen production), and three for the modular PEME-HPP configuration with the same optimization objectives. Table 5.2 summarizes the conducted six case studies that provide insights into system performance under the different objectives. Subsequently, the Pareto

Table 5.2: Summary of Case Studies

Cases	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6
PEME-HPP Configuration	Singular			Modular		
Minimizing LCOH	✓	✓	✗	✓	✓	✗
Maximizing H_2 Production	✗	✓	✓	✗	✓	✓

frontiers for the two configurations are derived to determine the trade-offs and identify the optimal balance (sweet spot) between the objectives. Subsection 5.3.4 considers different RES power profiles and examines their impact on the optimal number of SCMs, PEME’s parameters (cathodic pressure, membrane thickness, cell area), and PEME-HPP design. For all case studies and analyses in subsections 5.3.2, 5.3.3, and 5.3.4, the wind speed and solar radiation data for five years in Ontario, Canada [158] is used to generate a four-day typical power profile of a 100 MW and 200 MW wind and solar plants, respectively. The cost of electricity in the PPA is assumed to be fixed at a rate of 30\$/MWh as discussed in [160]. Other technical, cost, and simulation parameters are imported from previous techno-economic studies in the literature [36], [82], and are similar to those listed in Table 4.3.

5.3.1 Impact of PEME Modularization on PEME-HPP Performance

As explained earlier in subsection 5.1, PEME’s production and Faraday efficiencies vary with changes in the number of in-service SCMs, n . Accordingly, a sample numerical case is presented in Fig. 5.2 to illustrate the significance of varying n on each efficiency component at different loading levels. Fig. 5.2 (a) depicts the relationship between PEME production efficiency and the in-service SCMs (n), represented as a percentage of (N), at various loading levels. As shown in the figure, η_P increases non-linearly with the in-service SCMs $n = 30\% N$, after which it increases linearly. Further, the rate of increase in η_P with n/N escalates proportionally with the loading of PEME. Fig. 5.2 (b) depicts the relationship between PEME Faraday’s efficiency and the in-service SCMs at various loading levels. As shown in the figure, the decrease in Faraday’s efficiency becomes less significant as the

PEME loading increases.

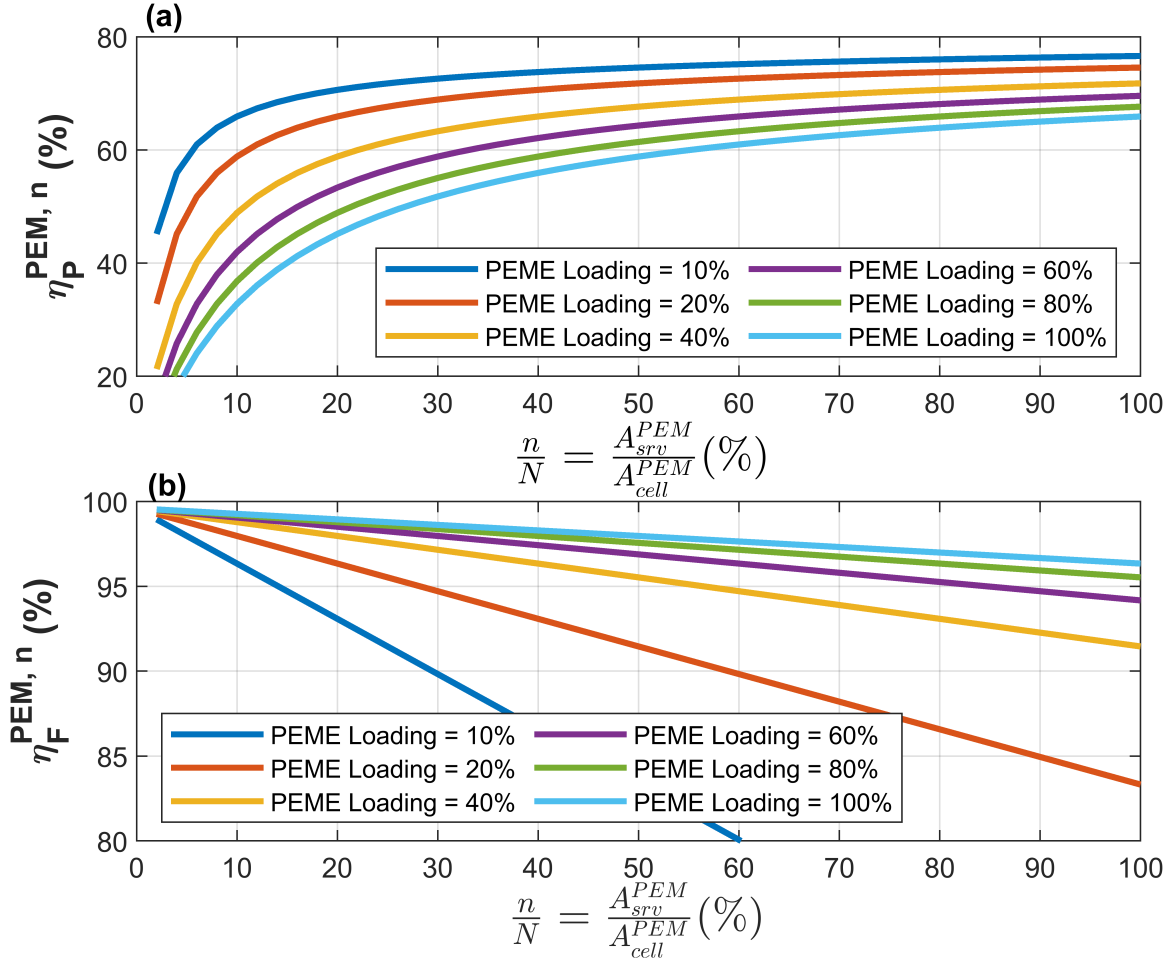


Figure 5.2: Variations of (a) PEME production efficiency, and (b) PEME Faraday efficiency with the number of in-service SCMs at different levels of PEME loading.

To further clarify the previous analysis, let us consider a PEME-HPP with a modular PEME that consists of four identical SCMs. The total PEME-HPP efficiency, η_T^n , at different numbers of in-service SCMs are depicted in Fig. 5.3 (a) as a function of the PEME loading. As illustrated in the figure, the total efficiency of the PEME-HPP varies with the number of in-service SCMs at each loading level. As shown, it is highly effective to wisely increase the number of in-service SCMs, n , with the increase of the PEME loading.

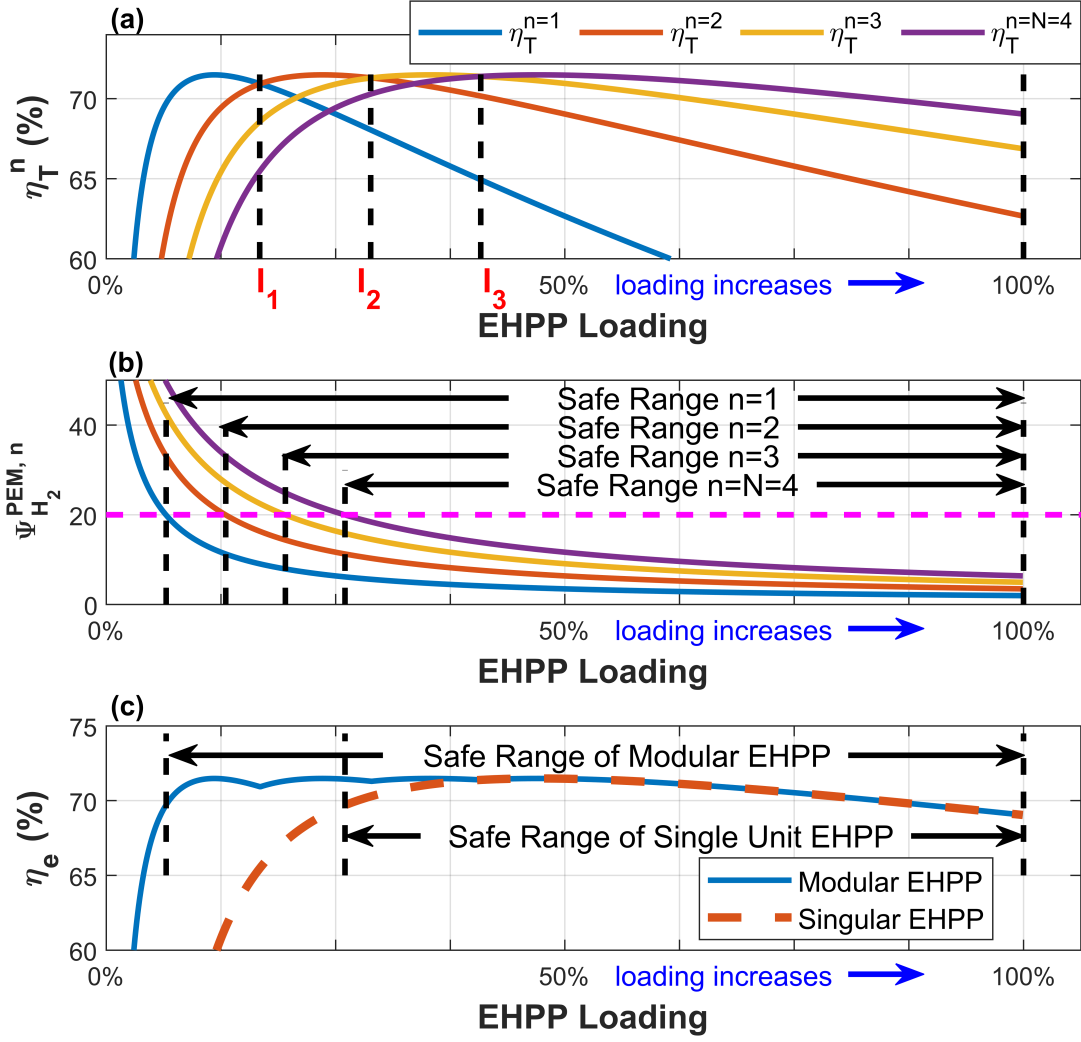


Figure 5.3: (a) Total efficiency, and (b) H_2 in O_2 ratio of a modular PEME-HPP at different n values. (c) Effective efficiency and safe operating range of modular and singular PEME-HPPs.

Therefore, n has to be changed dynamically with the change of the PEME loading to get

the highest possible efficiency as follows:

$$n = \begin{cases} 1 & \forall I^{PEM} \leq I_1 \\ 2 & \forall I_1 < I^{PEM} \leq I_2 \\ 3 & \forall I_2 < I^{PEM} \leq I_3 \\ N = 4 & \forall I_3 < I^{PEM} \end{cases} \quad (5.27)$$

Fig. 5.3 (b) shows the variation of H_2 in O_2 ratio at different numbers of in-service SCMs. As depicted in the figure, reducing the number of in-service SCMs at light loading accelerates the decay of $\Psi_{H_2}^{PEM, n}$, and hence the 20% safe limit, defined in [103], moves towards lower loading, this would, in turn, extend the safe operating range of the PEME-HPP. Fig. 5.3 (c) shows the effective efficiency and safe operating range of a modular PEME-HPP with N SCMs compared to a single unit PEME-HPP of the same size and PEME parameters. As shown in Fig. 5.3(c), a modular PEME-HPP offers a wider safe operating range and higher effective efficiency under light loading conditions compared to a singular PEME-HPP of the same size.

5.3.2 Cases 1 to 3: Design of PEME-HPPs with Singular PEME

Cases 1 to 3 consider a singular PEME-HPP configuration. In case 1, the objective is to minimize the LCOH. Case 2 has two objectives: minimizing the LCOH and maximizing H_2 production, with an equal weight assigned to each objective. In case 3, the objective is to maximize the H_2 production. Table 5.3 shows the results of the optimal design of the PEME-HPP in the different case studies. As shown in the table, the design of the PEME-HPP is highly sensitive to the selected optimization objective. For instance, case 1, aiming to minimize LCOH, utilizes a smaller cell area compared to cases 2 and 3 which helps reduce the capital expenditure of PEME and hence minimize the LCOH. This small cell area forces the PEME to operate at relatively high current densities, compared to other cases, thereby a moderate membrane thickness ($51\mu m$) is used to limit the decay in PEME-HPP efficiency at high loading levels. As the objective of maximizing H_2 production is given more weight, as in cases 2 and 3, a wider cell area is employed that leads the PEME to operate at lower

current densities. Therefore, a thicker membrane is used to improve the efficiency at these low current densities. Further, this thicker membrane enables the use of higher cathodic pressure, which allows for the utilization of a compressor with a lower rating compared to case 1. However, since the PEME capital cost is significantly higher than the compressor cost, the increase in PEME capital cost in cases 2 and 3 (due to increasing its cell area) dominates the CAPEX, ultimately leading to a higher LCOH for cases 2 and 3 compared to case 1.

These changes in PEME parameters of cases 2 and 3 reshape the effective efficiency of the PEME-HPP, as demonstrated in Fig. 5.4 (a), to improve the efficiency over the operating range of the PEME and hence increase the H_2 production. It is worth noting that cases 2 and 3 have the same membrane thickness and utilize a very close cathodic pressure, while the main difference is that case 3 has a much wider cell area. As a result, and as shown in Fig. 5.4 (a), the PEME-HPP effective efficiency curves are quite similar; however, case 2 exhibits higher efficiency at low loading levels and lower efficiency at high loading levels. This is a direct result of utilizing a smaller cell area than case 3 while keeping the other PEME parameters almost unchanged. The same observation of improving the effective efficiency is noted in Fig. 5.4 (b), which displays the hourly effective efficiency for cases 1 to 3. As depicted in the figure, the effective efficiency of cases 2 and 3 surpasses that of case 1 over the entire range of the four typical days. Therefore, the hourly energy consumption of the PEME-HPP, defined as the ratio between hourly PEME-HPP power and produced hydrogen ($P_{EHPP}^t/N_{H_2}^{PEM,t}$), is lower for cases 2 and 3 compared to case 1, as illustrated in Fig. 5.4 (c). It is also noted that the larger cell area selected to maximize hydrogen production in cases 2 and 3 reduces the PEME current density, J^{PEM} , compared to case 1, as depicted in Fig. 5.4 (d). This observation further clarifies the earlier discussions regarding the use of thicker membranes in cases 2 and 3 compared to case 1.

Table 5.3: Parameters of the Optimized PEME-HPP in Cases 1 to 6

Item	Parameter	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6
PEME	Configuration	Singular			Modular		
	$\delta_m^{PEM} (\mu m)$	51	183	183	51	127	183
	$\pi_{H_2(bar)}^{PEM}$	4	9	8	20	39	29
	$A_{cell}^{PEM} (m^2)$	2280	3840	5100	2640	4860	11220
	$P_{PEM}^{rate} (MW)$	132	144	142	151	158	154
	$\#Modules$	1	1	1	5	7	8
BoP	$P_{Conv}^{rate} (MW)$	136	148	147	156	163	159
	$P_{Cmp}^{rate} (MW)$	53	36	41	29	21	26
Outcomes	LCOH (\$/kg)	3.2	3.78	4.3	3	3.86	6.3
	Produced H_2 (Tonne)	8234	8610	8773	9149	9498	9741
	Consumption (kWh/kg)	63	61	60	57	55	53

5.3.3 Cases 4 to 6: Design of PEME-HPPs with Modular PEME

Cases 4 to 6 focus on the modular PEME-HPP configuration, with the following objectives, respectively: minimizing the LCOH, minimizing the LCOH while maximizing H_2 production (with equal weight assigned to each objective), and maximizing H_2 production. The results of cases 4 to 6 are summarized in Table 5.3. Similar to singular PEME-HPP (cases 1 to 3), as the weight of maximizing H_2 production increases a wider cell area with a thicker membrane is employed in the PEME design. As such, cases 5 and 6 have a wider cell area and thicker membrane and hence higher cathodic pressure than case 4. The modular PEME-HPP configuration in cases 4 to 6 showed significant enhancement to the PEME-HPP performance. In case 4, the modular PEME-HPP configuration achieved a 6% reduction in the LCOH compared to case 1. Additionally, in case 6, the modular configuration increased hydrogen production by 11% compared to case 3. Case 5, using

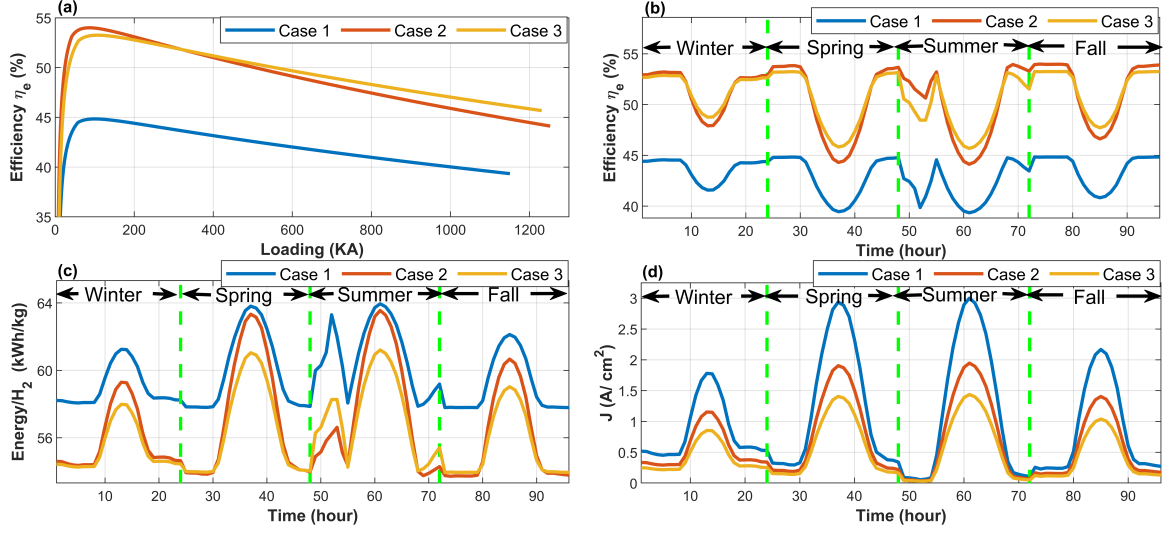


Figure 5.4: (a) Effective efficiency, (b) hourly effective efficiency, (c) hourly energy consumption, and (d) PEME hourly current density of the singular PEME-HPP in cases 1 to 3.

the modular PEME-HPP configuration, increases both the LCOH and H_2 production by 1.3% and 10%, respectively, compared to case 2. It is worth noting that, cases 2 and 5 have two contradictory objectives, making it impossible to improve one objective without deteriorating the other objective. To avoid repetition, the following discussion will focus on comparing the two extreme cases of the modular PEME-HPP (cases 4 and 6) with the corresponding extreme cases of the singular PEME-HPP (cases 1 and 3). Accordingly, the comparison between case 5 and case 2 will be omitted.

In case 1, with the singular PEME-HPP configuration, when the current supplied from RES decreases, the single unit PEME has to operate at a low current density which, in turn, results in lower efficiency. Yet, in case 4 with modular PEME-HPP configuration, PEME is divided into 5 SCMs, and hence the total efficiency curve changes with the number of in-service SCMs as shown in Fig. 5.5 (a). As such, in case 4, when the loading decreases, the number of in-service SCMs is reduced to keep a relatively high current density. Such an increase in the current density, due to reducing the number of in-service SCMs, enhances Faraday's efficiency of the modular PEME, especially at light loading. It is also noted that

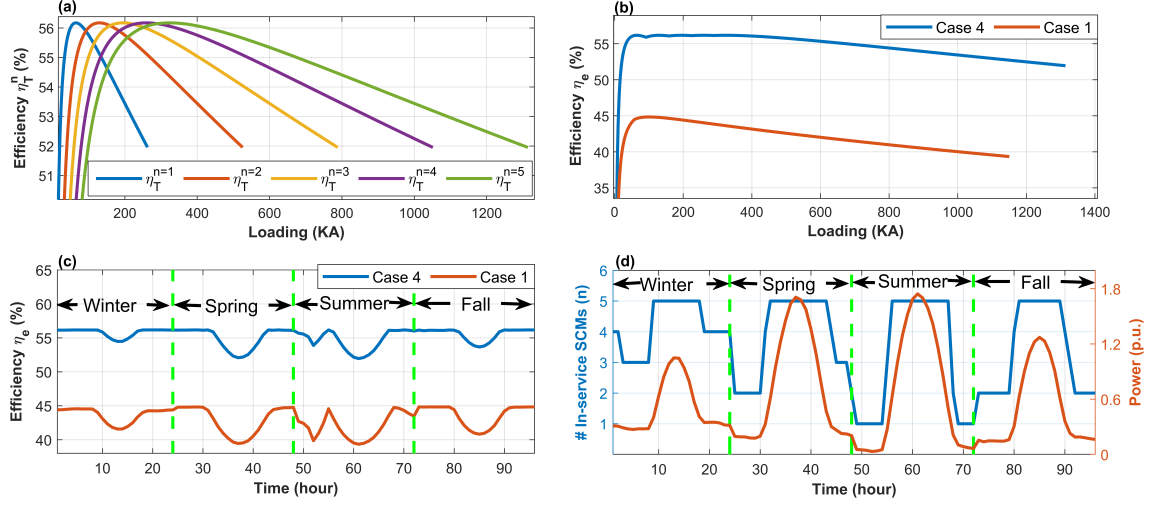


Figure 5.5: (a) Total efficiency curves of modular PEME-HPP with different number of in-service SCMs for case 4, (b) effective efficiency curves of PEME-HPP for cases 1 and 4, (c) hourly effective efficiency of PEME-HPP for cases 1 and 4, and (d) number of in-service SCMs at each hour for case 4 and the RES power profile feeding the PEME-HPP.

the voltage efficiency declines faster at high loading. Therefore, as PEME loading increases, more SCMs are switched on to reduce the current density and improve the voltage efficiency. Fig. 5.5 (b) depicts the effective efficiency of cases 1 and 4. As shown in the figure, the modular design utilized in case 4 enhances the PEME-HPP effective efficiency for the entire PEME loading range compared to case 1. Fig. 5.5 (c) shows the hourly effective efficiency of cases 1 and 4. As shown in the figure, the proposed modular design in case 4 significantly enhances the hourly effective efficiency compared to case 1. Fig. 5.5 (d) illustrates the number of in-service SCMs at each hour during the four-day simulation period, along with the RES power profile feeding the PEME-HPP, P_{RES}^t . As depicted in the figure, the number of in-service SCMs changes proportionally with the RES feeding power to maintain the highest possible efficiency. The number of in-service SCMs increases (additional SCMs are turned on) as the RES power increases, and decreases (turns off) as the RES power drops.

Similar results are obtained for case 6, however, the PEME is divided into 8 SCMs and its cell area is significantly oversized to achieve the highest efficiency regardless of the

LCOH. Fig. 5.6 (a) shows the total efficiency curves at the different numbers of in-service SCMs (from 1 to 8). As shown in the figure, each value of n (total efficiency curve) offers the highest efficiency for a specific loading range. Further, compared with case 3, the modular design of case 6 allows a wider cell area as the safety constraint can be expanded by increasing the number of SCMs, N , and there would be no limitations on operating at light loading conditions even with such a wide cell area. Consequently, as in Table 5.3, the LCOH of case 6 is 46% higher than that of case 3. Fig. 5.6 (b) presents the PEME-HPP effective efficiency in cases 3 and 6. As depicted in the figure, the modular PEME-HPP in case 6 has higher effective efficiency than the singular PEME-HPP of case 3 over the entire range of PEME loading. Fig. 5.6 (c) illustrates the hourly effective efficiency of cases 3 and 6, showing that the modular PEME-HPP in case 6 has higher effective efficiency than the singular PEME-HPP of case 3 over the entire typical four days (simulation period). Fig. 5.6 (d) depicts the hourly variations in the number of in-service SCMs in case 6 alongside the feeding RES power profile. As illustrated in the figure the hourly variations in the number of in-service SCMs in case 6 are also proportional to the variation in the RES feeding power exactly as in case 4.

Fig. 5.7 shows the Pareto frontier of the singular and modular PEME-HPPs. As illustrated in the figure, for the singular PEME-HPP, the LCOH and the produced H_2 , Q_{H_2} , increases from 3.2\$ to 4.3\$ and from 8234 tonnes to 8773 tonnes, respectively. The ultimate optimal solution, represented by the minimum LCOH and maximum H_2 production, is infeasible as the two objectives (LCOH minimization and H_2 production maximization) contradict each other. Yet, the designer can determine a suitable solution (design point) to partially optimize the two objectives. Similarly, in the modular PEME-HPP, the Pareto frontier exhibits a gradual proportional increase in both the LCOH and the produced H_2 , Q_{H_2} , as depicted in Fig. 5.7. Yet, as discussed in cases 1 to 4, the modular PEME-HPP offers lower LCOH and higher H_2 production at the two extremes. Further, modular PEME-HPP has a wider range of LCOH as it tends to oversize the PEME cell area while the safe operating range is expanded through increasing N . Additionally, in all instances, higher Q_{H_2} can be achieved by the modular design which offers higher effective efficiency

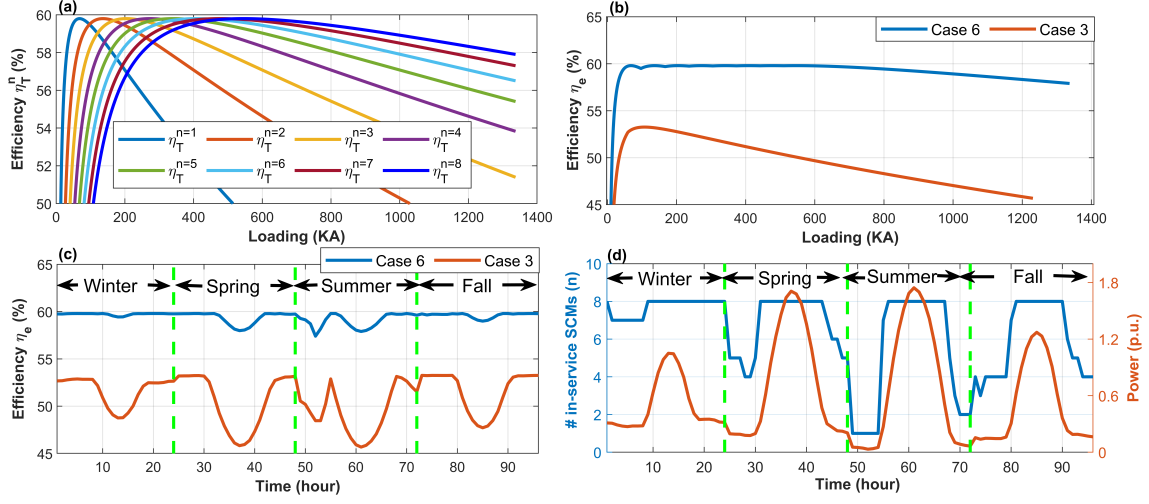


Figure 5.6: (a) Total efficiency curves of modular PEME-HPP with different number of in-service SCMs for case 6, (b) effective efficiency curves of PEME-HPP for cases 3 and 6, (c) hourly effective efficiency of PEME-HPP for cases 3 and 6, and (d) number of in-service SCMs at each hour for case 6 and the RES power profile feeding the PEME-HPP.

by increasing the number of SCMs whenever needed.

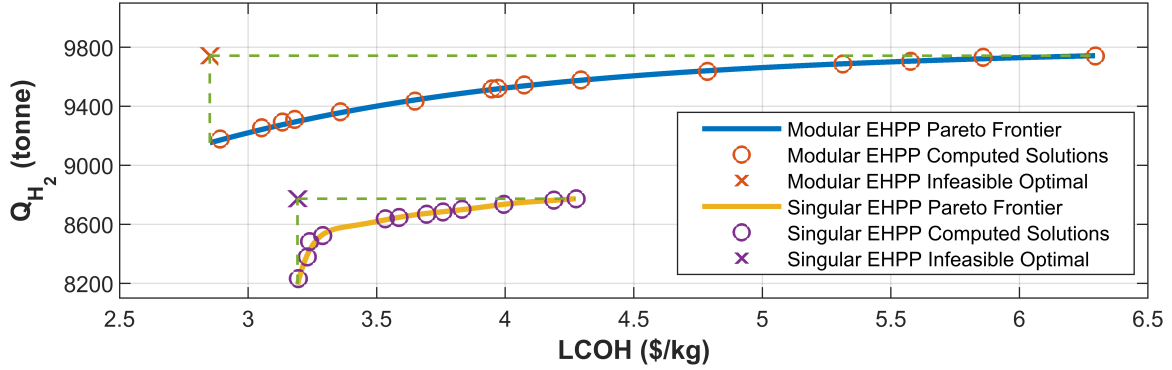


Figure 5.7: Pareto frontier for the singular and modular PEME-HPP.

5.3.4 Impact of the RES Power Profile on the Design of PEME-HPPs

This subsection investigates the impact of changing the power profile of the feeding RES (e.g., using wind RES instead of solar RES) on the design of PEME-HPPs, associated

Table 5.4: Parameters of Optimized PEME-HPP to Minimize LCOH with Different Solar and Wind Power Contribution Levels

RES	Solar	100 %	75 %	50 %	25 %	0 %
	Wind	0 %	25 %	50 %	75 %	100 %
PEME	$\delta_m^{PEM} (\mu m)$	51	51	51	51	51
	$\pi_{H_2}^{PEM} (bar)$	20	18	23	28	33
	$A_{cell}^{PEM} (m^2)$	3240	2760	2460	2340	2220
	$P_{PEM}^{rate} (MW)$	187	159	143	135	127
	$\#Modules$	8	6	4	3	3
BoP	$P_{Conv}^{rate} (MW)$	193	164	147	139	131
	$P_{Cmp}^{rate} (MW)$	35	32	25	21	18
Outcomes	LCOH (\$/kg)	3.6	3.17	2.9	2.7	2.6
	Produced H_2 (Tonne)	7525	8710	10022	11298	12513
	Consumption (kWh/kg)	57.2	57.4	56.7	56.4	56.4

PEME parameters (cathodic pressure, membrane thickness, cell area), and the number of SCMs. To avoid repetition, this subsection presents results for the case of LCOH minimization. Different contribution levels of solar and wind power resources (starting from 100% solar to 100% wind) have been utilized to drive the PEME-HPP as shown in Table 5.4. The difference in the equipment ratings is a result of the disparity in the peak values of the different profiles. Unlike the wind power profile, the solar profile decreases and increases gradually to and from zero. Therefore, as the contribution of solar power increases, more SCMs are needed to expand the PEME operation range to cover light loading conditions with current densities within the safe limits. Increasing the percentage of wind generation flats the power profile and reduces the peak of that profile. Hence, the PEME cell area and the number of SCMs, N , decrease with increasing wind contribution, which, in turn, results in reducing the capital cost and the LCOH. As wind penetration increases, the cathodic pressure also rises to enhance PEME-HPP efficiency, particularly under high loading conditions during which the plant operates most of the time. The cathodic pressure hits a low of 18bar at 25% wind contribution. As wind power generation decreases below 25%,

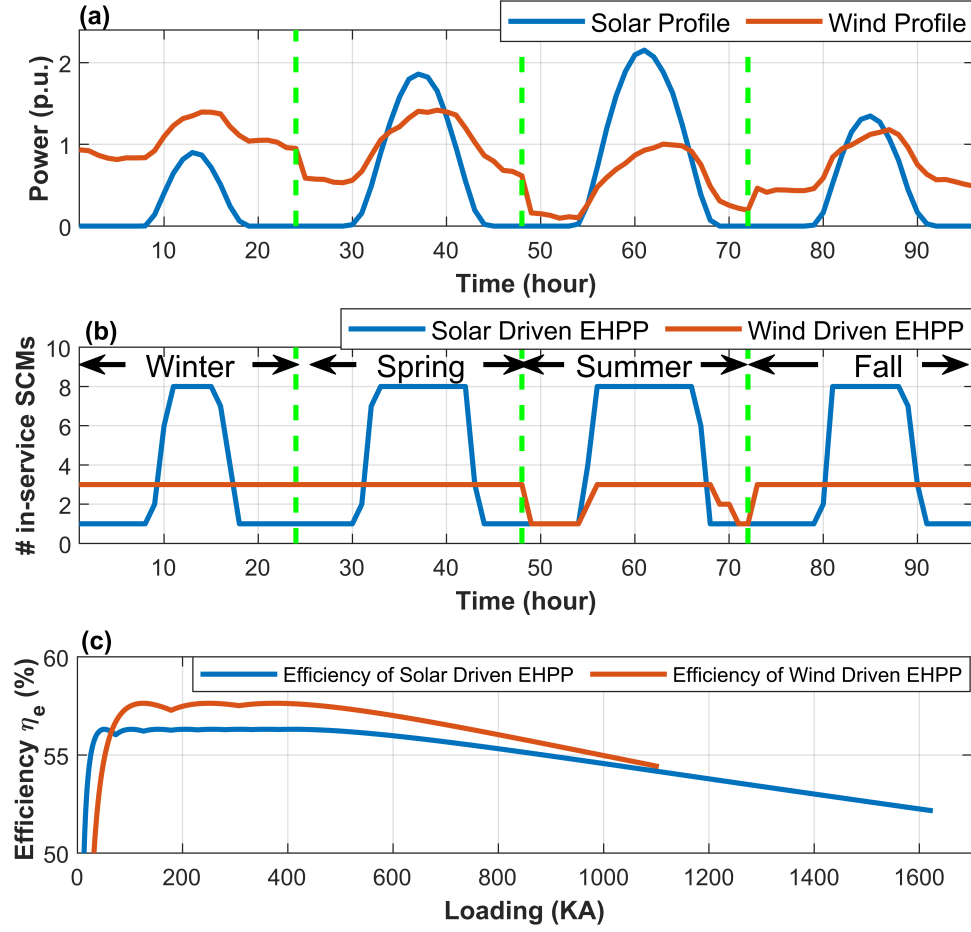


Figure 5.8: (a) Solar and wind power profiles, (b) number of in-service SCMs at each hour, and (c) effective efficiency for both solar and wind cases.

solar power becomes more dominant and the H_2 production during off-sun hours reduces significantly. Therefore, the cathodic pressure increases again allowing efficiency reduction at light loading and efficiency enhancement at high loading.

Fig. 5.8 (a) and (b) show the pure solar and wind power profiles and the hourly changes in the number of in-service SCMs for both 100% solar and 100% wind cases. For these two cases, Fig. 5.8 (c) depicts the effective efficiency curves. For the solar case, utilizing a high number of SCMs and moderate pressure increases the efficiency at low loading and the use of a wide cell area reduces the decay in the efficiency at high loading. For the

wind case, the low number of SCMs limits the safe operation under extremely light loading conditions whereas the small cell area enhances the efficiency at medium loading conditions while using a low number of SCMs. Yet, the small cell area decreases the efficiency faster at high loading conditions which is partially compensated by utilizing high cathodic pressure. Overall, the small cell area used in the wind case significantly reduces the LCOH compared to the solar case.

5.4 Summary

This chapter proposes an innovative modular design for PEME, which aims to enhance its efficiency, extend its operating range, and improve its integration with intermittent RES. The proposed modular configuration is formulated as a multi-objective optimization problem to determine the optimal i) number of PEME SCMs, ii) parameters of the PEME (cathodic pressure, membrane thickness, cell area), and iii) ratings of the PEME-HPP equipment (PEME, AC/DC converter, compressor). The proposed multi-objective formulation aims to minimize the LCOH while maximizing hydrogen production. The developed PEME modular design and multi-objective optimization formulation have been numerically validated. First, the impact of the proposed modular design of PEME-HPP is numerically evaluated compared to the conventional singular PEME-HPP design. Then, six optimization case studies are conducted: three for the singular PEME-HPP with varying weights for the optimization objectives (i.e., full weight for minimizing LCOH, equal weights for minimizing LCOH and maximizing H_2 production, and full weight for maximizing H_2 production) and three for the modular PEME-HPP using the same objectives' weights.

The results show that the modular design significantly enhances PEME-HPP efficiency at low loading levels and extends the plant's safe operating range. Further, the proposed modular design is capable of reducing the LCOH by 6% and increasing the produced H_2 by 11% in the studied wind and solar power profiles. Additionally, when the full weight is given to the objective of minimizing the LCOH, the PEME's parameters are designed in a way that tends to operate at higher current densities with lower PEME cell area to reduce

the PEME-HPP capital expenditure. As the weight of maximizing H_2 production increases, the optimal design of PEME parameters tends to favor a larger cell area to maintain the operating point at a low current density, thereby operating near the peak of the PEME efficiency curve. However, shifting the operating point towards lower current densities restricts PEME-HPP operation under low loading conditions, which limits the extent to which the cell area can be increased in the singular PEME configuration. In contrast, the modular PEME configuration allows increasing the number of SCMs to accommodate the need for a larger cell area as the weight of maximizing H_2 production increases. The Pareto frontiers of both singular and modular configurations exhibit a gradual increase in the LCOH as the produced H_2 increases, indicating that the two objectives contradict each other and hence the user has to specify the suitable design point. The Pareto frontiers also show that the proposed modular configuration always offers higher H_2 production compared to the singular one. Under different RES power generation profiles, the results show that compared to wind, the solar power profile requires lower cathodic pressure and a higher number of SCMs to enhance the modular PEME-HPP effective efficiency, especially at light loading conditions.

Chapter 6

Suitability of EHPP Technologies for Provision of Grid Services

The participation of EHPP in the provision of ancillary services has been investigated in prior studies, including those in [35, 37, 82, 117–125, 132, 133, 135]. However, these studies fail to incorporate a comprehensive electrochemical model of the electrolyzer, and most of them overlook the electrolyzer’s critical safety constraints, such as the hydrogen-to-oxygen ratio. Moreover, they do not identify the most suitable electrolyzer technology for each grid ancillary service. Additionally, a recent study in [169] indicates that the Output Pressure (π_{out}) of stored hydrogen varies by application. Yet, there is a lack of research on how this variation impacts the EHPP design and their ability to provide grid services.

Addressing the critical research gaps identified in previous studies, this chapter introduces a novel mathematical formulation for the optimal design of an EHPP integrated with power grids. The results and formulation presented in this chapter have been published by the author in [170]. The proposed model emphasizes the importance of considering the EHPP’s participation in various grid services, including CA, OR, and RS, as this can significantly affect its operational efficiency and cost-effectiveness. Different terminologies are introduced in the literature referring to various grid operators, and thus, to clarify these

terminologies, short definitions are provided for each service as follows: i) The CA is an offered service by the IESO of Ontario in which the IESO secures the capacity needed to balance the Ontario’s system during the peak hours. One form of the CA involves load participants who accept reducing their consumption during peak hours upon receiving a signal from the grid operator (i.e., IESO). The load participants, in return, receive a payment for their MW power/energy reduction. In this form involving load participants, the CA service is similar to the DR service discussed in the literature in [118] and those offered by other operators such as [171]. ii) The OR is a service offered by the IESO and is equivalent to real-time balancing. In OR service, participants receive a signal to either reduce their load or increase their generation within a few minutes to get a payment for each MWh they inject into the grid [172]. iii) RS is a potential service to be offered by the IESO in which participants receive setpoints that require instantaneously increasing/decreasing their consumption/generation by a certain amount of power to smooth the power output of a particular RES. A real-world case study is conducted by the authors of this work in collaboration with the IESO in [141] to prove the concept of this RS service. Additionally, it accounts for the application of the produced hydrogen, acknowledging that different applications require hydrogen at specific pressure ranges. Furthermore, the model incorporates the type of electricity source—whether a mix of conventional and renewable sources or purely renewable power—and the associated electricity prices, as these factors directly impact the EHPP’s design and performance. The objective of the formulated optimization problem is to minimize the LCOH by determining the optimal ratings for each EHPP component (including the bidirectional converter, electrolyzer, compressor, hydrogen storage, and fuel cell), selecting the most appropriate electrolyzer technology (AE or PEME), and specifying the internal design parameters of the electrolyzer (membrane thickness, cell area, cathodic pressure, and electrolyte concentration). The proposed formulation incorporates detailed electrolyzer models to assess the suitability of each technology for providing various grid services and for producing hydrogen for different applications across a range of power supply profiles and electricity pricing scenarios. The proposed framework provides a systematic approach to optimizing EHPP design and electrolyzer configuration, offering

practical insights for both electrolyzer manufacturers and grid operators. For manufacturers, the proposed framework supports the development of tailored electrolyzer designs optimized for specific pricing schemes, hydrogen applications, and grid service requirements. A practical outcome could be the introduction of a series of electrolyzer models, each designed to fit distinct operational conditions, thereby enhancing market adaptability and cost-effectiveness. Meanwhile, for grid operators, the framework facilitates the determination of appropriate grid service payments while assessing the likelihood of different EHPP configurations participating in these services.

Table 6.1 summarizes the key features of the proposed EHPPs design framework compared to previous works. As shown in the table, the following are the main contributions of the proposed model:

- The proposed mathematical model incorporates a detailed electrochemical electrolyzer model while considering the EHPP participation in different grid services.
- The used electrochemical electrolyzer model considers the impacts of electrolyzer safety constraints on its performance while participating in various grid services.
- The proposed model optimizes the electrolyzer’s internal design to enable effective participation in various grid services while supplying hydrogen for different applications.
- The proposed formulation considers different electrolyzer technologies (i.e., AE, PEME) and determines their suitability to provide various ancillary services and produce hydrogen for different applications across various power supply profiles and electricity pricing scenarios.

6.1 Problem Hypothesis and Formulation

This section presents the problem hypothesis and the mathematical formulation for the optimal design of the EHPP shown in Fig. 6.1. As illustrated in the figure, the EHPP

Table 6.1: Comparison of the Proposed EHPP Design Formulation with Others Work in Literature

Features of the Formulated Optimization Problem for EHPPs	[110, 111], [114]	[117, 118, 173] [121–123]	[133]	[132]	[135]	[87]	This Work
Consideration of electrolyzer's efficiency variation with loading	✗	✗	✓	✓	✓	✓	✓
Electrochemical electrolyzer model	✗	✗	✗	✗	✗	✗	✓
Design of electrolyzer parameters	✗	✗	✗	✗	✗	✗	✓
Electrolyzer safety constraint	✗	✗	✓	✗	✗	✓	✓
Participation in grid services	✗	✓	✓	✓	✓	✗	✓
Impact of hydrogen application on EHPP design	✗	✗	✗	✗	✗	✗	✓
Electrolyzer type	N/A	N/A	AE	PEME	AE/ PEME	AE/ PEME	AE/ PEME
Assessment of electrolyzer technology suitability in various grid services and hydrogen applications	✗	✗	✗	✗	✗	✗	✓

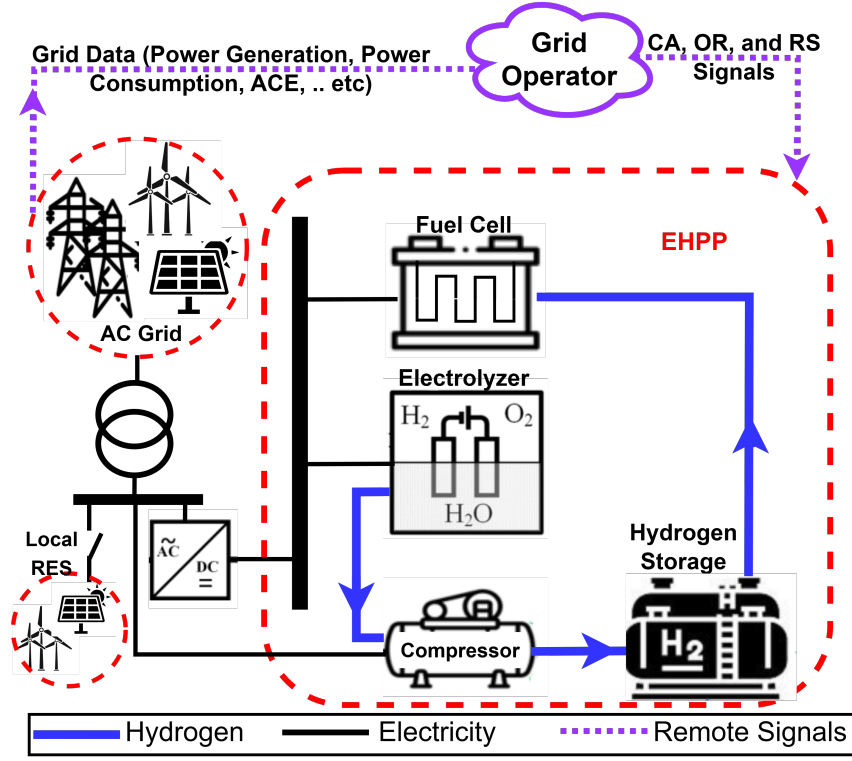


Figure 6.1: Example of an EHPP interacting with the grid operator to provide grid services.

consists of a bidirectional AC–DC converter, an electrolyzer, a compressor, HS, and an optional FC unit. As a grid-connected system, the EHPP interacts with the grid operator through communication signals to participate in the provision of grid services, such as CA and OR. Additionally, the EHPP may provide remote RS services to RES, such as solar and wind plants connected to the same AC grid, upon receiving a smoothing setpoint (RS signal) from the grid operator. The proposed optimization formulation also determines the most suitable electrolyzer technology for the identified grid services (CA, OR, and RS), while accounting for the desired hydrogen delivery pressure and operating conditions. The objective of the proposed formulation is to minimize the LCOH, considering the following assumptions:

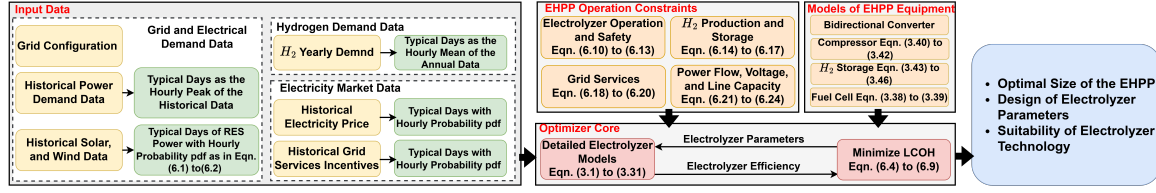


Figure 6.2: Block diagram of the proposed optimization model.

- EHPP participation in CA service is performed by reducing the plant consumption by the agreed amount of power for a number of hours per day. The CA payment is determined based on the amount of reduced power, regardless of how often the CA service is activated throughout the year [172].
- In OR service, the EHPP participation has two modes: reducing the EHPP consumption or increasing the FC power generation. The EHPP participation in OR is limited to 20% of the operating hours that offer the highest OR payment.
- To participate in RS, the EHPP functions as an energy storage system. The grid operator sends a setpoint to the EHPP to either increase the electrolyzer's loading or the FC's power generation, thereby compensating for power fluctuations from a remote RES connected to the same grid. Since the smoothing setpoint is sent with a sampling time of a few seconds, the hourly average of the smoothing setpoint is calculated for inclusion in the optimization problem.
- The desired output pressure, π_{out} , of the produced hydrogen depends on its specific application, with each one requiring a different pressure. To accommodate this, the output pressure from the EHPP is categorized into ranges from 25 to 600 bars, clustered according to the needs of each application.

Fig. 6.2 provides a block diagram of the proposed design framework. As depicted in the figure, the core of the optimization problem contains two main interdependent modules (minimization module and electrolyzer model), where electrolyzer efficiency is determined by its model based on the electrolyzer parameters sent by the minimization module. This

data exchange is repeated in each optimization iteration. The models of other components (compressor, converter, HS, and FC) are predefined and thus fed to the optimization core as inputs. The optimization core is also provided with a pre-specified yearly hydrogen demand profile, the configuration of the electrical grid to which the EHPP is connected, historical data for the electrical demand and RES power profiles, as well as historical data on electricity prices and grid services payment. Since the optimal EHPP design is based on these large historical datasets, capturing the seasonal variations in renewable generation, electricity demand, and hydrogen demand and the uncertainties in the electricity prices and grid services payments is crucial. To manage the complexity of this optimization problem, and following the approach of [156], the historical and annual datasets are condensed into a limited number of typical days (i.e., four typical days representing the four seasons of the year). This strategy reduces the number of decision variables and makes the optimization problem computationally feasible while still capturing the key seasonal characteristics that influence the sizing process. However, to maintain the model's accuracy, the reduction process of different datasets (i.e., RES power, electrical demand, hydrogen demand, electricity prices, grid services payment) is explained in the following paragraphs.

Following the approach of [156], the historical and annual data have been reduced to four typical days representing the four seasons of the year. The four typical days of the electrical demand are obtained as in [156], where each hour's demand is its peak demand at the corresponding hours in the historical data. The four typical days of the hydrogen demand are the mean of the demand during the corresponding hours in the annual data. To account for the intermittency of the RESs in the power grid, historical RES data (wind speed and solar irradiation data) is used to obtain typical days representing the four seasons. The pdf of each hour is calculated using Beta pdf (f_b) and Rayleigh pdf (f_r) for solar irradiation and wind speed, respectively [156]. The obtained pdf functions of each hour are discretized into h states covering the whole solar irradiation and wind speed ranges of that hour. Next, the probability of each irradiation state $\rho(SI^{i,t})$ and wind speed state $\rho(W S^{j,t})$ is calculated using the cumulative distribution function cdf as in [156]. Hence, the total number of the combined states at each hour is hxh , where the probability of each combined state is given

in (6.1), assuming no correlation exists between the renewable power generation in each hour and its adjacent ones.

$$\rho^{s,t} = \rho(SI^{i,t}) \rho(W S^{j,t}) \forall s = 1, \dots, h x h \wedge i, j = 1, \dots, h \wedge \forall t \in \mathbb{T} \quad (6.1)$$

Then, the power at each hour t in the typical days' power profile of any RES, P_{RES}^t , is calculated as the weighted average of the power of that RES in the $h x h$ combined states as follows:

$$P_{RES}^t = \frac{\sum_{s=1}^{h x h} \rho^{s,t} P_{RES}^{s,t}}{\sum_{s=1}^{h x h} \rho^{s,t}} \forall s = 1, \dots, h x h \wedge \forall t \in \mathbb{T} \quad (6.2)$$

To account for the uncertainty in electricity prices and OR payments, their historical data is analyzed to derive a normal pdf for each hour within the time period under study. These pdfs for electricity prices and OR payments are then discretized into multiple states, with the probability of each state being calculated. Following this, N_{MCS} MCS are generated, each with its corresponding hourly probabilities, $\rho_{ElecPrice}^{mc,t}$ for electricity prices, and $\rho_{OR}^{mc,t}$ for OR payments. The overall probability of each electricity price scenario, $\rho_{ElecPrice}^{mc}$, and each OR payment scenario, ρ_{OR}^{mc} , is then determined as the average of the hourly probabilities for the electricity prices and OR payments within that scenario, calculated as follows, respectively:

$$\rho_{ElecPrice}^{mc} = \frac{1}{\mathbb{T}} \sum_{t=1}^{\mathbb{T}} \rho_{ElecPrice}^{mc,t} \forall mc \in N_{MCS} \quad (6.3a)$$

$$\rho_{OR}^{mc} = \frac{1}{\mathbb{T}} \sum_{t=1}^{\mathbb{T}} \rho_{OR}^{mc,t} \forall mc \in N_{MCS} \quad (6.3b)$$

The objective function of the minimization module in the optimization core is formulated to minimize the LCOH as follows:

$$Min \quad \left(\frac{CAPEX + \sum_{y \in Y} (OPEX + C_{Deg} - C_{Inv}) / (1 + r)^y}{\sum_{y \in Y} (\sum_{t=1}^{\mathbb{T}} Q_d^t) / (1 + r)^y} \right) \quad (6.4)$$

where Y is the EHPP life time in years, and r is the yearly discount rate. The expression of the LCOH given in (6.4) includes capital expenditure CAPEX, operational expenditure OPEX, degradation cost C_{Deg} , grid services payment (C_{Inv}), and the output hydrogen from the EHPP, Q_d^t . The CAPEX is a function of the ratings of the electrolyzer (P_{PEM}^{rate}),

bidirectional converter (P_{Conv}^{rate}), FC (P_{FC}^{rate}), and compressor (P_{Cmp}^{rate}), as well as the HS capacity (E_{HS}), expressed as follows:

$$CAPEX = P_{Elz}^{rate} C_{Elz} + P_{FC}^{rate} C_{FC} + P_{Conv}^{rate} C_{Conv} + P_{Cmp}^{rate} C_{Cmp} + E_{HS} C_{HS} \quad (6.5)$$

where C_{Elz} , C_{FC} , C_{Conv} , C_{Cmp} , and C_{HS} are, respectively, the electrolyzer, FC, Converter, Compressor, and HS capital costs.

The total OPEX is the weighted average of the electricity and operational costs of the N_{MCS} MCS as given below:

$$OPEX = \frac{\sum_{mc=1}^{N_{MCS}} \rho_{Elec}^{mc} Price \left(\sum_{t=1}^{\mathbb{T}} P_{EHPP}^t Price_{Elec}^{t,mc} + N_{H_2}^{Elz,t} O_w + Q_{HS}^t O_{HS} + P_{Elz}^t O_{Elz} + P_{FC}^t O_{FC} + P_{Cmp}^t O_{Cmp} \right)}{\sum_{mc \in N_{MCS}} \rho_{Elec}^{mc} Price}, \quad \forall t \in \mathbb{T} \wedge mc \in N_{MCS} \quad (6.6)$$

where $Price_{Elec}^{t,mc}$ is the electricity price at hour t in scenario mc , while O_w , O_{HS} , O_{Elz} , O_{FC} , and O_{Cmp} are the operation costs of water consumption, HS, electrolyzer, FC, and compressor, respectively. The electricity cost depends on the EHPP's consumption, P_{EHPP}^t , which is the sum of the electrolyzer power, P_{Elz}^t , and compressor power, P_{Cmp}^t , as below:

$$P_{EHPP}^t = P_{Elz}^t + P_{Cmp}^t \quad \forall t \in \mathbb{T} \quad (6.7)$$

The C_{Deg} considers the electrolyzer and FC degradation, as expressed in (6.8), where D_{Elz} and D_{FC} are the degradation costs of the electrolyzer and FC, respectively.

$$C_{Deg} = \sum_{t=1}^{\mathbb{T}} P_{Elz}^t D_{Elz} + P_{FC}^t D_{FC}, \quad \forall t \in \mathbb{T} \quad (6.8)$$

The grid services payment, C_{Inv} , consists of three components: CA payment (CA_{Inv}), OR payment (OR_{Inv}), and RS payment (RS_{Inv}) as depicted in (6.9a). The CA payment, shown in (6.9b), has two obligation periods (Winter period and Summer period). Each period has its CA participation power (Pc_{CA}^W and Pc_{CA}^S) and CA payment price (CA_{prc}^W

and CA_{prc}^S). The superscripts W and S stand, respectively, for the winter and summer obligation periods, and N_{day} represents the number of days in the obligation period. The total OR payment, given in (6.9c), is the weighted average of the OR payment of the N_{MCS} Monte Carlo scenarios, that is a function of the hourly OR participation, Pc_{OR}^t , and the hourly OR payment price, $OR_{prc}^{t,mc}$. Similarly, as in (6.9d), the RS payment is a function of the summation of the RS participation, Pc_{RS}^t , and the RS payment price, RS_{prc} .

$$C_{Inv} = CA_{Inv} + OR_{Inv} + RS_{Inv} \quad (6.9a)$$

$$CA_{Inv} = N_{day}^W Pc_{CA}^W CA_{prc}^W + N_{day}^S Pc_{CA}^S CA_{prc}^S \quad (6.9b)$$

$$OR_{Inv} = \frac{\sum_{mc \in N_{MCS}} \rho_{OR}^{mc} \sum_{t \in \mathbb{T}} Pc_{OR,Elz}^t OR_{prc}^{t,mc}}{\sum_{mc \in N_{MCS}} \rho_{OR}^{mc}}, \quad \forall t \in \mathbb{T} \wedge \forall mc \in N_{MCS} \quad (6.9c)$$

$$RS_{Inv} = \sum_{t \in \mathbb{T}} Pc_{RS}^t RS_{prc} \quad \forall t \in \mathbb{T} \quad (6.9d)$$

6.1.1 Electrolyzer Operation and Safety Constraints

The operation of the electrolyzer includes constraints on the current densities, cell area, and cathodic pressure. The electrolyzer current density at any hour, $J^{Elz,t}$, is calculated by dividing the electrolyzer power consumption, P_{Elz}^t , by the electrolyzer cell voltage, V_{cell}^{Elz} , and cell area, A_{cell}^{Elz} . The electrolyzer hourly current density, $J^{Elz,t}$, must be limited by its maximum current density, J_{max}^{Elz} , as follows:

$$0 \leq J^{Elz,t} = \frac{P_{Elz}^t}{V_{Elz}^{rate} A_{cell}^{Elz}} \leq J_{max}^{Elz} \quad \forall t \in \mathbb{T} \quad (6.10)$$

The electrolyzer's cell area, A_{cell}^{Elz} , is also limited by a lower cell area bound, $A_{cell}^{Elz,min}$, and a upper cell area bound, $A_{cell}^{Elz,max}$, as given below:

$$A_{cell}^{Elz,min} \leq A_{cell}^{Elz} \leq A_{cell}^{Elz,max} \quad (6.11)$$

Similarly, the electrolyzer's cathodic pressure, $\pi_{H_2}^{Elz}$, is limited by a lower hydrogen pressure bound, $\pi_{H_2}^{Elz,min}$, and a upper hydrogen pressure bound, $\pi_{H_2}^{Elz,max}$, as shown hereunder:

$$\pi_{H_2}^{Elz,min} \leq \pi_{H_2}^{Elz} \leq \pi_{H_2}^{Elz,max} \quad (6.12)$$

For safety considerations, the percentage of hydrogen in oxygen is restricted by the safe limit of hydrogen in oxygen, $\Psi_{H_2}^{Elz, safe}$, as follows:

$$\Psi_{H_2}^{Elz} \leq \Psi_{H_2}^{Elz, safe} \quad (6.13)$$

6.1.2 Hydrogen Production and Storage Constraints

The SoH at each hour, SoH^t , is constrained by the minimum SoH, SoH^{min} , and maximum SoH, SoH^{max} , as given below:

$$SoH^{min} \leq SoH^t \leq SoH^{max} \quad \forall t \in \mathbb{T} \quad (6.14)$$

To guarantee the safe HS operation, hydrogen pressure inside the HS at each hour, π_{HS}^t , should not exceed the maximum design pressure, π_{HS}^{max} . Additionally, to meet the hydrogen application requirements, π_{HS} should not go below a specific threshold, π_{HS}^{min} . The constraints on π_{HS}^t is provided hereunder:

$$\pi_{HS}^{min} \leq \pi_{HS}^t \leq \pi_{HS}^{max} \quad \forall t \in \mathbb{T} \quad (6.15)$$

Further, to avoid HS explosion risks and prevent damage to the HS tank material and given the capability of the HS cooling system, the hydrogen temperature inside the HS at each hour, T_{HS}^t , has lower and upper bounds (i.e., T_{HS}^{min} and T_{HS}^{max}), as follows:

$$T_{HS}^{min} \leq T_{HS}^t \leq T_{HS}^{max} \quad \forall t \in \mathbb{T} \quad (6.16)$$

The hydrogen flow must satisfy the hydrogen balance equation where the sum of the electrolyzer hydrogen flow, $N_{H_2}^{Elz, t}$, and HS hydrogen flow, Q_{HS}^t , should equal the output hydrogen flow from the EHPP, Q_d^t and the flow of the FC hydrogen consumption, $N_{H_2}^{FC, t}$, as follows:

$$N_{H_2}^{Elz, t} + Q_{HS}^t = Q_d^t + N_{H_2}^{FC, t} \quad \forall t \in \mathbb{T}. \quad (6.17)$$

6.1.3 Grid Services Constraints

The consideration of each grid service requires additional constraints. For the CA service, the EHPP consumption has to be kept above the CA participation amount, Pc_{CA}^t , for the

whole availability window, $t \in CA_{Av}$, when there is no CA activation. However, when the activation signal is received, the consumption has to be reduced with the agreed CA participation, Pc_{CA}^t , during the CA activation hours, $t \in CA_{Act}$. These two constraints are formulated as follows:

$$P_{EHPP,CA}^{t,Av} \geq Pc_{CA}^t \quad \forall t \in \mathbb{T} \wedge t \in CA_{Av} \quad (6.18a)$$

$$P_{EHPP,CA}^{t,Act} + Pc_{CA}^t \leq P_{EHPP,CA}^{t,Av} \quad \forall t \in \mathbb{T} \wedge t \in CA_{Act} \quad (6.18b)$$

$$\text{where,} \quad Pc_{CA}^t = \begin{cases} Pc_{CA}^W & \forall t \in \mathbb{T}^W \\ Pc_{CA}^S & \forall t \in \mathbb{T}^S \end{cases} \quad (6.18c)$$

$P_{EHPP,CA}^{t,Act}$ and $P_{EHPP,CA}^{t,Av}$ are the EHPP power during the availability window when the CA service is activated and deactivated, respectively. Similarly, the participation in OR service adds further constraints. During the hours of participation in OR, $t \in OR_{Act}$, the sum of the EHPP power consumption, $P_{EHPP,OR}^t$, and the reduction in electrolyzer power (electrolyzer contribution in OR), $Pc_{OR,Elz}^t$, is limited by the EHPP normal consumption, P_{EHPP}^t , during these hours when there is no participation in any grid service as explained below:

$$0 \leq P_{EHPP,OR}^t + Pc_{OR,Elz}^t \leq P_{EHPP}^t \quad \forall t \in \mathbb{T} \wedge t \in OR_{Act} \quad (6.19)$$

The participation in RS requires fast response in terms of changing the consumed and produced power. As such, changes in the EHPP's participation in RS, Pc_{RS}^{ts} , should not exceed the electrolyzer ramp rate, RR_{Elz} , as outlined hereunder:

$$\frac{Pc_{RS}^{ts} - Pc_{RS}^{ts-1}}{\Delta t_s} \leq RR_{Elz} \quad \forall ts \in \mathbb{T}_s \quad (6.20)$$

6.1.4 Power Grid Constraints

The grid-connected operation of the EHPP requires considering the power flow constraints of the grid. As such, the objective function in (6.4) is subject to the voltage (V_b^t), thermal line capacity (S_b^t), active power (P_b^t) and reactive power (Q_b^t) flow constraints as

given in (6.21), (6.22), (6.23), and (6.24), respectively.

$$V_b^{min} \leq V_b^t \leq V_b^{max} \quad \forall t \in \mathbb{T} \quad (6.21)$$

$$S_b^t \leq S_b^{max} \quad \forall t \in \mathbb{T} \quad (6.22)$$

$$P_{b,g}^t = P_{b,d}^t + V_b^t \sum_{q=1}^B V_q^t \mathbb{Y}_{b,q} \cos(\delta_b^t - \delta_q^t - \theta_{b,q}) \quad \forall t \in \mathbb{T} \quad (6.23)$$

$$Q_{b,g}^t = Q_{b,d}^t + V_b^t \sum_{q=1}^B V_q^t \mathbb{Y}_{b,q} \sin(\delta_b^t - \delta_q^t - \theta_{b,q}) \quad \forall t \in \mathbb{T} \quad (6.24)$$

where $\mathbb{Y}$ and θ are the admittance matrix amplitude and angle, respectively. δ is the voltage angle. B and b are the total number of buses and the bus index, respectively. The subscripts g and d represent the generation and demand power, respectively.

6.2 Numerical Studies

This section evaluates the suitability of each electrolyzer technology (AE and PEME) based on their participation in various grid services, hydrogen production for different applications, and supply from sources with diverse power profiles. To account for different electricity pricing, two provinces with clean electricity systems in Canada are considered. Quebec benefits from abundant hydroelectric resources, allowing for a flat electricity rate, while Ontario's electricity prices are more variable due to a diverse energy mix that includes nuclear, hydroelectric, natural gas, and renewable sources. The hourly electricity prices in Ontario fluctuate based on market conditions and grid demand, as managed by the IESO. This variability can lead to higher and less predictable costs compared to the consistent pricing mechanism in Quebec. In this regard, three scenarios are considered to help assess the performance of AE and PEME technologies under different conditions, offering a comprehensive view of their operational flexibility and efficiency. The three scenarios are defined as follows:

- Scenario-I: The EHPP is drawing power from a mix of renewable and non-renewable sources. Hourly electricity prices are based on historical data from the IESO in

Ontario, with power delivered through the transmission system, adhering to power flow and line capacity constraints.

- Scenario-II: The EHPP is also fed through a transmission system as in scenario-I but with a flat electricity rate of 30 \$/MWh as defined by Hydro-Quebec [174].
- Scenario-III: The EHPP is co-located with an intermittent RES, with no power allowed to be injected into the grid. In this scenario, the EHPP consumes power through a PPA at a fixed rate of 44\$/MWh [175], with input power limited by the RES's availability.

Fig. 4.4 shows a single-line diagram of the IEEE 30-bus system used to validate the effectiveness of the proposed model. The EHPP is connected to bus 18. In scenarios I and II, two wind power plants, sized at 700 MW each, are connected to buses 20 and 30, while a 600 MW solar PV plant is connected to bus 26. In Scenario-III, 200 MW wind and 100 MW solar PV plants are connected to the same bus as the EHPP.

The IEEE-30 bus system is represented using its admittance matrix, which serves as the foundation for defining a set of nonlinear constraints that model the system's operational and power flow conditions, as previously discussed in Section 6.1.4. These nonlinear constraints comprise both inequality constraints—such as bus voltage limits and line capacity constraints, as specified in (6.21) and (6.22)—and equality constraints, which include active and reactive power flow equations. The equality constraints account for all connected generators, loads, and shunt elements, as detailed in (6.23) and (6.24).

Nine case studies are generated from the identified three scenarios as depicted in Table 6.2. Cases 1 to 3 study the three scenarios when the EHPP only meets the required hydrogen demand, i.e., the EHPP does not participate in grid services. Cases 4 to 5, 6 to 7, and 8 to 9 address scenarios I and II, considering the EHPP participation in CA, OR, and RS services, respectively. Five years of hourly historical data for solar irradiation and wind speed in the province of Ontario, Canada [158] is used to generate the hourly solar irradiation and wind speed profiles of the four typical days for different RESs in the grid as provided in (6.1) and

Table 6.2: Summary of Case Studies

Cases	1	2	3	4	5	6	7	8	9
Grid Service	-			CA		OR		RS	
Scenario	I	II	III	I	II	I	II	I	II

(6.2). Also, the historical electrical demand of five years in the province of Ontario [159] is used to obtain the four typical days of the electrical demand. Historical data on electricity prices, CA and OR payments given by the IESO [159] in Ontario is used to calculate the average CA payment and generate 1000 Monte Carlo scenarios for electricity prices and OR payments, where each scenario has its probability as given in (6.3). A whole-year hydrogen demand profile is obtained from [143] to find the four typical days of hydrogen demand. It is worth noting that while cathodic pressure varies between case studies, it remains constant during normal electrolyzer operation and does not change dynamically over time. Also, the electrolyzer cell temperature, T_{cell} , is assumed to remain constant at 353 K in the case studies. Maintaining the cell temperature at the required level could be practically realized using an active cooling system via circulating cooling water through the electrolyzer [103], [104]. The electrolyzer costs are obtained from [1], while other simulation parameters are imported from previous techno-economic studies [173], [143], and [141].

The proposed problem in section 6.1 is formulated as a nonlinear optimization problem. The formulated problem has been solved using the SQP algorithm, which is one of the most successful methods for solving nonlinear constrained optimization problems [176]. SQP is available in the Matlab Optimization Toolbox. For all case studies, the convergence, constraints, and decision variables tolerances are set to 10^{-6} while the maximum function evaluations and maximum iterations are set to 10^5 and 2500, respectively. The simulation platform has the following specifications: Core i7-10700K, 3.8 GHz CPU, 32 GB RAM, and 64-bit system.

6.2.1 Results of the Proposed Model Compared to Previous Models in the Literature

In this subsection, an example of numerical comparison is established between the literature-based optimization models used for optimal sizing of EHPP using different electrolyzer technologies and the proposed one. The comparison is conducted to highlight the significance of optimizing the electrolyzer internal design and considering its safety constraint in determining the electrolyzer technology suitability under different scenarios of the feeding power, electricity pricing, etc. As such, two literature-based optimization models are considered as follows:

- Model 1, adopted from [135], employs the different electrolyzer technologies models without optimizing the electrolyzer parameters (i.e., electrolyzer internal design/parameters are chosen as in the manufacturers' datasheets and previous studies in the literature) or considering the electrolyzer safety constraint on the hydrogen-to-oxygen ratio.
- Model 2, adopted from [87], employs the different electrolyzer technologies models without optimizing the electrolyzer parameters, as in Model 1, but it properly considers the electrolyzer's safety constraint.

Two case studies (Cases 1 and 3) are chosen to apply the different optimization models (1, 2, and the proposed one) at a selected output pressure ($\pi_{out} = 100 \text{ bar}$). AE and PEME internal parameters are selected as commonly used in some commercial units, as mentioned in [70] and [143], respectively. Table 6.3 presents the LCOH of Cases 1 and 3 at $\pi_{out} = 100 \text{ bar}$ with the different models for the two electrolyzer technologies (AE, PEME). According to Model 1, AE offers lower LCOH in Cases 1 and 3. However, according to Model 2, in Case 1, PEME offers a slightly lower LCOH than AE, while AE is the cheaper option in Case 3. According to the proposed model, PEME has a much lower LCOH than AE in Case 1 and almost the same LCOH as AE in Case 3. The presented comparison shows that the decision on electrolyzer technology suitability and its LCOH is highly affected by the optimization model. In fact, neglecting to optimize the electrolyzer's internal design and

its safety constraints, as in Model 1, results in misleading information and favors AE over PEME as it ignores the difference in safety limitations between AE and PEME. Similarly, in Model 2, using pre-defined (non-optimized) electrolyzer internal parameters may result in an unfair comparison of different electrolyzer technologies. For instance, the behavior of PEME using a pre-defined set of internal parameters (Model 2) may be unsuitable for certain cases (Case 1); however, optimizing its internal parameters significantly improves its behavior, resulting in much lower LCOH as in the proposed optimization model.

Table 6.3: The LCOH of Cases 1 and 3 at $\pi_{out} = 100 \text{ bar}$ with Different Optimization Models

Case #	Elz Type	Model		
		1 [135]	2 [87]	Proposed
1	AE	7.18	7.85	7.8
	PEME	7.33	7.67	7.3
3	AE	3.38	3.5	3.5
	PEME	3.55	3.55	3.5

6.2.2 Cases 1 to 3: EHPP Does Not Provide Grid Services

In Cases 1 to 3, the EHPP is designed for hydrogen production only without participating in grid services. Fig. 6.3 (a) shows a breakdown of the LCOH for both AE-HPP and PEME-HPP at all levels of π_{out} in Case 1. As shown in the figure, the use of PEME results in a lower LCOH compared to AE for all levels of π_{out} . As π_{out} increases, the difference in LCOH between AE-HPP and PEME-HPP also increases. Yet, the variations in CAPEX and other costs are relatively small compared to the increase in the electricity cost that occurs as π_{out} increases. Table 6.4 presents the optimal EHPP design parameters at π_{out} of 25 bar and 600 bar for all cases. It shows that PEME is the most suitable technology in Case 1. While the ratings of most EHPP equipment, except the compressor, remain relatively unchanged, resulting in minor CAPEX variations, the internal PEME design does change with π_{out} . Specifically, increasing π_{out} from 25 bar to 600 bar requires rising the cathodic pressure,

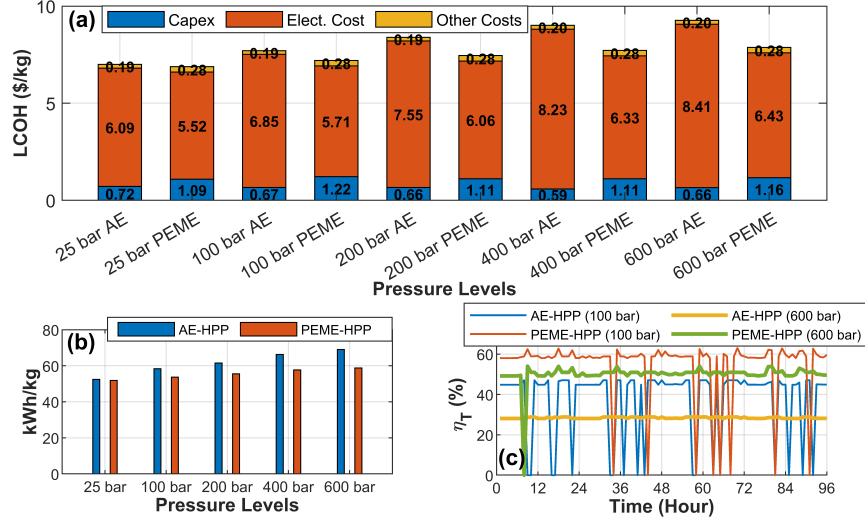


Figure 6.3: Case 1 AE-HPP and PEME-HPP (a) breakdown of LCOH, (b) average power consumption at different values of π_{out} , and (c) hourly total efficiency at π_{out} of 100 and 600 bar.

π_{H_2} , from 4 bar to 13 bar and the membrane thickness from $28 \mu m$ to $50 \mu m$. Fig. 6.3 (b) shows the AE-HPP and PEME-HPP power consumption at different π_{out} levels. The figure shows that at low pressure (25 bar), the power consumption of AE-HPP is slightly higher than PEME-HPP by 2%. However, increasing the π_{out} gradually increases the difference in power consumption between both technologies, making AE-HPP power consumption 15% higher than PEME-HPP at $\pi_{out} = 600$ bar. This observation explains that the increase in the electricity cost of AE-HPP compared to PEME-HPP is primarily due to the higher power consumption of AE-HPP, especially when high π_{out} is required. Fig. 6.3 (c) shows the hourly efficiency of both AE-HPP and PEME-HPP at π_{out} of 100 bar and 600 bar. As depicted in the figure, PEME-HPP efficiency is higher than that of AE-HPP, and the gap between the two technologies' efficiencies widens as π_{out} increases. PEME-HPP can operate with higher electrolyzer cathodic pressure, and thus, it has lower compressor power consumption compared to AE-HPP. Hence, the difference in power consumption can be attributed to the greater efficiency of PEME-HPP compared to AE-HPP.

For Case 2, Fig. 6.4 (a) presents the LCOH breakdown for both AE-HPP and PEME-

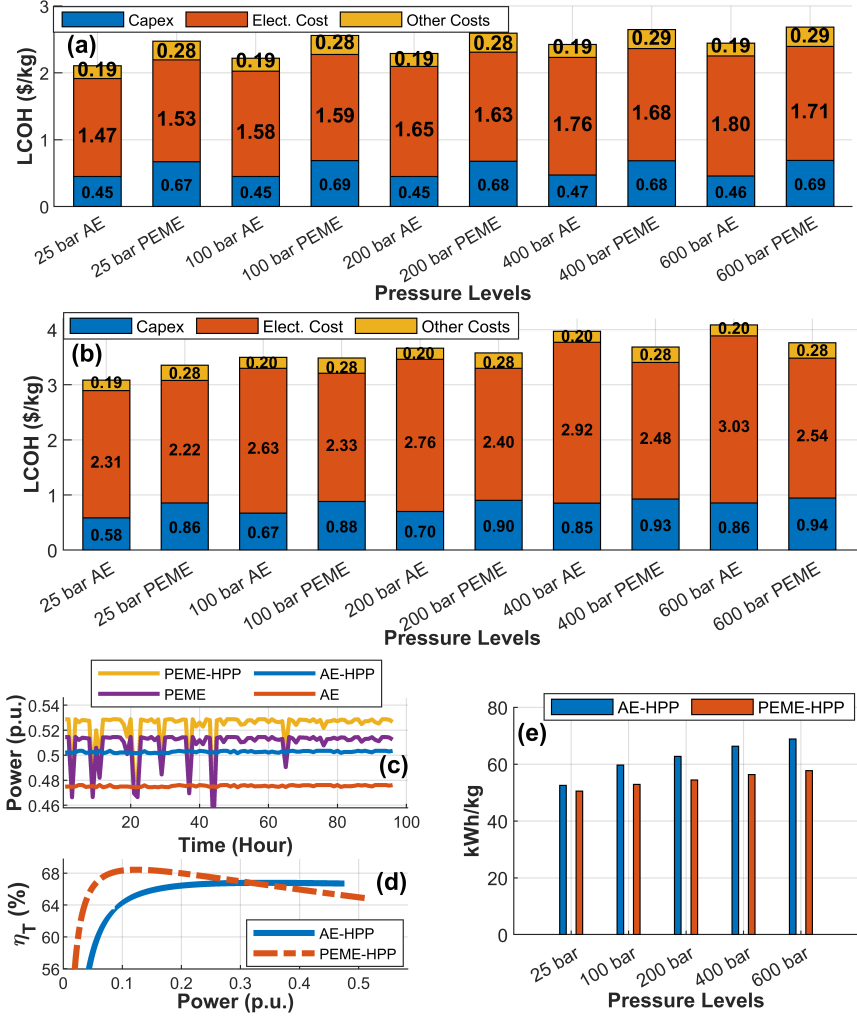


Figure 6.4: Breakdown of LCOH of EHPP at all π_{out} values in (a) Case 2 and (b) Case 3. Case 2 (c) hourly power consumption and electrolyzer loading at 25 bar, and (d) total efficiencies at 25 bar. (e) EHPP average power consumption in Case 3 at all π_{out} values.

HPP across various π_{out} levels. Unlike Case 1, the LCOH for AE-HPP is lower than that for PEME-HPP at all levels of π_{out} . However, as π_{out} increases, the advantage of AE-HPP diminishes; the difference in LCOH between AE-HPP and PEME-HPP decreases from 19% to 11% as π_{out} rises from 25 to 600 bar. This reduction is primarily driven by electricity costs, with PEME-HPP having lower electricity expenses than AE-HPP at pressures above 100 bar. Nevertheless, the savings in electricity costs for PEME-HPP are insufficient to

offset its higher CAPEX, resulting in a higher overall LCOH compared to AE-HPP. As shown in Table 6.4, in Case 2, increasing π_{out} only affects the compressor rating, with no impact on other EHPP design aspects or AE internal parameters.

The flat-rate electricity price used in Case 2 results in minimal hourly variation in EHPP power consumption, as shown in Fig. 6.4 (c), leading to a nearly constant electrolyzer loading at the rated capacity for both the EHPP and the electrolyzer. Such steady operation allows AE technology to compete effectively with PEME, as AE achieves higher efficiency when operating at relatively high cathodic pressure, ultimately resulting in lower electricity costs compared to PEME. Further, this steady operation increases the plant's capacity factor, resulting in an EHPP rating nearly half that of Case 1, as shown in Table 6.4. Fig. 6.4 (d) illustrates the efficiency curves of AE-HPP and PEME-HPP at $\pi_{out} = 25 \text{ bar}$. At lower power consumption levels (below 0.3 p.u.), AE exhibits higher hydrogen permeation than PEME, reducing its efficiency compared to PEME-HPP. Yet, at power levels close to the plant's rated capacity, PEME experiences a significant voltage drop across its membrane, reducing its efficiency. This makes AE-HPP more efficient than PEME-HPP under these conditions. Given that Case 2 requires the EHPP to operate at its rated capacity, AE-HPP emerges as the superior option, providing a lower LCOH due to its higher efficiency at full load compared to PEME-HPP.

In Case 3, the EHPP operates with a varying RES power, and the electricity price is lower than in Case 1. Therefore, the impact of electricity cost on the LCOH in Case 3 is less than in Case 1. Fig. 6.4 (b) depicts the LCOH breakdown for both AE-HPP and PEME-HPP. The high CAPEX of PEME-HPP makes its LCOH higher than that of AE-HPP at $\pi_{out} = 25 \text{ bar}$. However, at higher levels of π_{out} (100 to 600 bar), the electricity cost of AE-HPP increases, causing the LCOH of AE-HPP to surpass that of PEME-HPP by 9% at 600 bar. Similar to Case 1, the increase in the electricity cost of AE-HPP compared to PEME-HPP as π_{out} increases can be attributed to the growing difference in power consumption between AE-HPP and PEME-HPP, as illustrated in Fig. 6.4 (e). Although Case 3 uses a flat-rate electricity price like Case 2, the EHPP in Case 3 has a higher rating to account for RES fluctuations, leading to a lower capacity factor, as shown in Table 6.4. At 25 bar,

AE is designed with lower cathodic pressure and higher electrolyte concentration (M) than in Case 2 to reduce hydrogen crossover under low loading conditions imposed by RES. At 600 bar, the low cathodic pressure required for AE under low loading increases compressor consumption, making PEME more efficient and suitable for high π_{out} levels.

6.2.3 Cases 4 and 5: EHPP Provides CA Service

In Cases 4 and 5, the EHPP is designed for hydrogen production while participating in CA. Fig. 6.5 (a) depicts the changes in LCOH between Case 4 and Case 1 for both AE-HPP and PEME-HPP. The figure shows that participating in CA leads to an increase in LCOH for both electrolyzer technologies compared to Case 1. However, the impact of CA participation on LCOH is more pronounced for AE-HPP than for PEME-HPP. For example, at a pressure of 600 bar, the LCOH of AE-HPP in Case 4 increases by 9%, while for PEME-HPP, it increases by 5%, relative to Case 1.

Fig. 6.5 (b) provides a breakdown of the main components contributing to the LCOH in Case 4, namely CAPEX, electricity cost, and CA payment, for both AE-HPP and PEME-HPP at $\pi_{out} = 200 \text{ bar}$, compared to Case 1. As shown in the figure, participation in CA reduces CAPEX due to a shift in power consumption that flattens the power profile, resulting in a lower equipment rating, as in Table 6.4. However, this shift also causes the EHPP to consume more power during periods of high electricity prices, thereby increasing the overall electricity cost. Additionally, Fig. 6.5 (b) shows that AE-HPP receives higher CA payments than PEME-HPP due to its larger power reserve available for CA participation. Without CA, as explained in Case 1, AE-HPP's lower efficiency compared to PEME-HPP results in higher power consumption for the same hydrogen production, leading to greater CA participation when considered in Case 4.

Fig. 6.5 (c) shows the changes in the LCOH from Case 2 to Case 5 at various π_{out} levels. Unlike the trends observed in Case 4, where CA participation increased LCOH, in Case 5, the inclusion of CA services results in a decrease in LCOH compared to Case 2 for both AE-HPP and PEME-HPP. This reduction is primarily due to the substantial impact of CA

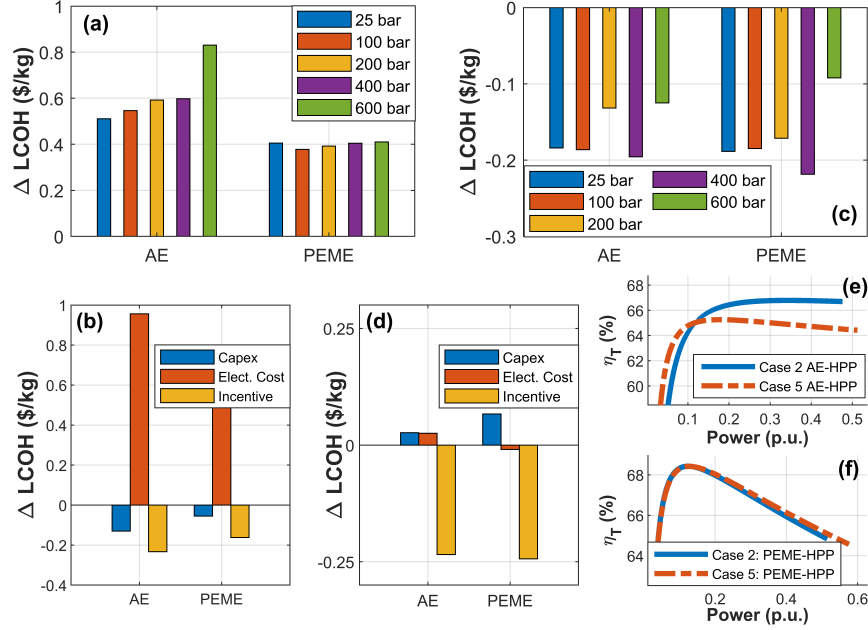


Figure 6.5: Deviation of Case 4 (a) LCOH from Case 1 for both AE and PEME at all π_{out} levels, and (b) LCOH breakdown from Case 1 at 200 bar. Deviation of Case 5 (c) LCOH from Case 2 for both AE and PEME at all π_{out} levels, and (d) LCOH breakdown from Case 2 at 25 bar. Total efficiency of (e) AE-HPP and (f) PEME-HPP in Cases 2 and 5 at 25 bar.

payments on lowering the overall LCOH. Unlike in Case 4, where power shifting increases electricity costs, Case 5 uses a flat-rate electricity price, allowing CA payments to reduce the LCOH. In both Case 2 and Case 5, a flat-rate electricity price is used, meaning that in the absence of grid services (as in Case 2), the EHPP operates at fixed power (its rated power), leaving little room for adjustments in power consumption without changing the plant capacity. However, in Case 5, CA services require increasing the plant's rating to accommodate shifting power consumption, as in Table 6.4, leading to a higher CAPEX compared to Case 2.

To further analyze these results, Fig. 6.5 (d) provides a breakdown of the changes in LCOH components from Case 2 to Case 5 at $\pi_{out} = 25 \text{ bar}$. As in the figure, CA payments are vital in reducing LCOH, while CAPEX increases for both AE-HPP and PEME-HPP. However, the increase in CAPEX is more pronounced for PEME-HPP due to its higher

capital cost. The variation in electricity costs between the technologies also differs.

For AE-HPP, electricity costs rise because the AE system is designed to operate over a wider loading range to accommodate CA requirements. In Case 5, compared to Case 2, AE is designed to operate at a lower cathodic pressure and higher electrolyte concentration to meet CA needs, as in Table 6.4. This limits hydrogen crossover under low loading conditions but also reduces EHPP efficiency, especially at high loading conditions. Fig. 6.5 (e) depicts the AE-HPP efficiency curves for Cases 2 and 5 at π_{out} of 25 bar. As shown, the lower cathodic pressure in Case 5 results in better efficiency at low loading conditions but significantly lower efficiency at high loading conditions compared to Case 2.

For PEME-HPP, the electricity cost slightly decreases in Case 5 due to improved efficiency from an increased PEME rating. The larger PEME setup uses a wider cell, which reduces voltage drop, resulting in slightly better efficiency at high loading conditions. Fig. 6.5 (f) shows the PEME-HPP efficiency curves for Cases 2 and 5 at $\pi_{out} = 25 \text{ bar}$, highlighting the slight improvement in efficiency in Case 5 over Case 2 at high loading conditions.

6.2.4 Cases 6 and 7: EHPP Participates in OR Service

In Cases 6 and 7, the EHPP is designed for hydrogen production while also participating in the provision of OR service. Fig. 6.6 (a) compares the LCOH for Cases 1 and 6 for both AE-HPP and PEME-HPP. At low π_{out} (up to 100 bar), the LCOH for AE-HPP in Case 6 is nearly identical to that in Case 1, indicating minimal participation in the OR service. This similarity arises because both cases use variable electricity prices, and during periods of high electricity prices, the EHPP's power consumption is very low. These periods also tend to offer high OR payments. At π_{out} up to 100 bar, the AE-HPP has limited power consumption during high OR payment periods, which restricts its ability to contribute to OR by reducing its consumption. At higher π_{out} , however, AE-HPP is required to increase its power consumption to meet the demands of high-pressure hydrogen production. This increased consumption allows AE-HPP to participate more effectively in the OR service by shifting its consumption away from periods of high electricity prices. As a result, the

LCOH for AE-HPP in Case 6 shows a noticeable reduction compared to Case 1 due to the received OR payments. However, as the π_{out} continues to rise, AE-HPP's ability to shift consumption diminishes, resulting in fewer hours of OR contribution but with higher levels of contribution per hour. This pattern is illustrated in Fig.6.6 (c) and Fig.6.6 (d), which display the AE-HPP's OR contributions at π_{out} of 400 bar and 600 bar, respectively. Consequently, OR payments for AE-HPP peak at π_{out} of around 200 bar and then gradually decrease as π_{out} increases further. Thus, the difference in LCOH between Case 1 and Case 6 is greatest at $\pi_{out} = 200 \text{ bar}$ and diminishes at higher π_{out} .

In contrast, for PEME-HPP, the LCOH in Case 6 is equal to that in Case 1 for all π_{out} levels, suggesting negligible participation in the OR service. The PEME-HPP's higher efficiency results in much lower power consumption compared to AE-HPP, even at high electricity prices. Additionally, due to its wider operating range, PEME-HPP can significantly reduce consumption during periods of high electricity prices and OR payments. Consequently, the PEME-HPP has very low power consumption during high OR payment hours, limiting its contribution to OR. Thus, the PEME-HPP's design in Case 6 is the same as Case 1, as in Table 6.4.

Fig. 6.6 (b) shows the LCOH for Cases 2 and 7 for both AE-HPP and PEME-HPP. Unlike in Case 6, participation in the OR service in Case 7 results in a reduction of the LCOH for both electrolyzer technologies compared to Case 2 at all π_{out} levels. However, despite this reduction, the LCOH of PEME-HPP remains higher than that of AE-HPP for all values of π_{out} , indicating that while OR payments do help reduce costs, they do not lower the PEME-HPP LCOH enough to make it more cost-effective than AE-HPP at any π_{out} . Similar to Case 5, in Case 7, AE is designed with relatively low cathodic pressure and high electrolyte concentration, as shown in Table 6.4, to minimize hydrogen crossover and thus expand the AE operating range for effective participation in OR services.

This analysis highlights the nuanced effects of π_{out} and power consumption on OR participation and cost efficiency, emphasizing the importance of optimizing these factors for each technology and use case.

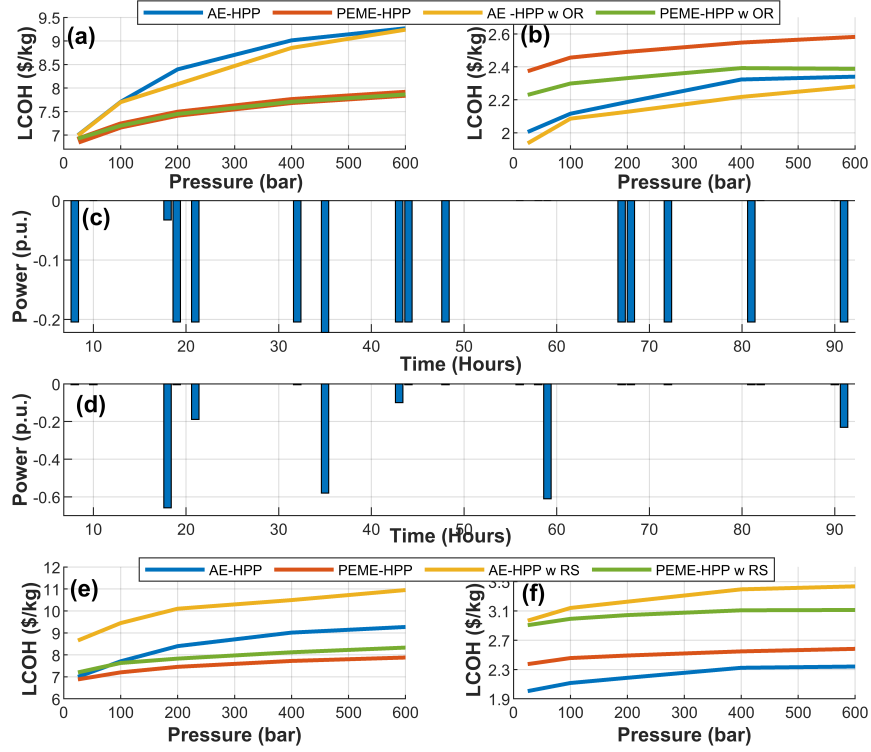


Figure 6.6: LCOH of AE-HPP and PEME-HPP at all π_{out} levels for (a) Cases 1 and 6, and (b) Cases 2 and 7. AE-HPP participation power in OR service at (c) 200 bar and (d) 400 bar. LCOH of AE-HPP and PEME-HPP at all π_{out} levels for (e) Cases 1 and 8, and (f) Cases 2 and 9.

6.2.5 Cases 8 and 9: EHPP Participates in RS Service

Fig. 6.6 (e) presents the LCOH for Cases 1 and 8 for both AE-HPP and PEME-HPP across various π_{out} levels. While there is no predefined payment for participating in the RS service, the impact of this participation on the LCOH is crucial in determining the appropriate compensation for RS service. The figure shows a substantial increase in the LCOH for AE-HPP in Case 8 compared to Case 1. Moreover, the increase in LCOH for AE-HPP is significantly higher than that for PEME-HPP.

This disparity between the two technologies can be attributed primarily to the operational characteristics of each electrolyzer. PEME is inherently capable of ramping up and

down much faster than AE, making it more adaptable to the rapid fluctuations required by RS services. As a result, to accommodate the fast response demands of RS service, AE needs to be oversized, leading to a significant increase in its CAPEX relative to Case 1. This overrating not only raises the initial investment but also diminishes AE's typical cost advantage over PEME, as the increased CAPEX erodes its lower cost structure.

Fig. 6.6 (f) compares the LCOH for Cases 2 and 9 for both AE-HPP and PEME-HPP at different levels of π_{out} . In contrast to the results of Case 2, where AE-HPP was more cost-effective, Case 9 demonstrates that PEME-HPP now offers a lower LCOH than AE-HPP when participating in RS service. This indicates that under the flat-rate electricity pricing scenario, AE-HPP is no longer the more suitable option if participation in RS service is required. This shift is primarily due to PEME-HPP's ability to handle the rapid power fluctuations associated with RS services more efficiently than AE-HPP. With a fixed input power and flat-rate electricity pricing scenario, the flexibility and fast response capability of PEME-HPP allow it to operate more efficiently and cost-effectively than AE-HPP, which struggles to adjust its output quickly without significant overrating. Consequently, AE-HPP loses its competitive edge under these conditions, highlighting the importance of matching the right electrolyzer technology to the specific requirements of grid services like RS.

The EHPP design in Cases 8 and 9, as shown in Table 6.4, reveals that the PEME's rating is slightly higher than in Case 1 and significantly higher than AE's rating in Case 2. In Case 8, the increased rating is to meet the RS power demand. In Case 2, with flat-rate electricity pricing, the EHPP operates at a high capacity factor with a relatively small electrolyzer rating. Therefore, in Case 9, participation in RS services requires overrating the PEME to enhance its ramp-up/down capabilities to meet both the RS power demand and RS rate of change. Meanwhile, the ratings of other EHPP equipment increase from Case 2 to only accommodate the RS power demand.

Table 6.5 provides the break-even values for RS payment, which restores the LCOH of Cases 8 and 9 to the LCOH of Cases 1 and 2, respectively, for both AE-HPP and PEME-HPP at different output pressures. The table shows that the break-even values are provided

in \$ per MW of the allocated capacity to participate in the RS service. In Case 8, PEME can effectively participate in RS service, regardless of the required output pressure, if the grid operator offers an RS payment exceeding 1,823 \$/MW. Conversely, AE requires a 400% higher payment to be a cost-effective technology for the provision of RS service. In Case 9, the PEME requires a slightly higher payment for participation in RS service when compared to Case 8. This is because Cases 2 and 9 belong to scenario-II, which has a flat rate electricity price. Hence, PEME's original size in Case 2 was smaller than being able to provide the fast response needed by the RS service in Case 9. Therefore, in Case 9, the PEME-HPP participation in RS requires a significant increase in PEME rating, making the PEME participation in RS service in Case 9 more expensive than in Case 8. On the other hand, in Case 9, the AE can participate in RS service with a 35% lower payment than in Case 8. Both Cases 8 and 9 require a significant increase in the AE rating to meet the ramp rate required for participation in RS service. Hence, the AE-HPP's CAPEX increase from Case 1 to Case 8 is close to that from Case 2 to Case 9. However, shifting AE-HPP's power consumption to participate in RS under the variable electricity pricing scheme in Case 8 is more expensive than in Case 9, which operates with a fixed electricity rate. As a result, AE-HPP participation in RS is more cost-effective in Case 9 than in Case 8.

6.2.6 Technology Suitability and Selection: AE versus PEME

The above analysis underscores the distinct differences between AE and PEME technologies across various scenarios, focusing on their suitability under different conditions. Table 6.6 provides a summary of the suitability of each electrolyzer technology based on the resulting LCOH for a wide range of hydrogen output pressure levels and participation in grid services. It also considers different input power profiles and electricity pricing schemes and reflects diverse hydrogen applications. The table provides the following findings:

- When EHPP is fed from the grid with variable electricity prices (scenario-I) or supplied by intermittent RES with a fixed PPA (scenario-III), and there is no participation in grid services, PEME is more cost-effective and outperforms AE, particularly

for high-pressure applications. This superiority of PEME is attributed to its higher efficiency and adaptability, as well as its ability to operate at high cathodic pressures with relatively limited gas crossover compared to AE.

- AE is more cost-effective and more suitable than PEME when EHPP is fed from the grid at a fixed electricity rate (scenario-II) except for the case of participating in RS service.
- When EHPP participates in OR grid service while being fed from the grid with variable electricity prices (scenario-I), AE becomes the more suitable technology compared to PEME. The suitability of AE, in that case, is due to its high power consumption -driven by its high gas crossover in high-pressure applications- at the hours of high electricity prices at which the grid operator usually offers high OR payment, allowing it to participate in OR service during these hours significantly.
- The EHPP's participation in RS requires a fast response, making PEME more suitable and cost-effective than the AE across all power feeding profiles, electricity pricing schemes, and output pressures.

Overall, AE is more cost-effective with fixed electricity pricing schemes, particularly for low-pressure applications. This cost-effectiveness and suitability become less obvious and even is lost in high-pressure applications. Yet, AE is also suitable for OR participation with a variable electricity pricing scheme at high-pressure applications where its power consumption allows it to participate effectively in OR service. Despite PEME's high capital cost, PEME is more cost-effective and suitable for variable electricity pricing schemes as well as fixed electricity pricing schemes with variable feeding power profiles, particularly for high-pressure applications, due to its high efficiency over a wide operating range and ability to operate at high cathodic pressures. Finally, PEME is the dominant technology for providing RS service due to its quick ramping capabilities.

6.3 Summary

This chapter introduces a novel optimization model designed to identify the most suitable electrolyzer technology for different electricity pricing schemes and various grid services—such as CA, OR, and RS—while meeting different hydrogen pressure requirements based on specific applications. The model aims to minimize the LCOH by optimizing EHPP equipment ratings, adjusting the internal parameters of the electrolyzer process, and selecting the most appropriate electrolyzer technology. Validation and results reveal that AE is generally more cost-effective at lower π_{out} levels and in scenarios with stable, flat-rate electricity pricing, especially when the electrolyzer does not participate in grid services. However, AE’s slower ramping capabilities and the need for overrated capacity in rapid response or RS scenarios lead to increased capital expenditures, making it less favorable in dynamic conditions. Conversely, PEME demonstrates superior adaptability and efficiency across a broader range of operating conditions. Despite its higher initial capital costs, PEME’s quicker ramp-up and ramp-down capabilities make it a favorable solution for scenarios with variable electricity pricing or intermittent input power from RESs. However, this higher capital cost reduces the economic viability of PEME for participating in CA and OR services compared to AE.

The proposed model significantly benefits the design and assessment of widespread EHPP deployment by providing a comprehensive framework to evaluate the economic and operational impacts of different electrolyzer technologies under varied conditions. This comprehensive model guides electrolyzer manufacturers to tailor the electrolyzer design to fit specific electricity pricing schemes, hydrogen applications, and grid services. A practical outcome could be the introduction of a series of electrolyzer models, each designed to fit distinct operational conditions, thereby enhancing market adaptability and cost-effectiveness. Additionally, the proposed framework assists grid operators in determining appropriate compensation for grid services and evaluating the likelihood of different EHPP configurations participating in these services. Overall, the proposed framework aids in identifying the optimal electrolyzer design, technology, and configuration for specific hydrogen applications.

and grid services, facilitating more informed decisions in EHPP deployment strategies. A key finding of this work is that the selection of electrolyzer technology and its internal design must account for multiple factors, including the electricity pricing scheme, the intended hydrogen application (e.g., required delivery pressure), and the potential grid services in which the EHPP may participate.

Table 6.4: Parameters of the Optimally Designed EHPP for Cases 1 to 9

π_{out}	Item	Parameter	Cases								
			1	2	3	4	5	6	7	8	9
25 bar	Electrolyzer	Technology	PEME	AE	AE	PEME	AE	PEME	AE	PEME	PEME
		l_m (μm)	28	500	500	28	400	28	500	28	30
		$\pi_{H_2(bar)}$	4	5	1	4	3	4	2	4	10
		$A_{elz}(m^2)$	1839	9861	13350	1675	10688	1839	12564	2002	1720
		$M(\%)$	–	15	45	–	42	–	44	–	–
		$P_{elz}^{rate}(MW)$	100	48	63	91	51	100	60	108	96
	Converter	$P_{Conv}^{rate}(MW)$	103	49	65	94	53	103	61	112	62
	Fuel Cell	$P_{FC}^{rate}(MW)$	–	–	–	–	–	–	–	15	15
	Compressor	$P_{Cmp}^{rate}(MW)$	8	3	12.5	6.6	5.5	8	9	8	2
	H_2 Storage	$E_{HS}(100kg)$	538	356	436	492	360	538	382	548	338
		$V_{HS}(m^3)$	20507	13569	16619	18753	13722	20507	14561	20888	12883
600 bar	Cost	$LCOH(\$/kg)$	7	2.1	3.1	7.4	1.9	7	2.0	7.32	3
	Electrolyzer	Technology	PEME	AE	PEME	PEME	AE	PEME	AE	PEME	PEME
		l_m (μm)	50	500	35	51	500	50	500	48	43
		$\pi_{H_2(bar)}$	13	5	13	14	3	13	3	13	30
		$A_{elz}(m^2)$	1880	9962	1357	1759	10103	1880	11246	1858	1720
		$M(\%)$	–	18	–	–	45	–	31	–	–
		$P_{elz}^{rate}(MW)$	106	48	75	99	56	106	54	105	96
	Converter	$P_{Conv}^{rate}(MW)$	109	50	77	103	58	109	55	108	59
	Fuel Cell	$P_{FC}^{rate}(MW)$	–	–	–	–	–	–	–	15	15
	Compressor	$P_{Cmp}^{rate}(MW)$	22	18	16	19	18	22	26	21	10
	H_2 Storage	$E_{HS}(100kg)$	554	364	414	516	370	554	380	532	340
		$V_{HS}(m^3)$	1231	809	920	1147	822	1231	845	1183	756
25 bar	Cost	$LCOH(\$/kg)$	8	2.45	3.76	8.4	2.3	8	2.39	8.44	3.18

Table 6.5: Break-even Values in \$/MW for RS Payment at Different Output Hydrogen Pressures

Case #	Elz	$\pi_{out}(bar)$				
		25	100	200	400	600
8	AE	6885	7060	7090	7210	7380
	PEME	1278	1530	1553	1598	1823
9	AE	4230	4416	4548	4707	4831
	PEME	2226	2255	2322	2385	2395

Table 6.6: Summary of Electrolyzer Technology Suitability at Various Scenarios, Grid Services, and Hydrogen Output Pressures^a

Scenario	Scenario-I					Scenario-II					Scenario-III				
$\pi_{out} \text{ (bar)}$	25	100	200	400	600	25	100	200	400	600	25	100	200	400	600
Cases 1 to 3	PEME/AE	PEME				AE					AE	PEME/AE		PEME	
Cases 4 and 5 (CA)	No Suitable Technology (NST)					AE					N/A				
Cases 6 and 7 (OR)	NST	AE				AE					N/A				
Cases 8 and 9 (RS)	PEME					PEME					N/A				

^a The cells color code is as follows. i) White: No suitable technology (NST) or not available (N/A) case study. ii) Yellow: PEME is the most suitable technology. iii) Blue: AE is the most suitable technology. iv) Green: Both AE and PEME are suitable.

Chapter 7

Optimal Operation and Control of PEME-HPP with Dynamic Cathodic Pressure and Temperature

The proposed models in previous chapters optimize PEME-HPP design and operation while incorporating PEME safety constraints and customizing the PEME’s internal design based on specific power supply and hydrogen demand profiles. However, previous chapters assume a fixed cathodic pressure throughout the operating period, without exploring adjustments of PEME cathodic pressure and temperature on an hourly basis. To alleviate these shortcomings, this chapter develops an optimization model to determine the optimal setpoints for the cathodic pressure and cell temperature of a PEME at each operating hour concurrently with the optimization of the PEME-HPP sizing and scheduling. The model also assesses the impact of optimizing these setpoints on the overall system performance. Furthermore, it employs the unified dynamic model of large-scale PEME systems presented in 3.2.2 to examine the limitations of conventional decoupled control strategies—i.e., regulating power, pressure, and temperature independently—in running a PEME with the proposed varying operating conditions. Such decoupled control strategies overlook the

physical coupling between PEME's domains and might lead to inefficient, conflicting, or even unsafe behavior under varying operating conditions (i.e., cathodic pressure and/or temperature). Motivated by these insights, it also introduces a coordinated control scheme that jointly regulates PEME loading and operating conditions across the three domains (i.e., electrical, mass transfer, and thermal). The formulation and results of this chapter have been published in [177,178].

7.1 Impact of Cathodic Pressure and Temperature on PEME Performance

This section highlights the significance of varying the PEME cathodic pressure and cell temperature on both the PEME efficiency and its safe operating range. While the detailed model of the PEME is presented in Section 3.2.1, this section focuses specifically on the key performance characteristics influenced by variations in cathodic pressure and cell temperature.

The PEME efficiency, η_{PEM} , consists of two components: the production efficiency, η_p^{PEM} , and the Faraday efficiency, η_F^{PEM} , expressed as follows:

$$\eta_{PEM} = \eta_p^{PEM} \eta_F^{PEM}. \quad (7.1)$$

The production efficiency is defined, as previously introduced in (3.29), as the ratio between the hydrogen LHV equivalent voltage and the PEME cell voltage. Since $V_{LHV}^{H_2}$ is a characteristic property of hydrogen gas, it is completely independent of variations in the cathodic pressure and cell temperature of the PEME. The cell voltage, V_{cell}^{PEM} , as presented earlier in (3.19), consists of three main components: the open-circuit voltage V_{oc}^{PEM} , the activation overpotential V_{act}^{PEM} , and the resistive overpotential V_{res}^{PEM} . The impacts of cathodic pressure and cell temperature on each of these voltage components are investigated systematically.

The open-circuit voltage, provided in (3.20), is composed of two terms. The first term is

the reversible voltage, V_{rev}^{PEM} , which varies slightly with the temperature. The maximum change in V_{rev}^{PEM} is $0.07V$ corresponding to an operating temperature range from $20^\circ C$ to $90^\circ C$ [23, 104], and thus, V_{rev}^{PEM} is assumed to be constant in this work. Assuming the PEME is operating at anodic pressure $\pi_{O_2}^{PEM} = 1 \text{ bar}$ and the standard pressure $\pi_o = 1 \text{ bar}$, the the second term in the open-circuit voltage is proportional to $T_{cell}^{PEM} \ln(\pi_{H_2}^{PEM})$, making temperature the dominant factor since $\ln(\pi_{H_2}^{PEM})$ tends to saturate at higher π_{H_2} values. Yet, this variable term in V_{oc}^{PEM} remains much smaller than the fixed term V_{rev} . As such, the impact of operating temperature and cathodic pressure on V_{oc}^{PEM} is as follows:

$$(V_{oc}^{PEM} - V_{rev}^{PEM}) \propto T_{cell}^{PEM} \ln(\pi_{H_2}^{PEM}) \quad (7.2)$$

The relation for the activation overpotential, V_{act}^{PEM} , as provided in (3.21), is more complex than that of the open-circuit voltage, since the exchange current density, J_o^{PEM} , is temperature-dependent, as expressed below [104]:

$$J_o^{PEM} = J_{o,ref}^{PEM} e^{\left(\frac{E_a}{RT_{cell}^{PEM}} \left(1 - \frac{T_{cell}^{PEM}}{T_{ref}^{PEM}} \right) \right)} \quad (7.3)$$

where $J_{o,ref}^{PEM}$ denotes the reference exchange current density at the reference temperature, T_{ref}^{PEM} . Considering that the remaining parameters (e.g., α^{PEM}) are independent of both the cathodic pressure and cell temperature, the complex relationship between V_{act}^{PEM} and T_{cell}^{PEM} can be simplified by defining three mathematical constants, A , B , and C , as follows:

$$V_{act}^{PEM} = A + B(\ln(J^{PEM}) - C)T_{cell}^{PEM} \quad (7.4a)$$

$$(V_{act}^{PEM} - A) \propto B(\ln(J^{PEM}) - C)T_{cell}^{PEM} \quad (7.4b)$$

where,

$$A = \frac{E_a}{z\alpha^{PEM}F}, \quad B = \frac{R}{z\alpha^{PEM}F}, \quad C = \ln(J_o) + \frac{E_a}{RT_{ref}^{PEM}} \quad (7.4c)$$

$$A > B(\ln(J^{PEM}) - C)T_{cell}^{PEM} \quad (7.4d)$$

$$C > \ln(J_{max}^{PEM}) \quad (7.4e)$$

Although establishing a strictly linear relationship between V_{act}^{PEM} and T_{cell}^{PEM} is challenging, the inequalities in (7.4d) and (7.4e) helps concluding that increasing T_{cell}^{PEM} leads to a slight reduction in the activation overpotential V_{act}^{PEM} . However, this reduction becomes less pronounced as the current density, J^{PEM} , increases and approaches its maximum value, J_{max}^{PEM} .

The resistive overpotential, V_{res}^{PEM} , consists of the voltage drop across the electrodes and the voltage drop across the membrane, as expressed in (3.23). While most of the parameters associated with V_{res}^{PEM} are independent of both cathodic pressure and cell temperature, the membrane conductivity is strongly dependent on the cell temperature, as expressed below [104]:

$$\sigma_m = (0.6877 + a_{H_2O})^3 e^{\left(\frac{-10440}{R T_{cell}^{PEM}} \sqrt{a_{H_2O}}\right)} \quad (7.5)$$

Given that the PEME operates within a limited T_{cell}^{PEM} range and that the water activity a_{H_2O} is unity, the membrane conductivity σ_m is approximately proportional to T_{cell}^{PEM} . Further, as the electrodes' resistance, R_o^{PEM} , is very small, the relation between V_{res}^{PEM} and T_{cell}^{PEM} is approximated as in (7.6). Consequently, the impact of T_{cell}^{PEM} becomes more significant at higher current densities.

$$V_{res}^{PEM} \underset{\sim}{\propto} \sigma_m^{-1} J^{PEM} \underset{\sim}{\propto} T_{cell}^{PEM, -1} J^{PEM} \quad (7.6)$$

By combining the relationships in (7.2), (7.4b), and (7.6), and noting that V_{res}^{PEM} is the component most significantly affected by $(T_{cell}^{PEM})^{-1}$ —particularly at high current densities—the dependence of the production efficiency η_p^{PEM} on T_{cell}^{PEM} can be approximated as shown in (7.7a). Meanwhile, since $\pi_{H_2}^{PEM}$ influences V_{oc}^{PEM} only logarithmically, the η_p is almost independent of $\pi_{H_2}^{PEM}$ as in (7.7b).

$$\eta_p^{PEM} \underset{\sim}{\propto} \frac{V_{LHV}}{V_{res}} \underset{\sim}{\propto} T_{cell}^{PEM} (J^{PEM})^{-1} \quad (7.7a)$$

$$\eta_p^{PEM} \underset{\sim}{\perp\!\!\!\perp} \pi_{H_2}^{PEM} \quad (7.7b)$$

The Faraday's efficiency is a function of the gas crossover equivalent current density, J_{loss}^{PEM} , as provided in (3.27). However, when the PEME operates under dynamic tem-

perature conditions, J_{loss}^{PEM} must be updated to account for the effect of cell temperature variations, as expressed below [104, 145]:

$$\begin{aligned} J_{loss}^{PEM} &= 2 \left(\frac{F Pr_{H_2}^{PEM} (\pi_{H_2}^{PEM} + \pi_{O_2}^{PEM})}{s_m^{PEM} \delta_m^{PEM}} + \frac{a_x}{s_m^{PEM} \delta_m^{PEM}} J^{PEM} \right) \cdot e^{\left(\frac{E_m}{R} \left(\frac{1}{T_{ref}^{PEM}} - \frac{1}{T_{cell}^{PEM}} \right) \right)} \\ &= 2 \left(\frac{F Pr_{H_2}^{PEM} (\pi_{H_2}^{PEM} + \pi_{O_2}^{PEM})}{s_m^{PEM} \delta_m^{PEM}} + \frac{a_x}{s_m^{PEM} \delta_m^{PEM}} J^{PEM} \right) \cdot e^{\frac{\mathfrak{M}}{T_{ref}^{PEM}}} \cdot e^{\frac{-\mathfrak{M}}{T_{cell}^{PEM}}} \end{aligned} \quad (7.8)$$

where E_m is the activation energy while $\mathfrak{M}$ is a constant defined as $\mathfrak{M} = \frac{E_m}{R} \approx 2500$.

As provided in (7.8), the term $\frac{a_x}{s_m^{PEM} \delta_m^{PEM}} J^{PEM}$ is negligible compared to the term $\frac{F Pr_{H_2}^{PEM} (\pi_{H_2}^{PEM} + \pi_{O_2}^{PEM})}{s_m^{PEM} \delta_m^{PEM}}$. Additionally, this work assumes the anodic pressure, $\pi_{O_2}^{PEM}$, is fixed at atmospheric pressure and can therefore be omitted compared to the cathodic pressure, $\pi_{H_2}^{PEM}$. Thus, J_{loss}^{PEM} is approximated as follows:

$$J_{loss}^{PEM} \approx \left(\frac{2F Pr_{H_2}^{PEM}}{s_m^{PEM} \delta_m^{PEM}} \right) \cdot e^{\frac{\mathfrak{M}}{T_{ref}^{PEM}}} \cdot \pi_{H_2}^{PEM} \cdot e^{\frac{-\mathfrak{M}}{T_{cell}^{PEM}}} \quad (7.9)$$

The term, $e^{-\mathfrak{M}/T_{cell}^{PEM}}$, can also be simplified using Taylor expansion as below:

$$e^{\frac{-\mathfrak{M}}{T_{cell}^{PEM}}} \Big|_{T_{cell}^{PEM}=T_{ref}^{PEM}=293} \approx e^{\frac{-\mathfrak{M}}{T_{ref}^{PEM}}} \cdot \left(1 + \frac{\mathfrak{M} T_{cell}^{PEM}}{(T_{ref}^{PEM})^2} \right) \quad (7.10)$$

Thus, by substituting (7.10) into (7.9), and considering that $\frac{\mathfrak{M} T_{cell}^{PEM}}{(T_{ref}^{PEM})^2} > 1$, J_{loss}^{PEM} is approximately directly proportional to $\pi_{H_2}^{PEM} \cdot T_{cell}^{PEM}$, as hereunder:

$$J_{loss}^{PEM} \approx 2 \left(\frac{F Pr_{H_2}^{PEM} \pi_{H_2}^{PEM}}{s_m^{PEM} \delta_m^{PEM}} \right) \cdot \left(1 + \frac{\mathfrak{M} T_{cell}^{PEM}}{(T_{ref}^{PEM})^2} \right) \approx \frac{2F Pr_{H_2}^{PEM} \mathfrak{M}}{s_m^{PEM} \delta_m^{PEM} (T_{ref}^{PEM})^2} \cdot \pi_{H_2}^{PEM} \cdot T_{cell}^{PEM} \quad (7.11a)$$

$$J_{loss}^{PEM} \propto \pi_{H_2}^{PEM} \cdot T_{cell}^{PEM} \quad (7.11b)$$

Accordingly, by substituting (7.11b) into (3.30), the relationship between η_F^{PEM} , $\pi_{H_2}^{PEM}$, and T_{cell}^{PEM} can be expressed as follows:

$$\eta_F^{PEM} \propto \begin{cases} J^{PEM} \cdot \pi_{H_2}^{PEM-1} \cdot T_{cell}^{PEM-1}, & \text{for small to moderate } J^{PEM} \\ 1, & \text{for large } J^{PEM} \end{cases} \quad (7.12)$$

Similar to J_{loss}^{PEM} , the hydrogen-to-oxygen current density $J_{H_2,loss}^{PEM}$, which is a component of J_{loss}^{PEM} , exhibits a similar proportional relationship with $\pi_{H_2}^{PEM}$ and T_{cell}^{PEM} as below:

$$J_{loss,H_2}^{PEM} \propto \pi_{H_2}^{PEM} \cdot T_{cell}^{PEM}, \quad (7.13)$$

Therefore, considering that $0.5J^{PEM} > J_{loss,H_2}$, and by substituting (7.13) into (3.28), the relationship between the hydrogen-to-oxygen percentage, $\Psi_{H_2}^{PEM}$, and $\pi_{H_2}^{PEM}$ and T_{cell}^{PEM} can be expressed as follows:

$$\Psi_{H_2}^{PEM} \propto \begin{cases} (J^{PEM})^{-1} \cdot \pi_{H_2}^{PEM} \cdot T_{cell}^{PEM}, & \text{for small to moderate } J^{PEM} \\ 0, & \text{for large } J^{PEM} \end{cases}. \quad (7.14)$$

From the preceding analysis, the following insights can be made: i) η_p^{PEM} is directly proportional to the cell temperature, especially at high current densities where V_{res}^{PEM} is the dominant component in V_{cell}^{PEM} . ii) η_F^{PEM} is inversely proportional to both cathodic pressure and temperature while being directly proportional to the current density. As such, an increase in either cathodic pressure or temperature will decrease η_F^{PEM} . However, as current density increases, the effect of cathodic pressure and temperature on η_F^{PEM} becomes less significant. iii) $\Psi_{H_2}^{PEM}$ is directly proportional to both cathodic pressure and temperature, and inversely proportional to current density at low and moderate current densities. Yet, the effects of pressure and temperature on $\Psi_{H_2}^{PEM}$ become nearly negligible at higher current densities.

7.2 Formulation of the Optimization Problems

The layout of the PEME-HPP under design is illustrated in Fig. 7.1. As shown in the figure, the proposed PEME-HPP is grid-connected and it comprises four components: the PEME, AC/DC converter, compressor, and local hydrogen storage. The electricity price is assumed to vary on an hourly basis. Consequently, the optimal design and operation of the PEME-HPP have to consider hourly adjustments to the plant's power consumption, along with the PEME's cathodic pressure and cell temperature.

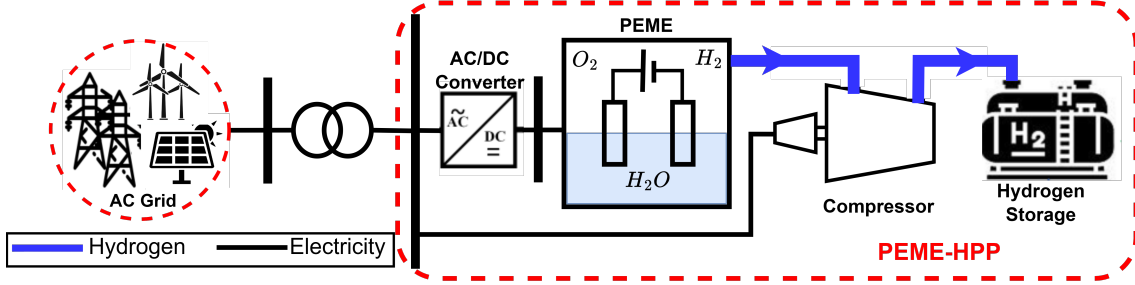


Figure 7.1: Layout of the PEME-HPP.

Two optimization problems are formulated, as illustrated in Fig. 7.2. The first is a design optimization problem that minimizes the LCOH by determining the optimal ratings of the EHPP equipment and the internal parameters of the PEME, using typical days composed of T hours that represent historical datasets of power and hydrogen demands, RES profiles, and electricity prices. The second is a scheduling optimization problem that, based on the optimal design obtained from the first problem, minimizes the combined operational and degradation costs per unit of hydrogen produced by determining the optimal hourly PEME power, cathodic pressure, and cell temperature setpoints over a rolling horizon of $\mathcal{H}$ hours.

7.2.1 Formulation of the Design Problem

The optimal design of PEME-HPP requires the utilization of large historical datasets to capture the seasonal variations in renewable generation, electricity demand, and hydrogen demand, and the uncertainties in the electricity prices. To manage the complexity of this optimization problem, and following the approach of [156] and [170], the historical datasets are condensed into a limited number of typical days composed of T hours. This strategy reduces the number of decision variables and makes the optimization problem computationally feasible while still capturing the key seasonal characteristics that influence the sizing process.

The typical days of the electrical demand are obtained as in [156], where each hour's

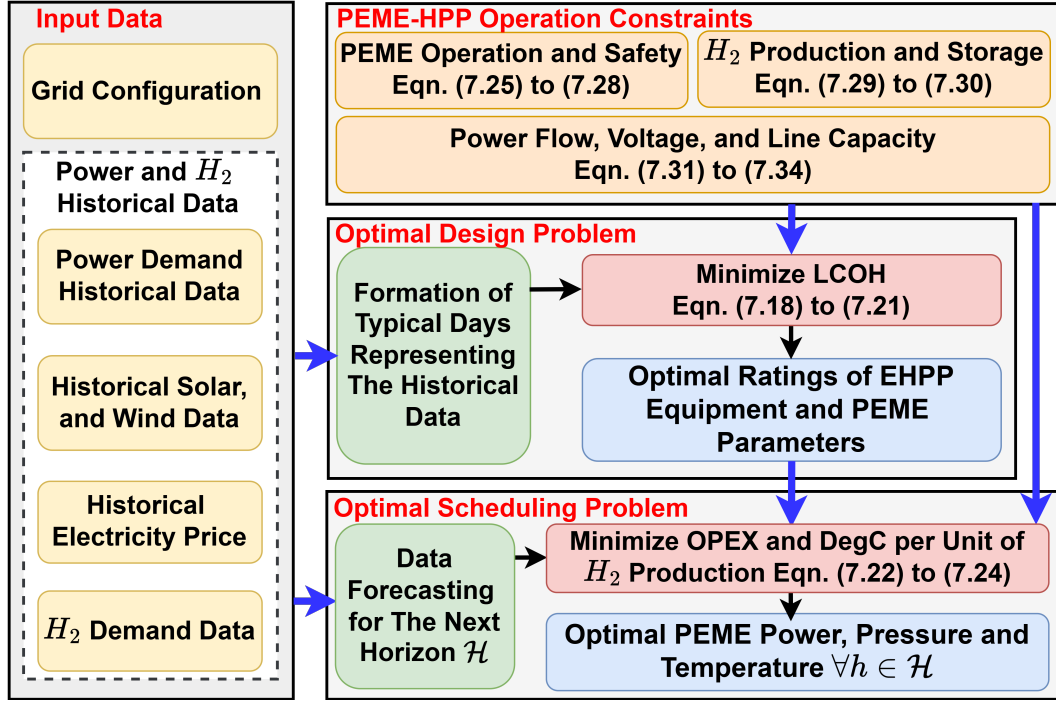


Figure 7.2: Block diagram of the proposed optimization formulations.

demand is its peak demand at the corresponding hours in the historical data. The typical days of the hydrogen demand are the mean of the demand during the corresponding hours in the annual data. To account for the intermittency of the RESs in the power grid, historical RES data (wind speed and solar irradiation data) is used to obtain typical days representing the four seasons. The pdf of each hour is calculated using Beta pdf (f_b) and Rayleigh pdf (f_r) for solar irradiation and wind speed, respectively [156]. The obtained pdf functions of each hour are discretized into h states covering the whole solar irradiation and wind speed ranges of that hour. Next, the probability of each irradiation state $\rho(SI^{i,t})$ and wind speed state $\rho(W S^{j,t})$ is calculated using the cdf as in [156]. Hence, the total number of the combined states at each hour is $h \times h$, where the probability of each combined state is given in (7.15), assuming no correlation exists between the renewable power generation in each

hour and its adjacent ones.

$$\rho^{s,t} = \rho(SI^{i,t}) \rho(WS^{j,t}) \quad \forall t \in \mathbb{T} \wedge s = 1, \dots, h \wedge i, j = 1, \dots, h \quad (7.15)$$

Then, the power at each hour t in the typical days' power profile of any RES, P_{RES}^t , is calculated as the weighted average of the power of that RES in the $h \times h$ combined states as follows:

$$P_{RES}^t = \frac{\sum_{s=1}^{h \times h} \rho^{s,t} P_{RES}^{s,t}}{\sum_{s=1}^{h \times h} \rho^{s,t}} \quad \forall t \in \mathbb{T} \wedge s = 1, \dots, h \times h \quad (7.16)$$

To account for the uncertainty in electricity prices, their historical data is analyzed to derive a normal probability distribution function pdf for each hour within the time period under study. These pdfs for electricity prices are then discretized into multiple states, with the probability of each state being calculated. Following this, $\mathcal{N}_{MCS}$ MCS are generated, each with its corresponding hourly probabilities, $\rho_{Elec}^{mc,t}$ for electricity prices. The overall probability of each electricity price scenario, ρ_{Elec}^{mc} , is then determined as the average of the hourly probabilities for the electricity prices within that scenario, calculated as follows:

$$\rho_{Elec}^{mc} = \frac{1}{\mathbb{T}} \sum_{t \in \mathbb{T}} \rho_{Elec}^{mc,t} \quad \forall mc \in \mathcal{N}_{MCS} \quad (7.17)$$

Inputs: The inputs of the proposed design formulation are the i) configuration of the grid to which the PEME-HPP is connected; ii) typical days hourly profile of the power; iii) typical days hourly profile of the RESs (P_{RES}^t) connected to the grid; iv) $\mathcal{N}_{MCS}$ MCSs for the typical days hourly profile of the electricity price ($Price_{elec}^t$); and v) typical days hourly profile of the hydrogen demands (Q_d^t).

Decision Variables: The decision variables are the i) sizes of the four main components in the PEME-HPP (AC/DC converter, PEME, compressor, and HS), ii) hourly power consumption of the PEME (P_{PEM}^t) over the entire typical days period, iii) hourly hydrogen flow to the storage (Q_{HS}^t) over the entire typical days period, iv) PEME's internal parameters (i.e., cell area, and membrane thickness), and v) PEME's cathodic pressure ($\pi_{H_2}^{PEM,t}$) and operating temperature ($T_{cell}^{PEM,t}$) at each hour in the typical days.

Objective Function: The optimization model aims to minimize the LCOH expressed as:

$$Min \left(\frac{CAPEX + \sum_{y \in Y} \left(\frac{\sum_{mc=1}^{N_{MCS}} \rho_{Elec}^{mc} OPEX(mc)}{\sum_{mc=1}^{N_{MCS}} \rho_{Elec}^{mc}} + C_{Deg} \right) / (1+r)^y}{\sum_{y \in Y} (\sum_{t \in \mathbb{T}} N_{H_2}^{PEM,t}) / (1+r)^y} \right) \quad (7.18)$$

where Y is the PEME-HPP life time in years, r is the yearly discount rate, and CAPEX is the capital expenditures obtained as:

$$CAPEX = P_{Conv}^{rate} C_{Conv} + P_{PEM}^{rate} C_{PEM} + P_{Cmp}^{rate} C_{Cmp} + E_{HS} C_{HS} \quad (7.19)$$

where C_{Conv} , C_{PEM} , C_{Cmp} , and C_{HS} are the capital costs of the AC/DC converter, PEME, compressor, and HS, respectively.

The $OPEX(mc)$, based on the electricity price of scenario mc , is calculated as shown in (7.20), while C_{Deg} represents the degradation cost of the PEME, determined according to (7.21).

$$OPEX(mc) = \sum_{t \in \mathbb{T}} (P_{PEM}^t + P_{Cmp}^t) Price_{elec}^t(mc) + N_{H_2}^{PEM,t} O_w + P_{PEM}^t O_{PEM} + P_{Cmp}^t O_{Cmp} + Q_{HS}^t O_{HS} \quad (7.20)$$

$$C_{Deg} = \sum_{t \in \mathbb{T}} P_{PEM}^t D_{PEM} \quad (7.21)$$

where $Price_{elec}^t(mc)$ is the electricity price at hour t in scenario mc , O_w represents the water consumption cost, O_{PEM} , O_{Cmp} , and O_{HS} are the operation costs of the PEME, compressor, and HS, respectively. D_{PEM} is the PEME degradation cost. $N_{H_2}^{PEM,t}$ is the hydrogen flow produced from PEME, which is a function of its efficiency as explained earlier in (3.41), and hence it depends on $\pi_{H_2}^{PEM,t}$ and $T_{cell}^{PEM,t}$. P_{Cmp}^t is the compressor power consumption as given in (3.40).

7.2.2 Formulation of the scheduling Problem

The real-time optimal scheduling is performed using a rolling time horizon approach with a horizon window of $\mathcal{H}$ hours. In this method, the scheduling problem is formulated

as a multi-interval optimization, where the optimal setpoints for PEME power, cathodic pressure, and operating temperature are determined for the current hour (h) as well as for a look-ahead window of $(\mathcal{H} - 1)$ future hours, as illustrated in Fig. 7.3. At each hour, the optimization problem is re-solved, and the setpoints are updated recursively. This rolling horizon approach enables the optimization model to incorporate anticipated variations within the look-ahead window—such as changes in RESs’ power generation, electrical demand, and electricity prices—while implementing the optimal setpoint for the current hour (h). The Optimal scheduling formulation inputs, decision variables, and objective function are summarized as follows.

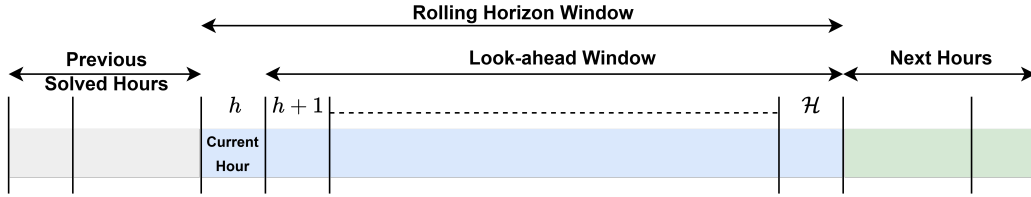


Figure 7.3: Rolling horizon approach with a horizon window of $\mathcal{H}$ hours.

Inputs: The inputs of the scheduling optimization formulation for each rolling horizon window are the i) configuration of the grid to which the PEME-HPP is connected; the hourly profile over the rolling horizon window $\mathcal{H}$ of ii) the renewable plants’ power connected to the electric grid; iii) electric demand; iv) the hydrogen demand (Q_d^h); and v) the electricity price ($Price_{elec}^h$).

Decision Variables: The decision variables are the setpoints of i) the PEME power (P_{PEME}^h); ii) the PEME’s cathodic pressure ($\pi_{H_2}^{PEM,h}$); and iii) the PEME’s operating temperature ($T_{cell}^{PEM,h}$) at each hour in the rolling horizon window $\mathcal{H}$.

Objective Function: The optimization model aims to minimize the operational cost per unit of the produced hydrogen over the rolling horizon window $\mathcal{H}$ as expressed below:

$$\text{Min} \left(\frac{OPEX + C_{Deg}}{\sum_{h \in \mathcal{H}} N_{H_2}^{PEM,h}} \right) \quad (7.22)$$

where OPEX and C_{Deg} are the operation expenditures and PEME degradation cost over

the horizon window $\mathcal{H}$ as calculated in (7.23) and (7.24), respectively.

$$OPEX = \sum_{h \in \mathcal{H}} (P_{PEME}^h + P_{Cmp}^h) Price_{elec}^h + F_{PEME}^h O_w + F_{HS}^h O_{HS} + P_{PEME}^h O_{PEME} + P_{Cmp}^h O_{Cmp} \quad (7.23)$$

$$C_{Deg} = \sum_{h \in \mathcal{H}} P_{PEME}^h D_{PEM} \quad (7.24)$$

$N_{H_2}^{PEM, h}$ and P_{Cmp}^h represent the hydrogen flow produced by the PEME and the compressor power consumption, respectively, in each hour h , and are calculated similarly to (3.41) and (3.40).

7.2.3 Constraints of the Optimization Problems

The objective functions provided in (7.18) and (7.22) are subject to PEME operation, hydrogen production, and electric grid constraints as follows.

PEME Operation Constraints: The PEME current density is limited to the minimum and maximum current densities as given below:

$$0 \leq J^{PEM, i} = \frac{P_{PEM}^i}{V_{PEM}^{rate} A_{cell}^{PEM}} \leq J_{max}^{PEM} \quad \forall i \in \mathcal{H} \vee \mathbb{T} \quad (7.25)$$

Additionally, the PEME cathodic pressure and cell temperature have to be limited within the practical minimum and maximum PEME pressure and temperature as provided in (7.26) and (7.27), respectively.

$$\pi_{H_2}^{PEM, min} \leq \pi_{H_2}^{PEM, i} \leq \pi_{H_2}^{PEM, max} \quad \forall i \in \mathcal{H} \vee \mathbb{T} \quad (7.26)$$

$$T_{cell}^{PEM, min} \leq T_{cell}^{PEM, i} \leq T_{cell}^{PEM, max} \quad \forall i \in \mathcal{H} \vee \mathbb{T} \quad (7.27)$$

The hydrogen in oxygen percentage has to be within the safe threshold, $\Psi_{H_2}^{PEM, safe}$, as follows:

$$\Psi_{H_2}^{PEM, i} \leq \Psi_{H_2}^{PEM, safe} \quad \forall i \in \mathcal{H} \vee \mathbb{T} \quad (7.28)$$

Hydrogen Production Constraints: The state of hydrogen in the storage is constrained by the minimum and maximum permissible limits as below:

$$SoH^{min} \leq SoH^i \leq SoH^{max} \quad \forall i \in \mathcal{H} \vee \mathbb{T} \quad (7.29)$$

Further, the hydrogen flow must satisfy the hydrogen balance equation where the sum of the hydrogen flow produced from PEME and HS flow should equal the flow of the hydrogen demand as follows:

$$N_{H_2}^{PEM,i} + Q_{HS}^i = Q_d^i \quad \forall i \in \mathcal{H} \cup \mathbb{T} \quad (7.30)$$

Power Grid Constraints: The grid-connected operation of the PEME-HPP requires considering the power flow constraints of the grid. As such, the objective functions in (7.18) and (7.22) is subject to the voltage (V_b), thermal line capacity (S_b), active power (P_b) and reactive power (Q_b) flow constraints as given in (7.31), (7.32), (7.33), and (7.34), respectively.

$$V_b^{min} \leq V_b^i \leq V_b^{max} \quad \forall i \in \mathcal{H} \cup \mathbb{T} \quad (7.31)$$

$$S_b^i \leq S_b^{max} \quad \forall i \in \mathcal{H} \cup \mathbb{T} \quad (7.32)$$

$$P_{b,g}^i = P_{b,d}^i + V_b^i \sum_{q=1}^B V_q^i \mathbb{Y}_{b,q} \cos(\delta_b^i - \delta_q^i - \theta_{b,q}) \quad \forall i \in \mathcal{H} \cup \mathbb{T} \quad (7.33)$$

$$Q_{b,g}^i = Q_{b,d}^i + V_b^i \sum_{q=1}^B V_q^i \mathbb{Y}_{b,q} \sin(\delta_b^i - \delta_q^i - \theta_{b,q}) \quad \forall i \in \mathcal{H} \cup \mathbb{T} \quad (7.34)$$

where $\mathbb{Y}$ and θ are the admittance matrix amplitude and angle, respectively. δ is the voltage angle. B and b are the total number of buses and the bus index, respectively. The subscripts g and d represent the generation and demand power, respectively.

7.3 Numerical Studies for PEME-HPP Design and Scheduling with Dynamic Cathodic Pressure and Temperature

This section numerically evaluates the influence of cathodic pressure and cell temperature on PEME-HPP performance, specifically in terms of efficiency and safety limits. Such analysis is crucial for understanding how variations in pressure and temperature govern maximizing the PEME-HPP efficiency. Subsequently, the section validates the proposed optimal design and scheduling formulations, which incorporate the hourly optimization of the PEME's cathodic pressure and cell temperature.

Table 7.1: Summary of Case Studies

Cases	Case 1	Case 2	Case 3	Case 4	Case 5
Pressure Optimization	No	Fixed	Hourly Optimized	Fixed	Hourly Optimized
Temperature Optimization	No	Fixed		Hourly Optimized	

The validation is conducted using the modified IEEE 30-bus benchmark transmission system, shown in Fig.4.4, where two wind plants are connected to buses 20 and 30, a PV plant is connected to bus 26, and the PEME-HPP is coupled to bus 18. Five years of actual historical solar irradiation and wind speed data, with hourly resolution, were obtained from the province of Ontario, Canada [158], to generate the power profiles of the various RESs. Additionally, five years of historical electrical demand and electricity price data were collected from the IESO in Ontario, Canada [159]. The historical hydrogen demand data were adopted from the techno-economic study in [82]. Following the approach of [156], the typical days used in the optimal design problem are selected such that each represents one season of the year, thereby accounting for seasonal variations in RES profiles, hydrogen and electricity demands, and electricity prices. In contrast, and consistent with the methodology in [36], the optimal scheduling problem uses real data as inputs, under the assumption of perfect forecasting of RES profiles, electrical and hydrogen demands, and electricity prices over the rolling horizon window. Five case studies for the optimal design and scheduling of PEME-HPP have been conducted as summarized in Table 7.1. In all case studies, the safety limit for the hydrogen in oxygen percentage, $\Psi_{H_2}^{safe}$, is set at 10% assuming a recombination catalyst layer is employed. The cathodic pressure and operating temperature in Case 1 are chosen, as widely used by manufacturers and reported in literature, to be 30 *bar* and 80°C, respectively. All other technical and economic parameters are adopted from the previous techno-economic studies in [36, 143].

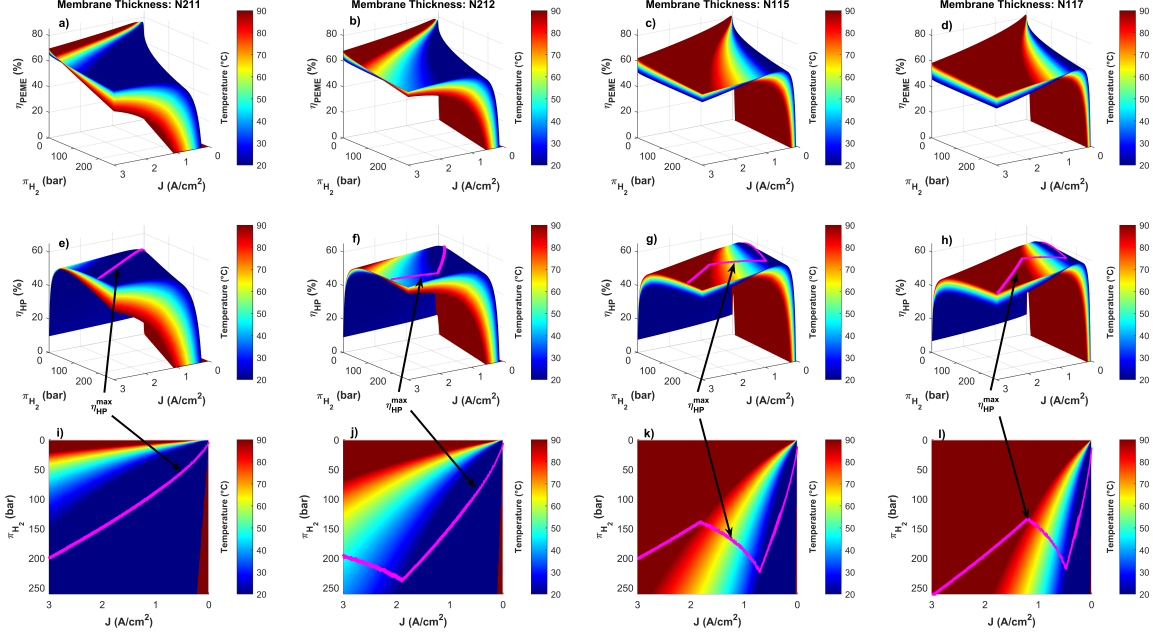


Figure 7.4: (a)–(d) Variation of PEME efficiency with current density, cathodic pressure, and temperature for membranes N211, N212, N115, and N117, respectively. (e)–(h) Variation of PEME-HPP efficiency with current density, cathodic pressure, and temperature for the same membranes. (i)–(l) Top view of the PEME-HPP efficiency variations shown in (e)–(h).

7.3.1 Illustrative Numerical Analysis of Cathodic Pressure and Cell Temperature Effects

To numerically analyze the impact of cathodic pressure and temperature variations, the PEME efficiency η_{PEM} is evaluated over the operating range of current density $J^{PEM} = 0\text{--}3\text{ A/cm}^2$, considering four commercially available membrane thicknesses ($N211$: $25.4\text{ }\mu\text{m}$, $N212$: $51\text{ }\mu\text{m}$, $N115$: $127\text{ }\mu\text{m}$, and $N117$: $183\text{ }\mu\text{m}$), under various combinations of cathodic pressure (1–260 bar) and temperature (20–90°C). Fig.7.4 (a)–(d) illustrates the variations in PEME efficiency for the four membrane thicknesses. As shown in Fig.7.4 (a), a low operating temperature ($T_{cell}^{PEM} = 20^\circ\text{C}$) yields higher efficiency, particularly at high cathodic pressures. However, consistent with the analytical assessment insight (i), as the membrane thickness increases, V_{res}^{PEM} becomes the dominant component of V_{cell}^{PEM} . Consequently, as

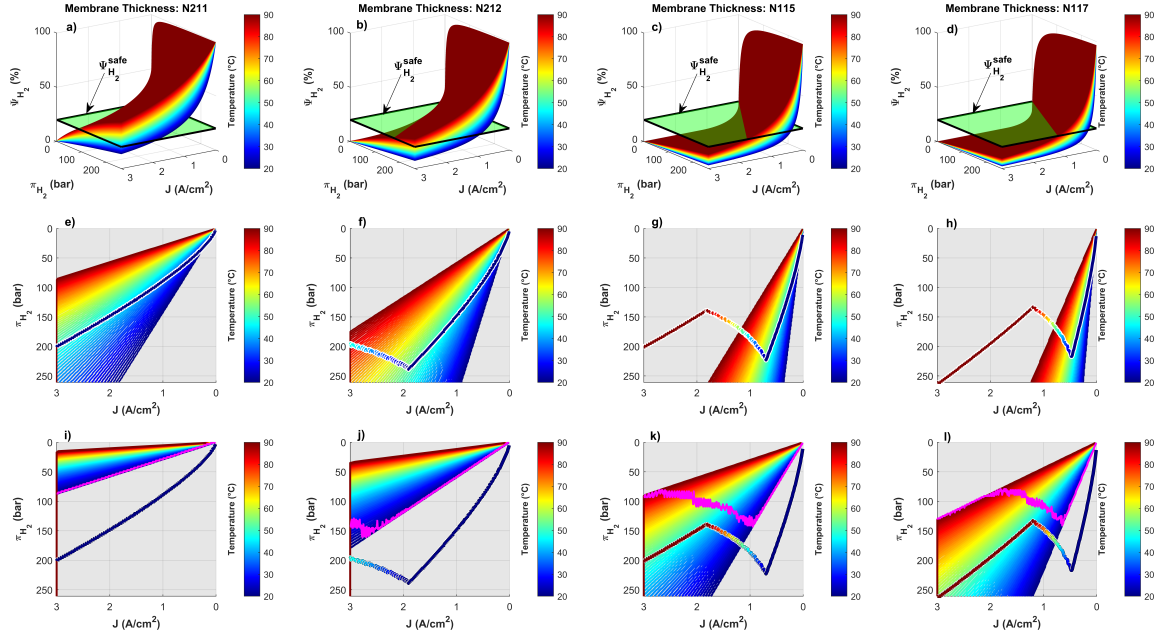


Figure 7.5: (a)–(d) Variation of the hydrogen-to-oxygen percentage, $\Psi_{H_2}^{PEM}$, with current density, cathodic pressure, and temperature for membranes N211, N212, N115, and N117, respectively. (e)–(h) Cross-sectional views of Ψ_{H_2} given in (a)–(d) at the safety limit $\Psi_{H_2}^{PEM,safe} = 20\%$, along with the trajectories of η_T^{max} , color-coded by temperature, for the same membranes N211, N212, N115, and N117, respectively. (i)–(l) Cross-sectional views of $\Psi_{H_2}^{PEM}$ given in (a)–(d) at the tighter safety limit $\Psi_{H_2}^{PEM,safe} = 5\%$, along with the trajectories of η_T^{max} (color-coded by temperature) and $\eta_T^{max,safe}$ (shown as pink lines) for membranes N211, N212, N115, and N117, respectively.

shown in Fig. 7.4 (b)–(d), higher temperatures yield higher η_p^{PEM} , and thus higher η_{PEM} , initially at low cathodic pressures and progressively extending to higher pressures. Ultimately, at the maximum thickness (i.e., N117), elevated temperatures provide the highest efficiency across the entire cathodic pressure range for the medium and high current densities. Nevertheless, at low current densities, where the influence of η_p^{PEM} on η_{PEM} is minimal and η_F^{PEM} is inversely proportional to the operating temperature according to the analytical assessment insight (ii), the lowest operating temperature ($T_{cell}^{PEM} = 20^\circ\text{C}$) yields the highest efficiency across all membrane thicknesses and cathodic pressures. Furthermore, it is worth noting that, for the same current density and operating temperature,

the lowest cathodic pressure yields the highest η_{PEM} , since it produces hydrogen at low pressure, which would require additional mechanical compression to reach the utilization pressure. Therefore, analyzing the impact of cathodic pressure variations on η_{PEM} alone can be misleading unless the overall PEME-HPP efficiency—including the mechanical work of the compressor—is taken into account.

The PEME-HPP efficiency, η_T , which also accounts for the mechanical work of the compressor and converter efficiency, is calculated as follows:

$$\eta_T = \eta_{PEM} \eta_{Conv} \eta_{mc} \quad (7.35)$$

where η_{mc} is obtained as in (3.31), while η_{Conv} is assumed to be fixed.

Fig. 7.4 (e)–(f) depicts the PEME-HPP efficiency for the four commercially available membrane thicknesses over the operating ranges of current density, cathodic pressure, and temperature. As shown in the figure, the same general trends observed in η_{PEM} are also evident in η_T ; however, unlike η_{PEM} , for the same current density and temperature, η_T is very low at low cathodic pressures and then gradually increases as the cathodic pressure rises to a peak, before decreasing again. The maximum PEME-HPP at each current density, η_T^{max} , is indicated by a pink line. Fig. 7.4 (e)–(f) provides the top view of Fig. 7.4 (i)–(l). As illustrated in Fig. 7.4 (i), for the thin membrane *N211*, the η_T^{max} line is always achieved by operating at the lowest temperature, $T_{cell}^{PEM} = 20^\circ\text{C}$, with the corresponding cathodic pressure gradually increasing as the current density rises. For the thicker membrane *N212*, as shown in Fig. 7.4 (j), η_T^{max} is also obtained at $T_{cell}^{PEM} = 20^\circ\text{C}$ up to a current density of 2 A/cm^2 , beyond which the operating temperature corresponding to η_T^{max} begins to increase while the cathodic pressure decreases. A similar trend is observed for the even thicker membranes *N115* and *N117*, as illustrated in Fig. 7.4 (k)–(l): at low current densities, the highest efficiency occurs at $T_{cell}^{PEM} = 20^\circ\text{C}$ with increasing cathodic pressure, but as the current density rises, the operating temperature shifts upward while the pressure decreases, until it eventually reaches $T_{cell}^{PEM} = 90^\circ\text{C}$, where the cathodic pressure starts to increase again with current density.

The hydrogen-to-oxygen percentage, $\Psi_{H_2}^{PEM}$, for the four membrane thicknesses is shown

in Fig. 7.5 (a)–(d). As illustrated, and consistent with the analytical assessment insight (iii), $\Psi_{H_2}^{PEM}$ increases with higher cathodic pressure and operating temperature, but decreases with the increase of current density. Additionally, as the membrane becomes thicker, $\Psi_{H_2}^{PEM}$ decreases overall and falls below the safety limit, $\Psi_{H_2}^{safe}$, at lower current densities. Fig. 7.5 (e)–(h) provide horizontal cross-sectional views of $\Psi_{H_2}^{PEM}$ at the safety limit, $\Psi_{H_2}^{PEM, safe}$, for the 3D plots in Fig. 7.5 (a)–(d). For each temperature, a dividing line separates the $(J^{PEM} - \pi_{H_2}^{PEM})$ domain into two regions: 1) an unsafe region located southeast of the line, representing combinations of J^{PEM} and $\pi_{H_2}^{PEM}$ where PEME operation is unsafe; and 2) a safe region located northwest of the line, representing the allowable operating combinations for that temperature. Fig. 7.5 (e)–(h) also show the $\eta_T^{\max}$ curve, introduced earlier in Fig. 7.4 (e)–(l), now color-coded by temperature. By comparing the temperature-colored $\eta_T^{\max}$ curve with the safety limit dividing lines, it becomes possible to determine whether the maximum efficiency at a given temperature falls within the safe operating region. For example, in Fig. 7.5 (f), the $\eta_T^{\max}$ curve appears in dark blue (corresponding to $T_{cell}^{PEM} = 20^\circ\text{C}$) up to $J^{PEM} = 2 \text{ A/cm}^2$. However, a small segment of this curve lies in the unsafe region southeast of the $T_{cell}^{PEM} = 20^\circ\text{C}$ safety limit for $J^{PEM} < 0.22 \text{ A/cm}^2$, while the remaining portion lies safely northwest of the safety limit dividing line. To further illustrate the impact of safety limits on defining the safe maximum efficiency, $\eta_T^{\max, safe}$, Fig. 7.5 (i)–(l) considers a stricter safety limit ($\Psi_{H_2}^{PEM, safe} = 5\%$). The results show that, for all membrane thicknesses, large portions of $\eta_T^{\max}$ fall within the unsafe region. As an alternative, and in compliance with the safety limit, the safe maximum efficiency (shown as pink lines), $\eta_T^{\max, safe}$, can be determined. This adjustment typically involves lowering the cathodic pressure to return the operation to the safe region.

7.3.2 Cases 1 and 2: PEME-HPP Design and Scheduling with Fixed Cathodic Pressure and Temperature

In Case 1, the PEME-HPP is optimally designed under the assumption that the PEME operates at a fixed cathodic pressure of $\pi_{H_2}^{PEM} = 30 \text{ bar}$ and a temperature of $T_{cell}^{PEM} =$

Table 7.2: Optimized Parameters and Operating Conditions of a PEME-HPP

Item	Parameter	Case 1	Case 2	Case 3	Case 4	Case 5
PEME	δ_m^{PEM}	N115	N212	N211	N212	N211
	$A_{cell}^{PEM}(m^2)$	1737	1446	1290	1337.5	1290
	$\pi_{H_2}^{PEM}(bar)$	30	38	69 ^a	37.4	69 ^a
	$T_{cell}^{PEM}(K)$	353	309	293	325.7 ^a	305 ^a
	$P_{PEM}^{rate}(MW)$	105	80.7	70.3	74.6	70.3
Elec. Devices	$P_{Conv}^{rate}(MW)$	63.5	65	68.8	64.5	68.8
	$P_{Cmp}^{rate}(MW)$	10.5	9.3	10.2	9.7	10.2
H_2 Storage	$E_{HS}(100kg)$	193	191	189	195	189
Cost	$LCOH(\$/kg)$	8.876	8.46	7.945	8.265	7.9

^a These values are the averages of the set-points throughout the entire simulation period, while the actual set-points vary from hour to hour.

353K. The corresponding optimal parameters are summarized in Table 7.2. As shown, the PEME is significantly overrated, with a rated power of $P_{PEM}^{rate} = 105$ MW compared to the AC/DC converter rated power of $P_{Conv}^{rate} = 63.5$ MW. The AC/DC converter rating reflects the actual power consumption of the PEME, whereas the PEME rating represents the use of a larger cell area and operation at a lower loading level to achieve an optimal LCOH. This overrating—approximately 65% above the PEME maximum actual power consumption—substantially increases the CAPEX. Moreover, operating the PEME at a low loading level requires the use of a thick membrane (N115), which maintains the hydrogen in oxygen ratio within the safety limit, $\Psi_{H_2}^{PEM, safe}$. Although the N115 membrane exhibits lower efficiency at higher loading, this drawback is negligible since the converter’s rated power constrains the overrated PEME, and it will not operate at such high loading conditions.

In Case 2, the PEME cathodic pressure and cell temperature are optimized but fixed over the PEME lifetime at specific optimal values of 38 bar and 309K, respectively, as shown in Table 7.2. Under these optimized conditions, the PEME rated power is decreased by 23% compared to Case 1, reflecting a corresponding reduction in PEME cell area. Therefore, in

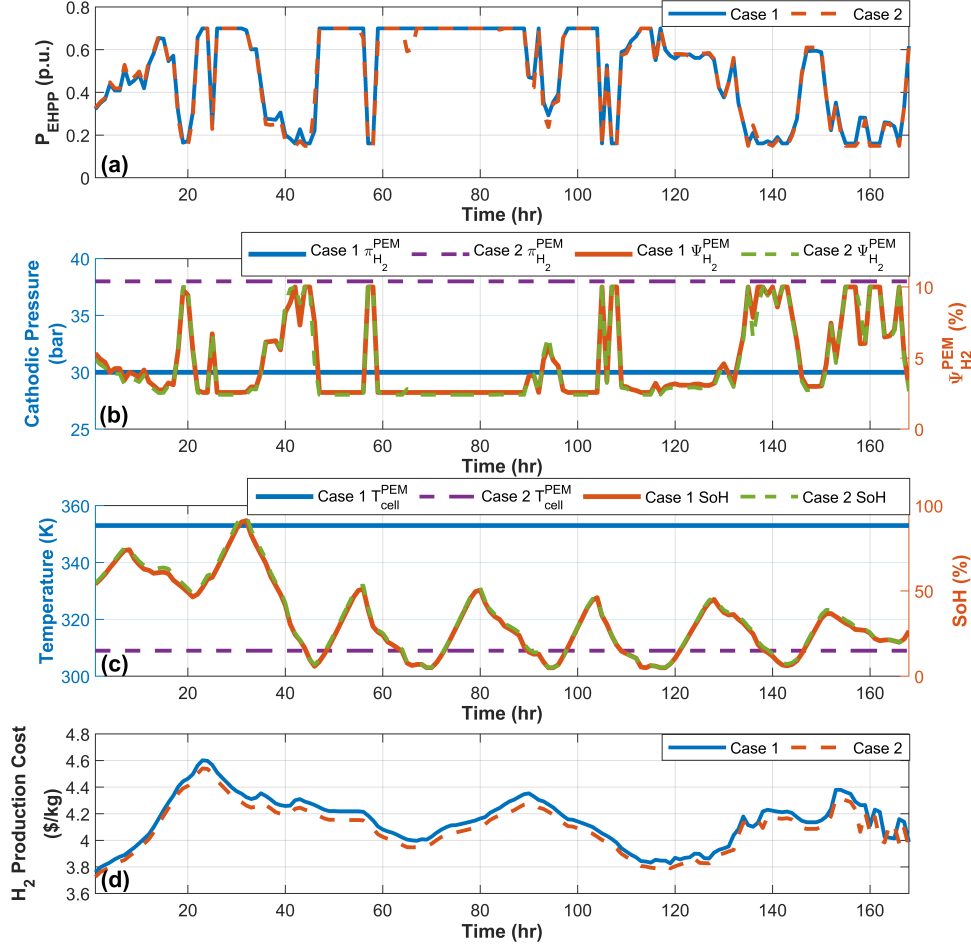


Figure 7.6: (a) PEME-HPP power consumption, (b) PEME cathodic pressure and hydrogen in oxygen percentage, (c) PEME operating temperature and the SoH of the HS, and (d) H_2 production cost throughout a week of operation of PEME-HPP for Cases 1 and 2.

Case 2, the PEME operates at higher loading levels, allowing the use of a thinner membrane (N_{212}) while maintaining the hydrogen-to-oxygen ratio within the safety limit, $\Psi_{H_2}^{PEM, safe}$, despite the higher cathodic pressure relative to Case 1. This is achieved by lowering the operating temperature to $T_{cell}^{PEM} = 309K$. It is worth noting that, as discussed earlier in the subsection 7.3.1, the thick membrane (N_{117}) is the optimal thickness to achieve the highest η_T when a high operating temperature is utilized in Case 1. However, a thinner membrane (N_{212}) is optimal when a lower temperature of $T_{cell}^{PEM} = 309K$ is utilized as in

Case 2.

Fig. 7.6 (a) presents the PEME-HPP power consumption for Cases 1 and 2 over one week of operation. In both cases, the power consumption, P_{EHPP} , is nearly identical, as it follows the lowest electricity prices. Fig. 7.6 (b) illustrates the PEME cathodic pressure and hydrogen-to-oxygen percentage. The cathodic pressure remains fixed in both cases, while $\Psi_{H_2}^{PEM}$ shows similar variations, with Case 2 exhibiting slightly lower values for the same P_{EHPP} . In both cases, however, $\Psi_{H_2}^{PEM}$ remains within the safety limit of $\Psi_{H_2}^{PEM, safe} = 10\%$. Fig. 7.6 (c) shows the PEME operating temperature and hydrogen storage SoH . The temperature is constant throughout the week for both cases, and SoH follows an identical profile. Despite these similarities in P_{EHPP} , $\Psi_{H_2}^{PEM}$, and SoH , the H_2 production cost in Case 2 is noticeably lower, as shown in Fig. 7.6 (d), reflecting the improved PEME-HPP efficiency in Case 2 compared to Case 1.

The substantial reduction in PEME cell area and rated power in Case 2, compared to Case 1, led to a notable decrease in the CAPEX of the PEME-HPP. Furthermore, optimizing the PEME's cathodic pressure and temperature enhanced PEME-HPP efficiency, thereby reducing OPEX. Together, these reductions in both CAPEX and OPEX led to a 4.5% decrease in LCOH in Case 2 relative to Case 1.

7.3.3 Cases 3 and 4: PEME-HPP Design and Scheduling with Varying Cathodic Pressure or Temperature

Case 3 considers optimizing the PEME cathodic pressure on an hourly basis, while fixing the operating temperature over the PEME lifetime at its optimal value. The optimal PEME-HPP parameters for Case 3 are given in Table 7.2. It is worth noting that, as the pressure varies hourly, the value given in the table is the average pressure over the optimization period. As provided in the table, such hourly optimization of PEME cathodic pressure increases PEME-HPP operational flexibility and allows the use of a PEME with a rated power 12.5% lower than Case 2 and 33% lower than Case 1, thereby requiring a significantly smaller cell area. As a result, the PEME operates at higher loading levels

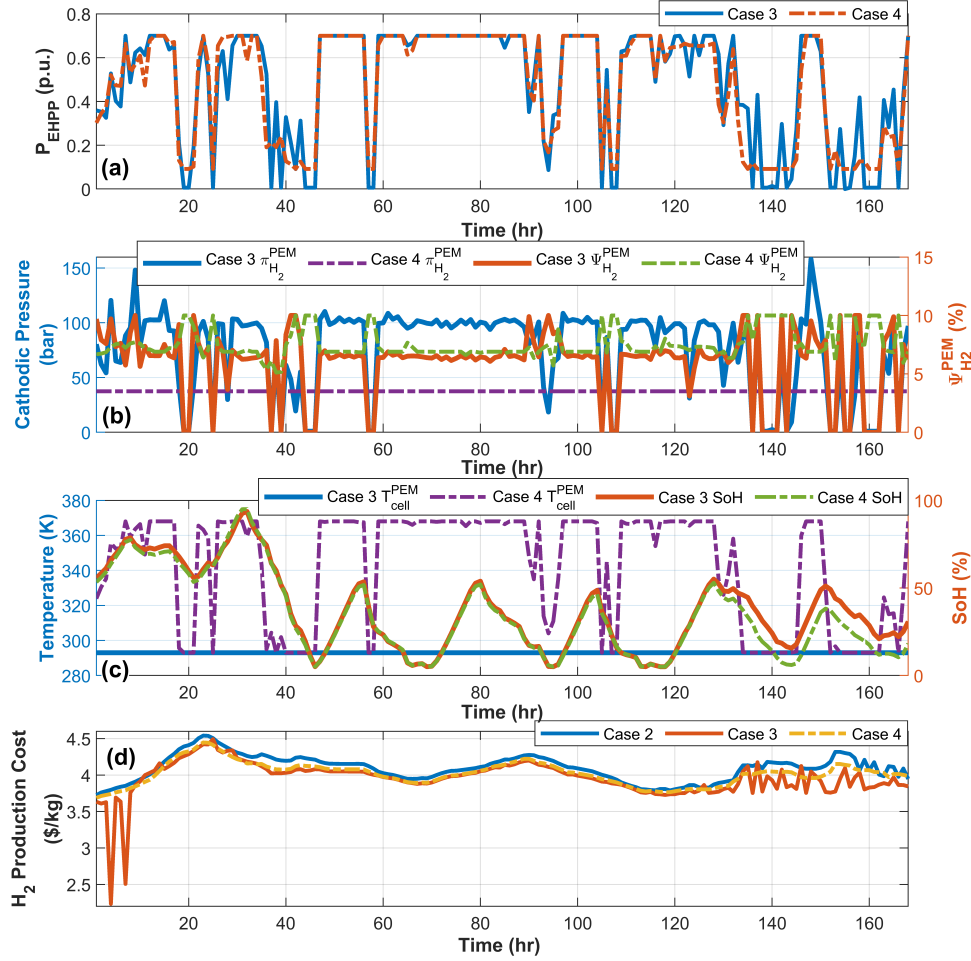


Figure 7.7: (a) PEME-HPP power consumption, (b) PEME cathodic pressure and hydrogen in oxygen percentage, (c) PEME operating temperature and the SoH of the HS, and (d) H_2 production cost throughout a week of operation of PEME-HPP for Cases 3 and 4.

compared to Cases 1 and 2. The combination of high-loading operation and the added flexibility introduced by the hourly variation of the cathodic pressure enables the use of the thinnest membrane ($N211$), which reduces the voltage drop across the membrane and enhances both PEME voltage efficiency and overall PEME-HPP efficiency, η_{HP} . Moreover, the optimized operating temperature is set to a low value of 293 K , minimizing $\Psi_{H_2}^{PEM}$ and providing a wider range for cathodic pressure variation even with that thin membrane. This

outcome is consistent with Section 7.3.1, which shows that the highest η_T is achievable with the *N211* membrane at very low temperatures. Although the average cathodic pressure in Case 3 is higher than in Case 2, it can drop to very low values at certain instances, particularly under low loading conditions. As a result, the mechanical compressor power consumption increases by about 5% compared to Case 2. Nevertheless, since the PEME capital cost is significantly higher than that of the compressor, the reduction in PEME rated power drives the overall CAPEX in Case 3 to be substantially lower than in Case 2.

In Case 4, the PEME operating temperature is optimized on an hourly basis, while the cathodic pressure is fixed at its optimal value throughout the PEME lifetime. The corresponding optimal PEME-HPP parameters are summarized in Table 7.2. In terms of rated power and cell area, the PEME is slightly overrated, with its rated power being 7% higher than in Case 3. Unlike Case 3, Case 4 employs a thicker membrane (*N212*), which is better suited to the lower current density operation introduced by overrating the PEME in this case. The optimal cathodic pressure is set to *37 bar*, very close to that of Case 2, and significantly lower than the average cathodic pressure in Case 3. Although the average operating temperature in Case 4 is higher than in Case 2, it drops significantly at certain times, allowing the PEME to operate at lower loading levels without exceeding the hydrogen-to-oxygen safety limit. Overall, the CAPEX in Case 4 is lower than in Case 2 due to the use of a smaller PEME, but remains higher than in Case 3.

In terms of the optimal scheduling of PEME-HPP, Fig. 7.7 (a) illustrates the PEME-HPP power consumption throughout a week of operation. Unlike Cases 1 and 2, which have similar PEME-HPP power consumption, Cases 3 and 4 have apparent variation in their power profiles. Obviously, Case 3 has more flexible power variations that easily vary from no load to full load compared to Case 4, which has less flexible power variations that barely reach a low of 0.1 p.u., still showing better flexibility than Cases 1 and 2. Fig. 7.7 (b) depicts the cathodic pressure variations and hydrogen-to-oxygen percentage of the same week for Cases 3 and 4. As shown in the figure, in Case 3, the cathodic pressure varies significantly, where it generally increases with the increase of PEME-HPP power to achieve the highest PEME-HPP efficiency while decreasing with the PEME-HPP power drop to

avoid exceeding the safety limit at lower loading levels, as proven in the corresponding $\Psi_{H_2}^{PEM}$ changes. For Case 4, the cathodic pressure is fixed all over the operating time, while the hydrogen-to-oxygen variations are limited and tends to vary close to the safety limit $\Psi_{H_2}^{PEM, safe} = 10\%$, indicating that the impacts of temperature variation, specifically at such cathodic pressure ($\pi_{H_2}^{PEM} = 37 \text{ bar}$), on hydrogen-to-oxygen percentage is limited as previously presented in Fig. 7.5 (b). PEME temperature and hydrogen storage SoH are demonstrated in Fig. 7.7 (c). For Case 3, the PEME temperature is fixed at its lowest value $T_{cell}^{PEM} = 293 \text{ K}$. In contrast, for Case 4, the PEME temperature varies significantly and tends to operate at the highest temperature when the PEME is running at high loading levels to achieve the highest efficiency; however, at lower loading levels, the temperature drops significantly to maintain the high efficiency and safe operation. Fig. 7.7 (d) depicts the H_2 production cost throughout a week of operation for Cases 2 to 4. As shown in the figure, Cases 3 and 4 clearly provide lower H_2 production costs compared to Case 2. Additionally, Case 3 can introduce significantly lower H_2 production cost in some instances compared to Cases 3 and 4, as those between 140 and 160 operating hours.

7.3.4 Case 5: PEME-HPP Design and Scheduling with Varying Cathodic Pressure and Temperature

In Case 5, the PEME-HPP optimal design incorporates the optimization of both cathodic pressure and operating temperature on an hourly basis. While the overall design is similar to that of Case 3, the key difference lies in the operating temperature, whose average value in Case 5 is higher than that of Case 3. The additional hourly adjustment of operating temperature in Case 5 results in a modest improvement in LCOH, reducing it by 0.6% compared to Case 3. This improvement is primarily driven by lowering OPEX, achieved through enhanced PEME-HPP efficiency by dynamically varying the operating temperature on an hourly basis.

In terms of optimal scheduling, since the PEME-HPP designs in Cases 3 and 5 are identical, their power consumption is nearly the same. The differences arise from the temperature

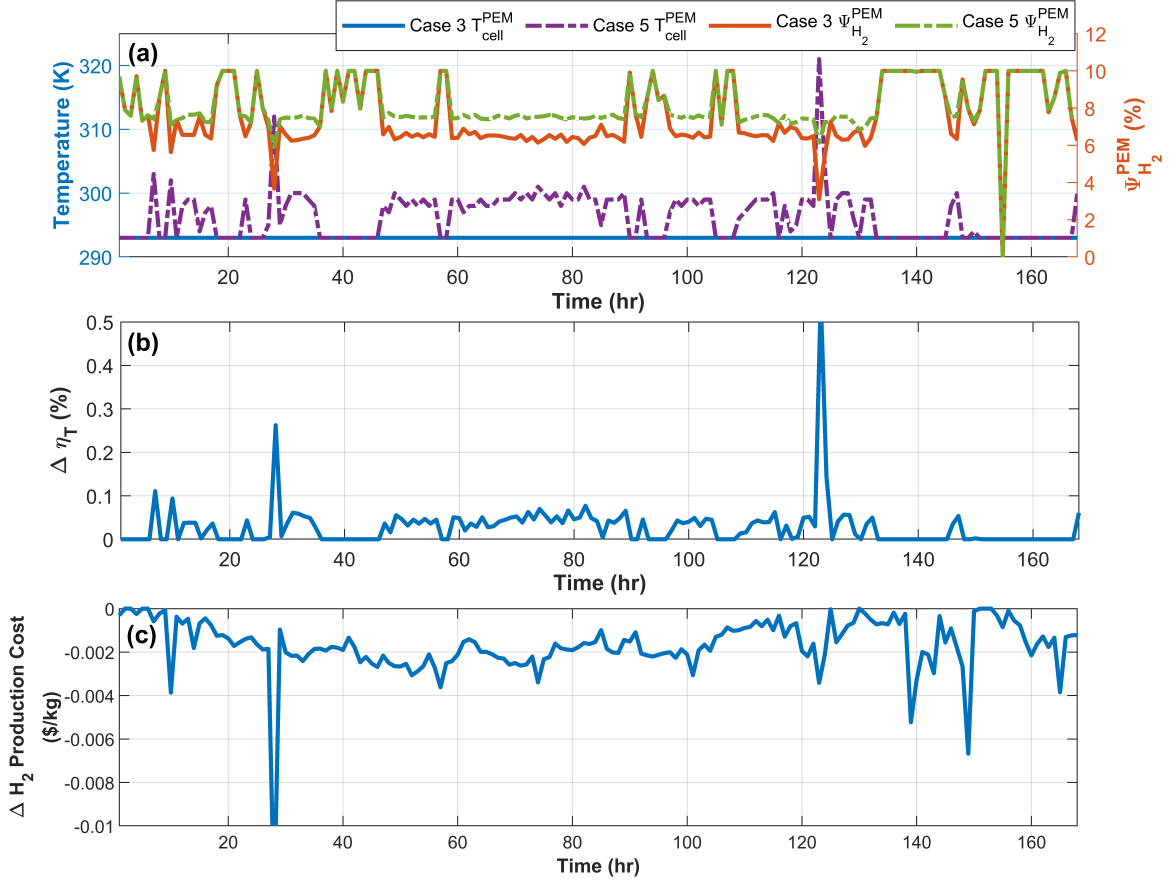


Figure 7.8: (a) PEME operating temperature and hydrogen in oxygen percentage for Cases 3 and 5 throughout a week of operation of PEME-HPP. Difference between Case 5 and Case 3 (b) PEME efficiency, and (c) H_2 production cost throughout a week of operation of PEME-HPP.

variations in Case 5, which influence the hydrogen-to-oxygen percentage, PEME-HPP efficiency, and consequently the H_2 production cost compared to Case 3. Fig.7.8(a) presents the PEME operating temperature and $\Psi_{H_2}^{PEM}$ for both cases. As shown, the operating temperature in Case 5 is slightly higher than in Case 3, particularly when $\Psi_{H_2}^{PEM}$ remains below the safety limit $\Psi_{H_2}^{PEM, safe}$, allowing safe temperature increases. However, when $\Psi_{H_2}^{PEM}$ in Case 3 is at the safety limit, no further temperature increase is possible. Fig.7.8(b) and (c) illustrate the differences in PEME-HPP efficiency and H_2 production cost between the two

cases. As depicted, the higher temperatures in Case 5 lead to proportional improvements in PEME-HPP efficiency and, in turn, a corresponding reduction in H_2 production cost relative to Case 3.

7.4 Control of PEME with Dynamic Cathodic Pressure and Temperature

As shown in Sections 7.2 and 7.3, the operation of PEME with dynamic cathodic pressure and/or cell temperature results in a noticeable reduction in the LCOH, particularly in the case of dynamic cathodic pressure operation. Although the steady-state analysis and numerical results presented in Section 7.3 demonstrate the technical feasibility of such operating strategies, the dynamic behavior of PEME under varying cathodic pressure and/or cell temperature may introduce additional operational challenges. Accordingly, building upon the dynamic PEME model developed in Section 3.2.2, this section investigates the real-time dynamic operation of the PEME using the optimal power input and cathodic pressure profiles obtained from the steady-state optimal design formulation of Section 7.2.

In this section, and given that the impact of dynamic temperature operation is less significant compared to that of dynamic cathodic pressure, the analysis focuses on the case where the PEME operates at a fixed optimal cell temperature while the cathodic pressure varies dynamically. First, the conventional control strategy for PEME is examined, and its limitations are identified. Subsequently, a coordinated control approach is proposed to ensure safe and reliable operation of the PEME under dynamic cathodic pressure conditions.

7.4.1 Conventional Decoupled Control of PEME

Despite the inherent coupling between the electrical, thermal, and mass transfer dynamics in PEME, most deployed control strategies adopt decoupled, domain-specific control loops. This section presents the conventional control architecture and demonstrates its key limitations, particularly under dynamic operating conditions.

Fig. 7.9 illustrates a conventional control architecture employed in PEME, where each physical domain is governed by an independent, decoupled control loop. The electrical, thermal, and mass transfer subsystems are typically controlled separately, with limited or no coordination between them.

The main controllers are as follows:

- **Electrical domain controller:** Governs the loading of the electrolyzer by controlling the back-to-back converters. It modulates the AC/DC converter to follow an active power setpoint P_{PEM}^* and the DC/DC converter to control the DC bus voltage. Further details on the electrical domain controller are provided in [179,180].
- **Mass transfer domain controller:** Manages the hydrogen pressure in the cathodic compartment, $\pi_{H_2}^{PEM}$, by controlling the hydrogen outlet flow $Q_{H_2}^{out}$. In this study, a simple proportional controller is used to follow the pressure setpoint $\pi_{H_2}^*$:

$$Q_{H_2}^{out} = -0.03(\pi_{H_2}^* - \pi_{H_2}^{PEM}). \quad (7.36)$$

- **Thermal domain controller:** Ensures that the electrolyzer temperature T_{cell}^{PEM} remains at the desired level T_{cell}^* by controlling the coolant or heating flow Φ_{th} . A proportional controller is deployed in this study:

$$\Phi_{th} = 5 \times 10^5 (T_{cell}^* - T_{cell}^{PEM}). \quad (7.37)$$

While this structure simplifies controller design and supports modular implementation, it inherently overlooks the strong interdependence among the different physical domains. As a result, system-wide performance and safety can be compromised under dynamic or large-scale operation.

7.4.2 Limitations of the Conventional Decoupled Control Approach

To evaluate the performance of the decoupled control architecture under varying PEME operating conditions, a dynamic scheduling profile is applied to the system, wherein the

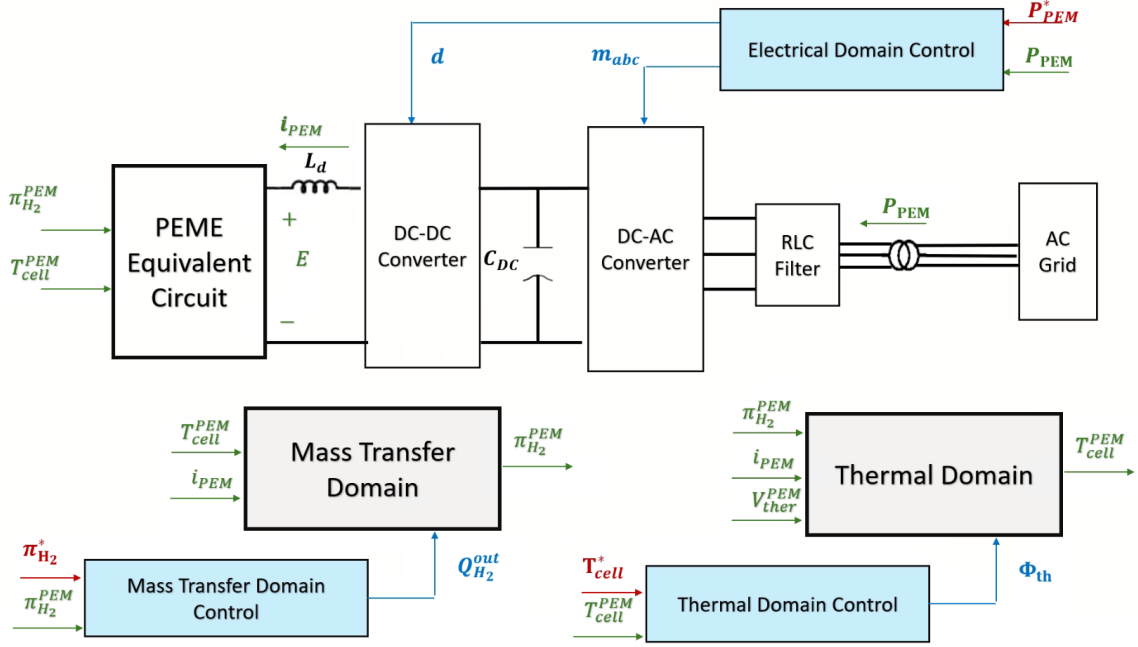


Figure 7.9: Conventional control architecture of PEME

power and pressure setpoints are optimized to minimize the LCOH as proposed in 7.2. The temperature setpoint is assumed to remain constant throughout the simulation period. Fig. 7.10 shows the PEME system response over a 96-hour period under this strategy.

As observed in Fig. 7.10 (a) and (b), the power and pressure controllers successfully track their respective setpoints under steady-state conditions. A small discrepancy between the power setpoint P_{PEM}^* and the actual PEME power P_{PEM} is evident in Fig. 7.10 (a), primarily due to losses in the power electronic converters. However, Fig. 7.10 (c) reveals a critical safety issue that arises during transients: the hydrogen in oxygen percentage transiently exceeds the acceptable safety limit $\Psi_{H_2}^{PEM, safe}$.

These excursions occur due to the lack of coordination between the electrical, mass transfer, and thermal domains. In particular, rapid power changes lead to immediate variations in hydrogen generation, which the slower-responding pressure controller cannot accommodate quickly enough. This results in a temporary accumulation of hydrogen within

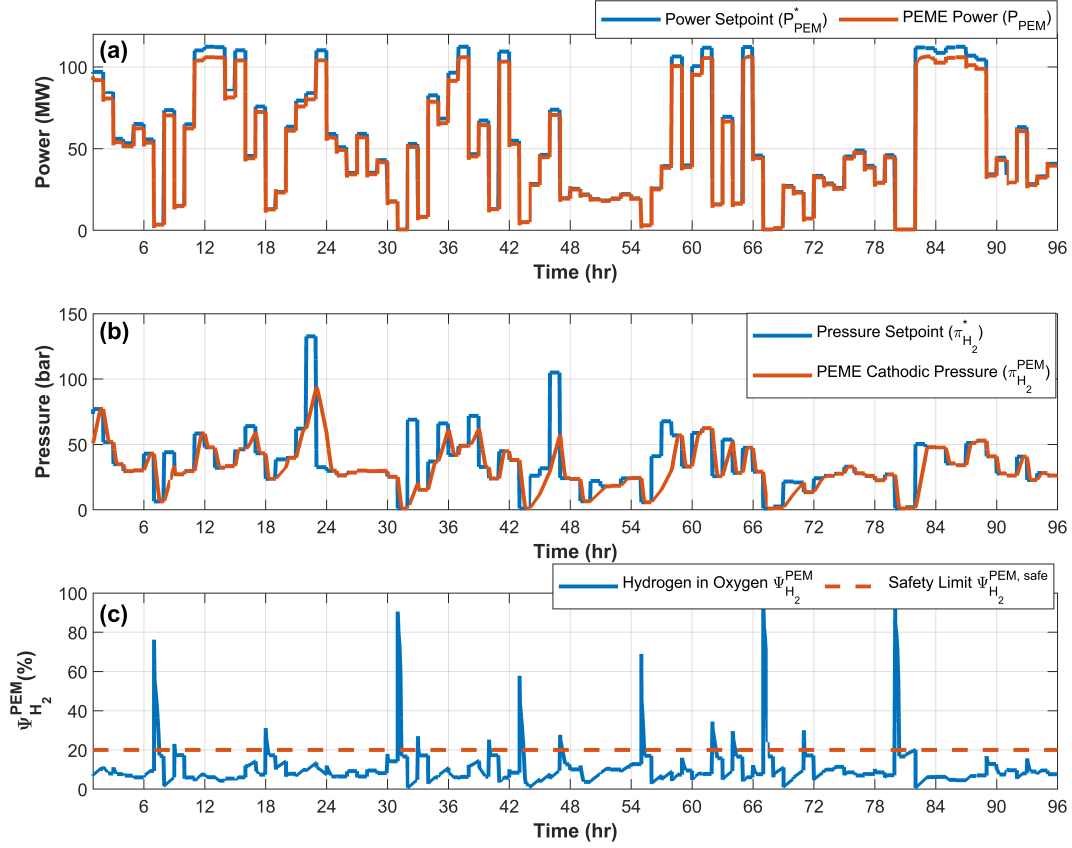


Figure 7.10: Under conventional control: (a) power setpoints and PEME power, (b) pressure setpoints and PEME cathodic pressure, and (c) hydrogen concentration in oxygen.

the oxygen compartment, violating safety constraints. Although the steady-state performance of the system appears acceptable, these transient violations underscore a critical limitation of the decoupled control strategy: its inability to guarantee safe operation under dynamically changing conditions. An integrated control approach that accounts for the interdependencies between physical domains is therefore necessary to ensure both efficiency and safety.

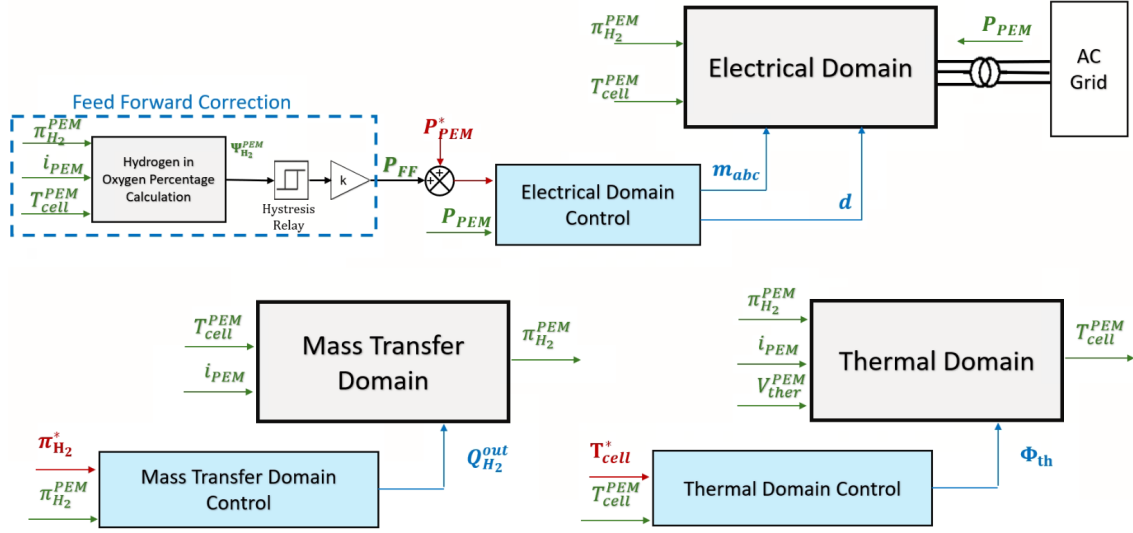


Figure 7.11: Coordinated control architecture of PEME

7.4.3 Coordinated Control of PEME

This subsection develops a coordinated control for PEME to mitigate the limitations of conventional decoupled control in maintaining the hydrogen in oxygen percentage, $\Psi_{H_2}^{PEM}$, within safe limits. Fig. 7.11 illustrates the coordinated control architecture, in which a feedforward correction component for the power setpoint is applied during the transients to coordinate the PEME electrical domain with both the mass transfer and thermal domains. A feedback measurement from $\Psi_{H_2}^{PEM}$ is used to generate the feedforward power correction P_{FF} , which is then added to the original power setpoint P_{PEM}^* . A hysteresis relay is used to limit the application of the feedforward correction to the transients where the $\Psi_{H_2}^{PEM}$ is about to exceed the safe limits. P_{FF} is calculated as follows:

$$P_{FF}(t) = \begin{cases} k \Psi_{H_2}^{PEM} & , \Psi_{H_2}^{PEM} > \xi_U \Psi_{H_2}^{PEM, safe} \\ 0 & , \Psi_{H_2}^{PEM} \leq \xi_L \Psi_{H_2}^{PEM, safe} \\ P_{FF}(t^-) & , otherwise \end{cases} \quad (7.38)$$

where $k = 50 \times 10^6$ is the feedforward gain, and ξ_U and ξ_L are the upper and lower threshold ratios, respectively, defining the hysteresis relay limits as percentages of the hydrogen in

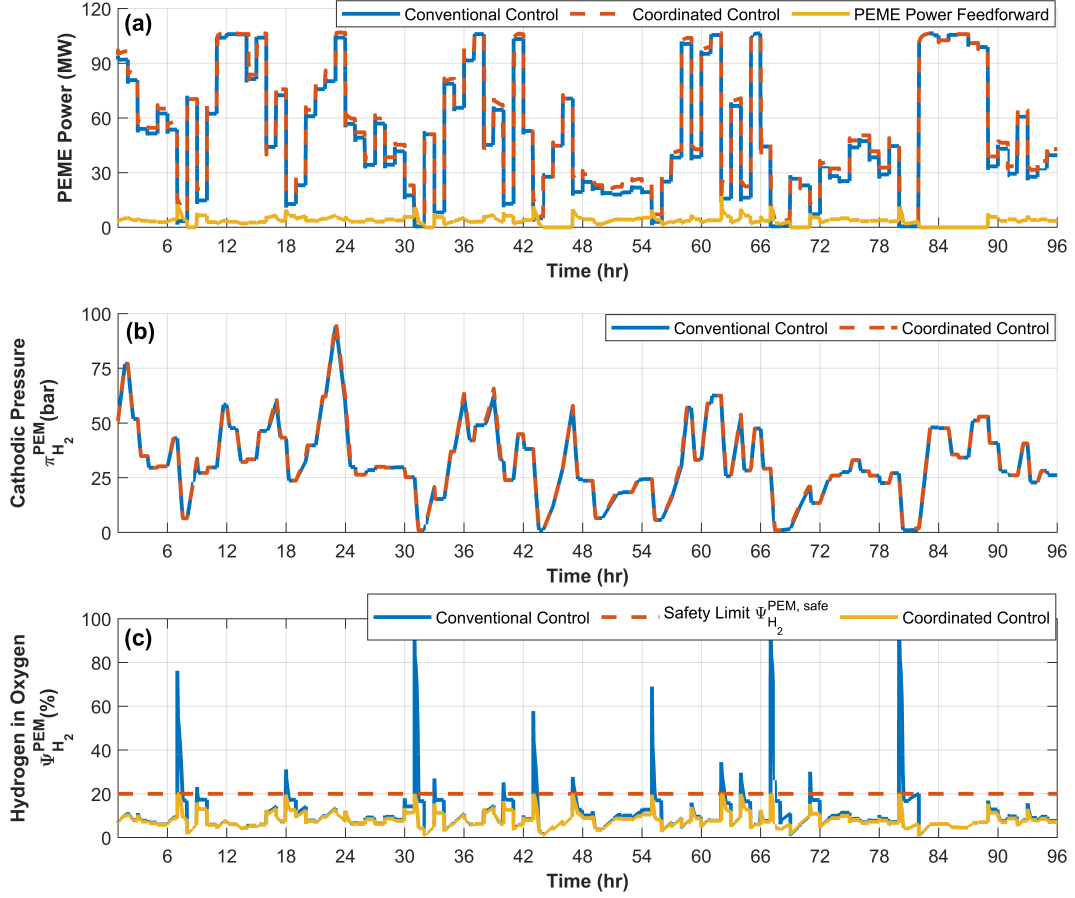


Figure 7.12: Comparison of PEME (a) power, (b) cathodic pressure, and (c) hydrogen in oxygen percentage under conventional and coordinated control.

oxygen safety limit $\Psi_{H_2}^{PEM, safe}$. As in (7.38), the feedforward power correction at time t , $P_{FF}(t)$, keeps its last status, $P_{FF}(t^-)$, while transitioning between the hysteresis relay thresholds (i.e., $\xi_U \Psi_{H_2}^{PEM, safe}$ and $\xi_L \Psi_{H_2}^{PEM, safe}$).

Fig. 7.12 presents the time response of the PEME system over a 96-hour period under both conventional and coordinated control approaches. Fig. 7.12 (a) illustrates the PEME power, P_{PEM} , for both control approaches, along with the feedforward power correction, P_{FF} , applied in the coordinated control. As shown in the figure, the PEME power in coordinated control slightly deviates from that in conventional control, particularly during

the transient stages. This deviation is mainly caused by the feedforward power correction, which changes the PEME power setpoint. Fig. 7.12 (b) depicts the PEME cathodic pressure, $\pi_{H_2}^{PEM}$, for both control approaches, exhibiting nearly identical behavior. This similarity is expected, as the feedforward power correction has only a minor influence on the PEME power, primarily during transients. Consequently, the impact of the feedforward correction on the cathodic pressure can be considered negligible. Fig. 7.12 (c) shows the hydrogen-to-oxygen ratios, $\Psi_{H_2}^{PEM}$, under both control strategies. The figure reveals that coordinated control significantly reduces the $\Psi_{H_2}^{PEM}$ spikes observed during transients with conventional control and keeps them within the safety limit, $\Psi_{H_2}^{PEM, safe}$.

The previous results demonstrate that the proposed coordinated control effectively incorporates the hydrogen in oxygen ratio dynamics, arising from the interaction of PEME's three domains, into the electrical domain controller, which responds fast enough to maintain this ratio within safe limits. Beyond ensuring safe operation, the proposed strategy stands out for its simplicity and practical applicability, requiring no specialized controllers or complex theoretical formulations. This makes it a promising solution for the real-world deployment of PEME systems under dynamic operational conditions, such as dynamic cathodic pressure.

7.5 Summary

This chapter investigates the impact of cathodic pressure and cell temperature on the performance, design, and operation of PEME-HPP. The results demonstrated that dynamically adjusting these operating conditions can significantly enhance PEME efficiency across varying loading conditions. To this end, a comprehensive optimization framework was developed to simultaneously address the design and operation of PEME-HPP. The proposed formulation minimizes the LCOH by optimally determining the system sizing (including PEME, converter, compressor, and hydrogen storage), internal PEME parameters (cell area and membrane thickness), and the corresponding operating set-points (cathodic pressure and temperature). In addition, a rolling-horizon scheduling model was formulated

to optimize real-time operation based on the optimal design parameters.

The results revealed that adopting hourly optimization of the operating temperature with a fixed optimal cathodic pressure achieves a 28% reduction in PEME rated power and a 7% reduction in LCOH, while hourly optimization of the cathodic pressure with a fixed optimal operating temperature achieves even greater improvements—33% reduction in rated power and 10.6% reduction in LCOH. Finally, jointly optimizing both cathodic pressure and cell temperature on an hourly basis provides only a modest additional improvement, yielding a total LCOH reduction of 11.2%. These findings highlight that dynamic optimization of the PEME cathodic pressure is more critical than that of the operating temperature. However, optimizing the cell temperature dynamically along with the cathodic pressure still provides additional benefits.

To ensure the practical feasibility of such dynamic operation, the detailed multiphysics dynamic model of PEME, previously developed in Chapter 3, is employed in conjunction with a conventional decoupled control strategy. The results show that conventional control strategies are insufficient for handling dynamically varying operating conditions, as they may lead to violations of hydrogen in oxygen safety limits. Accordingly, a coordinated control strategy is proposed and validated, demonstrating its effectiveness in maintaining safe operation under dynamic cathodic pressure conditions.

Overall, this chapter confirms that dynamic optimization of PEME operating conditions can substantially improve both economic and operational performance, thereby enhancing the viability of PEME-HPP in future low-carbon energy systems. Further, the developed models assist PEME manufacturers in optimizing their internal parameters and help hydrogen production plant operators determine the optimal operating conditions.

Chapter 8

Conclusions and Future Work

This dissertation investigated the optimal design, configuration, operation, and control of EHPPs integrated with modern power systems. Motivated by the increasing global demand for low-carbon hydrogen and the need to improve the economic competitiveness of water electrolysis technologies, the research focused on developing comprehensive modeling and optimization frameworks for EHPP deployment. In particular, the work emphasized PEME technology due to its high efficiency, compact design, and superior dynamic response, while also considering AE for comparative analysis. The developed methodologies aim to reduce the LCOH, improve operational flexibility, and enable effective integration of hydrogen production systems with renewable energy sources and electricity markets.

The research began by developing detailed mathematical models for the main components of EHPPs, including electrolyzers, compressor, HS, BESS, and FC. Both steady-state and dynamic models were developed to accurately capture the electrochemical, thermal, and mass-transfer characteristics of PEME. These models provided the foundation for the optimization frameworks developed throughout the thesis.

Building upon these models, the thesis introduced a novel optimization formulation for the optimal design of grid-connected PEME-HPPs. Unlike conventional approaches that consider that the PEME has a fixed internal design, the proposed formulation integrates

the internal design parameters of PEME—such as membrane thickness, cell area, and cathodic pressure—directly within the system sizing problem. The framework simultaneously determines the optimal ratings of major plant components, including the PEME, AC/DC converters, compressors, HS, and optional BESS, while minimizing the LCOH. The results demonstrated that incorporating the internal design optimization of PEME can significantly reduce hydrogen production costs. In particular, optimizing PEME parameters yielded up to a 20% reduction in LCOH compared with using commercially available PEME designs. Additionally, the integration of a BESS improved operational flexibility and provided further reductions in LCOH. The analysis also highlighted the importance of incorporating PEME safety constraints, particularly hydrogen in oxygen crossover limits, as neglecting these constraints may lead to impractical or unsafe EHPP designs.

To further improve electrolyzer performance under intermittent renewable power conditions, the thesis proposed an innovative modular configuration for PEME-HPPs. In this configuration, the PEME is divided into multiple SCMs, allowing flexible operation across a wide range of loading levels. A multi-objective optimization formulation was developed to determine the optimal number of modules, PEME internal parameters, and other EHPP equipment ratings while simultaneously minimizing the LCOH and maximizing hydrogen production. The results showed that the proposed modular configuration significantly enhances plant efficiency at low loading levels and extends the safe operating range of PEME systems. Compared with conventional singular PEME configurations, the modular architecture achieved up to a 6% reduction in LCOH and an 11% increase in hydrogen production under the studied renewable power profiles. Furthermore, Pareto frontier analysis revealed the inherent trade-off between minimizing hydrogen production costs and maximizing hydrogen output, providing decision-makers with valuable insights into selecting appropriate design points based on operational priorities.

In addition to system design improvements, this thesis investigated the suitability of different electrolyzer technologies for providing grid services while supplying hydrogen to various applications. A comprehensive framework was developed to determine the optimal electrolyzer technology and internal design based on electricity pricing schemes, hydrogen

pressure requirements, and participation in ancillary grid services such as CA, OR, and RS. The results indicated that AE is generally more cost-effective under stable electricity pricing conditions and low hydrogen pressure requirements. However, their slower dynamic response and the need for oversizing to address fast-response grid services reduce their economic attractiveness in dynamic operating environments. Conversely, PEME exhibit superior operational flexibility and faster ramping capabilities, making them more suitable for applications involving variable electricity prices, intermittent renewable generation, or rapid grid service responses. These findings emphasize that the selection of electrolyzer technology and design must consider multiple interacting factors, including electricity market conditions, hydrogen demand characteristics, and grid service requirements.

The thesis also addressed the operational optimization and control of PEME-HPPs. A novel optimization framework was developed to optimize the PEME loading and operating conditions (cathodic pressure and cell temperature) on an hourly basis, along with optimizing the PEME internal parameters. The results demonstrate that dynamically adjusting the PEME cathodic pressure and operating temperature across varying loading levels (i.e., current density) can reduce hydrogen production costs compared to conventional fixed operating conditions. In particular, dynamic operation can reduce the LCOH by up to 11.2%, while also decreasing the PEME-HPP ratings by up to 33%. To support the implementation of dynamic operating conditions, the thesis further developed a multiphysics dynamic model of PEME systems that captures the interactions among electrical, thermal, and mass-transfer processes. Using this model, the thesis demonstrated that conventional decoupled control strategies are insufficient for managing a PEME when its operating conditions vary dynamically. As a result, a coordinated control strategy was proposed to simultaneously regulate PEME loading, cathodic pressure, and operating temperature while maintaining the hydrogen in oxygen percentage within the safe limits.

Overall, this dissertation provides comprehensive frameworks for the design, operation, and technology selection of EHPPs integrated with power systems. By combining detailed electrolyzer modeling with system-level optimization, the proposed methodologies significantly improve the economic and operational performance of EHPPs. The results

demonstrate that optimizing electrolyzer internal parameters, adopting modular system architectures, dynamically adjusting operating conditions, and strategically selecting electrolyzer technologies based on market conditions can substantially reduce the LCOH and enhance EHPP flexibility. The developed frameworks provide valuable tools for multiple stakeholders involved in the emerging hydrogen economy. Electrolyzer manufacturers can use the developed frameworks to tailor electrolyzer designs to specific operating environments and applications. Hydrogen plant developers and operators can employ the proposed optimization models to determine economically optimal system configurations and operational strategies. Furthermore, grid operators and policymakers can benefit from the results by better understanding the role of EHPP in providing grid services and supporting renewable energy integration.

Building upon the contributions of this work, several opportunities remain for further research and development. These potential extensions are outlined as follows:

- Incorporate detailed electrolyzer degradation models, including membrane aging and catalyst deterioration, to enable more accurate long-term planning and cost assessment.
- Expand the modeling framework to include the full hydrogen value chain, including transportation, pipeline networks, and end-use applications such as mobility and industrial processes.
- Investigate the integration of EHPP within multi-energy systems, including coupling with natural gas networks, district heating systems, and electricity grids, to enhance sector coupling and system flexibility.
- Enhance the proposed coordinated control strategy by incorporating advanced control techniques, such as model predictive control (MPC), adaptive control, or data-driven approaches, to improve real-time performance under dynamic conditions.
- Explore the capability of EHPP to provide additional grid services, such as voltage support, black-start capability, and synthetic inertia, particularly in systems with

high penetration of inverter-based resources.

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Appendix A: List of Publications

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- [5] El-Hamalawy, A.F., Farag, H.E. and Asif, A., 2025. Optimal Design and Technology Selection for Electrolyzer Hydrogen Plants Considering Hydrogen Supply and Provision of Grid Services. *IEEE Transactions on Sustainable Energy*.
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- [9] El-Hamalawy, A.F., Farag, H.E. and Asif, A., Optimal Pressure and Temperature Management in PEM Electrolyzers for Efficient Integration with the Electric Grid under High Renewable Energy Penetration. Journal of Power Sources (Under Review).