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Uncertainty-Aware Design and Operation of Hydrogen-
Integrated Multi-Energy Systems for Hard-to-Abate Sectors

Progettazione e gestione in condizioni di incertezza di
sistemi multi-energetici integrati con idrogeno per i settori
hard-to-abate

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“All models are wrong, but some are useful.”

George E. P. Box

*A mia mamma Diana, al mio babbo Marco e a mio fratello Stefano,
alla mia nonna Luana, agli zii e ai cugini,
e ai nonni che non ci sono più ma che sento ancora vicini.*

DECLARATION

I hereby declare that this submission is my own work and, to the best of my knowledge and belief, it contains no material previously published or written by another person, nor material which to a substantial extent has been accepted for the award of any other degree or diploma at University of Florence or any other educational institution, except where due references are provided in the thesis itself.

Any contribution made to the research by others, with whom I have been working at the University of Florence or elsewhere, is explicitly acknowledged in the thesis.

Andrea Ademollo
30/11/2025

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ABSTRACT

Green hydrogen is a promising option to decarbonise hard-to-abate industrial and remote energy systems, yet plant-level design and operation are affected by multiple uncertainties. In this thesis, uncertainty is treated explicitly in two ways: (i) long-horizon variability of renewable availability for capacity planning (two-stage stochastic design), and (ii) short-horizon uncertainty in PV output and electricity prices revealed sequentially across market gates (multi-stage stochastic scheduling). Regulatory and certification uncertainty is treated through explicit constraints and sensitivity analysis.

This thesis develops and applies a modelling toolbox for power-to-hydrogen (PtH) plants embedded in multi-energy systems, built chronologically from rule-based simulation to deterministic and, ultimately, two-stage and multi-stage stochastic mixed-integer linear programming (MILP), with the explicit aim of understanding the strengths and limitations of each modelling layer.

The work begins with the development and use of the Multi Energy System Simulator (MESS), which couples detailed component models (electrolysers, fuel cells, hydrogen storage, batteries and auxiliaries) with multi-carrier mass and energy balances and rule-based controllers. Applied to industrial cogeneration and to grid-connected, PV-based PtH plants serving constant hydrogen demand across Italian bidding zones, MESS highlights how plant design and operation react to changes in the PV-to-electrolyser ratio, component degradation and green-hydrogen certification rules. The rule-based approach is transparent and flexible but offers no guarantee of optimality and requires extensive parameter tuning. These limitations motivate a shift towards optimisation-based methods.

A deterministic MILP formulation is first introduced for joint design and operation of PtH plants, with particular emphasis on hydrogen storage technology selection. By enforcing techno-economic constraints over a representative year, it provides cost-optimal designs under perfect foresight and enables a consistent comparison of compressed-gas, underground and metal-hydride storage. This reveals that different technologies can deliver similar levelised cost of hydrogen (LCOH), with the preferred option that could be driven more by geology, footprint and mass requirements. At the same time, the deterministic formulation exposes its own weakness: by assuming known future conditions, it cannot capture the cost of hedging against variability in renewable availability and electricity prices.

To address this, the thesis advances to a two-stage stochastic MILP applied to the joint sizing and operation of an off-grid hybrid renewable energy system for the island of Pantelleria in Italy. Here, investment decisions are taken before uncertainty is revealed, while hourly operation is optimised in the second stage under multiple renewable energy production scenarios. Results show that, at zero emissions, the deterministic design costs 8.10 M€/yr while the two-stage stochastic design increases the mean to 9.37 M€/yr (+15.7%). Comparing two-stage solutions with perfect-foresight designs quantifies the cost of robustness, defined as the scenario-weighted increase in costs of the two-stage solution relative to the deterministic perfect-foresight solution under the same CO₂ cap, and shows how deterministic sizing can underestimate both total cost and emissions when variability is ignored. At this point, the focus is still primarily on design: uncertainty is treated to make better sizing choices and

reduce LCOH at the planning stage, but operational decisions remain aggregated into a single recourse block.

In practice, however, once a PtH plant has been built, the main lever left to reduce effective hydrogen cost and improve economic performance lies in its day-to-day interaction with electricity markets. The methodological path therefore culminates in a multi-stage stochastic MILP for market-coupled scheduling of a grid-connected PtH plant, already in place, serving a hydrogen refuelling station. Scenario trees for electricity prices and renewable generation represent day-ahead, intraday and reserve markets with non-anticipativity constraints and detailed device dynamics. This formulation captures how information is gradually revealed and optimises bidding and dispatch decisions so as to maximise operating profit and implicitly lower ex-post LCOH. The case studies show that co-optimised bidding and recourse operation can increase expected operating profit while reducing downside risk compared with strategies that treat prices as deterministic or ignore reserve-market participation, and provide a consistent way to value flexibility from batteries, fuel cells and hydrogen storage once the plant configuration is fixed. In the Barcelona case study, the electrolyser delivers the contracted 1440 kgH₂/day at an average load factor of about 42% while the fuel cell remains mainly in standby to monetise reserve capacity.

An appendix finally sketches how agrivoltaic layouts can be introduced as an alternative PV siting option in land-constrained PtH projects by modifying land-use and cost parameters without altering the core optimisation structure. In the Tuscany case study, agrivoltaics yields a positive net present value of 781 k€ per hectare and an internal rate of return of 13% (vs. 1330 k€ and 21% for ground-mounted PV), while preserving crop revenues.

Overall, the thesis offers a chronologically developed and internally consistent framework for moving from rule-based simulation to market-aware stochastic optimisation of green-hydrogen-enabled multi-energy systems, clarifying when each modelling layer is appropriate and how neglecting uncertainty or market coupling can materially affect both plant sizing decisions and operating economics.

Keywords: green hydrogen, power-to-hydrogen, multi-energy systems, stochastic optimisation, electricity markets

PROPOSITIONS

Motivation

- Decarbonising hard-to-abate sectors requires plant-scale models of green-hydrogen systems that connect detailed technology behaviour with economically meaningful indicators such as the levelised cost of hydrogen and emissions.
- To support real decisions on power-to-hydrogen plants, it is not sufficient to use either simple rule-based models or purely deterministic optimisation; a consistent methodological path, from detailed simulation to stochastic optimisation, is needed to treat design and operation under uncertainty and market exposure in a unified way.

Original contribution

- The thesis extends the Multi Energy System Simulator (MESS) into a hydrogen-centred, multi-energy simulation framework with detailed component models, enabling transparent rule-based analyses of industrial cogeneration and grid-connected power-to-hydrogen plants under green-hydrogen certification rules.
- A deterministic mixed-integer linear programming (MILP) model is developed for the joint design and operation of power-to-hydrogen plants, providing a consistent benchmark to compare hydrogen storage technologies.
- A two-stage stochastic MILP framework is introduced for the sizing and operation of an off-grid hybrid renewable–hydrogen system, quantifying the cost of robustness and demonstrating how deterministic designs can misrepresent total cost and emissions when uncertainty in renewable generation is ignored.
- A multi-stage stochastic MILP model is formulated for the market-coupled operation of a grid-connected power-to-hydrogen plant serving a hydrogen refuelling station, showing how sequential participation in day-ahead, intraday and reserve markets can increase expected profit, reduce downside risk and reveal the economic value of operational flexibility once the plant is built.

Open questions

- How can high-fidelity physical and degradation models of hydrogen technologies be embedded into large-scale optimisation frameworks without losing tractability, for example through systematic piecewise-linearisation or hybrid simulation–optimisation schemes?

- How can data-driven and machine-learning-based forecasting be combined with scenario generation to construct scenario trees that better capture temporal correlations, regime changes and rare but impactful events for prices and renewable production?
- How should power-to-hydrogen plants be co-designed with electricity networks, accounting for congestion, locational pricing and grid reinforcement needs, rather than treating the grid connection as a single unconstrained node?
- Which combinations of market products, tariff structures and risk-aware objective functions are most suitable to characterise the long-term profitability and effective hydrogen cost of power-to-hydrogen projects under evolving policy and market conditions?

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SYNOPSIS

The transition towards a low-carbon energy system requires deep emissions reductions in hard-to-abate sectors such as chemicals, steel, cement and paper. In this context, green hydrogen produced from renewable electricity is increasingly considered as an enabling energy carrier, particularly where direct electrification is not immediately feasible. Power-to-hydrogen (PtH) plants, however, are capital-intensive assets that must be designed and operated under multiple sources of uncertainty: fluctuating renewable generation, variable hydrogen demand, evolving regulatory frameworks for green-hydrogen certification, and volatile electricity markets. This thesis addresses these challenges by developing a coherent methodological path for modelling PtH plants embedded in multi-energy systems, starting from rule-based simulation and progressing to deterministic, two-stage and multi-stage stochastic mixed-integer linear programming (MILP). Along this path, the focus moves from design-level decisions that shape the levelised cost of hydrogen (LCOH) at planning stage to operational decisions that exploit market opportunities once a plant is built.

Scope and objectives. The overarching goal of the thesis is to build and apply a toolbox that can (i) represent PtH plants and their coupling with other energy carriers at component level; (ii) support the techno-economic design of such plants under realistic technical and policy constraints; and (iii) optimise their operation under uncertainty and electricity-market exposure. Rather than advocating a single “best” model, the work investigates the strengths and weaknesses of different modelling layers and clarifies when each is appropriate. This is done through a sequence of case studies that cover industrial cogeneration, grid-connected PtH plants supplying steady hydrogen demand, off-grid hybrid renewable-hydrogen systems, and a grid-connected plant serving a hydrogen refuelling station with access to day-ahead, intraday and reserve markets.

Rule-based simulation with MESS. The thesis begins with the development and use of the Multi Energy System Simulator (MESS), a rule-based simulation framework for multi-energy systems. MESS couples detailed component models for electrolyzers, fuel cells, compressors, hydrogen storage, batteries and conventional units with multi-carrier mass and energy balances. Control strategies are implemented through priority rules that emulate industrial control philosophies. This layer is used to study two main configurations. First, a solid oxide fuel cell (SOFC) cogeneration system for a paper mill is analysed, in which natural gas is progressively replaced by hydrogen. Simulations quantify how this substitution affects fuel consumption, emissions and approximate LCOH, demonstrating that hydrogen-fed SOFCs can deliver significant CO₂ reductions while maintaining high electrical self-sufficiency. Second, MESS is extended and coupled with a genetic algorithm to size grid-connected, PV-based PtH plants supplying a constant industrial hydrogen demand across Italian bidding zones. Here the simulator is used to explore how PV-to-electrolyser ratios, component degradation and different temporal-correlation rules between renewable generation and hydrogen consumption influence grid dependence and the share of hydrogen that may be certified as green.

These rule-based studies are transparent and flexible: they allow rapid exploration of alternative layouts, control rules and policy constraints, and provide valuable intuition on

system behaviour. However, they also reveal the intrinsic limitations of rule-based approaches: there is no guarantee that the resulting designs or schedules are cost-optimal, the value of flexibility options (such as storage or modulating converters) is difficult to quantify, and the impact of alternative future conditions can only be explored through ad hoc parametric runs. These weaknesses motivate the transition to optimisation-based formulations.

Deterministic optimisation for joint design and operation. The next methodological step replaces rule-based control with a deterministic MILP formulation for joint design and operation of PtH plants. In this framework, decision variables represent plant capacities, hourly operating points and storage trajectories over a representative year, and constraints enforce techno-economic feasibility, hydrogen-delivery requirements and simplified green-hydrogen rules. The focus is placed on hydrogen storage technology choice: compressed-gas tanks, underground hydrogen storage and metal-hydride options are embedded into a common plant model and compared under consistent operating assumptions.

This deterministic model provides cost-optimal designs under perfect foresight and clarifies the drivers of LCOH differences between storage technologies. Results indicate that, once capital cost, operating profiles and coupled constraints are taken into account, multiple storage options can yield similar LCOH. In such cases, practical aspects such as geology, footprint and mass constraints could be the most limiting ones. The deterministic MILP thus offers a principled benchmark for design and a richer insight into trade-offs than rule-based simulation alone. At the same time, it assumes full knowledge of future loads and renewable generation, which is unrealistic for assets with long lifetimes and high exposure to variability, and can therefore produce designs and LCOH estimates that are overly optimistic.

Two-stage stochastic optimisation for design under uncertainty. To address design under uncertainty, the thesis then develops a two-stage stochastic MILP formulation. Here, first-stage variables represent capacity decisions (e.g. PV, wind, batteries, hydrogen storage, diesel backup), while second-stage recourse variables represent hourly operation under multiple scenarios. This framework is applied to an off-grid hybrid renewable-hydrogen system for the island of Pantelleria, where the objective is to minimise total annualised cost and emissions subject to reliability requirements and different CO₂ budgets.

By comparing two-stage designs with deterministic ones, the model explicitly quantifies the cost of robustness. It shows that, when variability in renewable availability and load is significant, deterministic designs tend to mis-size storage and backup capacity, leading to underestimation of both total cost and emissions, especially when tight emission caps are imposed. The two-stage formulation thus improves sizing decisions and yields more realistic LCOH estimates by internalising the cost of unfavourable operating conditions. Methodologically, this step retains the linear structure and interpretability of the deterministic MILP but introduces a clear separation between decisions that must be taken before uncertainty is realised and those that can adapt ex post. However, operational recourse is still represented as a single block, and the model does not explicitly address the temporal structure of electricity markets.

Multi-stage stochastic optimisation for market-coupled operation. In practice, once a PtH plant has been built, the main leverage left to reduce effective hydrogen cost and improve economic performance lies in operational decisions, in particular in how the plant interacts with electricity markets on a daily basis. This motivates the final methodological step: a multi-stage stochastic MILP for market-coupled scheduling of a grid-connected PtH plant serving a hydrogen refuelling station. In this setting, plant capacities and technical constraints are assumed known and fixed, and the optimisation problem focuses on operating schedules and market bids.

Scenario trees are used to represent the joint evolution of electricity prices and renewable generation across day-ahead, intraday and reserve markets. Non-anticipativity constraints ensure that decisions at each stage depend only on information that is actually available at that time, while state variables track the dynamics of batteries, hydrogen storage, electrolyser loading and, where relevant, fuel cells. The model captures both energy and reserve products and allows different flexibility portfolios to be compared on a consistent basis.

Case studies reveal that co-optimised bidding and recourse scheduling can increase expected operating profit and, crucially, reduce downside risk compared with strategies that treat prices as deterministic or ignore reserve-market participation. They also highlight how the presence of flexible assets reshapes operating strategies: for example, batteries and fuel cells can be used to hedge against price volatility and to capture reserve revenues, thereby indirectly lowering the ex post cost of hydrogen for a given plant configuration. This multi-stage model therefore complements the design-oriented deterministic and two-stage formulations by focusing on operational value creation for an existing plant.

Overall contributions. Taken together, the modelling layers developed in this thesis form a coherent toolbox for analysing green-hydrogen-enabled multi-energy systems. Rule-based simulation with MESS supports exploratory studies and stakeholder communication, deterministic and two-stage MILP formulations provide structured support for plant sizing and LCOH assessment under alternative uncertainty assumptions, and the multi-stage MILP offers a detailed view of how market-aware operation can exploit the flexibility of an already-built plant. Across the case studies, the work shows that (i) different hydrogen storage technologies can be nearly interchangeable at plant level once optimally sized and operated, with non-technical aspects often driving the final choice; (ii) ignoring uncertainty in design can lead to mis-sized assets and underestimation of costs and emissions; and (iii) explicit modelling of electricity markets and sequential decision-making reveals additional operational value streams and shapes both profitability and risk exposure.

An appendix finally sketches how agrivoltaic layouts can be introduced as an alternative PV siting option in land-constrained PtH projects by modifying land-use and cost parameters while preserving the core optimisation structure. Overall, the thesis contributes a chronologically developed and internally consistent framework that helps clarify when each modelling layer is appropriate and how neglecting uncertainty or market coupling can materially affect both the sizing of PtH plants and their operating economics once deployed.

NOMENCLATURE

Acronyms

AEL	Alkaline Water Electrolyser
AEMEL	Anion-Exchange Membrane Electrolyser
AF	Abandoned Farmland
aFRR	automatic Frequency Restoration Reserve
AV	Agrivoltaic
BESS	Battery Energy Storage System
BF-BOF	Blast Furnace-Basic Oxygen Furnace
BOP	Balance of Plant
CcH ₂	Cryo-compressed Hydrogen
CCUS	Carbon Capture, Utilisation and Storage
CF	Conventional Farming
CGH ₂	Compressed Gaseous Hydrogen
CHP	Combined Heat and Power
CO ₂	Carbon dioxide
COMP	Compressor
CRF	Capital Recovery Factor
CVaR	Conditional Value-at-Risk
DA	Day-Ahead
DC	Direct Current
DG	Diesel Generator
DRI	Direct Reduced Iron
EAF	Electric Arc Furnace
EH	Electric Heater
EL	Electrolyser

EOL	End of Life
EU	European Union
FC	Fuel Cell
FCS	Full-light Cropping System
GHG	Greenhouse Gas
GMPV	Ground-Mounted Photovoltaic
GT	Gas Turbine
H ₂	Hydrogen
H ₂ O	Water
HRES	Hybrid Renewable Energy System
HRS	Hydrogen Refuelling Station
HRSG	Heat Recovery Steam Generator
HS	Hydrogen Storage
HTA	Hard-to-Abate
IB	Imbalances
IEA	International Energy Agency
IES	Integrated Energy System
IM	Intraday Market
IPOPT	Interior Point OPTimizer
IRR	Internal Rate of Return
ISO	International Organization for Standardization
KPI	Key Performance Indicator
LH ₂	Liquid Hydrogen
LOHC	Liquid Organic Hydrogen Carrier
LP	Linear Programming
MESS	Multi Energy System Simulator
MH	Metal Hydride
MILP	Mixed Integer Linear Programming
MINLP	Mixed-Integer Nonlinear Programming
NFPA	National Fire Protection Association

NG	Natural Gas
NLP	Nonlinear Programming
NPC	Net Present Cost
NPV	Net Present Value
NREL	National Renewable Energy Laboratory
O ₂	Oxygen
OMIE	Operador del Mercado Ibérico de Energía (Iberian Electricity Market Operator)
PBT	Payback Time
PCM	Phase Change Material
PEMEL	Proton-Exchange Membrane Electrolyser
PEMFC	Proton-Exchange-Membrane Fuel Cell
PPA	Power Purchase Agreement
PtG	Power-to-Gas
PtH	Power-to-Hydrogen
PtHtP	Power-to-Hydrogen-to-Power
PtX	Power-to-X
PV	Photovoltaic
PVGIS	Photovoltaic Geographical Information System
PyPSA	Python for Power System Analysis
RED III	Renewable Energy Directive (recast)
RES	Renewable Energy Sources
RFNBO	Renewable Fuels of Non-Biological Origin
RM	Reserve Market
RT	Real-Time
RUE	Radiation Use Efficiency
SAA	Sample Average Approximation
SDDP	Stochastic Dual Dynamic Programming
SG	Steam Generator
SMR	Steam Methane Reformer

SOEC	Solid Oxide Electrolyser Cell
SOFC	Solid-Oxide Fuel Cell
SOS2	Special Ordered Set of type 2
SQP	Sequential Quadratic Programming
TAC	Total Annualised Cost
TES	Thermal Energy Storage
TMY	Typical Meteorological Year
TRL	Technology Readiness Level
TSFA	Time Series Factor Analysis
UHS	Underground Hydrogen Storage
VAR	Vector Autoregressive model
VPP	Virtual Power Plant
VRE	Variable Renewable Energy
WT	Wind Turbine

Greek symbols

α	Generic solar/incidence angle	[rad]
β	Array tilt angle	[rad]
χ	BESS calendar-ageing coefficient	[-]
δ	Binary variable	[-]
η	Efficiency	[-]
γ	Specific-heat ratio	[-]
ϕ	Weighting / mode-selection parameter	[-]
π	Scenario probability	[-]
σ	Discrete operating mode	[-]
θ	Rule parameters for the rule-based policy.	[-]
ξ	Exogenous inputs	[-]

Latin symbols

ΔG°	Standard-state Gibbs free energy change	[kJ/mol]
ΔH°	Standard-state reaction enthalpy change	[kJ/mol]

ΔS°	Standard-state reaction entropy change	[kJ/(mol K)]
ΔT	Temperature difference	[K]
Δt	Time-step length	[h]
$\dot{m}$	Mass flow rate	[kg/h]
$\dot{n}$	Molar flow rate	[mol/h]
$\dot{V}$	Volumetric flow rate	[m ³ /h]
ℓ	Characteristic thickness	[m]
κ_m	Membrane ionic conductivity	[S/m]
Λ	Air excess ratio	[-]
λ	Membrane hydration number	[-]
$\mathbb{EP}$	Expected profit over the multi-stage daily horizon	[€]
$\mathcal{A}$	Set of assets/technologies	[-]
$\mathcal{C}(n)$	Children of node n in the scenario tree.	[-]
$\mathcal{C}$	C-rate of the BESS	[h ⁻¹]
$\mathcal{D}$	Battery ageing damage increment	[-]
$\mathcal{F}(s)$	Genetic-algorithm (GA) fitness value	[€/kg]
$\mathcal{G}$	Ground-level irradiance field used in agrivoltaic shading	[W/m ²]
$\mathcal{H}(\cdot)$	Per-period inequality constraints	[-]
$\mathcal{I}$	Index set used for intraday interval partitioning	[-]
$\mathcal{I}_t$	Set of intraday sessions still covering delivery hour t	[-]
$\mathcal{L}(\cdot)$	Per-period operating-cost function	[€]
$\mathcal{N}_k$	Set of nodes at stage k in the multi-stage scenario tree	[-]
$\mathcal{P}$	Absolute pressure	[bar]
$\mathcal{R}$	Thermal resistance	[K/W]
$\mathcal{S}$	Set of ground pixels in the agrivoltaic layout	[-]
$\mathcal{T}$	Set of time steps over the planning horizon	[-]
$\mathcal{T}(n)$	Time indices aggregated at scenario-tree node n	[-]
$\mathcal{T}_i$	Set of delivery hours tradable in intraday session i	[-]
$\mathcal{T}_y$	Set of time steps belonging to calendar year y	[-]
$\mathcal{U}$	Admissible control/decision domain	[-]

$\mathcal{X}$	Feasible state/decision space for x_t	[-]
$\mathcal{Y}_k$	Admissible decision domain at stage k	[-]
$\mathcal{Z}$	Admissible design domain for s .	[-]
ARID	Agricultural Reference Index for Drought	[-]
ASR	Area-specific resistance	$[\Omega \text{ m}^2]$
DHI	Diffuse horizontal irradiance	$[\text{W}/\text{m}^2]$
DNI	Direct normal irradiance	$[\text{W}/\text{m}^2]$
DR	Real discount rate	[-]
ET_0	Reference evapotranspiration	$[\text{mm}/\text{day}]$
GHI	Global horizontal irradiance	$[\text{W}/\text{m}^2]$
GTI	Global tilted irradiance (plane-of-array)	$[\text{W}/\text{m}^2]$
LAOR	Land Area Occupation Ratio	[%]
LCOE	Levelised cost of electricity	$[\text{€}/\text{kWh}]$
LCOH	Levelised cost of hydrogen	$[\text{€}/\text{kg}]$
LC	Life-cycle count to end of life	[-]
LER	Land Equivalent Ratio combining crop and electricity outputs	[-]
LHV	Lower heating value	$[\text{kWh}/\text{kg}]$
LOH	Level of Hydrogen	[-]
OPEX	Operating expenditures	$[\text{€}]$
PAR	Photosynthetically Active Radiation	$[\text{W}/\text{m}^2]$
PR	PV performance ratio	[-]
REV	Revenue	$[\text{€}]$
RH	Relative humidity	[-]
SDR	Self-discharge rate of the battery	$[\text{h}^{-1}]$
SEC	Specific electric consumption	$[\text{kWh}/\text{kg}]$
SFC	Specific fuel consumption	$[\text{kg}/\text{kWh}]$
SOC	Battery state of charge	[-]
SOH	Battery state of health	[-]
TIT	Turbine inlet temperature	$[\text{K}]$
Tr	Actual daily crop transpiration	$[\text{mm}/\text{day}]$

XXX

TT	Cumulative thermal time (growing degree days)	[°C day]
Ω	Scenario set in the stochastic formulation	[-]
ω	Scenario index in the stochastic formulation	[-]
$\Phi_k(\cdot)$	Stage- k cost aggregation function	[€]
Π_k	Non-anticipativity pairing set at stage k	[-]
ρ	Density	[kg m ⁻³]
τ_P	Certification aggregation window.	[h]
ζ_n	Information revealed up to scenario-tree node n	[-]
A	Area	[m ²]
a_{alb}	Ground albedo	[-]
B	Electrolyte molality	[mol/kg]
b	Exhaust bypass fraction in HRSG duct	[-]
c	Commodity price or remuneration	[€/kWh], [€/Sm ³], [€/kg]
C_0	Upfront investment	[€]
$CAPEX$	Installed capital cost	[€]
CF_y	Operating cash flow in calendar year y	[€]
CI	Carbon intensity	[kg _{CO2eq} /kWh] or [kg _{CO2eq} /kg _{H2}]
cp	Specific heat capacity at constant pressure.	[kJ/(kg K)]
D	Diameter	[m]
d	Distance	[m]
$Diff$	Binary/multi-component diffusivity	[m ² /s]
E	Energy / capacity	[kWh]
F	Faraday constant	[C/mol]
$f(\cdot)$	State recursion / system dynamics	[-]
f_{Solar}	Fraction of daily PAR intercepted by the crop canopy	[-]
f_{Water}	Water-stress modifier in the SIMPLE model	[-]
G	Solar irradiance	[W/m ²]
$g(\cdot)$	Per-period equality constraints	[-]
h	Specific enthalpy	[kJ/kg]
I	Electric current	[A]

i	Current density	[A/m ²]
$J(s)$	Investment-cost function of the design s	[€]
k	Thermal conductivity	[W m ⁻¹ K ⁻¹]
L	Axial length	[m]
M	Molar mass	[kg/mol]
m	Mass	[kg]
N	Generic count / number / horizon length	[-]
N_T	Number of time steps in the planning horizon	[-]
P	Nameplate electrical power of a unit	[kW]
p	Instantaneous power	[kW]
q	Specific thermal energy	[kWh/kg]
r	Radius	[m]
R_{univ}	Universal gas constant	[J/(mol K)]
s	Time-invariant sizing / design decision vector	[-]
sc	Specific consumption	[Sm ³ kg ⁻¹]
T	Temperature.	[K]
u	Control vector	[-]
V	Electric voltage	[V]
v	Continuous scheduling decision vector	[-]
v_n	Decision vector associated with node n	[-]
Vol	Volume.	[m ³]
W	Width	[m]
w	Wind speed	[m/s]
x	Molar fraction	[-]
x_t	State vector	[-]
Y	crop yield per hectare	[t/ha]
Y^*	Discounted payback year	[-]
y_t	Output vector	[-]
z	Height	[m]

Subscripts

act	Activation
air	Air
aisle	Aisle
amb	Ambient
app	Approach
bed	Bed
cal	Calendar
ca	Cathode-side quantities
cell	Cell
ch	Charge
ci	Cut-in
col	Column
conc	Concentration
cont	Container
co	Cut-out
ct	Charge-transfer
cyc	Cycle
deg	Degradation
des	Desorption
dis	Discharge
edge	Module edge
elec	Electrolyte
es	Equivalent solid / thermal mass
exh	Exhaust
ext	External
Far	Faradaic
fw	Feedwater
hub	Hub
id	Ideal
ins, i	Inner insulation layer

ins, o	Outer insulation layer
int	Internal
in	Inlet conditions
ion	Ionic property
lim	Limiting value
max	Maximum
mem	Membrane
min	Minimum
mod	Module
nom	Nominal
ohm	Ohmic
op	Operating
out	Outlet conditions
pp	Pinch-point
rat	Rated
ref	Reference
rev	Reversible
row	Row
rt	Round-trip
sb	Standby
site	Site
stack	Stack
st	Steam
sub	Subcooling offset
tank	Tank
th	Thermal
tot	Total
ves	Vessel
<i>a</i>	Asset
<i>d</i>	Day index

j	Corner index
k	Stage index
n	Scenario-tree node index
p	Pixel index
s	Stream
t	time
y	Quantity aggregated over calendar year

Superscripts

age	Ageing-related quantity
ann	Annualised quantity
avail	Available
cert	Certified
ch	Charging
cold	Cold state
cov	Covered
crop	Crop
curt	Curtailement
dem	Demand
dis	Discharging
eff	Effective property/value
el	Electricity
eng	Engineering
eq	Equivalent
exp	Exported
fix	Fixed
FL	Full-light
gen	Generated
gnd	Ground-level quantity
grey	Grey

grid	Grid
imp	Imported
inst	Installation
ins	Insurance
irr	Irrigation
loss	Loss
net	Net value
O&M	Operations and maintenance
off	Off / not committed
on	On / committed
ray	Ray
RD	Reserved downward capacity
repr	Replacement
RU	Reserved upward capacity
sav	Savings
sold	Sold/exported portion
SUN	Sunlit
th	Thermal
var	Variable
warm	Warm state

1. INTRODUCTION

The contemporary energy–environment nexus is characterised by mutually reinforcing crises—climate change, biodiversity loss, and air pollution—that stem from two centuries of fossil-fuelled industrialisation over a finite biosphere. The 2024 global mean surface temperature was 1.55 °C above the 1850–1900 pre-industrial baseline, making it the warmest year on record; monthly and 12-month averages temporarily exceeded 1.5 °C during much of 2023–2024 [1–3]. Updated remaining-budget assessments indicate that, as of 1 January 2025, a 50 % chance of limiting warming to 1.5 °C corresponds to a remaining budget of ~ 235 Gt CO₂, and ~ 1110 Gt CO₂ for 2 °C (higher-likelihood budgets are smaller) [4]. Against this backdrop, total greenhouse gas emissions reached a new high of 57.1 Gt/yr CO₂-eq in 2023, and energy-related CO₂ emissions climbed to a record 37.8 Gt in 2024, underscoring the urgency of structural change [5, 6].

Within Europe, the transition is framed by binding legislation targeting climate neutrality by mid-century and deep reductions by 2030. The 2050 Long-Term Strategy, the European Climate Law, and the European Green Deal provide the legal and policy architecture, while successive packages (Fit for 55, including the recast Renewable Energy Directive (RED III) and related market reforms) align instruments, markets, and standards to deliver the targets [7–9]. Independent assessments continue to flag policy and investment gaps compatible with a 1.5 °C pathway, highlighting needs in renewable deployment, electrification, efficiency, flexibility, grids, and credible carbon pricing [9]. At the same time, the transition must contend with real-economy frictions: legacy asset vintages, technology learning curves, supply-chain constraints for critical materials, and institutional limits in permitting and planning. Regulatory clarity on renewable and low-carbon hydrogen has advanced via RED III and the Commission’s Delegated Acts that define Renewable Fuels of Non-Biological Origin (RFNBO) conditions and life-cycle methodology, tightening certification baselines for investment [10, 11].

In this context, hydrogen is not a panacea, but it is potentially decisive where direct electrification faces thermodynamic or process constraints (e.g., high-temperature industry, chemical feedstocks, long-haul mobility), and where long-duration storage is needed to integrate Variable Renewable Energy (VRE) at scale. Its effective deployment requires evidence-based prioritisation of end-uses coupled with rigorous planning and scheduling of Power-to-Hydrogen (PtH) plants.

The remainder of this introduction is organised as follows: Section 1.1 details the energy-transition and decarbonisation drivers behind the growing interest in hydrogen. Section 1.2 discusses hydrogen’s specific role in the broader energy system and the key system-integration

levers that can facilitate its deployment. Building upon this, Section 1.3 identifies the hard-to-abate sectors where hydrogen can have the greatest impact and classifies relevant archetypes for analysis. Section 1.4 provides an overview of the entire hydrogen value chain, from production to end-use. Finally, Section 1.5 outlines the specific structure and content of the subsequent chapters of this thesis.

1.1 Energy transition and decarbonisation drivers

Within the European Union (EU) policy architecture introduced in Chapter 1—climate neutrality by mid-century under Fit for 55, RED III and RFNBO rules with strengthened carbon pricing and trade safeguards—the immediate drivers of the transition are operationalised through pricing and planning tools: the 2023 European Union Emissions Trading System (EU ETS) revision tightens the cap and broadens scope for energy-intensive activities, while the carbon border adjustment mechanism aligns the effective carbon cost of selected imports to EU benchmarks, mitigating leakage and reinforcing low-carbon investment signals [12, 13]. Security of supply and network governance complement these price signals: REPowerEU accelerates renewable deployment and diversification, the revised Trans-European Networks for Energy steers cross-border infrastructure via projects of common interest / projects of mutual interest frameworks, and hydrogen-ready corridors appear in system planning (e.g., the European Hydrogen Backbone) to link coastal import/Renewable Energy Sources (RES) hubs with inland demand centres and storage basins [14–16].

Current system status. Despite policy momentum, system aggregates still reflect a structural mitigation gap: energy-related CO₂ rose again in 2024 to a record 37.8 Gt [6]; global total primary energy supply reached 592 EJ in 2024 and remained 86 % fossil-based (oil 34 %; coal 28 %; gas 25 %), with nuclear just over 5 % [17]. Power-sector progress is rapid—about 585 GW of renewable capacity added in 2024, led by Photovoltaic (PV) and wind—yet electricity is only part of final energy: renewables supplied a little over 8 % of total energy demand in 2024 and 13.5 % of total final energy consumption in 2023, while in Europe they reached 24.5 % of gross final energy with wide Member State heterogeneity [18–20]. These aggregates are summarised in Figure 1.1, which shows total world primary energy use.

Integration and flexibility. Deepening VRE shares stress operations and networks: temporal/spatial variability, limited coincidence with demand, and grid bottlenecks manifest as frequency excursions, congestion, and curtailment [22]. A credible response relies on a portfolio of flexibility resources—short-duration storage and fast reserves (increasingly batteries), responsive demand, interconnection, and grid reinforcement—supplemented by complementary long-duration options to bridge multi-day to seasonal imbalances; authoritative pathways (such as International Energy Agency (IEA) Net Zero Emissions) are consistent with this multi-lever approach [23–25]. Delivering a 1.5 °C-consistent trajectory hinges on scaled capital formation into clean supply, grids, flexibility, and demand-side efficiency, supported by carbon pricing and de-risking instruments; independent trackers still show heterogeneity in pledges and near-term delivery, reinforcing the need to prioritise measures with the highest abatement per euro and strong co-benefits while preserving affordability and security [9, 20, 26, 27].

Italian context. In Italy, the draft updated national energy and climate plan grounds these dynamics in industrial districts and logistics corridors, highlighting renewable siting, grid constraints, and flexibility needs; wholesale price formation and gas costs condition

Primary energy consumption by source, World

Primary energy¹ is measured in terawatt-hours², using the substitution method³.

Our World
in Data

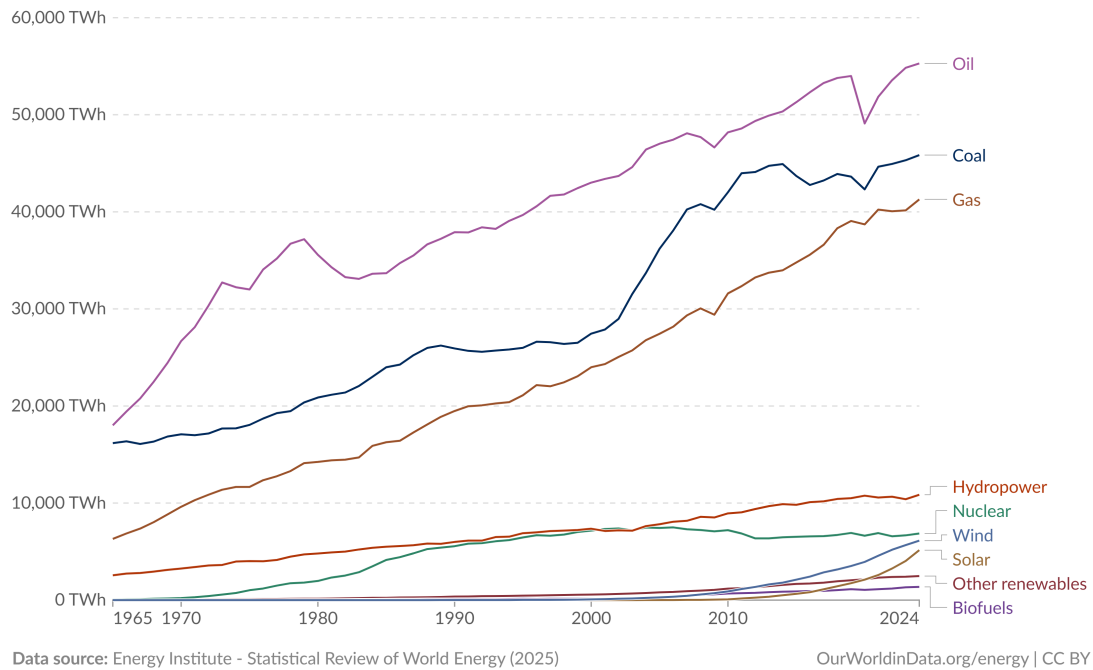


Figure 1.1: World primary energy use. Data retrieved from [21].

arbitrage and investment signals for grid-connected assets, while residual grid carbon intensity informs lifecycle appraisals of electrified configurations and end-use choices [28, 29].

1.2 Hydrogen’s role in the energy transition

Hydrogen is not a panacea, but it can be decisive where direct electrification is constrained by thermodynamics, process chemistry, or operational envelopes, and where long-duration flexibility is required to integrate high shares of VRE. A widely used framing of the relative competitiveness of hydrogen applications is Michael Liebreich’s *Hydrogen Ladder*, which ranks prospective end-uses from “unavoidable” (Category A) to “uncompetitive” (Category G) in a net-zero energy system [30]. A representative prioritisation consistent with this framing is shown in Figure 1.2.

In this thesis hydrogen’s role is structured along three levers: (i) feedstock substitution to displace unabated fossil-based H_2 in refineries and bulk chemicals and to enable Direct Reduced Iron (DRI) routes in steel with Electric Arc Furnaces (EAF); (ii) high-temperature fuel/Combined Heat and Power (CHP) carrier in process industries via hydrogen-ready gas turbines with heat-recovery or Solid Oxide Fuel Cell (SOFC)-based CHP; and (iii) flexibility resource that stores surplus renewable energy over days to seasons with reconversion to power [31–34].

Industry and refineries. Current H_2 demand is concentrated in ammonia, methanol, and hydroprocessing and remains largely supplied by unabated fossil routes; accelerating low-emission H_2 uptake here yields first-order abatement and builds scale for downstream applications. Flagship initiatives (e.g., H2 Green Steel) signal a shift to large electrolytic supply for DRI/EAF steelmaking alongside chemical pilots and CO_2 capture retrofits, though aggregate volumes still fall short of 2030 milestones and require bankable offtake and targeted

Hydrogen Ladder 5.0

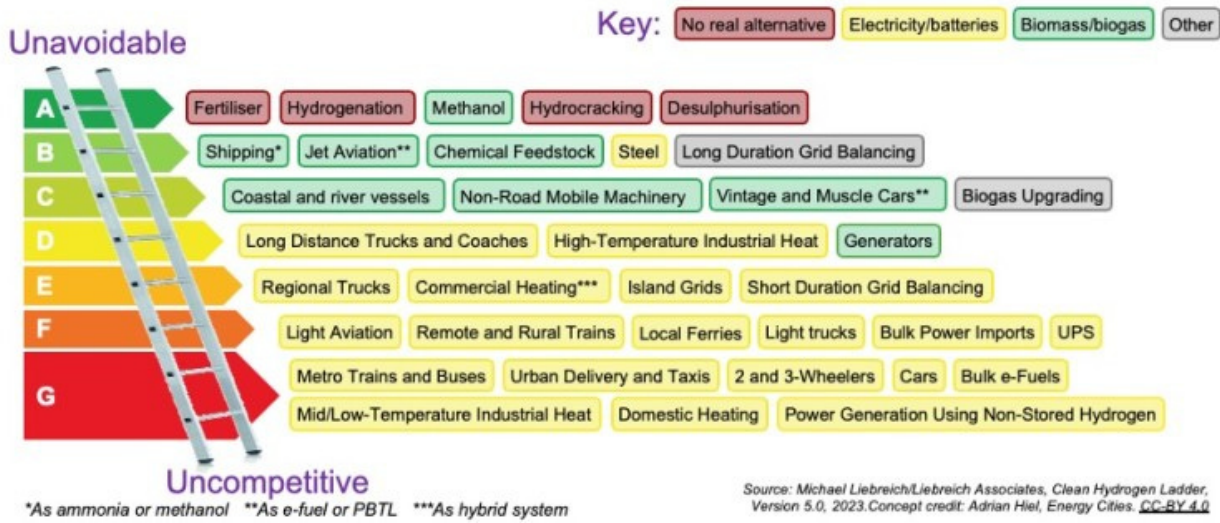


Figure 1.2: Hydrogen Ladder 5.0: prioritisation of hydrogen end-use sectors from A (“unavoidable”) to G (“uncompetitive”) in a prospective net-zero energy system. [30].

support [32, 33, 35].

Transport. While hydrogen’s aggregate transport share is modest, certain duty cycles—heavy-duty road, selected maritime segments, and non-electrified rail—benefit from high energy density and rapid refuelling. Demonstrators such as the MF Hydra ferry and the Coradia iLint train illustrate feasibility; broader scaling hinges on refuelling infrastructure, platform maturity, and total cost of ownership convergence [32, 36, 37].

Buildings. Pilots in the UK and Japan explore hydrogen boilers and residential fuel cells, yet infrastructure requirements and efficiency comparisons with heat pumps indicate a constrained near-term role under current policies [32].

Power and long-duration storage. Hydrogen and ammonia offer dispatchable options via gas turbines, internal combustion engines, and fuel cells; co-firing and dedicated firing have been demonstrated at increasing shares, with NO_x managed through dry-low- NO_x combustion and selective catalytic reduction. For seasonal adequacy, hydrogen stored in pressurised tanks or subsurface (e.g., salt caverns or suitable porous formations) and reconverted in high-efficiency fuel cells (stack electrical efficiency $> 60\%$) can hedge prolonged low-VRE periods alongside compressed air energy storage, pumped hydro, and advanced batteries across timescales [23, 32, 34].

Storage pathways and siting. Compressed gas favours modularity and dispersed siting; underground options unlock very large capacities where geology permits; selected metal hydrides offer compactness with thermal-management needs. Comparative syntheses of volumetric density, siting, safety, and cost inform technology selection by duty and scale are reflected in the modelling choices later in the thesis [38–40].

Regulatory certification. Delegated acts under the Renewable Energy Directive specify additionality and temporal/geographical correlation for electricity used in RFNBO and set life-cycle Greenhouse Gas (GHG) methodologies and thresholds. Because these definitions delimit admissible operating envelopes and contracting space (e.g., hourly matching windows, regional correlation, certificate accounting), they are encoded in the thesis as hard constraints rather than ex-post checks, ensuring policy-coherent sizing and scheduling [10, 11].

Modelling implications. The thesis prioritises feedstock replacement and industrial decarbonisation where hydrogen is indispensable and models hydrogen production, storage and reconversion as complements to battery- and network-based flexibility within uncertainty-aware optimisation that reflects technical envelopes, market participation rules, and certification [32, 33].

1.3 Hard-to-abate sectors and archetypes

Hard-to-Abate (HTA) sectors are characterised by large, continuous energy needs and process conditions—high-temperature heat, reducing atmospheres, strict product-quality constraints—that make direct electrification technically difficult, operationally risky, or cost-prohibitive at scale. Typical HTA domains include refining and bulk chemicals (ammonia, methanol), primary metals (iron and steel), cement and glass, and process industries such as pulp and paper, where heat recovery integration and high availability further limit disruptive fuel switching [41–43]. Across major economies with diverse structures (EU, USA, China), heavy industry constitutes a substantial fraction of national GHG emissions; in China, for example, heavy-industry emissions account for roughly one-third of the national total, while in the EU and USA they remain material even as power-sector decarbonisation advances [44–46]. Decarbonising these sectors therefore requires a portfolio of levers: demand- and material-efficiency (including circularity and quality-preserving substitution), process innovation, fuel switching to low-carbon electricity and clean molecules, and Carbon Capture, Utilisation and Storage (CCUS), sequenced under credible policy and infrastructure plans [41].

Hydrogen’s role in HTA. Even where electrical technologies exist, many HTA processes require $> 1000^{\circ}\text{C}$ heat or controlled reducing environments, and their plant-wide energy integration (e.g., cascade use of by-product heat, CHP) is optimised for continuous operation. Redesigning such systems around electricity-only solutions may forgo valuable waste-heat streams, impose significant grid reinforcement, and challenge product quality and availability. Hydrogen provides three complementary functions: (i) a molecular feedstock (ammonia, methanol, refinery hydroprocessing), (ii) a reducing agent (ironmaking), and (iii) a high-temperature fuel for kilns and furnaces; additionally, as an intermediate energy carrier it couples VRE to continuous industrial loads via conversion, compression, and storage [31–34]. Hydrogen is not a universal solution; rather, it complements electrification and CCUS where it yields higher abatement per euro, preserves product specifications and availability, and minimises system-level costs and risks [41, 46, 47].

Present hydrogen use and future pathways. Today, most hydrogen is consumed in oil refining and ammonia synthesis. In Europe, annual hydrogen demand is on the order of ~ 8.65 Mt, with Germany and the Netherlands among the largest users; refineries, ammonia, and methanol dominate the sectoral split, highlighting a near-term feedstock-substitution opportunity that is technologically mature and policy-relevant [48]. Medium-term growth in iron and steel is expected as hydrogen-based direct reduction (H_2 –DRI) with EAF melting scales from pilots and first-of-a-kind projects [49].

Globally, hydrogen demand reached just over 97 Mt in 2023 and remains overwhelmingly concentrated in established uses: refining, ammonia and methanol together account for the vast majority of demand, with fossil-based DRI and other industrial uses making up most of the remainder, while new “energy-transition” applications still contribute well below 1 % [50]. On the supply side, production is almost entirely derived from unabated fossil fuels: roughly two-thirds from natural gas, about one-fifth from coal gasification, and more than 15 % as by-product hydrogen in refineries and petrochemicals, with low-emissions routes (fossil with

CCUS and electrolysis) still below 1 Mt and under 1 % of global output [50]. Global hydrogen production by technology is summarised in Figure 1.3.

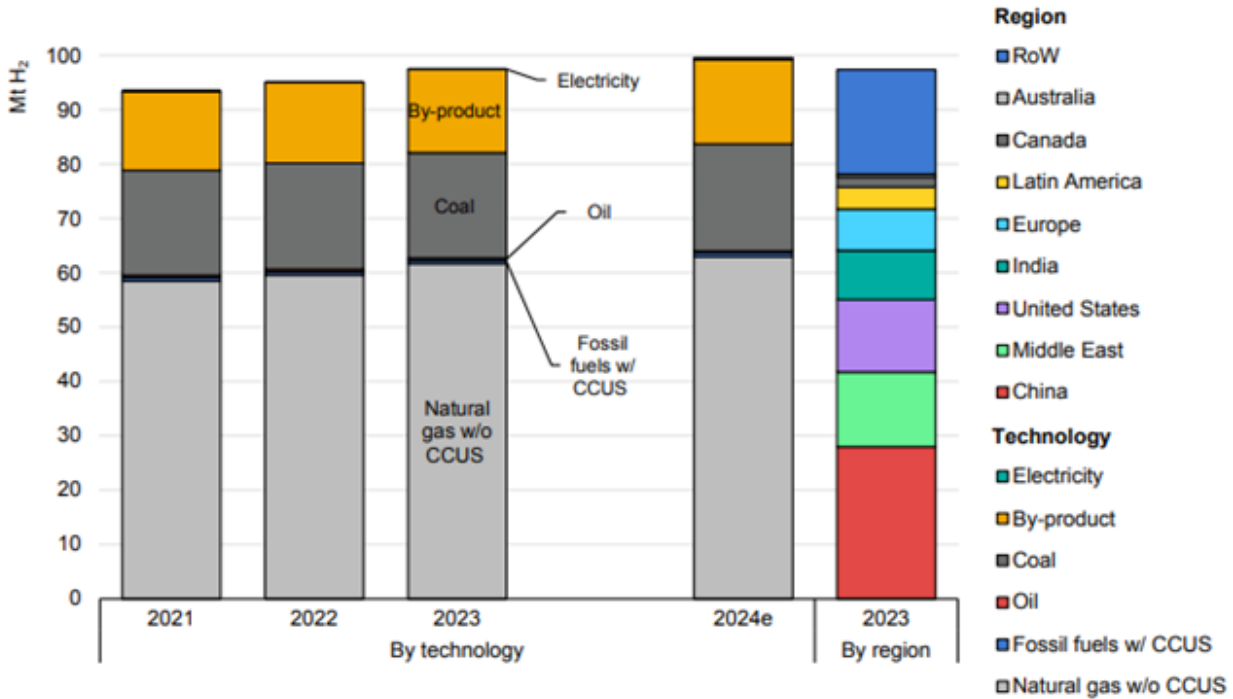


Figure 1.3: Global hydrogen production by technology. Data derived from the Global Hydrogen Review 2024 [50].

Archetypes used in this thesis. To capture the diversity of HTA use-cases while keeping the modelling tractable, three archetypes are defined and used throughout:

- **Steady industrial H₂ (base-load off-taker)**—continuous or slowly varying hydrogen draw typical of refineries, ammonia/methanol plants, and H₂–DRI steelmaking. The emphasis is on high electrolyser utilisation, continuity-oriented storage, and integration with site utilities [49, 51, 52].
- **Hydrogen Refuelling Station (HRS; variable H₂ demand)**—time-of-day-peaked service load driven by fleet logistics, requiring staged compression and cascade-bank management; electrolyser/compressor dispatch can couple to wholesale electricity prices to reduce operating costs [53].
- **Coupled electric–thermal demand**—simultaneous electricity and process-steam demand over long operating windows, favouring tightly integrated CHP (Gas Turbine (GT)–Heat Recovery Steam Generator (HRSG) or SOFC–CHP) layouts [34, 43].

The combination of these archetypes spans much of the techno-economic design space encountered in HTA sectors and supports generalisable insights on sizing, scheduling, and system value. For illustration, Figure 1.4 compares representative daily hydrogen demand profiles for the steady industrial off-taker and the HRS archetypes, normalised to a common peak and with equal daily hydrogen consumption.

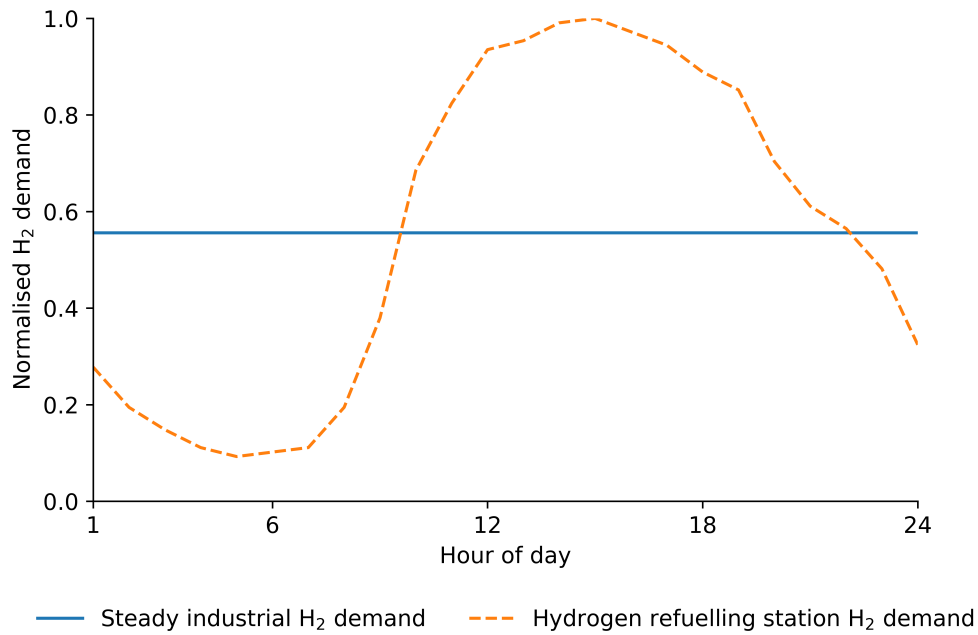


Figure 1.4: Representative daily hydrogen demand profiles: Steady industrial H₂ demand (constant load) and Hydrogen refuelling station H₂ demand (time-of-day-peaked). Both profiles are normalised by the maximum hourly demand of the refuelling-station profile, so that the areas under the curves correspond to the same daily hydrogen consumption.

1.3.1 Steady industrial hydrogen demand

This archetype captures continuous or slowly varying hydrogen demand typical of large process sites: refineries (hydrotreating, hydrocracking), bulk chemicals (ammonia via Haber–Bosch, methanol), and ironmaking via hydrogen direct reduction with Electric Arc Furnace (EAF) finishing (H₂–DRI–EAF). In refineries and chemicals, hydrogen is an essential feedstock whose shortfall immediately constrains throughput; in H₂–DRI, hydrogen is the primary reductant for iron ore in the shaft furnace, replacing syngas/natural gas (NG) [31, 49, 51]. The incumbent Blast Furnace–Basic Oxygen Furnace (BF–BOF) steel route exhibits high emissions (approximately 1.8 tCO₂/t_{crude steel}), while NG–DRI–EAF can roughly halve that to approximately 0.9 tCO₂/t_{crude steel}; deep decarbonisation requires switching to H₂–DRI–EAF and/or targeted CCUS on residuals [49]. Representative hydrogen intensities on the order of ~50 kg_{H₂}/t_{steel} are commonly adopted for H₂–DRI [52]. Refinery and chemical complexes typically draw multi-MW to multi-tens-of-MW hydrogen equivalents, operating 24/7 [31, 51].

Assurance of continuity. Because the off-take is steady, the preferred operating stance is high annual utilisation of the hydrogen supply to lower unit costs. In practice, sites consider three generic options whose detailed engineering is treated later in the thesis: (i) co-locating electrolyzers with the plant (sized against baseload with modest headroom), (ii) grid-coupled electrolysis backed by long-term power sourcing (e.g., Power Purchase Agreements (PPAs)), and/or (iii) delivered hydrogen from external producers. The mix chosen is context-specific (power prices, space, permitting, grid access) but, for base-load users, designs emphasise reliability and predictable scheduling rather than frequent cycling [31]. Additionally, some onsite buffer is typically provided even when supply is steady. At concept level this may be above-ground compressed storage or, where conditions allow, subsurface options; the purpose is continuity across short outages and maintenance rather than daily arbitrage [38–40].

System and market interfaces. When hydrogen is produced from electricity, site

economics hinge on electricity price formation and achievable utilisation. Even for base-load users, limited operational flexibility can help align with grid constraints or contractual conditions, but the economic optimum generally remains at high capacity factor. Under EU certification for RFNBO, additionality and temporal/geographical correlation rules bound admissible operating windows for renewable hydrogen claims; these guardrails are encoded as constraints in the modelling framework used later in the thesis [10, 11].

Early European initiatives illustrate the transition from pilots to first-of-a-kind plants: HYBRIT (Sweden) produced fossil-free sponge iron using hydrogen in 2021; ArcelorMittal (Hamburg) is advancing hydrogen-based DRI; additional programmes by Tata Steel, Baowu, Thyssenkrupp, and Voestalpine are tracked in public databases (e.g., the Green Steel Tracker) and inform the scaling trajectory for steady industrial offtakers [54–56].

1.3.2 Variable hydrogen refuelling station demand

HRS serving depot-based or corridor fleets (buses, trucks, light-duty vehicles) exhibit pronounced intra-day peaks tied to departures, returns, and logistics windows, with comparatively modest day-to-day variability once operations stabilise. The boundary draw seen by onsite production and storage is therefore a bursty service load driven by fast-fill events and minimum-wait constraints, rather than a smooth process demand [53]. This temporal asymmetry motivates designs that decouple hydrogen production from dispensing through intermediate compression and buffered storage. Usually two configurations are considered: (i) onsite production that feeds compression, and intermediate storage before dispensing, and (ii) delivered hydrogen (gaseous or liquid) that is conditioned onsite through comparable buffer and dispensing stages. Onsite routes reduce road deliveries and can couple to local renewables; delivered routes externalise production but add logistics and interface scheduling [53]. In both cases, staged compression and cascaded storage are used to meet short service windows reliably.

Scheduling and market coupling. Because demand is peaked while production assets favour steady, high utilisation, HRS operation co-optimises: (i) production timing (e.g., shifting into lower-price hours where feasible), (ii) compressor duty, and (iii) inventory trajectories in intermediate storage to guarantee service levels (queueing limits, first-fill times). Under EU renewable-fuel certification for road transport, Delegated Acts enforce additionality and hourly temporal/geographical correlation for electricity used to produce certified RFNBO hydrogen; these rules bound admissible operating windows and, in turn, the required production and buffer capacities for a given service profile [10, 11]. Compared with large industrial offtakers that require multiple tonnes per day, typical HRS throughputs are lower and more variable; as a result, the specific cost of hydrogen is more sensitive to fixed capital recovery on production, compression, and storage equipment. Co-optimising production hours (subject to certification windows), compressor duty, and buffer trajectories to concentrate operation in lower-price periods and to reduce idle time improves capacity factors and lowers unit cost; analogous utilisation gains are relevant for stations supplied by delivered hydrogen, where compression/dispensing assets still exhibit high fixed-cost intensity [53, 57].

1.3.3 Coupled electric–thermal demand

Some industries, such as pulp and paper mills, exhibit sustained, simultaneous demands for electricity and process steam (typically saturated in the medium-pressure range), making them prototypical CHP users with high annual operating hours and availability requirements

[43, 58, 59]. The site power-to-heat ratio depends on product mix and machine configuration, while heat-integration practices (e.g., multi-effect evaporation, cascade use of exhaust/waste heat) shape the feasible electricity–steam trade-off [43, 60]. Conventional CHP layouts rely on gas turbines with heat recovery, steam turbines, and, at larger sites, combined-cycle CHP [43, 61]. When sized to the mill’s steam curve and integrated with process heat recovery, CHP consistently outperforms separate generation on energy utilisation and life-cycle cost; upgrades typically target better heat recovery and process-side efficiency measures [60, 62–64].

Low-carbon pathways and hydrogen options. Decarbonisation strategies span fuel switching (biomass/biogas integration in suitable mills), targeted electrification where thermodynamically feasible, enhanced waste-heat valorisation, and—where applicable—carbon capture on concentrated flue points [59, 65, 66]. Hydrogen provides complementary routes that preserve the CHP logic: (i) adapting existing prime movers toward hydrogen-ready operation in the gas-turbine/heat-recovery pathway, with appropriate attention to combustion characteristics and emissions control; and (ii) deploying fuel-cell-based CHP (e.g., SOFC) that couples high electrical efficiency with useful heat for site services [34]. Where hydrogen is produced on site, an electrolyser and modest hydrogen storage can be scheduled against electricity prices and plant downtime; where hydrogen is delivered, planning focuses on secure offtake and on the interaction with the mill’s steam and power profiles.

Integration and operation. Within gas-turbine-based CHP, the HRSG is the integrating hinge between prime-mover exhaust and the site’s steam headers: HRSG configuration and approach/pinch choices determine achievable steam levels, stack temperature limits, and the electricity–steam trade-off that must match the mill’s composite steam curve [43, 67]. Operationally, mills may adopt a thermal-follow strategy (prime mover schedules to track steam demand; electricity imported/exported as needed) or an electric-follow strategy (prime mover optimised to power prices/constraints; steam balance completed via auxiliary boilers or Thermal Energy Storage (TES)). The former typically benefits from steam accumulators or hot-water TES to buffer short transients; the latter may require limited electrical storage for drive protection/short peak shaving or secure external supply contracts. Where hydrogen is produced on site, an electrolyser and modest hydrogen storage can be timed to electricity prices and maintenance windows; where hydrogen is delivered, planning focuses on firm offtake and interaction with the site’s steam/power profiles. Key KPIs include overall fuel utilisation, specific electricity/steam per tonne of product, and delivered cost metrics that reflect fuel/carbon prices and asset utilisation.

1.4 The hydrogen value chain

This section introduces the hydrogen value chain as a sequence of tightly linked functions that transform electricity and water into hydrogen delivered to a user with defined pressure, purity, and continuity requirements. For large industrial off-takers, a typical PtH supply comprises the following building blocks:

1. **Electricity provision** from on-site renewables (PV, wind) and, where permitted, limited grid import. Hybrid renewable portfolios are commonly considered to shape the production profile driving electrolyser utilisation [68–70].
2. **Short-term electrical buffering** using Battery Energy Storage System (BESS) optionally smooths minute-to-hour variability and mitigates RES ramps seen by the electrolyser; modest buffering can increase utilisation and reduce downstream storage needs when economically justified [70, 71].

3. **Hydrogen production: electrolysis** converts electricity to hydrogen. Three technologies dominate: Alkaline Electrolyser (AEL), Proton-Exchange Membrane Electrolyser (PEMEL), and Solid Oxide Electrolyser Cell (SOEC). They differ in maturity, operating temperature, dynamic response, efficiency, and water treatment needs, and are selected according to the driving electricity profile and integration opportunities (e.g., heat) [72].
4. **Hydrogen compression** brings the product to the plant’s handling pressure and purity: compression/pressurisation, gas drying and purification, and safety systems. The chosen delivery pressure depends on on-site distribution and end-use equipment [72, 73]. In the quantitative models developed in this thesis, compression is represented as an explicit electrical load (Section 3.2.2).
5. **Hydrogen storage** provides decoupling across time scales. Options include compressed-gas tanks (modular, mature), underground storage in suitable geology (bulk, low specific cost where available), and metal hydrides (high volumetric density when low-grade heat is present). Each option trades round-trip efficiency, footprint, cost, and operating temperature/pressure [40, 72].
6. **Delivery and end-use** complete the chain: on-site piping/tube trailers or short pipelines distribute hydrogen to users. End-uses include direct combustion in boilers and gas turbines (with growing co-firing/retrofit capabilities) and reconversion via fuel cells for electricity and CHP when flexibility is required [72, 73].

Because electricity supply, electrolysis, storage, and end-use are interdependent, design choices at one stage cascade to the others. For instance, the renewable mix and variability shape electrolyser sizing and operating mode; these, in turn, influence storage technology/pressure and distribution design. Integrated assessments therefore consider component interactions, local resource and space constraints, and any GHG intensity limits on grid electricity when defining “renewable hydrogen” pathways [68–70, 73]. A generic layout of such a hybrid on/off-grid PtH system is shown in Figure 1.5.

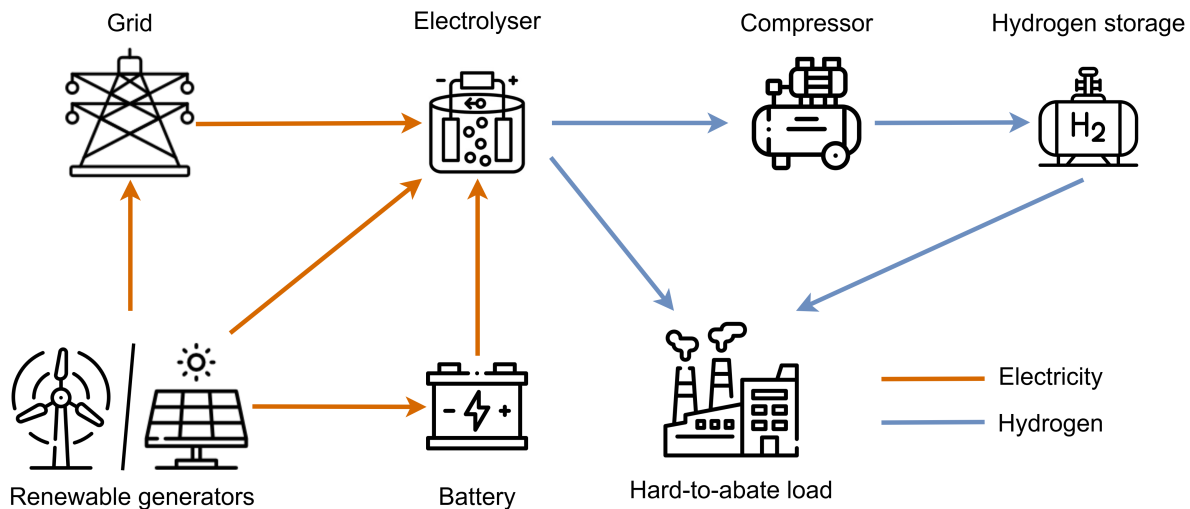


Figure 1.5: General schematic representation of a hybrid on/off-grid PtH system.

1.4.1 Renewable electricity supply

The RES block sets the energy input profile for electrolysis and thus strongly influences electrolyser capacity factor, storage requirements, and overall operating strategy. In industrial applications, PV–wind hybridisation is often adopted to exploit complementary diurnal and seasonal patterns (PV typically summer-peaked, wind frequently stronger in winter at many European/coastal sites), reducing curtailment and smoothing the input to electrolysis [68, 70]. PtH systems can operate fully off-grid (all electricity from RES and on-site buffers) or with a grid interconnection. Where policy allows, limited grid imports may be used to support continuity, subject to compliance with renewable-hydrogen GHG-intensity thresholds; conversely, strict limits drive larger on-site RES builds and greater reliance on hydrogen storage [69, 73]. Additionally, hourly variability of RES affects electrolyser ramping, start-up frequency, and partial-load operation. BESS integration can reduce fluctuations seen by the electrolyser, improving utilisation and potentially lowering required hydrogen storage mass; excessive BESS sizing generally raises system cost without commensurate benefit [70, 71]. Finally, practical design must account for land/roof availability, setback and safety distances, interconnection limits, and potential co-benefits (e.g., use of by-product oxygen, heat integration). The RES portfolio selected upstream influences downstream choices (electrolyser technology and operating set-points, storage type/pressure, delivery pressure), so RES sizing is treated consistently with the rest of the chain in techno-economic studies [68, 72].

1.4.2 Hydrogen production

Electrolysis splits water into hydrogen and oxygen in an electrochemical cell with two electrodes separated by an electrolyte. Practical plants assemble multiple cells into stacks and add Balance of Plant (BOP) (power conversion, water treatment, thermal management, gas processing) and, where required, on-stack or downstream pressurisation. Integration in PtH systems couples the electrolyser to the upstream electricity profile (RES and/or grid), targeted delivery pressure and purity, and the chosen storage/end-use pathway [72, 74, 75].

Four technology families are relevant for industrial applications, as represented in Figure 1.6.

Low-temperature units (AEL, PEMEL, Anion-Exchange Membrane electrolyser (AEMEL)) operate at 50 °C to 100 °C with aqueous or polymeric electrolytes and can be configured for differential pressure on the hydrogen side; high-temperature SOEC operates at 800 °C to 1000 °C with ceramic electrolytes conducting O^{2-} and usually delivers near-atmospheric product that is compressed downstream. Typical specific electricity use for modern PEMEL at nominal conditions is 50 kWh/kg_{H₂} to 55 kWh/kg_{H₂}, depending on load, temperature, and auxiliaries [69, 73]. Where suitable sinks exist, low-grade heat (50 °C to 80 °C) and by-product oxygen can be valorised to improve system-level performance [76, 77]. Indicative stack-level characteristics are summarised in Table 1.1.

- **AEL** uses an aqueous alkaline electrolyte (typically KOH) with nickel-based electrodes and separators. Strengths are maturity and comparatively low specific CAPEX; limitations include lower current density, slower transients, reduced efficiency at deep part-load, and gas-crossover constraints [72, 74].
- **PEMEL** employs a solid proton-conducting membrane with noble-metal catalysts (Pt, IrO₂). It offers compact designs, high current densities, and fast load following, and is well suited to variable RES profiles. Differential-pressure operation routinely delivers

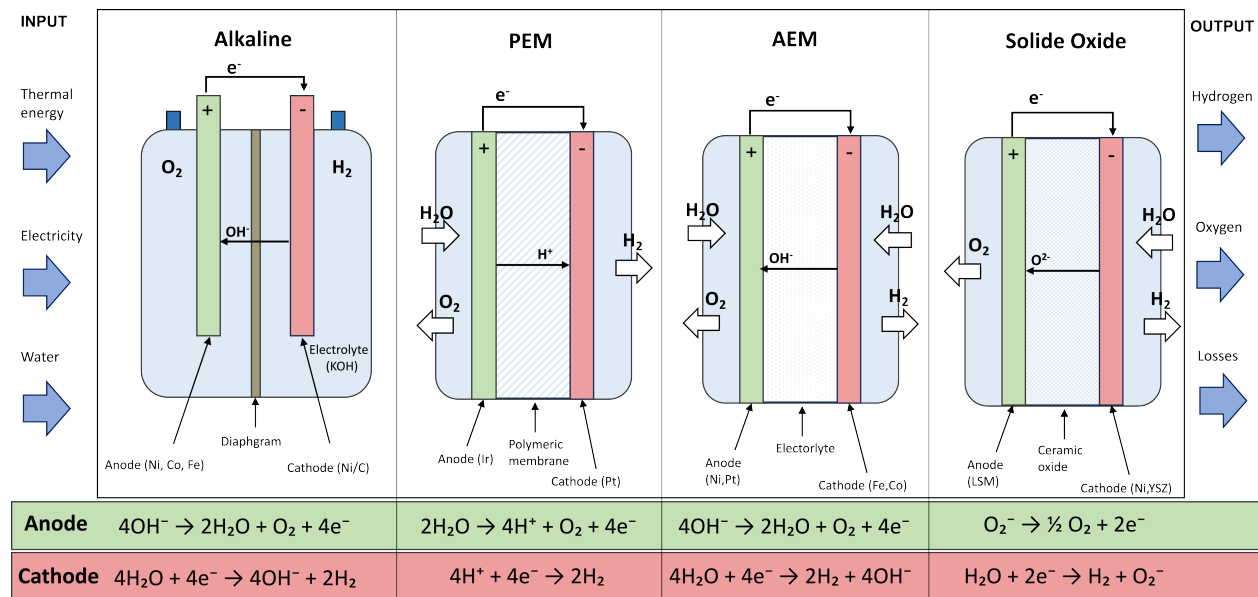


Figure 1.6: Comparison of electrolysis technologies: schematic principles and reactions of AEL, PEMEL, AEMEL, and SOEC.

Table 1.1: Indicative comparison of electrolysis technologies (stack-level ranges). Maturity refers to Technology Readiness Level (TRL).

	AEL	PEMEL	AEMEL	SOEC
Operating temperature (°C)	65–100	70–90	50–70	800–1000
Delivery pressure (bar)	25–30	30–80	~30	<30
Stack voltage efficiency (%)	60–80	60–80	40–65	80–95
Specific energy (kWh/N m ³)	4.5–7.5	5.8–7.5	4.8–5.2	2.5–3.5
Dynamic response	slow–moderate	fast	moderate	slow
H ₂ purity (vol., %)	99.3–99.9	99.999	99.99	99.999
Stack lifetime (h)	10 000	20 000	n/a	>20 000
Maturity (TRL)	Commercial	Commercial	R&D/pilot	Demo

30 bar to 80 bar hydrogen; heat recovery (50 °C to 80 °C) can preheat feedwater or serve local heat uses [75–77]. Iridium intensity and cost remain key challenges [74].

- **AEMEL**—Anion-Exchange Membrane electrolyser—targets PEM-like cell architecture with alkaline-side ion transport, enabling reduced precious-metal use. Current systems are limited by membrane conductivity and catalyst activity/durability; R&D focuses on membranes, electrodes, and cell design to close the gap with AEL/PEM [72].
- **SOEC** supplies part of the splitting energy as high-temperature heat, achieving high stack efficiencies at 800 °C to 1000 °C (ceramic electrolytes, e.g., yttria-stabilised zirconia (YSZ)). It is attractive where steady heat is available (industrial waste heat, nuclear). Challenges include materials stability, thermal-cycling sensitivity, sealing, and BOP complexity; pressurisation typically occurs downstream [72, 74].

Key cross-cutting decisions include: (i) delivery pressure—on-stack pressurisation versus downstream compression, (ii) operating strategy—balancing RES following with limits on cycling and low-load operation, (iii) heat and oxygen valorisation—recovering low-temperature heat and using O₂ in adjacent processes, and (iv) water management [72, 76]. Modest electrical buffering or RES hybridisation can raise utilisation and shrink hydrogen storage, whereas excessive battery sizing adds cost without proportional benefit [70, 71].

As controllable loads, electrolyzers can participate in ancillary services. Operation is conveniently described by three mutually exclusive states—on (producing), standby (holding at low power), and off—with distinct warm (standby→on) and cold (off→on) starts. PEM units typically ramp within sub-second to second-scale and cold-start within minutes; alkaline units respond in seconds–minutes with longer cold-starts. Properly scheduled, both meet secondary-reserve response windows (e.g., 15 min automatic Frequency Restoration Reserve (aFRR)) [78]. When on, stacks can offer bidirectional reserve around the set-point (within minimum-input limits); in standby, downward reserve dominates; when off, only cold-start upward modulation is feasible and must respect start-up time [79–81].

BOP shapes efficiency, availability, and site integration: (i) AC/DC conversion—transformer efficiency; (ii) water treatment—filtration and polishing to prevent contamination (typically 15 L/kg_{H₂}); (iii) thermal management—closed-loop cooling and dry coolers/chillers to remove low-grade heat; and (iv) gas processing—demisters and dryers for purity and safety. Local integration can upgrade BOP value, e.g., using low-grade heat for water preheating or nearby thermal users [76, 77].

Ageing influences scheduling and economics. Degradation correlates with cumulative operating hours and start/stop events. In PEM systems, catalyst dissolution/support corrosion and membrane hydration cycles dominate; in alkaline units, electrode corrosion and separator ageing are critical. Embedding degradation via usage costs (hours on) and start-up costs (warm vs. cold) steers schedules toward fewer starts (often favouring standby over repeated off/on), smoother profiles, and selective reserve provision when revenues exceed marginal ageing costs—consistent with experimental and review evidence that fast cycling and deep excursions accelerate wear, while steady operation extends life [72, 82].

1.4.3 Hydrogen compression

Hydrogen’s very low volumetric energy density makes compression indispensable whenever production and consumption are temporally or spatially decoupled. Target pressures depend on the use case (on-site buffer storage, pipeline injection, refuelling), and compression approaches fall into two broad families: mechanical and non-mechanical [83].

1. **Mechanical compression.** Positive-displacement machines dominate current practice for medium–high discharge pressures and moderate flows. Reciprocating (oil-free) compressors are widely deployed above 3 MPa, often in multistage layouts up to tens of MPa; they are mature but require careful materials selection (embrittlement) and robust thermal management and maintenance at high compression ratios. Diaphragm compressors hydraulically drive a metal diaphragm that isolates the gas from lubricants, providing very high purity at low–medium flow—typical of HRS—at the cost of diaphragm fatigue and limited throughput [83]. For high flows and intermediate ratios, centrifugal stages are attractive, but hydrogen’s low molecular weight forces very high impeller tip speeds; material and aero–thermo–mechanical constraints limit today’s adoption mainly to prototypes. Linear and liquid-piston concepts exist largely at R&D level for hydrogen (the latter better established for compressed-air service) [83].
2. **Non-mechanical compression.** Thermally or electrochemically driven concepts eliminate most moving parts and can integrate with site heat. Metal-hydride compressors absorb hydrogen at one condition and desorb at higher pressure when heated; they can leverage waste heat and deliver very pure gas, but overall efficiency is low (typically 2 % to 10 %) and multistage designs are needed beyond ~ 150 bar [84]. Electrochemical (PEM-based) compressors transport protons across a membrane under an applied potential and recombine them at elevated pressure; they are compact and oil-free, with demonstrations reported up to ~ 1000 bar, but durability at high differentials remains a challenge [85]. Cryogenic/cryo-compressed options combine deep cooling (near 20 K) with pressurisation to achieve very high densities; complexity and boil-off management restrict these to niche applications. Adsorption-based concepts are at an early stage with limited performance data [83].

Mechanical compressors remain standard for industrial and mobility deployments, yet compression energy is non-negligible: a substantial fraction of the stored hydrogen LHV can be consumed to reach high pressures, motivating careful staging and intercooling measures [83]. Non-mechanical routes can be advantageous where waste heat is available, purity is critical, or compactness and low maintenance are valued, but most are not yet broadly commercial. At elevated pressures hydrogen departs from ideal-gas behaviour; density and work estimates should therefore employ an appropriate equation of state or compressibility factor Z via $PV_{\text{ol}} = nZRT$. Ideal-gas estimates are generally adequate up to roughly ~ 100 bar; beyond that, tabulated $Z(p, T)$ or reference equations of state (e.g., Leachman et al.) are recommended for design and system modelling [86].

1.4.4 Hydrogen storage

Hydrogen storage technologies span physical options—compressed gaseous hydrogen (CGH₂), liquid hydrogen (LH₂), and cryo-compressed hydrogen (CcH₂)—and material-based options (metal hydrides (MH) and liquid organic hydrogen carriers (LOHC)). In PtH supply chains, storage decouples stochastic generation and end-use over time scales from intraday to seasonal, interacts with electrolyser operating strategy and compression choices, and constrains ancillary-service delivery through charge/discharge limits and pressure windows. The main storage pathways and their indicative characteristics are summarised in Table 1.2 [40, 83, 87, 88].

Upstream, electrolyser outlet pressure and dynamics determine the need for on-stack pressurisation versus downstream compression; midstream, storage selection fixes the pressure/temperature domain and the round-trip pathway (purely mechanical for CGH₂ tanks

Table 1.2: Summary of hydrogen storage pathways.

	CGH ₂	LH ₂	CcH ₂	UHS	Hydrides	LOHC
Pressure [bar]	100–1000*	~1	200–300	50–200	10–200	~1
Temperature [°C]	ambient	~ –253	~ –233	ambient	20–350	20–300
Density [kg/m ³]	8–50	~70	50–60	4–15	50–150	carrier-dependent
Duration	diurnal	transport	diurnal	week–season	diurnal	week
Ch./disch. rate	Fast	Fast	Fast	High	Mid	Mid
TRL	High	High	Demo	High	Mid	Mid–High

Note: * Most Type III/IV vehicle/industrial systems operate at 350 bar/700 bar; higher pressures refer to specialised applications.

and underground hydrogen storage (UHS) caverns, thermally assisted for metal hydrides, liquefaction plus boil-off control for LH₂/CcH₂); downstream, end-use pressure and continuity requirements drive minimum inventory and usable Level of Hydrogen (LOH) windows. Co-optimising these couplings is essential to avoid oversized compression, excessive cycling of electrolyzers, or underutilised storage [40, 83].

1. **Compressed gas (CGH₂).** CGH₂ cylinders are the standard modular choice for on-site buffers and mobility. Four tank types are typically used [89, 90], as illustrated schematically in Fig. 1.7: Type I (all-metal) and Type II (metal liner, hoop-wrapped) are heavy and typically limited to 175 bar to 300 bar; corrosion and mass penalise gravimetric capacity (approximately 1.7–2.1 wt%). Type III (metal liner, full composite wrap) and Type IV (polymer liner, full composite wrap) are used at 350 bar/700 bar with system gravimetric capacities approximately 5.0–5.7 wt%. Type III offers very high burst strength and negligible permeation; Type IV minimises mass and shows good cycling durability. System design balances compression work, footprint, and safety. Indicative system-level characteristics of the four tank types are summarised in Table 1.3 [83, 89, 90].

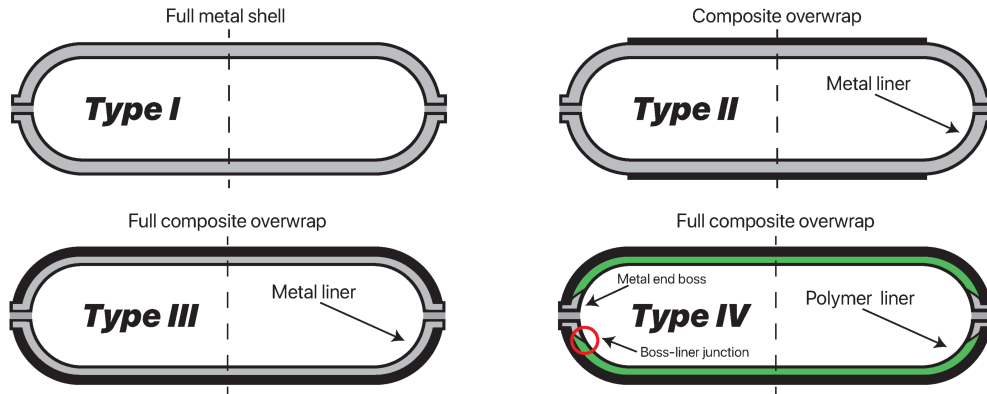


Figure 1.7: Schematic cross-sections of compressed hydrogen cylinder types: Type I (all-metal), Type II (metal liner with partial composite overwrap), Type III (metal liner with full composite overwrap) and Type IV (polymer liner with full composite overwrap).

2. **Liquid and cryo-compressed.** Liquefied hydrogen attains $\sim 70 \text{ kg/m}^3$ at 20 K, enabling high energy density for transport and some stationary buffers. Cryo-compressed tanks combine low temperature with elevated pressure (200 bar to 300 bar), further enhancing density and reducing boil-off losses. Integration requires liquefaction, vacuum

Table 1.3: Indicative characteristics of CGH₂ tank types (system level).

	Type I	Type II	Type III	Type IV
Pressure (bar)	175–200	200–300	350–700	350–700
Gravimetric density (% mass)	~1.7	~2.1	5.0–5.5	5.0–5.7

insulation, and boil-off gas management; economics hinge on duty cycle and utilisation [86, 91].

- Underground hydrogen storage (UHS).** Salt caverns provide large-scale, low-cost bulk storage with high deliverability, proven for natural gas and demonstrated for H₂. Key issues are suitable geology, cushion gas, permeability, and microbiological/chemical interactions (for aquifers/reservoirs). UHS naturally supports weekly to seasonal balancing and reduces the need for above-ground tank farms [40].
- Material-based storage.** Metal hydrides store hydrogen via reversible chemisorption with high volumetric density and near-ambient pressure operation; they require heat for desorption, making waste-heat coupling attractive. LOHC physically transport hydrogen bound in a liquid (e.g., toluene/methylcyclohexane); they offer ambient-condition logistics and fuel-like infrastructure at the cost of dehydrogenation energy and catalyst management [84, 87, 88].

Storage choice sets the optimal discharge pressure and thus the compression train (on-stack pressurisation vs. multi-stage downstream compression). For flexibility services, part of fast up/down regulation can be routed through storage charge/discharge within allowable pressure bands, limiting electrolyser cycling. Conversely, hydride/LOHC systems shift flexibility to thermal units (heaters/reactors), affecting reserve-provision speed. In all cases, storage ageing (cycling, thermal gradients, liner fatigue for tanks; cavern leaching cycles; hydride decrepitation; catalyst deactivation in LOHC) should be reflected in scheduling to avoid hidden OPEX and loss of availability [40, 83, 87].

1.4.5 Hydrogen utilisation

Hydrogen end-use blocks in this thesis cover two pathways to deliver electricity and process steam at industrial sites: fuel-cell CHP and Gas Turbine (GT) combustion with heat recovery.

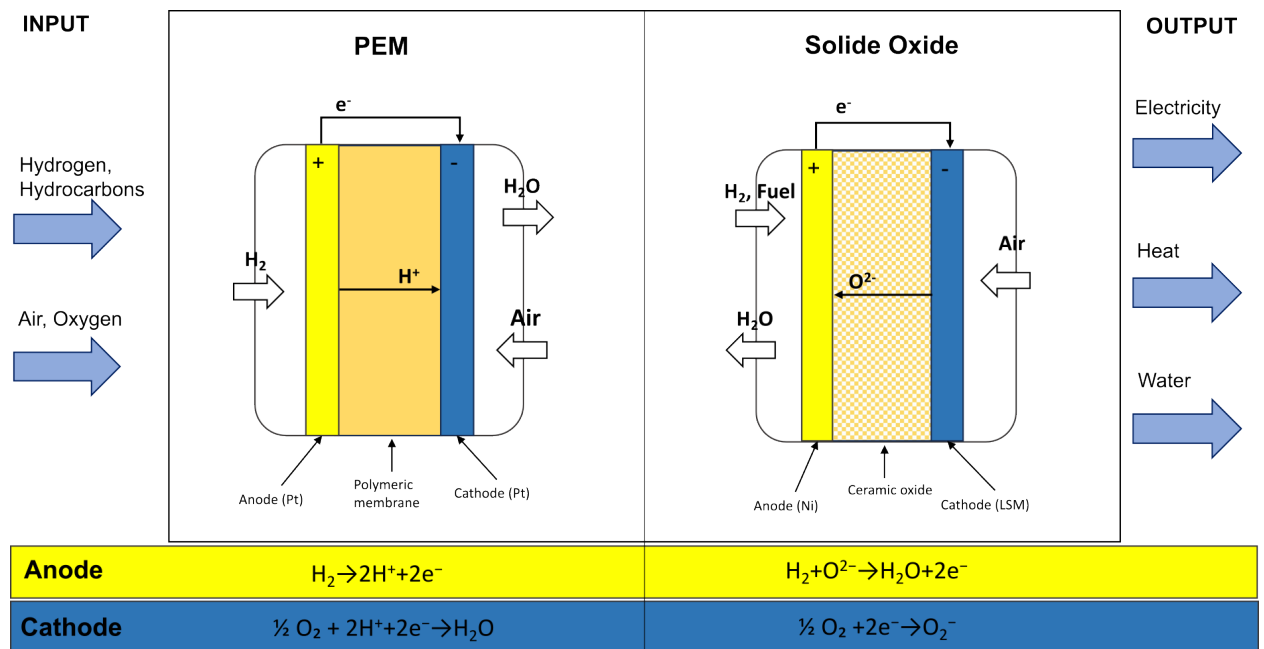
Fuel cell

Fuel cells (FCs) convert hydrogen and oxygen directly into electricity and heat through electrochemical reactions, producing water as the by-product. Their performance is governed by the Nernst potential and overpotential losses (activation, ohmic, concentration), rather than a thermodynamic cycle limit, and is therefore strongly dependent on cell design, materials, operating temperature, reactant quality, and current density [92]. In Power-to-Hydrogen-to-Power (PtHtP) settings, fuel cells supply firm electricity and co-generated heat for CHP; start-up time, ramping capability, part-load efficiency, and fuel purity requirements determine how they are dispatched alongside storage and other on-site units [93, 94]. Detailed numeric ranges are provided in Table 1.4.

The main technology families are distinguished by electrolyte and temperature, as represented in Figure 1.8.

Table 1.4: Indicative characteristics of stationary fuel-cell technologies.

	PEMFC	AFC	PAFC	MCFC	SOFC
Temperature (°C)	50–100	60–90	150–200	600–700	500–1000
Typical fuel	H ₂	H ₂	H ₂	H ₂ /NG/biogas	H ₂ /NG/biogas
Electrical efficiency (%)	40–60	50–70	37–45	45–55	45–60
CHP efficiency (%)	80–90	80–85	80–90	75–85	75–95
Dynamics	fast	fast	moderate	moderate	slow
Maturity	Commercial	Demo	Commercial	R&D/Demo	Demo/Commercial

**Figure 1.8:** Comparison of fuel cell types: schematic principles and reactions of PEM and Solid Oxide fuel cells, showing electrochemical reactions and general inputs and outputs.

The following bullets summarise indicative characteristics for stationary use:

- **Proton-Exchange-Membrane Fuel Cell (PEMFC):** low-temperature polymer electrolyte (50 °C to 100 °C) with noble-metal catalysts; high power density, rapid transients, and compact balance-of-plant; requires dry, high-purity H₂ and tight water/thermal management; stack cost and precious-metal intensity remain key constraints [93, 94].
- **Alkaline Fuel Cell (AFC):** aqueous KOH electrolyte (60 °C to 90 °C); high electrical efficiency and fast dynamics; sensitivity to CO₂ in the oxidant stream limits use with ambient air unless CO₂ is removed, making pure O₂ operation advantageous but costly [93].
- **Phosphoric Acid Fuel Cell (PAFC):** phosphoric-acid electrolyte (150 °C to 200 °C); tolerant to some fuel/air impurities and proven in CHP blocks at the 100 kW to 1000 kW scale; electrical efficiency lower than high-temperature options but with well-established durability in stationary duty [94].
- **Molten Carbonate Fuel Cell (MCFC):** molten-carbonate electrolyte at about 600 °C to 700 °C with internal reforming of natural gas or biogas; good fuel flexibility and scale for large stationary plants; corrosion and electrolyte management are central design issues [94].
- **Solid-Oxide Fuel Cell (SOFC):** solid-oxide electrolyte operating at 500 °C to 1000 °C; highest electrical efficiency potential among FCs and excellent quality heat for CHP; internal reforming and tolerance to multiple fuels (H₂, NG, biogas, syngas) enable flexible integration; start-up is comparatively slow and thermal cycling must be limited to protect materials [92, 94, 95].

SOFC and MCFC exhaust at 200 °C to 600 °C enable steam generation, and SOFC anode off-gas oxidation provides a controllable thermal source for HRSG or process heaters, whereas PEMFC heat at 50 °C to 80 °C serves low-grade loops [92, 94].

At plant level, fuel quality, pressure, and contaminant limits define the upstream interface. PEMFC stacks are typically fed with dry, high-purity H₂ at modest pressure; SOFC systems can accept H₂ or reformed fuels near atmospheric pressure with anode recycle, shifting BOP emphasis from compression to thermal integration [93, 94]. Heat valorisation is technology-dependent: PEMFC reject heat at 50 °C to 80 °C for low-grade uses, whereas SOFC/MCFC exhausts at 200 °C to 600 °C are suited to steam generation and process integration, raising overall efficiency and reducing hydrogen throughput for a given useful-energy target [92, 94].

Dispatch and flexibility depend on start-up and part-load behaviour. PEMFC units support fast ramps and short warm starts, enabling frequent cycling when required by variable renewables; SOFC units favour fewer thermal cycles and sustained operation near an efficient load band, with start-up costs and degradation considerations guiding schedules in PtH plants [92, 95]. Durability is shaped by operating stresses: for PEMFC, catalyst and support degradation, membrane hydration cycles, and fuel/air transients dominate; for SOFC, thermal gradients, interconnect corrosion, and anode re-oxidation are critical. Including usage- and start-related penalties in scheduling internalises ageing and nudges operation toward smoother profiles and fewer cold starts [94, 96].

Hydrogen-fired gas turbines (GT)

Gas turbines can be adapted to hydrogen-rich fuels to supply firm power and high-temperature heat, making them suitable end-uses within PtH chains for industrial campuses

and CHP. In retrofits, the compressor–turbine core is typically retained while combustors, fuel control, and selected BOP elements are modified for hydrogen; downstream, an HRSG recovers exhaust heat, with typical exhaust/stack temperatures constrained by pinch/approach and acid–dew-point limits (exhaust ~ 720 K to 870 K; stack >400 K) [97]. A simplified hydrogen-fired gas-turbine combined heat-and-power layout with heat-recovery steam generator (HRSG) and paper-mill steam supply is illustrated in Fig. 1.9.

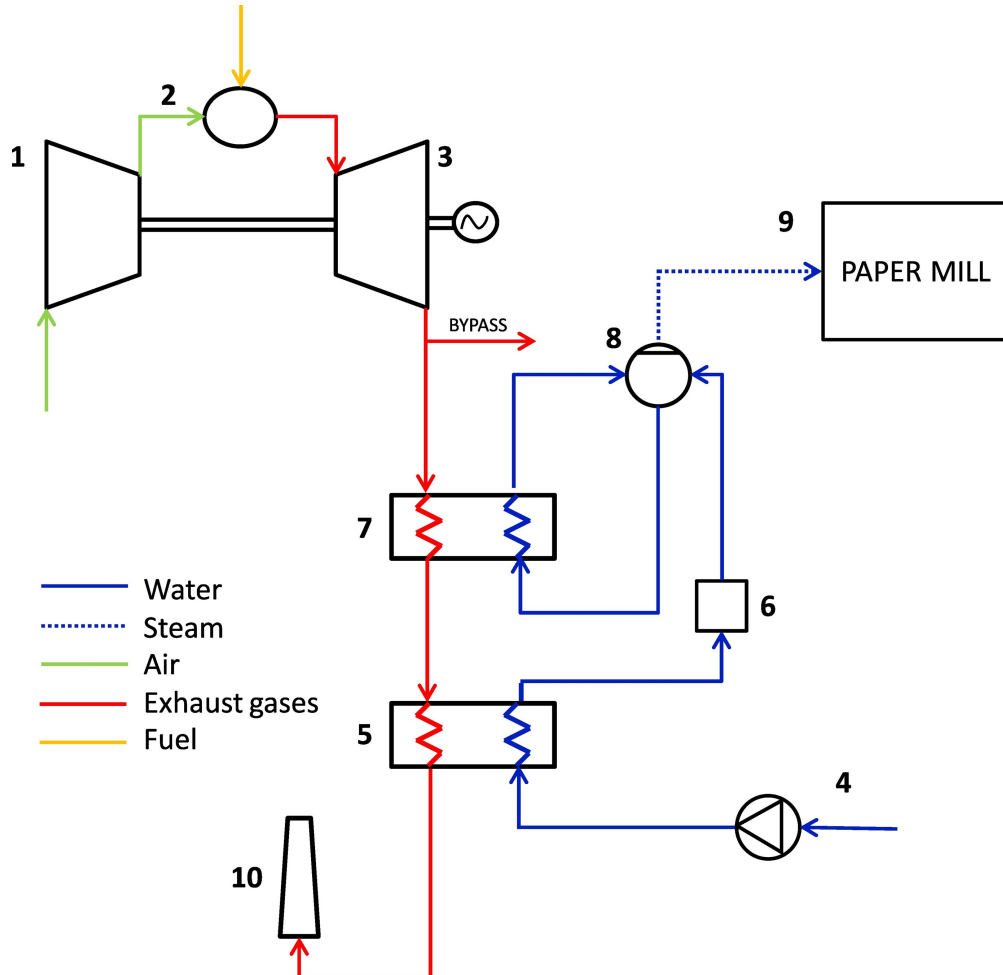


Figure 1.9: Simplified hydrogen-fired gas-turbine combined heat-and-power (CHP) system with heat-recovery steam generator (HRSG) supplying process steam to a paper mill. The coloured lines indicate air (green), fuel (yellow), exhaust gases (red), water/condensate (solid blue) and steam (dotted blue). Numbered components include: gas-turbine compressor (1), combustor (2), turbine and generator (3), feedwater pump (4), HRSG heat exchangers (5, 7), condensate tank or deaerator (6), steam drum (8), process steam user (9) and stack (10).

Combustion and hardware. Relative to natural gas, hydrogen’s higher laminar flame speed, wider flammability limits, lower ignition energy, and lower volumetric heating value enable ultra-lean operation but raise flashback and auto-ignition risks in premixed systems. Practical adaptations include micro-mixing or sequential lean-premixed burners, increased injector velocities and staged air/fuel to suppress flashback, and steam or nitrogen dilution for NO_x control where required. Materials and seals must be compatible with hydrogen to mitigate embrittlement and leakage. Original equipment manufacturer pathways range from certified co-firing (today typically 20 % to 65 % (vol.)) to 100 % hydrogen via burner swaps and control updates, with catalogued changes in pressure loss, fuel-flow capacity, and control logic [98, 99]. With appropriate combustor design, base-load shaft efficiency can be

comparable to natural-gas operation while maintaining low CO and managing NO_x through lean combustion and/or diluents; part-load stability depends on the chosen burner concept and must preserve HRSG constraints [97].

Retrofitting experience and system studies indicate technical feasibility for both hydrogen co-firing and neat-hydrogen operation in industrial frames. At plant scale, economics hinge on hydrogen cost and duty cycle; integrated PtH–GT assessments show viable operability envelopes when compression, storage, and GT firing limits are co-designed [73, 100]. In practice, burner replacement and control upgrades are a minor fraction of total project CAPEX relative to RES–electrolysis–storage, but they unlock high-value CHP service and fast electrical/thermal ramps [100].

Integration with PtH chains. GT fuel requirements (pressure, flow transients, allowable Wobbe index) co-determine the downstream compression train and storage pressure level to minimise recompression. Compared with SOFC blocks, GTs accept wider fuel-quality variation and offer faster start/ramp, which is useful when electrolyzers follow RES. Scheduling co-optimises (i) hydrogen production and storage (charging/discharging) to keep the turbine within efficient, low- NO_x regions and respect HRSG pinch/approach, and (ii) GT load changes for residual fast modulation, subject to combustor stability under high-hydrogen operation [73, 100].

1.5 Thesis structure

The remainder of the thesis is organised as follows. Chapter 2 reviews rule-based, deterministic, and stochastic approaches for joint sizing and scheduling of hydrogen-integrated energy systems and positions the contribution of this work within that literature. It highlights how different modelling choices embed technical detail, uncertainty, and market interaction, motivating the toolbox adopted in later chapters.

Chapter 3 presents the modelling framework used throughout the thesis. It is structured around two main families: (i) rule-based simulation, implemented via the Multi Energy System Simulator (MESS), and (ii) optimisation-based formulations. For the latter, deterministic Mixed Integer Linear Programming (MILP) and stochastic MILP (two-stage design and multi-stage scheduling) are developed on a common component library, with uncertainty and information-structure constraints layered on top.

Chapter 4 reports five application studies that draw on these methods. Two cases use the rule-based simulator: a like-for-like comparison of SOFC-based CHP against a gas-turbine-based benchmark at a paper mill, and a nation-wide PV–PtH screening for industrial hydrogen supply across Italian bidding zones. Three further cases use MILP formulations: a deterministic joint sizing–scheduling baseline comparing hydrogen storage technologies; a two-stage stochastic design study for a stand-alone island system under reliability and emissions constraints; and a multi-stage stochastic scheduling study for a hydrogen refuelling station operated as a hydrogen-enabled virtual power plant in coupled electricity markets.

Chapter 6 synthesises the main findings from the methodological and application chapters, drawing out implications for policy, market design, and investment in hydrogen-integrated systems, and outlining directions for future work.

An additional topic—agrivoltaic siting under land constraints—is documented in Appendix 7. It provides photovoltaic layout constraints and land-use/economic trade-offs relevant when conventional ground-mounted PV is infeasible, while leaving the core PtH sizing and scheduling methodology unchanged.

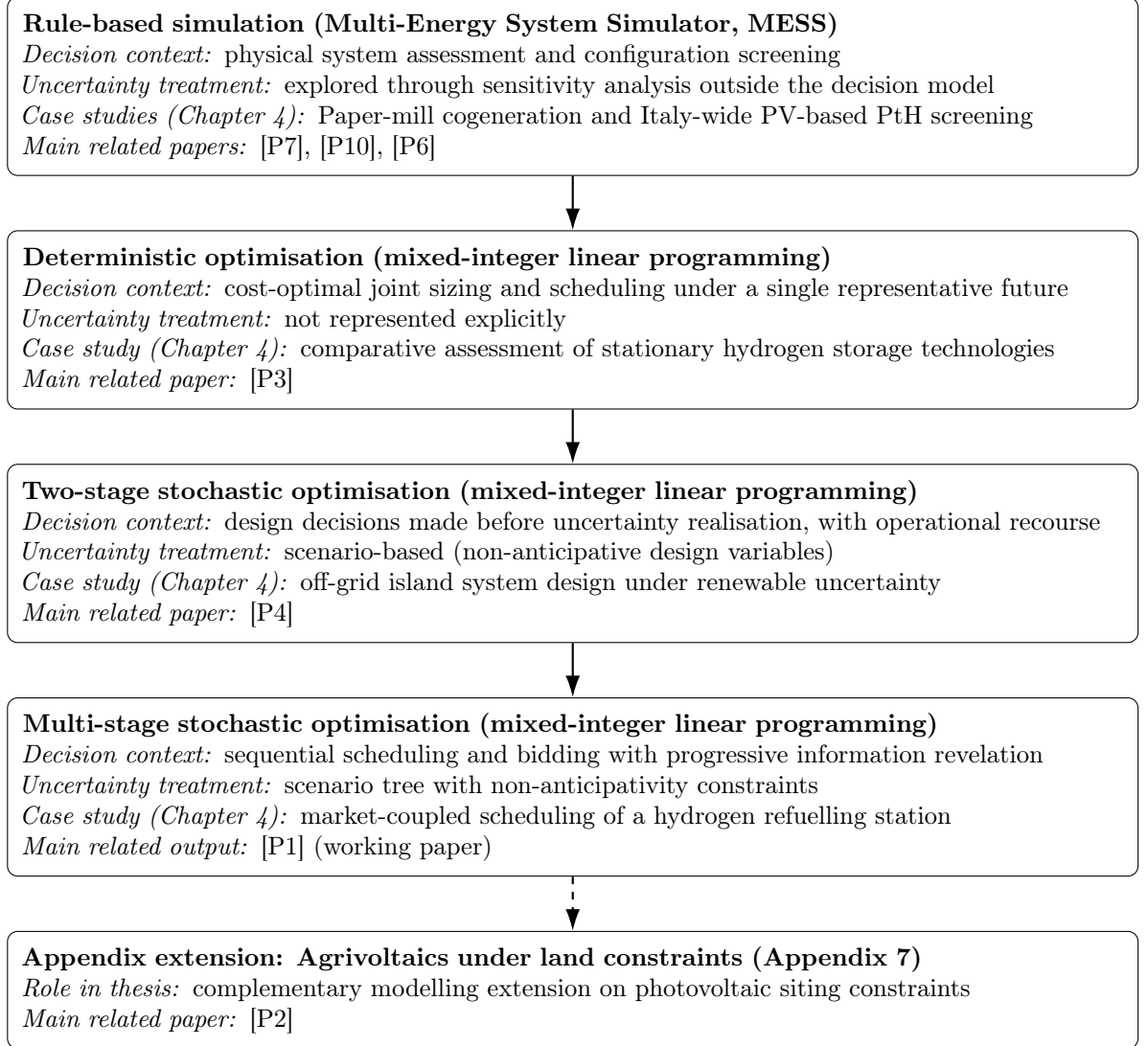


Figure 1.10: Conceptual map of the modelling families used in the thesis, the associated case studies, and their primary peer-reviewed publications (detailed in Chapter 5). The case studies are intentionally heterogeneous because each modelling layer targets a different decision context.

2. STATE OF THE ART

The decarbonisation mandate outlined in EU policy [7, 14] and the certification constraints governing renewable fuels [10] make the design and operation of PtH assets a time-coupled planning problem: capacity choices (e.g., PV/BESS/EL/HS/FC ratings) and hourly scheduling (dispatch, market participation, compliance) interact over long horizons. As established in the Introduction, component characteristics, duty profiles, and site rules shape feasibility and cost. The focus here is how the literature has modelled these intertwined decisions to screen concepts, quantify trade-offs, and cope with uncertainty.

A widely used lens in the energy-system-modelling literature distinguishes between optimisation and simulation models. Optimisation models formulate an objective (e.g., cost, emissions) and constraints to endogenously select designs and operations; simulation models reproduce system behaviour under specified designs and operating rules without seeking an internal optimum. Optimisation is typically used for normative pathways and least-cost portfolios, whereas simulation supports descriptive scenarios, feasibility, and operational detail; both are useful depending on the question and context [101]. This distinction also matters for hydrogen: absent explicit policy or technical constraints, least-cost formulations can under-select hydrogen technologies; simulation allows testing designs that reflect non-cost preferences or compliance needs before moving to formal optimisation.

- **Rule-based simulation.** Operating logics (priority rules, thresholds, module on/off, state updates) are propagated over full-year time series to test feasibility, explore technology mixes, and verify certification or temporal-matching constraints in a traceable manner. These studies favour speed and interpretability and readily accommodate detailed component modelling (including degradation) and site-specific rules; they do not guarantee economic optimality and expose multi-objective trade-offs only indirectly.
- **Deterministic optimisation.** Optimisation frameworks (typically LP/MILP) co-optimize components' sizes and hourly operation under perfect foresight, enforcing balances, capacity limits, and cyclic state constraints while quantifying trade-offs (e.g., total annualised cost vs. emissions). Certification requirements can be represented explicitly as hard constraints, enabling direct comparison of compliant vs. purely economic solutions. Tractability often calls for simplified plant dynamics or monetised degradation, and results are sensitive to forecast assumptions.
- **Stochastic optimisation.** Scenario-based models represent variability in weather, load, and prices. In PtH plants, two-stage stochastic formulations usually separate

first-stage sizing from second-stage operation to ensure feasibility across scenarios, while multi-stage scheduling aligns decisions with information revelation in sequential electricity markets. These approaches quantify the value of flexibility and hedging, at the expense of greater modelling and computational burden and a dependence on scenario generation and reduction choices.

Across these families, ageing and degradation (e.g., PV output decay, BESS cycling costs, electrolyser/fuel-cell usage and start-up wear) can shift the sizing/dispatch frontier and are therefore either simulated explicitly or monetised within optimisation. Certification and compliance (e.g., lifecycle GHG-intensity caps) can become binding, reshaping feasible designs relative to purely economic optima and motivating explicit constraints in models [10]. Uncertainty treatment is context-dependent: two-stage models are common when supply and demand variability dominate, whereas multi-stage formulations are preferred when sequential market offers and redispatch matter.

Representative tools—both commercial and open-source—developed for this scope are summarised below.

1. **Backbone** (implemented in the General Algebraic Modeling System (GAMS)). An adaptable framework for both investment planning and short- to mid-term scheduling across multiple energy carriers; it supports scenario-based uncertainty (stochastic parameters). *Pros:* broad multi-sector coverage in a single code base; usable for capacity expansion and for unit-commitment-style operation; documented features for handling uncertainty. *Cons:* requires commercial modelling software and solvers; not a turnkey model but a flexible framework that must be configured for each study [102].
2. **Balmorel** (implemented in GAMS; partial-equilibrium, welfare-maximising formulation). A deterministic model widely used for electricity and district-heating planning and market analysis, with a strong track record in Nordic and wider European applications. *Pros:* mature open-source code base; detailed representation of power/heat markets and cross-border trade. *Cons:* uncertainty is usually explored via separate scenario runs rather than within the model; detailed hydrogen and process-industry representations require user extensions [103].
3. **energyPRO** (commercial suite; simulation plus an analytical cost-optimal scheduler). A project-level tool for combined heat and power, district heating and cooling, and Power-to-X (PtX) applications, with dispatch simulation and a built-in analytical solver for cost-optimal operation (and optional solver-based optimisation). *Pros:* familiar interface for plant-level techno-economics; integrates operational and market constraints. *Cons:* closed-source; uncertainty is usually explored via separate scenario runs rather than within the model [104].
4. **oemof/solph** (open energy modelling framework in Python; LP and MILP). An open framework in which the *solph* library builds optimisation problems from a graph of components and connections. *Pros:* very extensible; active open-science ecosystem with many examples and add-ons. *Cons:* primarily geared to optimisation; purely simulation-style studies require custom components; uncertainty is usually explored via separate scenario runs rather than within the model [105].
5. **PyPSA** (Python for Power System Analysis; network simulation plus linear optimisation for operation and investment). Combines power-flow simulation with multi-period optimisation under linearised network equations and is frequently used at national

or continental scale; supports sector coupling. *Pros*: demonstrated scalability; rich electricity-sector features and open datasets. *Cons*: uncertainty is usually explored via separate scenario runs rather than within the model [106].

6. **REopt** (National Renewable Energy Laboratory (NREL); MILP). A techno-economic optimiser for sites and campuses that sizes and schedules distributed energy resources to minimise life-cycle cost. *Pros*: robust, well-documented workflow; broad library of technologies; widely used via a web interface. *Cons*: optimisation-centric; uncertainty is usually explored via separate scenario runs rather than within the model [107].
7. **SpineOpt** (implemented in the Julia language using the julia mathematical programming library; operational and planning horizons, with explicit uncertainty support). A flexible framework with rich temporal structures and options for representing uncertainty and decomposition. *Pros*: strong focus on detailed temporal resolution and uncertainty handling; modern open tooling. *Cons*: higher modelling complexity [108].

In what follows, Section 2.1 reviews rule-based simulation as a screening and compliance instrument, Section 2.2 covers deterministic joint sizing–scheduling, and Section 2.3 surveys stochastic optimisation under uncertainty, distinguishing two-stage sizing from multi-stage market-offer models. Formal model statements are deferred to Chapter 3.

2.1 Rule-based simulation

A rule-based simulator advances the system by executing a logic-driven mode selector and the associated mode dynamics at each time step, rather than optimising decisions. Figure 2.1 sketches the resulting time-marching loop: given the current state x_t , exogenous inputs ξ_t , and rule parameters θ , the simulator selects an operating mode σ_t , computes the corresponding controls u_t , and updates states and outputs before moving to the next step.

2.1.1 Mathematical formulation

Following the hybrid/switching-systems formalism [109, 110], the compact time-marching formulation is shown in Eq. 2.1:

$$\begin{aligned} \sigma_t &= \Gamma(x_t, \xi_t; \theta) \\ u_t &= \mu_{\sigma_t}(x_t, \xi_t; \theta) \\ x_{t+1} &= f_{\sigma_t}(x_t, u_t, \xi_t) \\ y_t &= y_{\sigma_t}(x_t, u_t, \xi_t), \quad t = 1, \dots, N_T. \end{aligned} \tag{2.1}$$

Reading 2.1 (general $\rightarrow$ PtH examples). *Implementation note.* In code, Γ is realised as an if/else rule tree evaluated at every step; the path taken is σ_t , whose effects are the chosen branch and set-points below.

State x_t . *General:* all memory variables propagated across time. *PtH examples:* hydrogen inventory, battery State Of Charge (SOC), unit statuses (on/off, warm/cold), start counters, degradation states, and certification ledgers that timestamp renewable provenance and certified quantities.

Exogenous inputs ξ_t . *General:* uncontrollable drivers supplied as time series. *PtH examples:* solar/wind availability, electricity/heat demands, wholesale and network tariffs, ambient conditions.

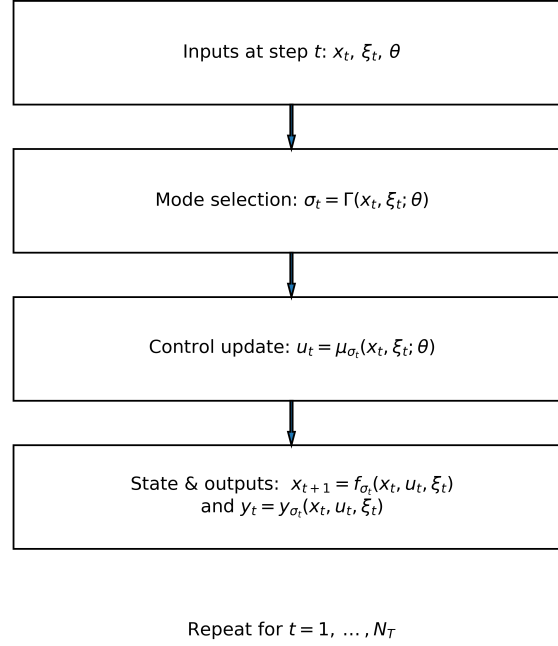


Figure 2.1: Rule-based time-marching scheme: at each step t , inputs (x_t, ξ_t, θ) feed the mode selector Γ , the control map μ_{σ_t} , and the mode-dependent dynamics/output maps $f_{\sigma_t}, y_{\sigma_t}$, yielding u_t, x_{t+1} and y_t .

Rule parameters θ . *General:* thresholds and priorities governing decisions. *PtH examples:* SOC bands, minimum loads/idle times, curtailment caps, import/export priorities, and compliance gates (e.g., “produce H_2 only when eligible RES is available”).

Mode selector $\sigma_t = \Gamma(\cdot)$. *General:* discrete operating situation chosen by evaluating predicates on $(x_t, \xi_t; \theta)$. *PtH examples:* surplus/deficit on the electric balance; charge vs. discharge for storage; produce vs. consume hydrogen; import vs. export at the grid interface; warm vs. cold-start regimes.

Control map $u_t = \mu_{\sigma_t}(\cdot)$. *General:* deterministic set-points/actions within the active mode, respecting instantaneous limits and guards. *PtH examples:* electrolyser production set-point, compressor mass flow, battery charge/discharge power, grid import/export.

Mode-dependent dynamics $x_{t+1} = f_{\sigma_t}(\cdot)$. *General:* physics-consistent updates of all states. *PtH examples:* energy/mass balances for H_2 , electricity and heat; start-up penalties; degradation increments; certification-ledger writes that attribute eligible RES to produced hydrogen with correct time alignment.

Outputs $y_t = y_{\sigma_t}(\cdot)$. *General:* variables of interest derived from states/actions. *PtH examples:* unmet-load hours, curtailed energy, hydrogen production/uses, cash flows; certified-green H_2 under annual/monthly/hourly correlation, instantaneous/aggregated GHG intensity, and KPIs such as Levelised Cost of Hydrogen (LCOH) or Net Present Value (NPV).

Domains and guards. *General:* $x_t \in \mathcal{X}$, $u_t \in \mathcal{U}$ with mode-dependent admissible sets; guards enforce invariants. *PtH examples:* electrolyser minimum load when online; tank pressure/volume limits; battery SOC bands; certification guards enforce the selected temporal-correlation mode.

Initial and boundary conditions. *General:* x_1 specified; optional cyclicity to avoid end effects. *PtH examples:* set initial hydrogen inventory, battery SOC, and certification-ledger state.

Structure and implementation. *General:* explicit time march. *PtH examples:* full-year (8760 h) traces with multiple carriers and certification ledgers are tractable. Implementation

order per step: refresh ξ_t ; evaluate Γ ; compute and clip u_t ; update states via f_{σ_t} ; settle grid via y_{σ_t} .

Running 2.1 for $t = 1, \dots, N_T$ with fixed $(\Gamma, \mu, f, y, \theta)$ yields a transparent, auditable trajectory. Replaying across scenarios, size vectors, and alternative rule sets builds a fast screening map for feasibility, certification, and levelised cost.

2.1.2 Scientific literature on rule-based simulation for PtH plants

Rule-based simulation has an important role in the hydrogen–renewables community and has been used to “play out” hourly (and often sub-hourly) operation of PtH plants without solving an optimisation problem. The common pattern is a supervisory energy-management strategy that applies simple if–then logics to decide when to run the electrolyser, when to charge or discharge short-term storage, and when to call on a fuel cell or the grid, while component-level dynamics are simulated with physics-based or empirical models. This makes it possible to explore feasibility, sizing sensitivities, and operational side-effects such as on/off cycling and round-trip losses with full time resolution and transparent control rules.

A representative and influential example is the dynamic model and validation of the Hydrogen Office demonstrator in Scotland. Valverde-Isorna et al. develop a whole-system model of a wind–electrolyser–storage–fuel-cell microgrid and validate it against operational data from the site. The supervisory control is threshold-based: surplus wind triggers electrolysis (subject to tank headroom), while deficits are covered by the fuel cell when the tank exceeds a minimum state; otherwise the grid bridges the shortfall. Their study reports realistic round-trip efficiencies and shows how wind variability propagates into electrolyser cycling and tank utilisation, providing a transparent baseline for design choices and for assessing autonomy under different wind regimes [111].

Earlier works established much of today’s modelling practice. Khan and Iqbal analyse a stand-alone small wind–hydrogen hybrid where an electrolyser absorbs surplus wind and a fuel cell covers deficits. Their MATLAB/Simulink study uses a simple supervisory rule to toggle between electrolysis and generation; results quantify the achievable load coverage and hydrogen balance as functions of wind resource and storage size [112]. In a grid-connected setting, Zhou et al. model the electrolyser and associated power electronics in detail and embed them in a wind–hydrogen–supercapacitor hybrid; on top of device-level control loops, they implement energy-management rules that prioritise wind capture while maintaining direct-current (DC) bus quality, demonstrating how rule parameters affect hydrogen throughput [113].

Many techno-economic screening studies use commercial simulators with rule-based dispatch engines. In Hybrid Optimisation of Multiple Energy Resources (HOMER), for example, the default controllers are load-following (generators produce only enough to meet the primary load) and cycle-charging (whenever a generator runs, it operates near full output and surplus power charges storage or feeds lower-priority sinks). These logics have been widely applied to PV/wind/battery/fuel-cell/electrolyser hybrids to explore sizing under representative time series. As a concrete example, Dawood et al. analyse a stand-alone 100 % renewable microgrid using HOMER with a PV–battery–hydrogen configuration; their results show how storage sizing influences reliability and cost, and that hydrogen storage becomes attractive when seasonal mismatches dominate and curtailment would otherwise be high [114]. Beyond off-the-shelf rules, Dufo-López and Bernal-Agustín explicitly tune rule parameters (e.g., switching thresholds) with a metaheuristic and then simulate the year-long operation of PV–wind–battery–hydrogen systems; they report how different rule sets shift unmet load, curtailment, and component utilisation, and how hydrogen storage improves autonomy for

weak seasonal solar resources [115]. In a more recent MATLAB/Simulink workflow, Wei et al. implement a PV–electrolyser–hydrogen-tank system with a rule that directly routes PV direct current to electrolysis while a low-pass filter determines the capacity of the auxiliary storage used to smooth PV fluctuations; the study quantifies how the controller’s time constant and storage size shape hydrogen production variability and smoothing efficiency [116].

Finally, hardware-focused demonstrations also rely on rules at the supervisory layer, even when lower-level loops are continuous. Little, Thomson and Infield discuss the electrical integration of a stand-alone wind/PV system with a DC bus linking the electrolyser, fuel cell and converters; while the paper’s emphasis is power-electronics integration and protection, the microgrid is operated under straightforward operating rules (bus regulation, electrolyser absorption of surplus, fuel-cell supply on deficit), and the authors report commissioning insights on converter interactions and safe operating envelopes—practical details that underpin many simulation rule sets used later in the literature [117]. A much-cited early feasibility study by Shakya, Aye and Musgrave couples such rule-based operation with economic analysis for a stand-alone wind–PV–hydrogen system in Australia; they show that hydrogen storage can enable high renewable penetrations in off-grid contexts, with viability hinging on electrolyser and storage costs as well as resource complementarity [118].

Advantages and drawbacks of rule-based approaches. Rule-based simulation is fast, transparent, and easy to extend with component detail or site-specific constraints (including start-up penalties and ledgering for eligible production). It yields auditable time traces that expose feasibility, cycling, and certification questions before one commits to a specific optimisation model. The trade-off is that there is no endogenous optimality: performance depends on the chosen rules and thresholds, and multi-objective trade-offs (cost vs. emissions vs. curtailment) are only observed ex post rather than solved for. For this reason, many studies use rule-based simulation to screen designs and stress-test controls, and then move to LP/MILP/nonlinear programming (NLP) formulations when endogenous trade-offs or strong policy constraints must be represented.

Recent surveys on hydrogen-based hybrid microgrids confirm that energy-management contributions span heuristic/rule-based schemes, deterministic optimisation, and stochastic formulations; rule-based controllers remain common when constraints are highly non-linear, policy-driven, or when fast screening across many design alternatives is required [119]. In parallel, sector-coupling reviews emphasise that electrolyser flexibility (load range, ramping, start-up/stand-by losses and lifetime effects) largely determines the system-level value of PtH as a controllable demand and storage pathway [120]. In this thesis, rule-based simulation is therefore used as a transparent baseline and feasibility/stress-test layer, while the optimisation layers quantify endogenous trade-offs and the value of hedging uncertainty.

2.2 Deterministic optimisation

In a deterministic setting, the optimiser solves a fixed mathematical programme for one specified set of data (forecasts and parameters). Both the quality of theoretical guarantees and the practical scalability depend on the modelling framework and on the chosen algorithms.

- **Linear programming (LP).** Problems with a linear objective, linear equality/inequality constraints, and continuous decision variables are convex and have polynomial-time algorithms. Modern solvers combine presolve and scaling with either the simplex method (pivoting on a basis) or interior-point/barrier methods (Newton steps within the feasible region) [121, 122]. These implementations exploit sparsity and block structure effectively.

- **Mixed-integer linear programming (MILP).** When some decision variables must take integer or binary values, the resulting problems are, in general, computationally hard in the worst case. The dominant paradigm builds on linear-programming relaxations with branch-and-bound or branch-and-cut, strengthened by cutting planes, primal heuristics, and problem decomposition [123, 124]. The tightness of the formulation (i.e., strong relaxations) is a key driver of performance.
- **Nonlinear programming (NLP).** With smooth nonlinear objectives and/or constraints and continuous variables, state-of-the-art algorithms include interior-point methods and sequential quadratic programming. These rely on first- and second-order derivative information [125–127]. Convex nonlinear programmes have globally optimal solutions under standard regularity conditions; for non-convex problems, algorithms return locally optimal, stationarity-certified solutions.

These methods differ in modelling expressiveness and solution guarantees:

- **Modelling expressiveness.** LP uses only linear relations and continuous variables; MILP keeps linear relations but adds integer/binary variables for discrete choices; NLP allows smooth nonlinear relations with continuous variables. In PtH terms: LP captures linearised physics and accounting; MILP captures on/off logic, mutually exclusive modes, and minimum up/down; NLP captures smooth part-load curves, thermodynamic couplings, and degradation maps.
- **Solution guarantees.** LP is convex with global optimality certificates. MILP can provide global optima but via combinatorial search; practitioners often accept a small optimality gap for speed. NLP is globally optimal only if convex; otherwise solvers return high-quality locally optimal, stationarity-certified solutions. For PtH: LP gives reproducible “best-response” schedules; MILP gives auditably optimal (or near-optimal) commitment schedules; NLP gives physics-faithful operating points with local-optimality certificates.

2.2.1 Mathematical formulation

The horizon is discretised into $t = 1, \dots, N_T$. At each step the optimiser chooses a vector of continuous scheduling decisions $v_t \in \mathbb{R}^{n_t}$, and—when joint sizing is studied—a vector $s \in \mathbb{R}^{n^{(s)}}$ of time-invariant design variables. All problem data (forecasts, parameters, prices) enter as coefficients in the constraints and objective. The formulation and algorithms follow the standard theory of linear [121, 122], mixed-integer linear [123, 124, 128], and nonlinear optimisation [125–127].

Linear programming (LP)

A compact, time-banded LP for joint sizing–scheduling is shown in Eq. 2.2

$$\begin{aligned}
\min_{s, v_1, \dots, v_{N_T}} \quad & \kappa^\top s + \sum_{t=1}^{N_T} c_t^\top v_t && \text{objective [121, 122]} \\
\text{s.t.} \quad & A_t v_t \leq b_t + U_t s && \text{per-period inequalities (availability)} \\
& E_t v_t = d_t + V_t s && \text{per-period equalities (balances)} \\
& G_t v_t + H_t v_{t+1} \leq r_t + W_t s, \quad t = 1, \dots, N_T - 1 && \text{intertemporal linear couplings [129]} \\
& \underline{s} \leq s \leq \bar{s} && \text{design bounds} \\
& \ell \leq v_t \leq u, \quad t = 1, \dots, N_T && \text{scheduling bounds}
\end{aligned}$$

2.2

Reading 2.2 (general $\rightarrow$ PtH examples):

Objective and sense. *General:* a linear scalarisation over design and scheduling; minimisation or maximisation according to the study aim [121, 122]. *PtH examples:* minimise total annualised cost where κ represents linearised CAPEX for stacks, storage vessels and interfaces, and c_t collects variable OPEX and tariffs (e.g., electricity purchases for electrolysis, fees for grid use, revenues from by-products). Multi-objective trade-offs (e.g., cost versus emissions) can be handled with the ε -constraint method on the same constraint set [130].

Decision vectors s and v_t . *General:* s are time-invariant design variables; v_t are per-period scheduling variables. *PtH examples:* s includes nameplate ratings such as electrolyser nominal capacity and hydrogen-storage working volume; v_t contains continuous operating levels such as electrolyser hydrogen-production flow, hydrogen-compression flow, BESS charge/discharge power, and grid import/export.

Objective coefficients κ and c_t . *General:* linear weights on s and v_t (costs, penalties, tracking terms, emissions factors, negative revenues). *PtH examples:* κ may encode annualised costs per kW of electrolyser and per kg of storage capacity; c_t may encode hourly electricity prices for electrolysis, revenues from selling oxygen, or penalties for curtailment.

Per-period inequalities $A_t v_t \leq b_t + U_t s$. *General:* linear admissible sets each period with design-coupled ceilings via $U_t s$. *PtH examples:* production or throughput ceilings that scale with installed sizes (e.g., electrolyser utilisation cannot exceed its nameplate; compressor flow cannot exceed rated power); eligibility ceilings (e.g., an hourly cap on eligible renewable electricity attributed to hydrogen).

Per-period equalities $E_t v_t = d_t + V_t s$. *General:* exact linear identities for balances, accounting, and definitions. *PtH examples:* carrier-wise balances (electric, hydrogen, heat) that express conservation at each hour; definitional equalities for KPIs (e.g., energy-attributed hydrogen, counted against a certification ledger within the same hour) so that eligible renewable input is consistently mapped to eligible hydrogen output.

Intertemporal links $G_t v_t + H_t v_{t+1} \leq r_t + W_t s$. *General:* linear couplings between consecutive periods that propagate memory variables (stocks, counters, rolling budgets) [129]. *PtH examples:* hydrogen-storage level between hours t and $t+1$; BESS state of charge; rolling counters for starts or cycling.

Bounds $\underline{s} \leq s \leq \bar{s}$ and $\ell \leq v_t \leq u$. *General:* box constraints exploited by solvers for presolve and scaling. *PtH examples:* admissible design ranges for electrolyser nameplate and storage size; non-negativity and operating ranges for all operating variables (e.g., hydrogen-production flows, compressor loads).

Data versus decisions. *General:* matrices $(A_t, E_t, G_t, H_t, U_t, V_t, W_t)$, vectors (b_t, d_t, r_t) and bounds $(\ell, u, \underline{s}, \bar{s})$ are data; only (s, v_t) are optimised. *PtH examples:* data include hourly

renewable availability, electricity and gas prices, tariffs for grid services, ambient conditions, and certification flags (e.g., hourly eligibility, monthly windows).

Structure and solvers. *General:* only neighbouring periods couple, yielding a block-banded, very sparse constraint matrix; modern LP solvers (revised simplex or interior-point) exploit this structure at scale [121, 122]. *PtH examples:* this enables full-year horizons with certification ledgers and multiple carriers while remaining auditable; representative periods or clustering can be used when N_T is very large, with care to preserve seasonal hydrogen shifts as in [129].

Piecewise-linear surrogates. When device maps are not constant (e.g., part-load efficiency, auxiliary consumption), they are commonly represented by convex piecewise-linear functions using Special Ordered Sets of type 2 (SOS2) or convex-combination variables, preserving the LP structure without binaries [128]. In PtH terms, electrolyser specific consumption or compressor power can be approximated over load bands with linear segments so that dispatch remains continuous and globally optimal for the surrogate.

Mixed-integer linear programming (MILP)

When discrete logic or modularity must be represented, binary/integer vectors are introduced while all relations remain linear. A prototypical MILP extension of Eq. 2.2 is shown in Eq. 2.3:

$$\begin{array}{ll}
 \min_{s, v_1, \dots, v_{N_T}, \delta_1, \dots, \delta_{N_T}} & \kappa^\top s + \sum_{t=1}^{N_T} (c_t^\top v_t + d_t^\top \delta_t) & \text{objective [123, 128]} \\
 \text{s.t.} & A_t v_t + B_t \delta_t \leq b_t + U_t s & \text{per-period linear limits with modes} \\
 & E_t v_t + F_t \delta_t = d_t^- + V_t s & \text{balances with mode selection} \\
 & G_t v_t + H_t v_{t+1} + K_t \delta_t + L_t \delta_{t+1} \leq r_t + W_t s & \text{intertemporal links incl. on/off} \\
 & M_t v_t + N_t \delta_t \leq q_t & \text{linking (big-M [128])} \\
 & \underline{s} \leq s \leq \bar{s} & \text{design bounds} \\
 & \ell \leq v_t \leq u, \quad t = 1, \dots, N_T & \text{scheduling bounds} \\
 & \delta_t \in \{0, 1\}^{n^{(\delta)}}, \quad t = 1, \dots, N_T & \text{binary/integer domains}
 \end{array}
 \tag{2.3}$$

Reading Eq. 2.3 (general $\rightarrow$ PtH examples):

Discrete mode variables δ_t . *General:* encode on/off, mutually exclusive operating regimes, or counts of identical modules. *PtH examples:* binaries for EL online/offline or HS charge/discharge selection; integer entries for the number of EL stacks chosen from a catalogue.

Linking constraints. *General:* ensure continuous decisions respect the active mode (upper/lower bounds, minimum levels) via big-M or stronger convex-hull formulations [128]. *PtH examples:* if the EL is online ($\delta_t = 1$) then hydrogen production lies within its stable operating range; if offline ($\delta_t = 0$) production is zero. For mutually exclusive routing, binaries select exactly one outlet and linear constraints enforce zero flow on non-selected paths.

Intertemporal logic with binaries. *General:* standard linear start/stop and minimum up/down inequalities are written on the δ_t sequence [123]. *PtH examples:* warm/cold behaviour (minimum idle times before restart), minimum run times for EL or compressors to limit cycling, and linear ramp-type inequalities to smooth large changes in hydrogen flows.

Cost terms and optimality gaps. *General:* mode-dependent costs (e.g., start-up costs) enter linearly through $d_t^\top \delta_t$; global optimality is provided by branch-and-bound/branch-and-

cut, typically within a user-set optimality gap [123]. *PtH examples*: start-up penalties for EL cold starts or fixed costs for bringing ancillary systems online.

Formulation strength. *General*: Once binary variables are introduced, different MILP formulations can represent the same underlying logic. Some of these are stronger, in the sense that their LP relaxations are tighter (smaller integrality gaps), so branch-and-bound can prune more nodes and solve the MILP more quickly, even though each node still solves a standard LP [128]. *PtH examples*: using convex-hull formulations instead of loose big-M inequalities for minimum-load zones or for mutually exclusive routing in hydrogen manifolds can materially reduce the number of explored nodes and the wall-clock time for year-long horizons with thousands of binary decisions.

Scalability notes. LP problems such as Eq. 2.2 scale to full-year horizons with multiple carriers thanks to sparsity and time banding [121, 122]. MILP problems such as Eq. 2.3 inherit sparsity but add combinatorial complexity; performance is governed by formulation strength, presolve, and decomposition. In practice, representative periods, rolling-horizon solves, or problem partitioning across carriers can be used while retaining deterministic guarantees on the chosen surrogate [128, 129].

Nonlinear programming (NLP) and mixed-integer nonlinear programming (MINLP)

When smooth nonlinear physics or performance maps must be retained (for example, load-dependent conversion efficiencies, compression power laws or temperature–pressure effects), the joint sizing–scheduling problem is formulated as an NLP; if discrete logic is simultaneously required (on/off modes, mutually exclusive routing, modular investments), the problem becomes a MINLP. The generic deterministic form is shown in Eq. 2.4:

$$\begin{aligned}
& \min_{s, v_1, \dots, v_{N_T}} && F(s, v_1, \dots, v_{N_T}) \\
& \text{s.t.} && g_t(s, v_t; \xi_t) = 0, \quad t = 1, \dots, N_T, \\
& && \mathcal{H}_t(s, v_t; \xi_t) \leq 0, \quad t = 1, \dots, N_T, \\
& && \Phi_t(s, v_t, v_{t+1}) = 0, \quad t = 1, \dots, N_T - 1, \\
& && s \in \mathcal{Z}, v_t \in \mathcal{U} \quad (\text{and } \delta_t \in \{0, 1\}^{n^{(\delta)}} \text{ in MINLP}).
\end{aligned} \tag{2.4}$$

Eq. 2.4 is the standard smooth constrained optimisation template: a differentiable objective $F(\cdot)$ with equality $g_t(\cdot) = 0$ and inequality $\mathcal{H}_t(\cdot) \leq 0$ constraints at each period, plus an intertemporal recursion $\Phi_t(\cdot) = 0$ that advances memory variables across time. For NLP, state-of-the-art solvers use interior-point or sequential quadratic programming (SQP) with derivative information [125–127]. For convex MINLP, outer-approximation and Generalised Benders provide deterministic guarantees; for non-convex MINLP, spatial branch-and-bound with convex relaxations is the classical deterministic approach [131].

Reading Eq. 2.4 (general $\rightarrow$ PtH examples):

Objective $F(s, v_1, \dots, v_{N_T})$. *General*: smooth cost or profit including investment terms and time-coupled operating terms; differentiable penalties can represent wear or auxiliary use. *PtH examples*: continuously differentiable operating cost including EL specific electricity consumption as a smooth function of utilisation; compressor power as a smooth function of flow and pressure ratio; differentiable surrogates for stack degradation as functions of operating point and hours.

Per-period smooth equalities $g_t(s, v_t; \xi_t) = 0$ [126]. *General*: algebraic balances, device performance relations and definitional identities that are smooth in the decision variables. *PtH examples*: a smooth map tying EL hydrogen production and electricity draw

via load-dependent efficiency; a compressor relation linking shaft power, hydrogen flow and pressure ratio with isentropic or polytropic exponents.

Per-period smooth inequalities $\mathcal{H}_t(s, v_t; \xi_t) \leq 0$ [125]. *General*: operating ranges, convex or non-convex envelopes, emission or power-quality limits represented by smooth functions. *PtH examples*: a differentiable upper envelope on EL current density as a function of temperature; a smooth maximum on compressor discharge temperature.

Intertemporal recursion $\Phi_t(s, v_t, v_{t+1}) = 0$ [126]. *General*: a smooth state update that advances inventories or other memory variables. *PtH examples*: HS level as a continuously updated state driven by production, compression and dispensing flows; BESS SOC as a smooth recursion if round-trip efficiency or losses are modelled with differentiable functions; a smooth rolling counter for usage-dependent degradation.

Domains and logical structure. *General*: $s \in \mathcal{Z}$ and $v_t \in \mathcal{U}$ impose box/convex domain constraints; discrete logic is captured by additional binaries δ_t in MINLP. *PtH examples*: continuous variables include EL hydrogen production, compressor mass flow, BESS charge/discharge and hydrogen dispensing rate; MINLP binaries switch operating modes (online/offline, warm/cold), choose exclusive routing (to HS versus to a dispenser), or select module counts from a catalogue.

Typical nonlinear blocks in the hydrogen chain.

- *Conversion maps*: specific electricity use for hydrogen production as a smooth function of normalised utilisation; FC electrical efficiency as a smooth function of load fraction. These enter $g_t(\cdot)$ and/or $\mathcal{H}_t(\cdot)$ and preserve differentiability for interior-point solvers (e.g., IPOPT) and SQP [126, 127].
- *Compression power*: shaft power as a smooth function of mass flow and pressure ratio (polytropic/isentropic models). This appears in $g_t(\cdot)$ and couples hydrogen and electric subproblems nonlinearly.
- *Thermal coupling*: differentiable relations for heat recovery and cooling loads, linking temperatures and duties; this allows co-optimising thermal and hydrogen subsystems with smooth constraints [126].
- *Smooth degradation surrogates*: differentiable penalties as functions of cumulative operating hours or distance from nominal load. These appear in $F(\cdot)$ or $\mathcal{H}_t(\cdot)$ and bias operation away from damaging regimes while keeping the problem smooth.

Why use NLP in PtH plants (fidelity gains). NLP retains smooth performance maps that are difficult to linearise without loss of fidelity: (i) load-dependent conversion efficiency in EL and FC; (ii) compression and expansion power laws as functions of flow and pressure ratio; (iii) temperature-coupled limits (e.g., discharge temperature, thermal management); (iv) smooth surrogates of ageing and degradation as functions of operating point. Keeping these maps differentiable allows interior-point/SQP solvers to compute high-quality stationary points with rigorous first-order optimality certificates [125, 127].

A large share of deterministic PtH formulations can be interpreted within the broader multi-energy systems (or energy hub) paradigm, where electricity, hydrogen (and optionally heat) are coupled through conversion and storage units and coordinated through a single optimisation model [132, 133]. This lens is useful to compare studies that differ in modelling fidelity (LP/MILP vs. NLP/MINLP), time resolution and policy constraints, and it provides a consistent baseline for the stochastic extensions discussed in Section 2.3.

2.2.2 Scientific literature on deterministic optimisation for PtH plants

LP

A large strand of the PtH literature uses linear programming to co-optimize design and operation under perfect foresight while keeping all decisions continuous and all constraints linear. In practice this means writing hourly energy and mass balances, capacity and availability limits, and simple intertemporal stock updates in linear form, and representing load-dependent device behaviour with convex piecewise-linear surrogates so that the overall problem remains an LP. The appeal is twofold: LPs scale to year-long horizons with many technologies and time-coupled inventories, and they deliver globally optimal solutions with economically interpretable dual variables (shadow prices).

On portfolio operations and markets, Voulkopoulos et al. build a pure LP for an aggregator that co-schedules renewables, EL, and participation in electricity, hydrogen and green-certificate markets [134]. Because all commitments are modelled as continuous, the result is a fast model that exposes where profit comes from (price spreads, certificate values, EL utilisation windows) and how the marginal value of capacity changes with policy and market conditions—LP dual variables (shadow prices) can make such margins transparent.

For design screening with multiple criteria, González Palencia et al. formulate a cradle-to-gate LP that compares hydrogen-production routes while trading off cost, energy and water use, and CO₂ intensity [135]. By keeping production levels and energy purchases continuous and by using linear resource and emission accounting, they quantify when renewable-electricity-based electrolysis becomes competitive, and how water constraints and grid mix affect route choice. The LP structure makes these trade-offs explicit and reproducible before introducing discrete investment choices.

Whole-system studies also rely on LP to integrate hydrogen as a carrier across sectors. Koirala et al. develop an integrated electricity–hydrogen–methane model for the Netherlands that couples production, transmission and storage across spatial nodes and long horizons using linear balances and stock equations [136]. They report how hydrogen pipelines and storage shift system costs and locational marginal values as renewable penetration rises, and they show spatial patterns in the utilisation of EL and methanation driven by nodal price signals obtained from the LP duals. Methodologically, Diéguez et al. publish a transparent LP formulation for high temporal and technological resolution energy-system models with hydrogen chains, presenting a linear formulation that assigns hourly, daily, or yearly temporal constraints by subsystem (e.g., hourly for electricity, daily for gas), which controls time coupling and preserves sparsity/tractability [137]. In the same spirit, the *TIMES* family is documented as a linear-programming generator for multi-sector planning; the reference documentation explains how hydrogen technologies, storage and end uses enter as continuous flows with linear stock and availability constraints, which is why *TIMES* remains a workhorse for policy scenarios where tractability and transparency are essential [138].

Finally, there is a growing literature on improving LP fidelity for EL without sacrificing tractability. Raheli et al. propose tight convex representations of EL part-load behaviour, including a fully linear relaxation and a second-order conic alternative [139]. They show that these relaxations can remove binaries, preserve convexity, and remain accurate under typical operating regimes, leading to near-LP solve times with better dispatch realism than constant-efficiency approximations.

Advantages and drawbacks of LP. Linear programming gives globally optimal solutions, scales to full-year horizons, and yields shadow prices that help explain marginal values of capacity, energy and policy constraints. It is therefore well suited to screening designs,

valuing certificates, and understanding the complementary roles of electricity, hydrogen and storage at plant-to-system scale. The main limitations are the need to linearise device maps, the inability to natively represent on/off or mutually exclusive operations without moving to MILP, and the risk of understating start–stop costs or nonlinear effects. In practice, LP provides a clean baseline that many studies then extend with MILP for commitment logic or with convex/nonlinear models where detailed physics materially affect the optimum.

MILP

MILP is the dominant deterministic framework when joint sizing and scheduling must capture discrete plant logic and modular investment while preserving linear relations elsewhere. In PtH settings, MILP turns on/off decisions, mutually exclusive routing, minimum up/down times, and start/stop costs into binary variables linked to continuous flows and capacities through linear constraints. This preserves scalability to year-long horizons and delivers globally optimal designs and hourly schedules under perfect foresight, while allowing richer operational realism than LP.

At the plant scale, Marocco et al. develop a year-long MILP for an off-grid island community integrating PV, BESS, EL, HS and FC [140]. The model uses piecewise-linear performance for EL and monetised wear for BESS and FC stacks; it co-optimises capacities and hourly operation. The main conclusions are that HS is critical for seasonal balancing when islanded, BESS remain essential for short-term smoothing, and the jointly optimised MILP policies outperform heuristic sizing/dispatch in total cost. Pushing seasonal storage further, Pilotti et al. co-design fully renewable, dispatchable plants for Sicily with wind, PV, BESS and hydrogen seasonal storage [141]. Their MILP quantifies how the advantage of hydrogen depends strongly on storage technology and cost: compressed tanks offer limited gains at current prices, whereas low-cost geological storage enables materially lower system costs and a dispatch that reliably meets load with high renewable shares.

Beyond single plants, MILP is widely used to design hydrogen supply chains and infrastructures with spatial detail. Seo et al. propose a centralised storage concept and solve a supply-chain MILP that consolidates production from multiple sites into an integrated bulk storage before distribution to HRS [142]. They compare alternative production and transport routes and show how centralisation reduces the total annual cost and accelerates a shift to central production/liquefaction; at mature demand levels, bulk storage with pipeline distribution becomes optimal; route selection remains sensitive to demand intensity and siting.

MILP also makes it straightforward to encode regulatory constraints and piecewise device behaviour. Graber et al. present a day-ahead MILP for PEMEL that explicitly enforces key elements of the EU green-hydrogen framework (additionality and temporal correlation translated into energy-source quotas over the day) and models part-load efficiency with linear segments [143]. They test full-load versus partial-load strategies against daily hydrogen targets and show how regulatory energy-source limits reshape optimal hours of operation and raise the delivered cost compared with unconstrained operation; the formulation offers a transparent way to quantify the cost of compliance while retaining fast solve times.

At the methodological end, the spatio-temporal MILP formulations by Samsatli and co-authors provide blueprints that have been adopted in many PtH studies. The 2015 framework sets out a general network model with storage and transport over space and time using linear balances with integer investment/logical choices, designed to scale to high temporal resolution [144]. The 2018 extension casts the design–operation problem as a multi-objective MILP, allowing explicit trade-offs (e.g., cost versus emissions) on integrated multi-vector networks [145]. Their application to Great Britain’s wind–hydrogen–electricity system for

decarbonising domestic transport shows how the MILP places EL, pipelines and stations while scheduling wind-coupled hydrogen production; outcomes include the identification of cost-effective siting patterns, infrastructure build-out phases, and the value of storage and network expansion under transport-demand scenarios [146]. Collectively, these works exemplify why MILP has become the workhorse for PtH joint sizing–scheduling when discrete choices matter across devices, networks, and policies.

Advantages and drawbacks of MILP. MILP inherits LP’s interpretability and scalability while adding the ability to model on/off logic, minimum run times, start-up costs and mutually exclusive routing—all central to realistic EL, compressor and HS operation, and to siting modular investments in plants and networks. Global optimality certificates (within a user-set optimality gap) support robust benchmarking and scenario studies. The trade-offs are increased computational burden compared with LP, sensitivity to formulation strength (e.g., tight linking constraints versus weak big-M), and a continuing need to linearise nonlinear device physics; when detailed thermodynamics or ageing laws dominate performance, practitioners either refine piecewise-linear approximations or adopt NLP/MINLP where fidelity is decisive.

NLP/MINLP

Although linear and mixed-integer linear formulations dominate the PtH literature, a growing thread uses NLP or MINLP when authors keep smooth device maps (for example, load-dependent EL performance, compression work as a function of flow and pressure) or must co-optimize discrete equipment choices together with nonlinear physics. These models are particularly visible in plant-level and microgrid settings where EL operation, HS, and sometimes power–gas coupling are optimised jointly.

At the plant scale, Saars et al. formulate the operation and sizing of an EL co-located with HS as an NLP driven by day-ahead electricity prices and an annualised-cost objective. They compare a NLP method with an LP approach for an EL+HS case, retaining explicit nonlinearities (e.g., compressor power). They obtain very similar costs of 5 €/kg while keeping smooth relations in the objective and compressor model, highlighting the value of preserving performance maps when capacity (EL nameplate) and hourly operation (run profiles and HS use) are co-optimised to exploit price arbitrage [147].

At system scale within a microgrid, Akülker and Aydin develop a deterministic MINLP for joint equipment selection and scheduling in a multi-energy microgrid that explicitly includes a PtG chain with electrolysis. The superstructure spans conventional and renewable generators, thermal units, storage, and a PtG block; integer variables select units while nonlinear relations capture part-load and process couplings. Their case studies show how carbon policy (cap-and-trade versus tax) reshapes the economically optimal portfolio and dispatch, and how adding the PtG route changes the sizing of other assets through sector coupling. A follow-up study focuses on which microgrid technologies to co-install with a PtG system and shows that coupling to chemical conversion shifts the microgrid towards higher renewable utilisation while meeting heat and gas service requirements [148, 149].

Coupled power–gas operation is another context where retaining nonlinear physics motivates MINLP. Abdallah et al. co-optimize a day-ahead schedule for an integrated electric and gas system with a PtH unit, modelling generator commitment logic alongside nonlinear power-flow and gas-network relations within a MINLP. Across seasonal cases on standard test networks, they report reductions in total operating costs and renewable curtailment when hydrogen conversion is co-optimised with the rest of the system, illustrating the multi-vector value of PtH when the nonlinear coupling between networks is retained [150].

While the focus here is plant and multi-energy optimisation rather than transmission planning, network-facing MINLP studies are relevant because they embed EL production and hydrogen blending decisions alongside nonlinear gas-flow physics. Ogbe et al. formulate a multi-period MINLP for placing PtH and methanation units and determining hydrogen and CO₂ blending levels in a natural-gas network, showing notable system-cost reductions and feasible hydrogen fractions when the full nonlinearity of blending and gas hydraulics is respected; this demonstrates how PtH design and operation interact with downstream transport constraints when the physics is not linearised [151].

Advantages and drawbacks of NLP/MINLP. Retaining smooth component maps improves physical fidelity for PtH chains, especially when compressor work, pressure–temperature effects, or load-dependent stack efficiency materially affect cost and feasibility; adding integer structure allows realistic equipment choice and on/off logic in the same model. These gains come with higher computational burden and, for non-convex NLP/MINLP, with local-optimality or global-optimisation effort; results also depend on model calibration for device maps. In practice, authors either scope the time horizon, decompose the problem, or mix continuous NLP plant models with discrete investment decisions, but the cited studies show that NLP/MINLP can deliver actionable insights on cost, sizing, and dispatch where linear surrogates would be misleading.

2.3 Stochastic optimisation

Deterministic optimisation assumes a single, fixed realisation of the inputs (renewable availability, demands, prices) and delivers capacities and schedules that are optimal for that forecast. In practice, PtH assets are exposed to substantial variability and forecast errors across multiple time scales: intra-hour ramps from clouds or wind shear, day-to-day weather shifts, multi-week low-renewable episodes, and price volatility across day-ahead, intraday and balancing markets. Solutions optimised for one nominal year can therefore underperform or even violate operational or certification constraints when realised conditions deviate. Stochastic optimisation addresses this by treating selected inputs as random variables and by splitting decisions into here-and-now choices (e.g., sizes, long-lived commitments) and recourse actions that adapt to the information revealed over time [152–154].

Two modelling patterns are prevalent in energy systems:

- *Two-stage models* choose capacities before uncertainty is realised and then, for each scenario of weather and prices, compute an adaptive operating schedule that respects physics and policy constraints. The objective is typically expected total cost (risk-neutral) or a risk-averse functional such as Conditional Value-at-Risk (CVaR) that penalises costly tails, thereby quantifying the premium for robustness (e.g., larger storage to ride through long low-renewable periods) [152, 155, 156].
- *Multi-stage models* mirror the offer–realisation sequence of electricity markets and forecast updates. Day-ahead offers are set with limited information, intraday redispatch updates the plan after new forecasts arrive, and real-time balancing handles residual error. Non-anticipativity constraints enforce that decisions at the same stage with the same revealed history coincide, while subsequent stages adapt by scenario node [153, 154].

Compared with the deterministic baseline, stochastic formulations provide three main benefits for PtH:

1. *Hedging and flexibility valuation.* They measure how much flexible capacity (e.g., additional HS, oversized interfaces, faster-ramping EL) reduces expected operating cost and exposure to tail events—effects that are often invisible in a single-forecast optimisation.
2. *Compliance under variability.* Certification rules (e.g., temporal correlation between eligible RES and hydrogen production) can be enforced scenario-wise, revealing the cost of compliance across years and the risk of infeasibility if designs are too tight for adverse realisations.
3. *Market-aligned decision-making.* Multi-stage models align with day-ahead/intraday/balancing timelines, enabling explicit trade-offs between offer conservatism and expected imbalance costs, and showing how storage/inertia improves the risk–return profile of market strategies.

These advantages come with costs and modelling choices:

- *Scenario design.* The fidelity of results depends on realistic scenarios for meteorology and prices. Standard practice samples multiple historical years and forward price paths, then applies scenario reduction to control computational size while keeping the reduced measure close to the original and retaining temporal patterns via multistage-tree construction when needed [157, 158]. Sample Average Approximation (SAA) provides consistency as the number of scenarios grows [159].
- *Risk attitude.* Risk-neutral objectives minimise expected cost; risk-averse objectives often use coherent measures such as CVaR, which can be modelled with auxiliary variables and linear/convex constraints to limit exposure to extremes. The choice affects optimal sizing and dispatch (e.g., risk-averse models tend to favour additional HS or curtailment flexibility) [155, 156].
- *Computational strategy.* Scenario trees and long horizons make the models large, so decomposition is used to split the problem into smaller pieces. Benders/L-shaped methods separate first-stage decisions from per-scenario subproblems [160]. Progressive hedging coordinates scenarios by adding penalties to encourage consistency across them [161]. For multistage linear/convex models, Stochastic Dual Dynamic Programming (SDDP) is also common in practice. In mixed-integer or highly detailed settings, these ideas are often combined with heuristic or problem-specific simplifications.
- *Model class.* As in the deterministic case, stochastic programmes may be LP, MILP, NLP or MINLP depending on device detail and logic. Linearity and piecewise linearity favour scalability and tighter decompositions; mixed-integer or nonlinear recourse increases difficulty and may require problem-specific strengthening or hybrid workflows.

For PtH specifically, the uncertain drivers typically include: (i) RES profiles (solar, wind), (ii) wholesale and imbalance prices across market stages and (iii) process demands for hydrogen/heat when co-sited with industry. Stochastic models allow all of these to vary across scenarios or tree nodes, while enforcing the same engineering and policy constraints scenario-wise.

2.3.1 Mathematical formulation

Two-stage stochastic optimisation

Two-stage stochastic optimisation for joint sizing–scheduling is summarised in Figure 2.2: the here-and-now design vector s is chosen once, while scenario-wise recourse trajectories $(x_{t,\omega}, v_{t,\omega})$ adapt to the realised inputs with probabilities π_ω . Formally, for a finite scenario set Ω with probabilities π_ω , the risk-neutral two-stage problem can be written as Eq. 2.5.

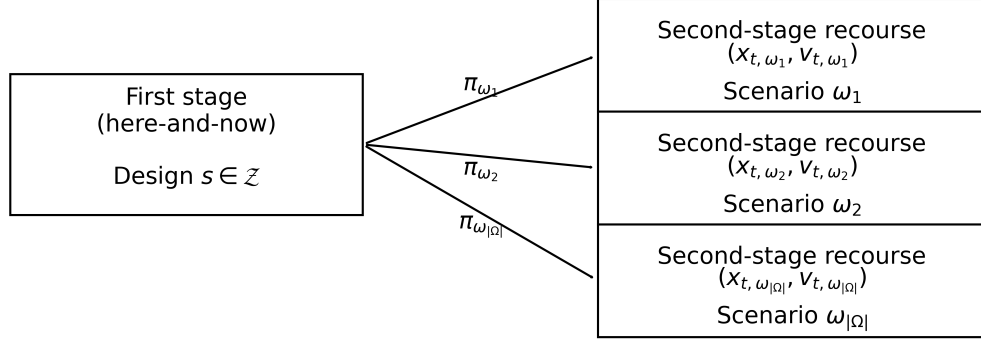


Figure 2.2: Two-stage stochastic formulation for joint sizing–scheduling: here-and-now design s and scenario-wise recourse trajectories $(x_{t,\omega}, v_{t,\omega})$ with probabilities π_ω .

As shown in Eq. 2.5, let Ω be a finite scenario set with probabilities π_ω (built from sampled and possibly reduced time series of uncertain inputs) [157–159]. Denote by $s \in \mathbb{R}^{n^{(s)}}$ the here-and-now design vector (time-invariant capacities), and by $\{x_{t,\omega}, v_{t,\omega}\}_{t=1}^{N_T}$ the per-scenario, per-period state and scheduling vectors. A risk-neutral two-stage programme is shown in Eq. 2.5:

$$\begin{aligned}
 \min_{s, \{x_{t,\omega}, v_{t,\omega}\}} \quad & J(s) + \sum_{\omega \in \Omega} \pi_\omega \sum_{t=1}^{N_T} \mathcal{L}(x_{t,\omega}, v_{t,\omega}; \xi_{t,\omega}) && \text{objective [152, 153]} \\
 \text{s.t.} \quad & x_{t+1,\omega} = f(x_{t,\omega}, v_{t,\omega}; \xi_{t,\omega}), \quad t = 1, \dots, N_T-1, \forall \omega && \text{state recursion per scenario} \\
 & g(x_{t,\omega}, v_{t,\omega}; \xi_{t,\omega}, s) = 0, \quad \forall t, \forall \omega && \text{per-period equalities (balances)} \\
 & \mathcal{H}(x_{t,\omega}, v_{t,\omega}; \xi_{t,\omega}, s) \leq 0, \quad \forall t, \forall \omega && \text{per-period inequalities (limits)} \\
 & x_{1,\omega} = \bar{x}_1, \quad x_{N_T+1,\omega} = x_{1,\omega}, \quad \forall \omega && \text{boundary (cyclic inventories)} \\
 & s \in \mathcal{Z}, \quad x_{t,\omega} \in \mathcal{X}, \quad v_{t,\omega} \in \mathcal{U}, \quad \forall t, \forall \omega && \text{domains and feasibility sets}
 \end{aligned} \tag{2.5}$$

Reading Eq. 2.5 (general $\rightarrow$ PtH examples):

Here-and-now s . *General:* time-invariant capacities common to all scenarios; chosen before uncertainty is realised [152]. *PtH examples:* EL nominal power, HS capacity, BESS capacity.

Recourse $\{x_{t,\omega}, v_{t,\omega}\}$. *General:* scenario- and time-indexed states and schedules that adapt to realised series $\xi_{t,\omega}$. *PtH examples:* hourly EL production set-point, HS charge/discharge, BESS charge/discharge, and grid import/export decided per weather/price scenario.

Objective. *General:* investment cost $J(s)$ plus expected operating cost $\sum_w \pi_w \sum_t \mathcal{L}(\cdot)$ [152]. *PtH examples:* annualised CAPEX for stacks, tanks and interfaces in $J(s)$; in $\mathcal{L}(\cdot)$, electricity purchases for electrolysis, O&M, market revenues/fees, imbalance/curtailment penalties, and monetised degradation where used.

State recursion $x_{t+1,w} = f(\cdot)$. *General*: per-scenario intertemporal update of inventories and other memory variables [153]. *PtH examples*: HS level carried across hours in each scenario; BESS SOC; rolling counters if used for simplified wear.

Per-period constraints $g(\cdot) = 0$, $\mathcal{H}(\cdot) \leq 0$. *General*: balances, operating limits and design couplings enforced scenario-wise [152]. *PtH examples*: carrier-wise conservation equalities and operating envelopes per hour and scenario.

Cyclic boundary $x_{N_T+1,w} = x_{1,w}$. *General*: closes yearly ledgers to avoid end effects; enforced scenario-wise. *PtH examples*: end-of-year HS equals the initial level for every scenario; same for BESS SOC and any rolling ledgers so that seasonal shifting is modelled consistently across realisations.

Model class and tractability. Problem 2.5 inherits the deterministic class: linear without binaries (LP); on/off or modularity (MILP); smooth nonlinear maps (NLP/MINLP).

Scenario design. Scenarios are typically built from multiple historical meteorological years and associated price trajectories (with resource correlation), then reduced to a tractable subset that preserves moments and persistence patterns important for long-duration HS utilisation [157, 158]. SAA provides statistical consistency as the number of scenarios grows [159]. In PtH studies this preserves clusters of low-renewable hours and seasonal effects that drive HS value.

Note on risk aversion. While Eq. 2.5 is written in risk-neutral form, risk-averse variants are common in PtH to hedge costly tails (e.g., long calm-and-cloudy periods with high prices). CVaR and related coherent measures can be embedded on the same physical constraints to reshape sizing and operating policies toward robustness [155, 156].

Multi-stage stochastic optimisation

The multi-stage extension aligns decisions with the chronology of day-ahead (DA), intraday (IM), and real-time (RT) markets, as sketched in Figure 2.3. Each node n in the scenario tree aggregates decisions v_n at a given information state, and non-anticipativity constraints enforce identical decisions at nodes that share the same history at a given stage k . A generic risk-neutral multi-stage formulation is given in Eq. 2.6.

When offers and redispatch decisions are made at several information stages, a scenario tree aligns the optimisation with the forecast–market chronology. Let stages be $k = 0, \dots, K$, with node sets $\mathcal{N}_k$ and probabilities p_n for each node $n \in \mathcal{N}_k$ (summing to one over terminal nodes). We take $p_{\text{root}} = 1$ and, for any internal node n , $\sum_{c \in \mathcal{C}((n))} p_c = p_n$; probabilities over terminal nodes sum to one. Each node aggregates the hours decided at that stage; $\mathcal{C}((n))$ denotes the children of node n , and ζ_n is the information revealed up to n . A risk-neutral multi-stage programme is shown in Eq. 2.6 [152–154]:

$$\begin{aligned}
\min_{\{v_n\}} \quad & \sum_{k=0}^K \sum_{n \in \mathcal{N}_k} p_n \Phi_k(v_n) && \text{objective (expected stage cost [152, 154])} \\
\text{s.t.} \quad & \mathcal{F}_k(v_n, \{v_c\}_{c \in \mathcal{C}((n))}; \zeta_n) = 0, \quad \forall n && \text{node physics \& recursion} \\
& \mathcal{H}_k(v_n, \{v_c\}_{c \in \mathcal{C}((n))}; \zeta_n) \leq 0, \quad \forall n && \text{operating limits \& capacities} \\
& v_n = v_{n'} \quad \forall (n, n') \in \Pi_k, \quad k = 0, \dots, K && \text{non-anticipativity constraints} \\
& v_n \in \mathcal{Y}_k \quad \forall n && \text{stage-specific domains}
\end{aligned} \tag{2.6}$$

Non-anticipativity. For each stage k , Π_k collects pairs of nodes in $\mathcal{N}_k$ that share the same information history up to k ; enforcing $v_n = v_{n'}$ for $(n, n') \in \Pi_k$ prevents using future information [154].

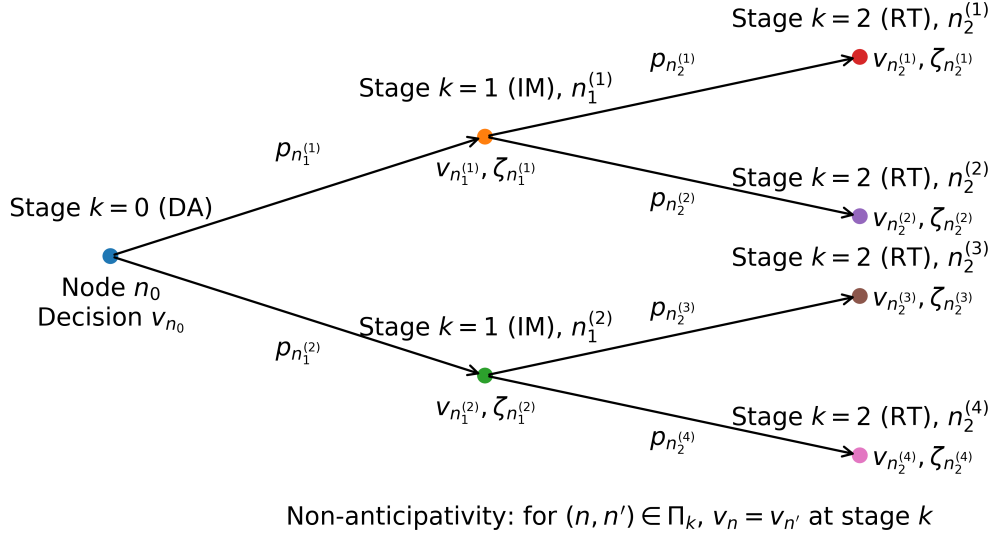


Figure 2.3: Multi-stage scenario tree aligned with day-ahead (DA), intraday (IM), and real-time (RT) decisions; non-anticipativity enforces identical decisions v_n at nodes sharing the same information history at a given stage k .

Reading 2.6 (general $\rightarrow$ PtH examples):

Scenario tree and stages. General: the tree encodes how information arrives and when decisions are committed; nodes represent decision points, and edges represent uncertainty realisations between stages [152, 154]. PtH examples: stage $k=0$ is day-ahead (DA) where hourly energy and reserve offers are set for the next day; stage $k=1$ is intraday (IM) where redispatch adapts to updated forecasts; stage $k=2$ is real-time (RT) where balancing actions are decided. A node $n \in \mathcal{N}_0$ aggregates the DA hours; its children in $\mathcal{N}_1$ reflect alternative IM forecast updates; terminal nodes reflect RT outcomes.

Stage decisions v_n . General: v_n are decisions available at node n given information ζ_n ; children decisions may depend on v_n and the subsequent information [154]. PtH examples: at DA nodes, v_n collects submitted offers (hourly schedules, reserve commitments) and coarse within-day setpoints; at IM nodes, v_n updates schedules and reserve activation windows; at RT nodes, v_n covers fine-grained dispatch, imbalance settlement and any curtailment.

Physics and intertemporal coupling $\mathcal{F}_k, \mathcal{H}_k$. General: functions $\mathcal{F}_k, \mathcal{H}_k$ assemble balances, device limits and state recursion across the hours grouped at each node and across parent-child links; they carry memory by linking node decisions v_n between stages [153, 154]. PtH examples: hydrogen inventory or battery state of charge; market rules are enforced at the appropriate stage.

Non-anticipativity. General: decisions at the same stage that share the same revealed history must be equal across nodes; this encodes that one cannot condition a stage- k decision on information revealed later [154]. PtH examples: all DA nodes that share the same DA forecast path must place identical DA bids (even though their IM and RT realisations later differ).

Objective. General: the expected sum of stage costs, $\sum_k \sum_{n \in \mathcal{N}_k} p_n \Phi_k(y_n)$, where Φ_k aggregates the cost terms associated with the hours decided at stage k [152]. PtH examples: at DA, Φ_k may include commitment costs and expected market revenues tied to offers; at IM/RT, Φ_k includes redispatch costs, imbalance charges, curtailment penalties and operating costs tied to the realised trajectory.

Model class and tractability. General: problem 2.6 inherits the LP/MILP/NLP character of the stage constraints. Tree size grows with horizon and branching, so decomposition and aggregation are essential. Progressive hedging provides a practical scenario-decomposition that enforces stage-wise non-anticipativity via quadratic penalties [161, 162]. PtH examples: a DA–IM–RT tree with hourly resolution remains tractable when device maps are linear/piecewise-linear (LP/MILP).

Tree construction and reduction. General: nodes are built from forecast-update processes (e.g., DA point forecast and error distribution, IM update distribution) and from market session timing; scenario reduction controls branching while keeping the reduced measure close (in a probability-metric sense) to the original and aiming to retain temporal patterns important for storage [157, 158]. PtH examples: DA nodes reflect daily solar/wind forecasts and price shapes; IM nodes reflect intraday markets prices; RT leaves capture residual errors. Reduction preserves clusters of consecutive low-renewable hours and correlated price spikes.

Note on risk aversion. While 2.6 is written in risk-neutral form, risk-averse preferences can be incorporated with stage-wise or nested coherent risk measures (for example, CVaR) on the same stage structure [153]; this often shifts PtH designs toward more storage or more conservative market offers without changing the physical constraint architecture.

2.3.2 Scientific literature on stochastic optimisation for PtH plants

Two-stage

A first stream of work casts PtH within two-stage scenario-based programmes where investment or day-ahead commitments are chosen here-and-now and hourly plant operation adapts by scenario. One of the earliest PtH-focused studies [163] develop a two-stage stochastic programming approach for an energy hub that explicitly contains a water electrolyser and compressed hydrogen storage. The first stage plans electrolyser and storage capacities alongside long-lived decisions; the second stage operates the hub across a large set of sampled scenarios capturing uncertainty in hourly electricity prices, the number of fuel-cell vehicles to be refuelled, and the dispensed hydrogen quantity. Using a scenario-based two-stage programme with uncertainty in hourly electricity prices and hydrogen refuelling events, the study quantifies the hedging value of PtH flexibility: sizing an electrolyser and hydrogen tank improves expected operating cost and increases revenue opportunities by shifting electricity consumption to low-price hours while meeting stochastic hydrogen demand; sensitivity analyses show that both electrolyser capacity and storage volume co-determine the value captured under volatile prices and demand variability. More generally, two-stage stochastic programming is widely adopted for microgrid planning problems in which long-lived topology/investment decisions precede daily operation under renewable uncertainty; for instance, Han and Lee [164] couple first-stage interconnection decisions with second-stage operational dispatch using data-based renewable scenario models.

At the multi-energy system scale, two-stage models are used to coordinate electricity and gas systems with embedded PtG conversion. [165] formulate a two-stage day-ahead scheduling model for an integrated electricity–natural gas system in which PtG facilities and gas-fired units provide flexibility to accommodate wind variability. The first stage clears day-ahead commitments; the second stage redispatches by scenario (e.g., 1000 scenarios reduced to 7) to meet realisations of wind and loads while enforcing the coupled gas–electric constraints and explicit ramping costs. Results demonstrate that incorporating PtG as a recourse option reduces wind curtailment and ramping costs, and helps satisfy flexibility

requirements compared with a system without PtG, thereby evidencing a systemic value of hydrogen conversion even without long-term geological storage.

At the plant/community scale, two-stage formulations have been applied to multi-energy microgrids that include electrolyzers, hydrogen storage and hydrogen mobility. [166] propose a two-stage risk-aware MILP where the first stage determines market positions and operational commitments, and the second stage adapts the hourly schedule for each scenario of solar/wind availability, electricity prices, and tri-vector demands (electrical, thermal, and hydrogen). The microgrid comprises PV, wind, CHP, a boiler, a hydrogen electrolyser, electrical/thermal/hydrogen storage, and both electric- and hydrogen-vehicle charging stations. Uncertainty is represented by thousands of scenarios reduced via backward reduction, with CVaR used to control tail risk. Using a 24-hour case study solved with CPLEX, it is shown that enabling bilateral contracts alongside pool participation significantly mitigates risk exposure; specifically, the CVaR metric drops by about 50% relative to a pool-only strategy, while hydrogen conversion and storage are actively used in adverse renewable/price realisations to hedge imbalance cost.

Beyond operations, two-stage structures have also been exploited for design and operation (sizing–scheduling) of hydrogen-enabled hubs. [167] build a two-stage design–operation model for an energy hub with hydrogen storage (electrolyser, tank, and FC pathway) and propose a clustering framework to keep long-horizon stochastic instances tractable while preserving temporal features that drive hydrogen utilisation. The study shows that careful multiscale time-series aggregation recovers near-optimal designs and dispatches at a fraction of the computational cost, and highlights the role of hydrogen storage in arbitraging multi-carrier energy flows while maintaining near-optimal performance.

Advantages and drawbacks of two-stage stochastic optimisation. Two-stage models provide a clear separation between here-and-now sizing/commitment and scenario-wise recourse, making them well suited to quantify the hedging value of electrolyzers and hydrogen storage under volatility. They readily incorporate policy or market features (e.g., risk measures, bilateral contracts) and support transparent sensitivity studies on prices and hydrogen demand. Their limitations mirror their strengths: results depend on the quality of scenario generation and reduction; stage aggregation may hide finer market chronologies; and when the recourse includes integer variables (on/off logic, network commitments) or detailed physics, decomposition and aggregation choices become critical for tractability and fidelity.

Multi-stage

Multi-stage stochastic formulations have been used to align PtH scheduling and market participation with the actual chronology of information revelation (e.g., day-ahead offers, intraday updates, real-time balancing) while respecting the intertemporal physics of hydrogen inventories, electrolyser start/stop logic, and storage couplings to BESS or heat. Scenario trees are constructed to mirror the chronology of day-ahead → intraday → real-time revelation, with non-anticipativity enforced at each stage. From a methodological viewpoint, multi-stage stochastic programming is a standard tool to represent sequential electricity-market decisions under uncertainty and partial information revelation, and to enforce non-anticipativity consistently across stages [168]. A representative example is the multi-stage bidding and operation strategy for an HRS proposed by [169]. In that study, the plant comprises an electrolyser, hydrogen storage and dispensing, and participates simultaneously in energy and reserve markets. Uncertainties include day-ahead energy price, secondary reserve price, system imbalance price, and hydrogen demand; non-anticipativity constraints enforce that decisions at a given stage depend only on information available up to that point. The model shows how the combination of reserve commitments and energy arbitrage, enabled by the

electrolyser and on-site storage, increases expected profit relative to energy-only baselines and simpler single-stage setups, and it quantifies the value of flexibility from shifting electricity consumption across market stages while meeting hydrogen service requirements.

Complementary strands of the literature address PtH value through ancillary-service participation and hybridisation with BESS: Maluenda et al. [170] propose a scenario-based (chance-constrained) day-ahead and intra-day scheduling model for a PV–BESS–electrolyzer plant participating in energy and frequency regulation markets, while recent surveys highlight that electrolyzer-based ancillary services are a rapidly growing but still fragmented research area [171].

Beyond single-plant stations, multi-stage models have been extended to electricity–hydrogen Integrated Energy Systems (IES). [172] develop a multi-stage dispatching framework that explicitly links a day-ahead schedule with intraday corrective actions under uncertainty, while embedding the flexibility of hydrogen production and consumption on both source and load sides. The approach combines deep-learning-based online security monitoring with a chance-constrained intraday correction atop a model-based day-ahead schedule, leveraging hydrogen’s ability to decouple renewable generation and final use across the day. Case results indicate lower operating costs and improved security margins versus deterministic scheduling, with the hydrogen layer absorbing forecast errors that would otherwise translate into imbalances or curtailment.

At a larger mesoscale, [173] propose a multi-stage and multi-timescale management strategy for hydrogen-based IES in which decisions are layered across markets and within-day timescales. Although the paper emphasises algorithmic structure (e.g., hierarchical coordination across timescales) rather than market clearing per se, it treats electricity–heat–hydrogen couplings and demonstrates that explicitly staging commitments and recourse improves renewable-energy utilisation and reduces total cost compared with single-stage or purely myopic controllers. The study underscores a recurring outcome in multi-stage PtH models: hydrogen inventories and electrolyser ramping provide the temporal shock absorbers that allow conservative day-ahead positions to be reconciled with aggressive intraday corrections when forecasts improve.

Recent work has pushed the multi-stage paradigm toward high-fidelity hydrogen infrastructure operation with policy constraints. [174] formulate a multi-stage stochastic optimisation for a mono-site hydrogen system (electrolyser, compressor, storage) supplied by variable renewables and grid power under an eligibility rule that limits the fraction of non-renewable electricity so that the site qualifies for public subsidy. Decomposition strategies are tailored to the stage structure and show on realistic instances that the method attains near-optimal solutions with small duality gaps while preserving the chronology of market and forecast updates. This is relevant for EU-style certification and subsidy schemes, where non-anticipativity across stages is essential to avoid ex-post infeasibility.

Finally, multi-stage stochastic optimisation has also been used on longer planning horizons where expansion or sequencing decisions (e.g., staged addition of electrolyser capacity or storage) must be coordinated with uncertain renewable availability and prices. [175] present a multi-stage long-term planning model for a grid-connected hydrogen-based energy system and propose an improved stochastic dual dynamic integer programming variant to handle the stagewise structure efficiently. Results highlight that staging investments while accounting for uncertainty yields more robust and cost-effective plans than static single-stage designs in the tested cases, especially when hydrogen serves seasonal and multi-week balancing roles.

Advantages and drawbacks of multi-stage stochastic optimisation. The multi-stage literature for PtH and electricity–hydrogen IES consistently reports three qualitative outcomes: (i) explicitly modelling market stages with non-anticipativity improves the expected value of flexible hydrogen assets (electrolysers and storage) compared with deterministic or

single-stage benchmarks; (ii) hydrogen inventories are pivotal in reconciling conservative day-ahead commitments with intraday and real-time corrections; and (iii) when policy or eligibility rules apply, enforcing them at every stage avoids optimistic bias and reveals the true cost of compliance. The main challenge is preserving persistence patterns in the scenario-tree construction phase.

2.4 Scope and novelty

Scope. This thesis is concerned with how to make electrolysis-based power-to-hydrogen (PtH) plants economically viable for real industrial users, by systematically reducing the levelised cost of hydrogen (LCOH) under realistic technical, market and regulatory constraints. The plants considered couple variable renewable electricity generation, battery-based electrical energy storage, water electrolyzers, hydrogen compression and hydrogen storage, and back-conversion technologies such as solid oxide fuel cells or gas turbines with heat-recovery steam generators, together with industrial electricity and heat demands in both grid-connected and off-grid settings.

The central question is not whether PtH plants can be engineered in principle, but how they should be designed and operated so that, over a 20–25 year project horizon, the delivered hydrogen is cheap, certifiable and bankable enough to compete with incumbent fossil-based options. To answer this, the thesis develops a single decision-analytics workflow that follows the same logic as real project development: it moves from understanding physics and control logics, through deterministic optimisation, to uncertainty-aware sizing and finally to market-based operation once the plant has been built.

The workflow is staged as follows. First, high-resolution, physics-faithful rule-based simulations are used to understand how individual components in the hydrogen chain behave, how simple operating rules affect efficiency and equipment ageing, and which physical levers are most effective in driving the LCOH down for a given layout. Second, these insights are embedded in a deterministic mixed-integer linear optimisation model of the whole plant that jointly optimises sizing and scheduling under perfect foresight, in order to search systematically for low-cost combinations of capacities and operating strategies for representative years. Third, recognising that 20–25 year forecasts of renewable output, electricity prices and hydrogen demand are inherently uncertain, the same plant model is extended into a two-stage stochastic capacity-planning framework, in which long-lived capacity decisions are made before uncertainty is realised and are then tested across scenarios while short-term scheduling remains flexible. Finally, once a plant is in the ground, a multi-stage stochastic market-scheduling layer is formulated for grid-connected designs, co-optimising participation in day-ahead, intraday, reserve and imbalance electricity markets while meeting hydrogen off-take, and quantifying how informed bidding and hydrogen-based flexibility can further reduce the realised LCOH.

Across all layers, the same component equations, degradation descriptions and European renewable-fuel certification rules are reused, and the same finance-consistent performance indicators (including LCOH, net present value, emissions intensity and certification compliance) are evaluated.

Chapter 3 formalises rule-based, deterministic and stochastic methods into a unified workflow while Chapter 4 applies that workflow to multiple PtH contexts to quantify achievable reductions in the LCOH.

When siting becomes a binding constraint for photovoltaic generation, an additional agrivoltaic option is introduced to signal land-use trade-offs; the agrivoltaic methodology and results are documented in Appendix 7, while the core chapters remain focused on PtH sizing

and scheduling.

Novelty. The main original contribution of this thesis is a coherent workflow for lowering the LCOH from electrolysis-based plants, which links physical understanding, mathematical optimisation and electricity-market operation within a single modelling spine. Rather than proposing isolated models or case studies, the work builds a sequential decision-analytics workflow for PtH projects:

- *From physics-faithful simulation to cost drivers.* The workflow starts with detailed rule-based simulations of industrial combined heat-and-power integration and grid-connected photovoltaic PtH layouts. These physics-faithful models are used not only to reproduce behaviour, but to pinpoint where costs arise along the hydrogen chain and which simple control logics help or hinder LCOH reduction.
- *From heuristics to deterministic co-optimisation of sizing and scheduling.* The same component models and cost structures are then embedded, with minimal simplification, into a deterministic mixed-integer linear optimisation model that treats plant sizing and scheduling in a single problem. Hydrogen production, storage and conversion technologies, as well as battery capacity become endogenous decisions chosen explicitly for their impact on LCOH, rather than fixed by assumption or tuned ex post.
- *From perfect foresight to two-stage stochastic capacity planning.* Building on this deterministic layer, the plant model is lifted into a two-stage stochastic capacity-planning formulation for an islanded hybrid renewable energy system, where investment decisions are made once and must perform well across many long-term realisations of renewable generation and demand. This step shows how design choices such as overbuilding renewables or shifting between battery and hydrogen storage can hedge against uncertainty and thereby improve the cost of hydrogen over the project life.
- *From static design to multi-stage market-coupled operation.* Finally, for grid-connected plants, the same physical and economic representation is embedded in a multi-stage stochastic scheduling model that co-optimises participation in day-ahead, intraday, reserve and imbalance markets while respecting hydrogen off-take commitments and detailed equipment dynamics and degradation. This last layer quantifies how much additional cost reduction can be unlocked purely by smarter operation in real electricity markets once the plant is built.

Table 2.1: Literature positioning, research gaps, and thesis contributions across the four modelling layers (rule-based → deterministic → two-stage → multi-stage).

Layer	State of the art	Research gap	Contribution	Ref
Rule-based simulation	Component-level simulation and heuristic EMS for hybrid RES-H ₂ systems; feasibility screening; fast sensitivity analysis; simple dispatch rules.	(i) No endogenous optimality: trade-offs are imposed by rules, not optimised. (ii) Limited quantification of the value of flexibility. (ii) Hard to compare consistently with optimisation layers when component abstractions change.	Uses rule-based simulation explicitly as a baseline layer to generate feasible operating trajectories and to stress-test component assumptions; then carries component abstractions forward into optimisation layers to enable cross-layer comparison of KPIs.	[112, 115, 116] [114, 119, 120]
Deterministic optimisation (LP - MILP - NLP - MINLP)	Sizing and dispatch under point forecasts; storage selection; policy constraints; typical energy-hub / multi-energy coupling with one objective (cost / LCOH / profit).	(i) Uncertainty mostly reduced to sensitivities. (ii) Market chronology simplified (single market or aggregated time).	Provides a deterministic optimisation baseline with consistent device models and KPIs, used as the reference point for (a) robustness premia in the two-stage model and (b) the incremental value of market chronology and non-anticipativity in the multi-stage model.	[134, 135, 140] [141, 143, 147] [132, 133]
Two-stage stochastic optimisation	Here-and-now design decisions and scenario-based operational recourse; typically used for renewable variability in planning problems.	(i) Limited linkage between robustness cost and decarbonisation stringency (CO ₂ caps / full decarbonisation). (ii) Limited comparison to deterministic baselines.	Quantifies the cost of robustness against a deterministic benchmark under identical component modelling and KPIs, and shows how the robustness premium changes across emission constraints.	[163, 165, 166] [164, 167]
Multi-stage stochastic optimisation	Sequential decision-making with scenario trees and non-anticipativity; day-ahead - intraday - real-time coupling; increasingly includes ancillary services and hybridisation (e.g., BESS-electrolyser).	(i) Fragmented treatment of revenue stacking (energy + reserve) and of operational constraints (start-up, ramps, standby). (ii) Often no explicit connection back to simpler layers (rule-based / deterministic / two-stage) to clarify when the added complexity is justified.	Develops a market-aware multi-stage framework with explicit non-anticipativity and sequential market chronology, highlighting when multi-stage complexity adds value versus deterministic/two-stage layers.	[169, 172, 173] [168, 174, 175] [170, 171]

Research gap and thesis contributions. The literature above evidences three recurring gaps for PtH plants operated as flexibility assets: (i) fragmentation across modelling layers, where rule-based, deterministic and stochastic formulations often rely on different component abstractions and assumptions, limiting traceability and comparability of results [119, 133]; (ii) partial alignment between uncertainty modelling and the true chronology of electricity-market decision-making, with two-stage models aggregating timelines and multi-stage models remaining computationally demanding and case-specific [163, 168, 169]; and (iii) an only-

recent integration of certification/policy constraints and ancillary-service value streams into optimisation-based PtH operation [143, 171]. This thesis addresses these gaps by developing a consistent four-layer modelling stack (rule-based $\rightarrow$ deterministic $\rightarrow$ two-stage $\rightarrow$ multi-stage), and by quantifying trade-offs and uncertainty-hedging value on common KPIs across realistic case studies and market chronologies.

Taken together, these steps constitute a single, transferable decision-analytics workflow for PtH projects: from early screening, through robust capacity planning, to market-coupled operation, all evaluated with consistent physics, degradation and finance. The novelty does not lie in any one case study in isolation, but in showing that a complex and uncertain problem such as lowering the LCOH can be tackled by a unified modelling approach that keeps the same technical detail across rule-based simulation, deterministic optimisation and stochastic market scheduling, and that is explicitly structured around the economic and regulatory conditions required for real-world adoption.

3. METHODS

This chapter is organised in two parts that mirror the algorithmic families introduced in the State of the Art: (i) rule-based simulation and (ii) optimisation-based methods. In each part, component models are first presented and then their system integration is explained. For optimisation-based studies, deterministic MILP and stochastic MILP (two-stage and multi-stage) are distinguished later; the stochastic layer reuses the same MILP component blocks and only augments them with scenario indices and information-structure constraints. Here the rule-based side is detailed up to the solver architecture that implements it.

Terminology (variability, uncertainty, risk, robustness). Throughout the thesis, the following terms are used with specific meanings:

- **Variability** denotes observed fluctuations of exogenous signals (e.g., PV, wind, prices, demand) across time or across historical years; it is a property of data.
- **Uncertainty** denotes the lack of knowledge, at the time decisions are made, about which future realisation of those signals will occur; it is represented via scenario sets $\omega \in \Omega$.
- **Risk** denotes the exposure of performance (cost, emissions, profits) and feasibility to uncertainty (e.g., tail outcomes, constraint violations, adverse price–volume realisations). Unless explicitly stated otherwise, the stochastic formulations in this thesis are risk-neutral, i.e., they minimise/maximise the expected objective value across scenarios.
- **Robustness** denotes the ability of decisions—especially non-anticipative ones (e.g., design variables common to all scenarios)—to remain feasible and to deliver stable performance across the considered scenario set Ω . Unless explicitly stated, “robust” is used in this scenario-based sense and not as worst-case robust optimisation.

3.1 Rule-based simulation: Multi Energy System Simulator (MESS)

The Multi Energy System Simulator (MESS) is a modular, in-house developed Python-based framework that realises the rule-based formulation from Section 2.1 with detailed

component logic across electricity, heat/cooling, hydrogen (and by-products), steam, gas and process water. It targets single-site studies and integrates a generic carrier/stream structure with unit-state logic and a full PtH chain (EL, COMP, HS, FC/GT) [176]. An overview of MESS workflow is represented in Figure 3.1.

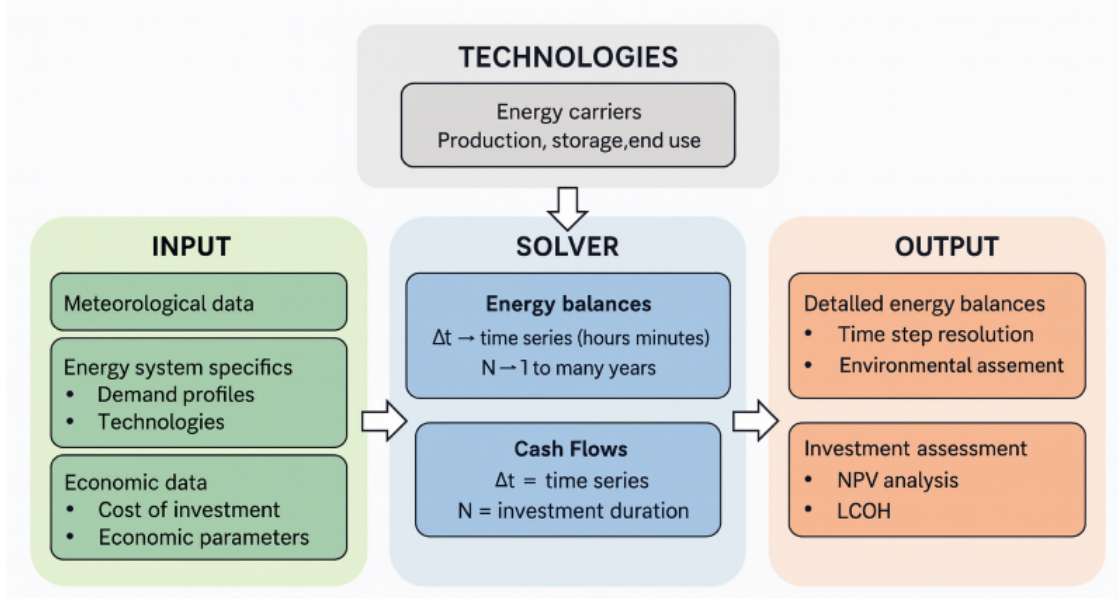


Figure 3.1: MESS workflow overview.

A compact statement of the MESS time march is shown in Eq. 3.1:

$$\begin{aligned}
 \sigma_t &= \Gamma(x_t, \xi_t; \theta) \\
 u_t &= \mu_{\sigma_t}(x_t, \xi_t; \theta) \\
 x_{t+1} &= f_{\sigma_t}(x_t, u_t, \xi_t) \\
 y_t &= y_{\sigma_t}(x_t, u_t, \xi_t), \quad t = 1, \dots, N_T.
 \end{aligned} \tag{3.1}$$

Symbols.

- x_t — memory states (e.g., LOH_t , SOC_t).
- ξ_t — time-series drivers injected at the start of the step (demands, tariffs, weather conditions).
- θ — rule parameters (bands, minimum loads, priorities).
- σ_t — branch selected by Γ (the realised operating situation for step t).
- u_t — feasible set-points/actions issued by μ_{σ_t} after clipping.
- f_{σ_t} — state-update maps applying physics and (optionally) degradation writes.
- y_{σ_t} — output maps that close balances and produce the time series used for KPIs calculation highlighted in Section 3.1.2.

Execution order.

1. **Refresh** ξ_t . Load the current electric, thermal or hydrogen demands, electricity/natural gas/hydrogen prices and weather conditions.

2. **Mode selection** $\sigma_t = \Gamma(x_t, \xi_t; \theta)$ (**priority rule tree**). Check admissibility and priorities in order; the first satisfied branch is the active mode. *Examples:*
 - *RES surplus* $\Rightarrow$ charge BESS $\rightarrow$ run EL $\rightarrow$ export if allowed.
 - *RES deficit* $\Rightarrow$ discharge BESS $\rightarrow$ run FC $\rightarrow$ import from grid.
 - *H₂ demand spike* $\Rightarrow$ pause EL if RES production is not available $\rightarrow$ prioritise FC if LOH_t is high, otherwise import.
3. **Control map** $u_t = \mu_{\sigma_t}(x_t, \xi_t; \theta)$ **with clipping**. Compute device set-points for the chosen mode (e.g., EL power, COMP flow, BESS charge/discharge, FC power, grid exchange) and clip them to what is feasible given ratings, minimum loads and the current x_t . *Examples:*
 - In *RES surplus*: target EL at the rule's priority; if LOH_t is near its upper band, redirect to BESS or to export per θ .
 - In *RES deficit*: aim FC at the requested power; if LOH_t is low, reduce FC and escalate to grid import per θ .
 - If a minimum load makes a set-point inadmissible, drop to the next priority action in the same mode.
4. **Mode dynamics** $x_{t+1} = f_{\sigma_t}(x_t, u_t, \xi_t)$. Translate u_t into physical flows with the device maps and update all states, and (if enabled) degradation/ageing. *Examples:*
 - EL operating: LOH_t increases; any water/oxygen states advance.
 - FC operating: LOH_t decreases and electrical/thermal outputs materialise.
 - BESS charging/discharging: SOC moves considering efficiencies and self-discharge.
5. **Output** $y_t = y_{\sigma_t}(x_t, u_t, \xi_t)$. Close residual balances per carrier at the grid interface according to site policy (import, export, curtail, or flag unmet load). Record per-technology/per-carrier series, curtailment/unmet-load flags and grid exchanges; expose any additional streams required for KPIs (see Section 3.1.2). *Examples:*
 - If the electrical balance is positive and export is allowed: log an export; if export is disallowed: log curtailment.
 - If the balance is negative and import is capped: log an unmet-load flag; otherwise record an import.
 - Store time series for utilisation, cashflow terms, emissions and certified quantities to support LCOH/NPV and compliance reporting.

3.1.1 Components modelling

The simulator adopts a modular, object-oriented representation of each technology as a physics-faithful block embedded in the hybrid rule-based loop of Section 3.1. Each block specifies: (i) admissible inputs/outputs (power, mass and heat flows), (ii) instantaneous constraints and guards (efficiency maps, part-load ranges), and (iii) internal state updates for inventories (e.g., SOC, degradation markers).

Demands. Demands for electricity, heat/steam and hydrogen are treated as exogenous time series in ξ_t at the simulator resolution (minutes to hours). Electrical demand is denoted by $p_t^{\text{el,dem}}$ [kW], thermal/steam demand by $p_t^{\text{th,dem}}$ [kW], and hydrogen demand by $\dot{m}_t^{\text{H}_2,\text{dem}}$ [kg/h]. Series may stem from measurements, industrial partners or open repositories and are pre-processed to match the model horizon and time step.

Renewables

Meteorological drivers (irradiance components, sun geometry, wind speed/direction, ambient conditions) and renewable production are treated as exogenous time series in ξ_t . When the Photovoltaic Geographical Information System (PVGIS) is used, site time series (including Typical Meteorological Year, TMY) are retrieved and, where available, the specific AC power per installed kWp series provided by PVGIS is used directly [177]. The resulting electrical outputs are denoted p_t^{PV} for the PV field and p_t^{WT} for the Wind Turbine (WT).

Photovoltaics. PV electrical power p_t^{PV} at time step t is obtained, for fixed and single-axis tracking PV systems, directly from PVGIS [177] as shown in Eq. 3.2:

$$p_t^{\text{PV}} = P_{\text{nom}}^{\text{PV}} \bar{p}_t^{\text{PV,1kW}}, \quad 3.2$$

where p_t^{PV} [kW] is the AC electrical power output of the PV array at time step t , $P_{\text{nom}}^{\text{PV}}$ [kWp] is the installed peak capacity, and $\bar{p}_t^{\text{PV,1kW}}$ [kW/kWp] is the PVGIS time series of specific AC power per kWp computed for the chosen array tilt β and azimuth α_a , mounting, technology and total system losses.

Otherwise, when only global horizontal irradiance GHI_t and diffuse horizontal irradiance DHI_t are available, the incident plane-of-array irradiance, that is, the Global Tilted Irradiance GTI_t , is obtained via the Hay–Davies transposition [178], and PV power (for fixed-tilt arrays) follows the Durisch model [179] as shown in Eq. 3.3:

$$p_t^{\text{PV}} = \eta_{\text{mod}}^{\text{PV}} \text{PR} A^{\text{PV}} \text{GTI}_t, \quad 3.3$$

where $\eta_{\text{mod}}^{\text{PV}}$ [–] is the PV module efficiency, PR [–] is the performance ratio of the PV system, A^{PV} [m²] is the total active area of the PV modules, and GTI_t [W/m²] is the global tilted irradiance on the array plane at time step t .

The Hay–Davies relation for GTI_t from its horizontal components is represented in Eq. 3.4:

$$\text{GTI}_t = \text{DNI}_t K_{b,t} + \text{DHI}_t (f_{\text{HD},t} K_{b,t} + (1 - f_{\text{HD},t}) \frac{1 + \cos \beta}{2}) + \text{GHI}_t a_{\text{alb}} \frac{1 - \cos \beta}{2}, \quad 3.4$$

where DNI_t [W/m²] is the direct normal irradiance, $K_{b,t}$ [–] is the geometric factor relating beam irradiance on the tilted and horizontal planes, $f_{\text{HD},t} = \text{DNI}_t / G_{\text{on},t}$ is the Hay–Davies anisotropy index, $G_{\text{on},t}$ [W/m²] is the extraterrestrial irradiance on a plane normal to the solar beam, β [rad] is the array tilt angle, and a_{alb} [–] is the ground albedo.

Geometric relations used in Eq. 3.4 are given in Eq. 3.5:

$$\text{DNI}_t = \frac{\text{GHI}_t - \text{DHI}_t}{\cos \alpha_{z,t}}, \quad K_{b,t} = \frac{\cos \alpha_{\text{inc}}}{\cos \alpha_{z,t}}, \quad \cos \alpha_{\text{inc}} = \cos \alpha_{z,t} \cos \beta + \sin \alpha_{z,t} \sin \beta \cos(\alpha_{s,t} - \alpha_a), \quad 3.5$$

where α_{inc} [rad] is the incidence angle on the tilted plane, $\alpha_{z,t}$ [rad] is the solar zenith angle, $\alpha_{s,t}$ [rad] is the solar azimuth angle, and α_a [rad] is the array azimuth; all angles are in radians. Near sunrise and sunset, $\cos \alpha_{z,t}$ is clipped away from zero to avoid division blow-up. Eqs. 3.3–3.5 yield GTI_t and p_t^{PV} at the simulator timestep for arbitrary array geometry and meteorological inputs [178, 179].

Agrivoltaic parenthesis. When agrivoltaic (AV) is considered, the PV power block remains unchanged. AV affects site feasibility and economics (installable MW per hectare, CAPEX per kW, and layout constraints) but not the per-kW PV production model used for PtH scheduling. AV modelling is included in Appendix 7 of the thesis.

Wind turbine. Wind power is obtained from the characteristic turbine power curve as a function of hub-height wind speed $w_{h,t}$. A standard three-region curve is adopted [180], as

shown in Eq. 3.6:

$$p_t^{\text{WT}} = \begin{cases} 0, & w_{h,t} \leq w_{\text{ci}}, \\ P_{\text{nom}}^{\text{WT}} \frac{w_{h,t}^3 - w_{\text{ci}}^3}{w_{\text{rat}}^3 - w_{\text{ci}}^3}, & w_{\text{ci}} < w_{h,t} < w_{\text{rat}}, \\ P_{\text{nom}}^{\text{WT}}, & w_{\text{rat}} \leq w_{h,t} \leq w_{\text{co}}, \\ 0, & w_{h,t} \geq w_{\text{co}}, \end{cases} \quad 3.6$$

where p_t^{WT} is electrical power at time t [kW], $w_{h,t}$ is hub-height wind speed [m/s], w_{ci} is cut-in speed [m/s], w_{rat} is rated speed [m/s], w_{co} is cut-out speed [m/s], and $P_{\text{nom}}^{\text{WT}}$ is the WT nameplate power [kW].

If wind speed is provided at a reference height z_{ref} (e.g., from PVGIS), it is extrapolated to the hub height z_{hub} by the power law [180], as represented in Eq. 3.7:

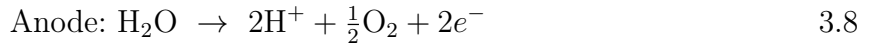
$$w_{h,t} = w_{\text{ref},t} \left(\frac{z_{\text{hub}}}{z_{\text{ref}}} \right)^{\alpha_{\text{shear}}}, \quad 3.7$$

where $w_{\text{ref},t}$ is the wind speed at the reference height [m/s], z_{hub} is the turbine hub height [m], z_{ref} is the anemometer/reference height [m], and α_{shear} is the wind-shear exponent reflecting surface roughness [-]. A representative $\alpha_{\text{shear}} = 0.17$ is used for open terrain in Italy, consistent with the Italian Wind Atlas, unless site-specific measurements indicate otherwise [180, 181].

Hydrogen production: electrolysis

The electrolysis unit is a mode-aware conversion block. The selector $\Gamma(\cdot)$ and policy $\mu_{\sigma}(\cdot)$ determine when electrolysis is enabled (e.g., minimum-load guards, storage availability) and dispatch a feasible power setpoint p_t^{EL} (electrical input) or an equivalent hydrogen-production request. The device dynamics $f_{\sigma}(\cdot)$ then map (x_t, ξ_t, u_t) to an operating point on the stack polarisation curve; mass/energy balances, by-products, and inventory updates are applied; the output map $y_{\sigma}(\cdot)$ exposes $\dot{m}_t^{\text{H}_2, \text{EL}}$, p_t^{EL} , water consumption $\dot{m}_t^{\text{H}_2\text{O}, \text{EL}}$, and (optionally) recoverable thermal power $p_t^{\text{EL}, \text{th}}$ [182–184].

Electrolysis thermodynamics and performance metrics. Low-temperature water electrolysis splits liquid water into hydrogen and oxygen via the half-reactions, as shown in Eqs. 3.8–3.9, and the overall reaction, as shown in Eq. 3.10:



where e^- denotes electrons. The reversible (Nernst) cell voltage at reference conditions is V_{rev} . The minimum molar electrical work is $zF V_{\text{rev}}$, with z the number of electrons per mole of H_2 and F the Faraday constant. Using $\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ$ and $\Delta G^\circ = zF V_{\text{rev}}$ at standard conditions, the theoretical minimum voltage is V_{rev} [182]. Practical operation requires activation, ohmic, and concentration overpotentials, yielding the cell/stack relations, as shown in Eq. 3.11:

$$V_{\text{cell}} = V_{\text{rev}} + V_{\text{act}} + V_{\text{ohm}} + V_{\text{conc}}, \quad V_{\text{stack}} = N_{\text{cell}} V_{\text{cell}}, \quad 3.11$$

where V_{cell} is the single-cell voltage [V], V_{act} , V_{ohm} , V_{conc} are overpotentials [V] and N_{cell} is the number of series cells [-].

Over any interval Δt , the specific electric consumption and the electrical efficiency are defined as in Eq. 3.12:

$$\text{SEC}^{\text{EL}} = \frac{\int_{\Delta t} p_t^{\text{EL}} dt}{\int_{\Delta t} \dot{m}_t^{\text{H}_2, \text{EL}} dt}, \quad \eta^{\text{el}} = \frac{\text{LHV}_{\text{H}_2}}{\text{SEC}^{\text{EL}}}, \quad 3.12$$

where SEC^{EL} is the electrolyser specific electric consumption [kW h/kg]; p_t^{EL} is the electrical input power [kW]; $\dot{m}_t^{\text{H}_2, \text{EL}}$ is the hydrogen production rate [kg/h]; η^{el} is the electrical efficiency on an LHV basis [-]; and LHV_{H_2} is the lower heating value of hydrogen [kW h/kg] [185]. Representative ranges are reported in Table 3.1.

Table 3.1: Typical electrolysis numerical values referenced in the text.

Quantity	Description	Value / Source
V_{rev} (std. cond.)	Reversible voltage at 25 °C, 1 atm	1.229 V [182]
z	Electrons per mole of H_2	2 [182]
F	Faraday constant	96 485 C/mol [182]
ΔH°	Standard-state enthalpy change	285.84 kJ/mol [182]
ΔG°	Standard-state Gibbs free energy	237.21 kJ/mol [182]
ΔS°	Standard-state entropy change	0.1631 kJ/(mol K) [182]
Commercial SEC range	Typical SEC^{EL} for devices	50 kW h/kg to 83 kW h/kg [185]
Applied cell voltage	Typical operating voltage window	1.8 V to 2.6 V [186]

PEM electrolyser model

Proton-exchange-membrane (PEM) electrolysers are favoured here for fast dynamics, high current density, compact BOP, and product purity [184, 186]. The stack is characterised by a polarisation curve $V_{\text{cell}}(i)$ assembled from physically grounded loss terms and parameterised by operating temperature and pressures [187, 188]. A temperature- and pressure-corrected Nernst expression is adopted, as shown in Eq. 3.13:

$$V_{\text{rev}}(T, \mathcal{P}) = 1.229 - \frac{\Delta S^\circ}{2F} (T - 298.15) + \frac{R_{\text{univ}} T}{2F} \ln \left(\frac{\mathcal{P}_{\text{H}_2} \mathcal{P}_{\text{O}_2}^{1/2}}{\mathcal{P}_{\text{H}_2\text{O}}} \right). \quad 3.13$$

where $V_{\text{rev}}(T, \mathcal{P})$ is the reversible (Nernst) cell voltage [V]; T is absolute temperature [K]; R_{univ} is the universal gas constant [J/(mol K)]; F is the Faraday constant [C/mol]; ΔS° is the standard-state entropy change per mole of H_2 [J/(mol K)]; and $\mathcal{P}_{\text{H}_2}$, $\mathcal{P}_{\text{O}_2}$, $\mathcal{P}_{\text{H}_2\text{O}}$ are partial pressures [bar] (so the logarithm is dimensionless). The water-vapour term is computed with an Antoine-type relation (in bar), as represented in Eq. 3.14:

$$\ln(\mathcal{P}_{\text{H}_2\text{O}}) = 11.676 - \frac{3816.44}{T - 46.13}, \quad 3.14$$

and electrode partial pressures follow $\mathcal{P}_{\text{H}_2} = \mathcal{P}_{\text{ca}} - \mathcal{P}_{\text{H}_2\text{O}}$ and $\mathcal{P}_{\text{O}_2} = \mathcal{P}_{\text{an}} - \mathcal{P}_{\text{H}_2\text{O}}$ [186].

Activation overpotential. A Butler–Volmer/Tafel form merges the two electrodes into an effective pair $(\alpha_{\text{ct}}, i_0)$, as shown in Eq. 3.15:

$$V_{\text{act}}(i, T) = \frac{R_{\text{univ}} T}{2 \alpha_{\text{ct}} F} \ln \left(\frac{i}{i_0} \right), \quad 3.15$$

where $V_{\text{act}}(i, T)$ is the activation overpotential [V]; i the current density [A/m^2]; α_{ct} the effective charge-transfer coefficient [-]; and i_0 the exchange current density [A/m^2]. Calibration follows [187] (representative values in Table 3.2).

Ohmic overpotential. The membrane area-specific resistance ASR yields the ohmic loss, as shown in Eq. 3.16:

$$\begin{aligned} V_{\text{ohm}}(i, T) &= \text{ASR } i, \\ \text{ASR} &= \frac{\ell_{\text{mem}}}{\kappa_m(\lambda, T)}, \\ \kappa_m(\lambda, T) &= 100 (0.005139 \lambda - 0.00326) \exp \left[1268 \left(\frac{1}{303} - \frac{1}{T} \right) \right]. \end{aligned} \quad 3.16$$

where $V_{\text{ohm}}(i, T)$ is the ohmic overpotential [V]; ASR the membrane area-specific resistance [Ωm^2]; ℓ_{mem} the membrane thickness [m]; and $\kappa_m(\lambda, T)$ the membrane conductivity [S/m] as a function of temperature T [K] and membrane hydration number λ [-]. The empirical correlation and typical $\ell_{\text{mem}}, \lambda$ ranges follow [189].

Concentration overpotential. At high i , a mass-transport term avoids exceeding a limiting current, as shown in Eq. 3.17:

$$V_{\text{conc}}(i, T) = -\frac{R_{\text{univ}} T}{2F} \ln \left(1 - \frac{i}{i_{\text{max}}} \right), \quad 3.17$$

where $V_{\text{conc}}(i, T)$ is the concentration overpotential [V] and i_{max} is the limiting current density [A/m^2]. The expression is evaluated only for $0 \leq i < i_{\text{max}}$.

Geometry. When detailed geometry is unknown, the single-cell active area can be inferred from nameplate data, as shown in Eq. 3.18:

$$A_{\text{cell}} = \frac{P_{\text{nom}}^{\text{EL}}}{V_{\text{max}} i_{\text{max}}}, \quad I_{\text{cell}} = i A_{\text{cell}}, \quad V_{\text{stack}}(i) = N_{\text{cell}} [V_{\text{rev}} + V_{\text{act}} + V_{\text{ohm}} + V_{\text{conc}}], \quad 3.18$$

where A_{cell} is the single-cell active area [m^2]; $P_{\text{nom}}^{\text{EL}}$ the nominal electrical power [W]; V_{max} the rated cell voltage at i_{max} [V]; I_{cell} the cell current [A]; and $V_{\text{stack}}(i)$ the stack voltage [V]. The operating point i_t is obtained by solving $p_t^{\text{EL}} = 10^{-3} V_{\text{stack}}(i_t) I_{\text{cell},t}$ with $I_{\text{cell},t} = i_t A_{\text{cell}}$, where p_t^{EL} is the instantaneous electrical input power [kW]. For robustness in the rule-based loop, $V_{\text{stack}}(i)$ is tabulated (i-V spline) and inverted once per configuration; at runtime a bounded 1-D search on i ensures feasibility and guards against clipping [183].

Hydrogen production. Faraday's law gives the molar and mass production rates, as shown in Eq. 3.19:

$$\dot{n}_t^{\text{H}_2, \text{EL}} = \frac{N_{\text{cell}} \eta_{\text{Far}}(i, T) I_{\text{cell},t}}{2F} 3600, \quad \dot{m}_t^{\text{H}_2, \text{EL}} = \dot{n}_t^{\text{H}_2, \text{EL}} M_{\text{H}_2}, \quad 3.19$$

where $\dot{n}_t^{\text{H}_2, \text{EL}}$ is the molar hydrogen production rate [mol/h]; $\eta_{\text{Far}}(i, T)$ the Faradaic efficiency [-]; $\dot{m}_t^{\text{H}_2, \text{EL}}$ the mass production rate [kg/h]; M_{H_2} the molar mass of hydrogen [kg/mol]; and F the Faraday constant [C/mol], with the factor 3600 converting from s to h. The correlation in [192] is adopted for $\eta_{\text{Far}}(i, T)$.

A constant specific water-use parameter is adopted, $sc_{\text{H}_2\text{O}} = 0.015 \text{ m}^3/\text{kg}$ (i.e., 15 L/kg) [191]. The corresponding volumetric and mass flows to the PEM electrolyser are given, as shown in Eq. 3.20:

$$\dot{V}_t^{\text{H}_2\text{O}, \text{EL}} = sc_{\text{H}_2\text{O}} \dot{m}_t^{\text{H}_2, \text{EL}} \quad [\text{m}^3/\text{h}], \quad \dot{m}_t^{\text{H}_2\text{O}, \text{EL}} = \rho_{\text{H}_2\text{O}} \dot{V}_t^{\text{H}_2\text{O}, \text{EL}} \quad [\text{kg}/\text{h}], \quad 3.20$$

where $\dot{V}_t^{\text{H}_2\text{O}, \text{EL}}$ is the process-water volumetric flow [m^3/h], $\dot{m}_t^{\text{H}_2\text{O}, \text{EL}}$ its mass equivalent [kg/h], and $\rho_{\text{H}_2\text{O}} \approx 1000 \text{ kg}/\text{m}^3$.

Table 3.2: PEM electrolyser: numerical values.

Quantity	Description	Value / Source
V_{rev}	Reversible voltage at 25 °C, 1 atm	1.229 V [182]
ΔS°	Standard-state entropy change per mol H ₂	0.1631 kJ/(mol K) [182]
T	Nominal operating temperature	70 °C [186]
$\mathcal{P}$	Typical operating pressure	30 bar [190]
Applied V_{cell}	Typical operating window	1.8 V to 2.6 V [186]
α_{ct}	Charge-transfer coefficient	0.45 [187]
i_0 (eff.)	Exchange current density	10^{-3} A/cm ² [187]
ℓ_{mem}	Membrane thickness	150 μm [189]
λ	Membrane hydration number	20 [189]
i_{min}	Minimum current-density guard	$\gtrsim 0.05$ A/cm ² [190]
i_{max}	Limiting / rated current density	2.5 A/cm ² (sizing) [183, 186]
N_{cell}	Cells per stack	30 (user-defined)
$sc_{\text{H}_2\text{O}}$	Process water per H ₂ mass	0.015 m ³ /kg (15 L/kg) [191]

Instantaneous electrical efficiency and specific electric consumption (SEC) derive from Eq. 3.12, with $p_t^{\text{EL}} = V_{\text{stack}}(i_t) I_{\text{cell},t}$. The stack thermal power (heat release) for thermal integration follows the LHV convention, as shown in Eq. 3.21:

$$p_t^{\text{EL,th}} = p_t^{\text{EL}} - \dot{m}_t^{\text{H}_2,\text{EL}} \text{LHV}_{\text{H}_2} \quad [\text{kW}], \quad 3.21$$

where LHV_{H_2} is in [kW h/kg] and $\dot{m}_t^{\text{H}_2,\text{EL}}$ in [kg/h], so that Eq. 3.21 is in [kW]. Site-level use of this low-grade heat can improve overall performance [184].

Operational guards and multi-module logic. Rule-based guards enforce a minimum current density and flow bounds (Table 3.2).

Capacity scaling uses identical modules, sequentially committed as p_t^{EL} grows; at each step, the dispatcher activates modules respecting activation thresholds and shares load to avoid inefficient regions. When a hydrogen demand-following mode is selected by Γ , the same mapping is solved for I_{cell} subject to the instantaneous admissible power bound $P_{\text{nom}}^{\text{EL}}$ and available PV/WT or grid import. Figure 3.2 illustrates the resulting PEM stack characteristics, namely the cell polarisation curve and the implied efficiency and hydrogen production versus power, together with the minimum-load guards used in the rule-based dispatcher.

Alkaline water electrolyser (AEL)

Alkaline water electrolysis (AEL) is represented as a mode-aware conversion block, analogous to the PEMEL case. The steady operating point solves $p_t^{\text{EL}} = 10^{-3} V_{\text{stack}}(i_t) I_{\text{cell},t}$, subject to technology-specific guards (e.g., minimum load) to limit gas crossover and ensure safe operation. Here, p_t^{EL} is the plant electrical input power [kW], V_{stack} the stack voltage [V], and $I_{\text{cell},t}$ the cell current [A], so the factor 10^{-3} converts W to kW.

Unless otherwise noted, all equations in this subsection refer to a single AEL module ($P_{\text{nom,mod}}^{\text{EL}} = 500$ kW). Let $N_{\text{mod},t}$ be the number of identical modules operating at time t (integer), with homogeneous dispatch across active modules. Plant-level quantities aggregate as shown in Eq. 3.22:

$$p_t^{\text{EL}} = N_{\text{mod},t} p_t^{\text{EL,mod}}, \quad \dot{m}_t^{\text{H}_2,\text{EL}} = N_{\text{mod},t} \dot{m}_t^{\text{H}_2,\text{EL,mod}}, \quad P_{\text{nom}}^{\text{EL}} = N_{\text{mod}} P_{\text{nom,mod}}^{\text{EL}}. \quad 3.22$$

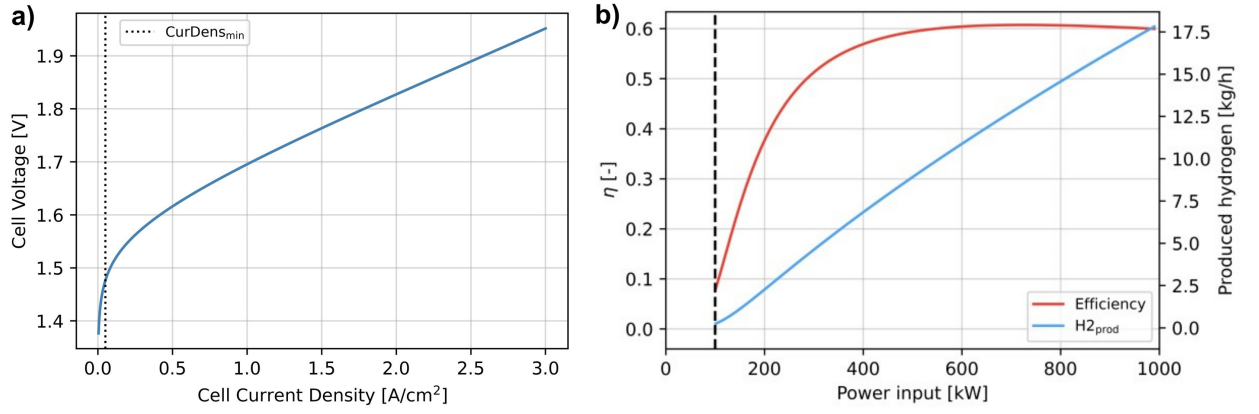


Figure 3.2: PEM electrolyser characteristics used in the rule-based model: (a) cell polarisation curve (cell voltage versus current density) with the minimum current-density guard indicated; (b) stack electrical efficiency and hydrogen production rate versus input electrical power, with the corresponding minimum-load guard.

The stack voltage follows the standard decomposition, as shown in Eq. 3.23:

$$V_{\text{stack}}(i, T) = N_{\text{cell}} [V_{\text{rev}}(T, \mathcal{P}) + V_{\text{act}}(i, T) + V_{\text{ohm}}(i, T)], \quad 3.23$$

where $V_{\text{stack}}(i, T)$ is the stack voltage [V], N_{cell} the number of series cells [-], $V_{\text{rev}}(T, \mathcal{P})$ the Nernst (reversible) cell voltage [V], $V_{\text{act}}(i, T)$ the activation overpotential [V], and $V_{\text{ohm}}(i, T)$ the ohmic overpotential [V].

A Nernst term that accounts for water–electrolyte interactions is adopted, as shown in Eq. 3.24:

$$V_{\text{rev}} = 1.23 - \frac{\Delta S^\circ}{zF} (T - T_{\text{ref}}) + \frac{R_{\text{univ}} T}{2F} \ln \left[\left(\frac{\mathcal{P}_{\text{tot}} - \mathcal{P}_{\text{H}_2\text{O}}}{\mathcal{P}_{\text{H}_2\text{O}}} \right)^{\frac{3}{2}} \frac{\mathcal{P}_{\text{H}_2\text{O}}^\circ}{\mathcal{P}_{\text{H}_2\text{O}}} \right], \quad z = 2, \quad 3.24$$

where T is the absolute temperature [K], T_{ref} a reference temperature [K], $\mathcal{P}_{\text{tot}}$ the total pressure [bar], $\mathcal{P}_{\text{H}_2\text{O}}$ the water vapour partial pressure over the electrolyte [bar], and $\mathcal{P}_{\text{H}_2\text{O}}^\circ$ the vapour pressure of pure water at the same temperature [bar]. All pressures in Eq. 3.24 are in bar so that the logarithm is dimensionless [193, 194].

The vapour pressures are obtained from empirical relations, as shown in Eqs. 3.25–3.26:

$$\ln \mathcal{P}_{\text{H}_2\text{O}} = 0.016214 - 0.13802 B + 0.19330 \sqrt{B} + 1.0239 \ln \mathcal{P}_{\text{H}_2\text{O}}^\circ, \quad 3.25$$

$$\ln \mathcal{P}_{\text{H}_2\text{O}}^\circ = 37.043 - \frac{6275.7}{T} - 3.4159 \ln T, \quad 3.26$$

where B is the electrolyte molality [mol/kg], itself a function of the KOH mass fraction [193].

Activation and ohmic contributions are represented with compact empirical forms, as shown in Eqs. 3.27–3.28 [193]:

$$V_{\text{act}}(i, T) = k \ln \left((t_1 + t_2/T + t_3/T^2) i + 1 \right), \quad 3.27$$

$$V_{\text{ohm}}(i, T) = (r_1 + r_2 T) i, \quad 3.28$$

where i is the current density [A/m²], and $k, t_1, t_2, t_3, r_1, r_2$ are stack-specific empirical coefficients. Coefficient ranges and calibration guidance are given in [193, 194].

Faradaic efficiency for AEL decreases at low current density and improves with temperature; a convenient correlation is used, as shown in Eq. 3.29:

$$\eta_{\text{Far}}(i, T) = \frac{i^2}{f_1 + f_2 i^2}, \quad 3.29$$

with f_1, f_2 temperature-dependent empirical coefficients [-]. Hydrogen production, oxygen co-production, water consumption, and instantaneous SEC^{EL} follow the same balances as in Section 3.1.1, with $\eta_{\text{Far}}(i, T)$ from Eq. 3.29. Guards enforce a minimum load and respect $\mathcal{P}/T$ bounds to limit impurity risk [195].

The specific water-use parameter is taken as $sc_{\text{H}_2\text{O}} = 0.015 \text{ m}^3/\text{kg}$ [191], yielding the volumetric and mass flow relations, as shown in Eq. 3.30:

$$\dot{V}_t^{\text{H}_2\text{O},\text{EL}} = sc_{\text{H}_2\text{O}} \dot{m}_t^{\text{H}_2,\text{EL}} \quad [\text{m}^3/\text{h}], \quad \dot{m}_t^{\text{H}_2\text{O},\text{EL}} = \rho_{\text{H}_2\text{O}} \dot{V}_t^{\text{H}_2\text{O},\text{EL}} \quad [\text{kg}/\text{h}], \quad 3.30$$

where $\dot{V}_t^{\text{H}_2\text{O},\text{EL}}$ is the process-water volumetric flow [m^3/h], $\dot{m}_t^{\text{H}_2,\text{EL}}$ its mass equivalent [kg/h], and $\rho_{\text{H}_2\text{O}}$ the water density [kg/m^3]. Instantaneous electrical efficiency and specific electric consumption follow from the stack polarisation and hydrogen-production balances shown in the following block which considers even ageing. Figure 3.3 illustrates the resulting alkaline stack characteristics at the beginning of life.

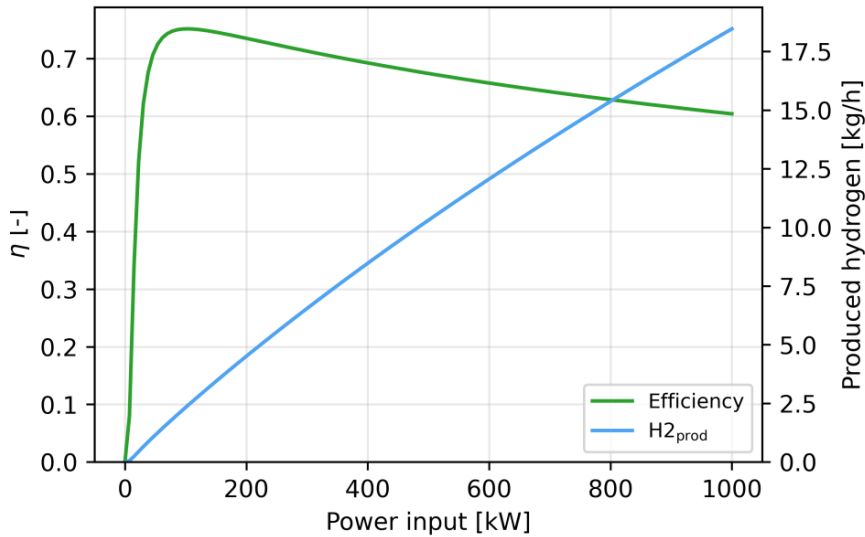


Figure 3.3: Stack electrical efficiency and hydrogen production rate versus input electrical power for the alkaline water electrolyser.

Rule-based multi-module logic. Identical modules are committed sequentially; per-module power obeys the guard

$$p_t^{\text{EL},\text{mod}} \in \{0\} \cup [u_{\text{min},\text{mod}}^{\text{EL}} P_{\text{nom},\text{mod}}^{\text{EL}}, P_{\text{nom},\text{mod}}^{\text{EL}}],$$

where $p_t^{\text{EL},\text{mod}}$ is the per-module electrical input [kW], $P_{\text{nom},\text{mod}}^{\text{EL}}$ the module nameplate power [kW], and $u_{\text{min},\text{mod}}^{\text{EL}}$ the minimum input-power fraction [-]. Let $N_{\text{mod},t}$ be the active module count; then $P_{\text{nom}}^{\text{EL}} = N_{\text{mod}} P_{\text{nom},\text{mod}}^{\text{EL}}$ and plant flows aggregate via Eq. 3.22. In H_2 -demand following, the controller first adjusts $N_{\text{mod},t}$ to satisfy the minimum-load guard and then inverts for $I_{\text{cell},t}$ on each active module under stack limits, mapping to $\dot{m}_t^{\text{H}_2,\text{EL},\text{mod}}$ via SEC_t^{EL} from Eq. 3.36.

Electrolyser ageing and integration in the rule-based loop (AEL). Ageing is represented as slow internal states in x_t and updated by $f_{\sigma_t}(\cdot)$ on a coarser grid. Two additive mechanisms act on the AEL cell voltage: (i) time-induced drift and (ii) thermal deviation from design [193, 196]. The operating-voltage relation is used, as shown in Eq. 3.31 [196]:

$$V_{\text{op},t} = V_{\text{id}} + \Delta V_{\text{deg},t} t + \Delta V_{\text{deg},T} (T_{\text{id}} - T_{\text{op},t}). \quad 3.31$$

Here, $V_{\text{op},t}$ is the degraded operating cell voltage [V]; V_{id} is the ideal (fresh) operating voltage at design conditions [V]; $\Delta V_{\text{deg},t}$ is the voltage drift rate due to time-induced degradation [V/h]; t is time along the ageing clock [h]; $\Delta V_{\text{deg},T}$ is the thermal-sensitivity coefficient [V/K]; T_{id} is the design temperature [K]; and $T_{\text{op},t}$ is the instantaneous operating temperature [K]. A module is replaced when the degraded operating voltage reaches $V_{\text{op},t} \geq V_{\text{op,EOL}}$; upon replacement, ageing states are reset and V_{op} returns to the fresh value V_{id} . In this work $V_{\text{op},t}$ denotes the single-cell voltage (so that the stack voltage is $V_{\text{stack}} = N_{\text{cell}} V_{\text{op},t}$). The adopted drift rate $\Delta V_{\text{deg},t} = 3 \mu\text{V/h}$ is applied at cell level, which corresponds to an increase of about 0.24 V over 80 000 h (i.e., roughly 10–15% of a typical 2 V operating voltage). This magnitude is consistent with literature-reported alkaline voltage-rise trends used in techno-economic lifetime models [196]. Accordingly, the replacement threshold $V_{\text{op,EOL}}$ is defined as a cell-voltage limit.

Stack temperature advances via a lumped balance, as shown in Eq. 3.32:

$$\Delta T = \frac{(p_t^{\text{EL,th,gen}} - p_t^{\text{EL,th,loss}}) \Delta t}{m_{\text{es}} c p_{\text{es}}}, \quad 3.32$$

where ΔT is the discrete temperature change over the ageing step [K]; $p_t^{\text{EL,th,gen}}$ is the internal heat-generation rate [kW]; $p_t^{\text{EL,th,loss}}$ is the heat loss to ambient [kW]; Δt is the ageing-step duration [h]; m_{es} is the equivalent thermal mass [kg]; and $c p_{\text{es}}$ is its specific heat capacity, expressed consistently with the power and time units (e.g., converted from kJ/(kg K) to kW h/(kg K) inside the implementation).

The internally generated heat is modelled as shown in Eq. 3.33:

$$p_t^{\text{EL,th,gen}} = \frac{N_{\text{cell}} (V_{\text{op},t} - V_{\text{LHV}}) I_{\text{cell,op},t}}{10^3}, \quad 3.33$$

where N_{cell} is the number of series cells [-], $I_{\text{cell,op},t}$ is the operating cell current [A], and $V_{\text{LHV}} = \text{LHV}_{\text{H}_2}/(zF)$ is the LHV-equivalent voltage [V]. Division by 10^3 expresses power in kW for consistency with $p_t^{(\cdot)}$.

Thermal losses through the cylindrical vessel (internal convection, steel and insulation conduction, external convection) are computed via the total series thermal resistance, as shown in Eqs. 3.34–3.35 [196]:

$$\mathcal{R}_{\text{th}} = \frac{1}{h_{\text{in}} 2\pi r_{\text{in}} L_{\text{ves}}} + \frac{\ln\left(\frac{r_{\text{st,o}}}{r_{\text{in}}}\right)}{2\pi k_{\text{st}} L_{\text{ves}}} + \frac{\ln\left(\frac{r_{\text{ins,o}}}{r_{\text{ins,i}}}\right)}{2\pi k_{\text{ins}} L_{\text{ves}}} + \frac{1}{h_{\text{out}} 2\pi r_{\text{ins,o}} L_{\text{ves}}}, \quad 3.34$$

$$p_t^{\text{EL,th,loss}} = \frac{T_{\text{int},t} - T_{\text{ext},t}}{\mathcal{R}_{\text{th}}} \frac{1}{10^3}, \quad 3.35$$

where $\mathcal{R}_{\text{th}}$ is the total thermal resistance [K/W]; $h_{\text{in}}, h_{\text{out}}$ are the inner/outer convective heat-transfer coefficients [W/(m² K)]; r_{in} is the inner radius [m]; $r_{\text{st,o}}$ is the outer radius of the steel wall [m]; $r_{\text{ins,i}}$ and $r_{\text{ins,o}}$ are the inner/outer radii of the insulation layer [m]; $k_{\text{st}}, k_{\text{ins}}$ are thermal conductivities [W/(m K)]; L_{ves} is the vessel length [m]; and $T_{\text{int},t}$ and $T_{\text{ext},t}$ are internal and ambient temperatures [K]. The factor $1/10^3$ converts W to kW.

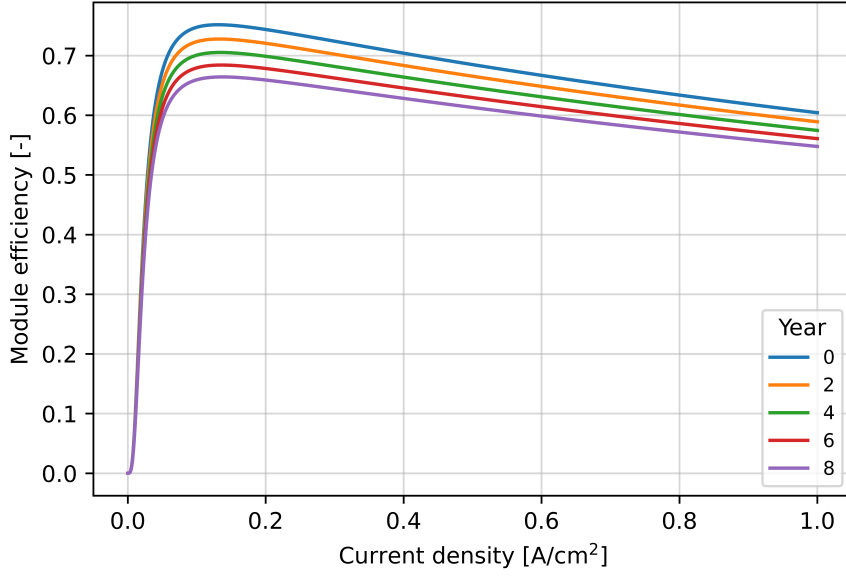


Figure 3.4: Example of alkaline electrolyser module efficiency as a function of current density for different ageing times showing the progressive downward shift in efficiency over the stack lifetime.

An instantaneous specific electric consumption for AEL, consistent with Faraday’s law at the current degraded point, is written as shown in Eq. 3.36:

$$\text{SEC}_t^{\text{EL}} = \frac{2F V_{\text{op},t}}{M_{\text{H}_2} \eta_{\text{Far}}(i_t, T_{\text{op},t})} \frac{1}{3.6 \times 10^6}, \quad 3.36$$

where SEC_t^{EL} is the instantaneous specific electric consumption of the electrolyser [kW h/kg]; F is the Faraday constant [C/mol]; $V_{\text{op},t}$ is the degraded operating cell voltage [V]; M_{H_2} is the molar mass of hydrogen [kg/mol]; and $\eta_{\text{Far}}(i_t, T_{\text{op},t})$ is the Faradaic efficiency [-]. The factor $1/(3.6 \times 10^6)$ converts from J/kg to kW h/kg. Figure 3.4 illustrates the resulting degradation of module efficiency as a function of current density for different ageing times, according to Eqs. 3.31 and 3.36 under nominal operating conditions.

In the loop, hydrogen production follows

$$\dot{m}_t^{\text{H}_2, \text{EL}} = \frac{p_t^{\text{EL}}}{\text{SEC}_t^{\text{EL}}},$$

with p_t^{EL} in [kW] and $\dot{m}_t^{\text{H}_2, \text{EL}}$ in [kg/h]. Rule-based guards prevent operation below a configured minimum load and apply temporary derating whenever $T_{\text{op},t}$ departs from T_{id} . The policy $\mu_{\sigma_t}(\cdot)$ reads the ageing states to adjust future dispatch.

Hydrogen compression

The compressor is modelled as a conversion/conditioning block that raises the hydrogen pressure from an inlet value $\mathcal{P}_{\text{in}}$ to a target outlet value $\mathcal{P}_{\text{out}}$ across a fixed absolute pressure span. The selector $\Gamma(\cdot)$ enables compression when storage constraints warrant it (e.g. when upstream hydrogen mass flow $\dot{m}_t^{\text{H}_2}$ is available and the target storage level is not yet reached). For an ideal gas, the shaft work of a single-stage compressor can be related to the thermodynamic pressure ratio

$$\mathcal{PR} = \frac{\mathcal{P}_{\text{out}}}{\mathcal{P}_{\text{in}}},$$

Table 3.3: AEL subsection: numerical values and typical ranges.

Quantity	Description	Value / Range / Source
$P_{\text{nom,mod}}^{\text{EL}}$	AEL module nominal power	500 kW
$u_{\text{min,mod}}^{\text{EL}}$	Per-module min. input power fraction	10%
$V_{\text{op,nom}}$	Nominal operating cell voltage (fresh)	1.95 V
$V_{\text{op,EOL}}$	EoL cell voltage threshold (replacement)	2.20 V
T	Nominal operating temperature	70 °C [194]
$\mathcal{P}$	Typical operating pressure	30 bar [194]
KOH mass fraction	For computing B in 3.25	30% [193]
Ageing: $\Delta V_{\text{deg},t}$	Voltage rise per hour of operation	3 $\mu\text{V/h}$ [196]
Ageing: $\Delta V_{\text{deg},T}$	Voltage rise per K below design	5 mV/K [196]
Overpotential coeff. k	In 3.27	0.185 V [193]
$s_{\text{CH}_2\text{O}}$	Specific water use	0.015 m ³ /kg [191]
h_{in}	Internal convection (electrolyte side)	100 W/(m ² K) [196]
h_{out}	External convection (ambient air)	20 W/(m ² K) [196]
k_{st}	Steel thermal conductivity	52 W/(m K) [196]
k_{ins}	Insulation thermal conductivity	0.05 W/(m K) [196]
r_{in} (example)	Vessel inner radius	0.30 m [196]
Wall thickness	Steel wall ($r_{\text{st,o}} - r_{\text{in}}$)	5 mm [196]
Insulation thickness	($r_{\text{ins,o}} - r_{\text{ins,i}}$)	5 mm [196]

and to the inlet temperature T_{in} . Assuming polytropic compression with effective heat-capacity ratio $\gamma = c_p/c_v$, the isentropic outlet temperature is

$$T_{\text{out}}^{\text{is}} = T_{\text{in}} \mathcal{PR}^{(\gamma-1)/\gamma}, \quad 3.37$$

and the corresponding specific isentropic work sw_{is} [J/kg] is

$$sw_{\text{is}}(T_{\text{in}}, \mathcal{PR}) = c_p(T_{\text{out}}^{\text{is}} - T_{\text{in}}) = c_p T_{\text{in}} \left[\mathcal{PR}^{(\gamma-1)/\gamma} - 1 \right], \quad 3.38$$

where c_p is the specific heat at constant pressure [J/(kg K)] and γ is the ratio of heat capacities c_p/c_v [-]. The actual specific shaft work is larger than sw_{is} and can be written as

$$sw_{\text{shaft}} = \frac{sw_{\text{is}}}{\eta_{\text{is}}}, \quad 3.39$$

where η_{is} is the isentropic efficiency of the compressor stage [-]. After accounting for mechanical and motor/drive efficiencies, lumped into η_{el} , the specific electrical work sw_{el} [J/kg] becomes

$$sw_{\text{el}}(T_{\text{in}}, \mathcal{PR}) = \frac{sw_{\text{is}}(T_{\text{in}}, \mathcal{PR})}{\eta_{\text{is}}\eta_{\text{el}}}. \quad 3.40$$

In principle, Eqs. 3.37–3.40 could be evaluated explicitly for each timestep and each compression stage, keeping track of temperature rise and intercooling.

For the present rule-based plant model, a simpler but thermodynamically consistent representation is adopted. The electrical demand of the compressor is expressed via a pressure-span-dependent specific electricity consumption SEC^{COMP} , as shown in Eq. 3.41:

$$p_t^{\text{COMP}} = \text{SEC}^{\text{COMP}} \dot{m}_t^{\text{H}_2, \text{COMP}}, \quad 3.41$$

where p_t^{COMP} is the compressor electrical power demand [kW], $\dot{m}_t^{\text{H}_2, \text{COMP}}$ is the hydrogen mass flow through the compressor [kg/h], and SEC^{COMP} is the specific electric consumption [kWh/kg] on an electrical basis (including motor and auxiliaries). The quantity SEC^{COMP} is conceptually related to sw_{el} via

$$\text{SEC}^{\text{COMP}} = \frac{sw_{\text{el}}(T_{\text{in}}, \mathcal{PR})}{3.6 \times 10^6},$$

but in practice is taken from the engineering dataset of Tractebel (ENGIE) and Hincio [197], which reports typical specific electricity consumptions for hydrogen compression between relevant pressure levels (e.g. production, storage and dispensing), accounting for realistic multi-stage designs, intercooling and auxiliary loads. For each simulated scenario, SEC^{COMP} is thus treated as a parameter that depends on the chosen inlet and outlet pressures, while the detailed thermodynamic temperature evolution inside the compressor is not explicitly tracked.

The compressor nameplate power $P_{\text{nom}}^{\text{COMP}}$ [kW] is sized against the expected peak hydrogen mass flow $\dot{m}_t^{\text{H}_2}$ with a design margin, ensuring that

$$P_{\text{nom}}^{\text{COMP}} \geq \max_t (\text{SEC}^{\text{COMP}} \dot{m}_t^{\text{H}_2, \text{COMP}}),$$

and rule-based guards in the plant controller prevent operation beyond this limit.

Hydrogen storage

Each storage technology is a bounded inventory block. The selector $\Gamma(\cdot)$ and policy $\mu_{\sigma}(\cdot)$ read the instantaneous hydrogen surplus/deficit and dispatch a technology-specific charge/discharge command u_t^{HS} together with a setpoint (mass flow or power). The device map $f_{\sigma}(\cdot)$ advances the storage state LOH_t (level of hydrogen), while the output map $y_{\sigma}(\cdot)$ reports delivered/absorbed hydrogen and footprint for KPI accounting. The exogenous inputs ξ_t may include ambient conditions and time-varying availability of waste heat for metal-hydride systems.

Common inventory logic. The storage state is the level of hydrogen $\text{LOH}_t \in [0, 1]$ (dimensionless). Charging and discharging mass flows are $\dot{m}_t^{\text{HS, ch}}$ and $\dot{m}_t^{\text{HS, dis}}$ [kg/h], and Δt is the simulation time step [h]. The LOH update follows Eq. 3.42:

$$\text{LOH}_{t+1} = \text{LOH}_t + \frac{\Delta t}{m_{\text{nom}}^{\text{HS}}} \left(\eta^{\text{HS, ch}} \dot{m}_t^{\text{HS, ch}} - \frac{\dot{m}_t^{\text{HS, dis}}}{\eta^{\text{HS, dis}}} \right), \quad 3.42$$

where $m_{\text{nom}}^{\text{HS}}$ is the nominal hydrogen mass capacity of the storage [kg], and $\eta^{\text{HS, ch}}, \eta^{\text{HS, dis}} \in (0, 1]$ are charge/discharge efficiencies (default $\eta^{\text{HS, ch}} = \eta^{\text{HS, dis}} = 1$).

In practice, operation is further restricted to a technology-specific window as shown in Eq. 3.43:

$$\text{LOH}_{\min} \leq \text{LOH}_t \leq \text{LOH}_{\max}, \quad 0 \leq \text{LOH}_{\min} < \text{LOH}_{\max} \leq 1, \quad 3.43$$

for example to keep a minimum buffer for security of supply or to avoid very high or very low pressure in physical vessels.

Compressed-gas hydrogen (CGH₂) vessels: Type I–IV

Compressed-gas hydrogen (CGH₂) tanks are pressure-constrained inventories. $\Gamma(\cdot)$ and $\mu_{\sigma}(\cdot)$ enforce interface-pressure compatibility (post-compressor discharge); $f_{\sigma}(\cdot)$ updates the

level LOH_t ; $y_\sigma(\cdot)$ reports payload, power and site footprint. Vessels follow the standard taxonomy: Type I (all-metal), Type II (hoop-wrapped metal), Type III (full composite, metal liner), and Type IV (full composite, polymer liner) [198]. Operating bands are selected according to code and design practice; higher pressure improves volumetric density but increases composite content and applicable siting distances per National Fire Protection Association (NFPA) [199]. *Note:* NFPA 2 is a U.S. code; it is used here only as a transparent proxy for stand-off distances when estimating land footprint. Actual designs must comply with the country-specific fire-safety authority and applicable local regulations.

Geometry, payload, footprint. A practical envelope uses external diameter D_{ext} and cylindrical length L_{tank} , compatible with stacking in an International Organization for Standardization (ISO) container [200]. With wall thickness δ_{wall} from type/pressure specifications [201–203], the internal diameter and volume are obtained as shown in Eq. 3.44:

$$D_{\text{int}} = D_{\text{ext}} - 2 \delta_{\text{wall}}, \quad \text{Vol}_{\text{int}} = \frac{\pi}{4} D_{\text{int}}^2 L_{\text{tank}}, \quad 3.44$$

where D_{int} is the internal diameter [m]; D_{ext} the external diameter [m]; δ_{wall} the wall thickness [m]; Vol_{int} the internal volume [m^3]; and L_{tank} the cylindrical length [m].

The per-vessel payload is represented in Eq. 3.45:

$$m_{\text{ves}}^{\text{H}_2} = \rho_{\text{H}_2}(\mathcal{P}^{\text{HS}}, T^{\text{HS}}) \text{Vol}_{\text{int}}, \quad 3.45$$

where $m_{\text{ves}}^{\text{H}_2}$ is the hydrogen mass per vessel [kg] and $\rho_{\text{H}_2}(\mathcal{P}^{\text{HS}}, T^{\text{HS}})$ is the real-gas density of hydrogen at storage conditions [kg/m^3] (from *CoolProp* [204]). The array footprint is calculated as in Eq. 3.46 and shown in Figure 3.5:

$$A_{\text{site}} = L_{\text{site}} W_{\text{site}} = [N_{\text{row}} L_{\text{cont}} + (N_{\text{row}} - 1) d_{\text{aisle}} + 2 d_{\text{NFPA}}] [N_{\text{col}} W_{\text{cont}} + (N_{\text{col}} - 1) d_{\text{aisle}} + 2 d_{\text{NFPA}}], \quad 3.46$$

where A_{site} is the site footprint area [m^2]; $N_{\text{row}}, N_{\text{col}}$ are the numbers of containers per row and per column [-]; d_{aisle} is the service-corridor spacing between containers [m]; d_{NFPA} is the perimeter clearance required by NFPA 2 [m] [199]; and $L_{\text{cont}}, W_{\text{cont}}$ are, respectively, container length and width [m] [200]. Each container packs N_v vessels [-]; plant-level nominal mass $m_{\text{nom}}^{\text{HS}}$ is the product of N_v , the number of containers and $m_{\text{ves}}^{\text{H}_2}$.

Charging raises the electrolyser outlet to the storage pressure using the compressor block; the tank itself is modelled as an isothermal inventory at $(\mathcal{P}^{\text{HS}}, T^{\text{HS}})$. Discharge to end-use may require throttling/pressure regulation; Joule–Thomson effects for hydrogen are neglected under the considered regimes.

Underground hydrogen storage (UHS) in salt caverns

At moderate depths, operation commonly spans tens to a few hundred bar; studies and projects report representative maximum cavern pressure $\mathcal{P}_{\text{max}}^{\text{UHS}} \approx 200$ bar and cushion-gas fraction of order 30 % [205, 206]. In this integration, the subsurface is abstracted as a large inventory with negligible surface footprint. Surface balances include wellhead-compression electric power p_t^{COMP} only, and the storage state is the level LOH_t (dimensionless) updated via Eq. 3.42 with an appropriately large $m_{\text{nom}}^{\text{HS}}$.

Metal hydride (MH) storage

MH storage is a thermally coupled inventory. Γ, μ_σ verify charge/discharge feasibility (electrolyser outlet pressure $\geq \mathcal{P}^{\text{eq, MH}}(T)$ for absorption; external Phase Change Material

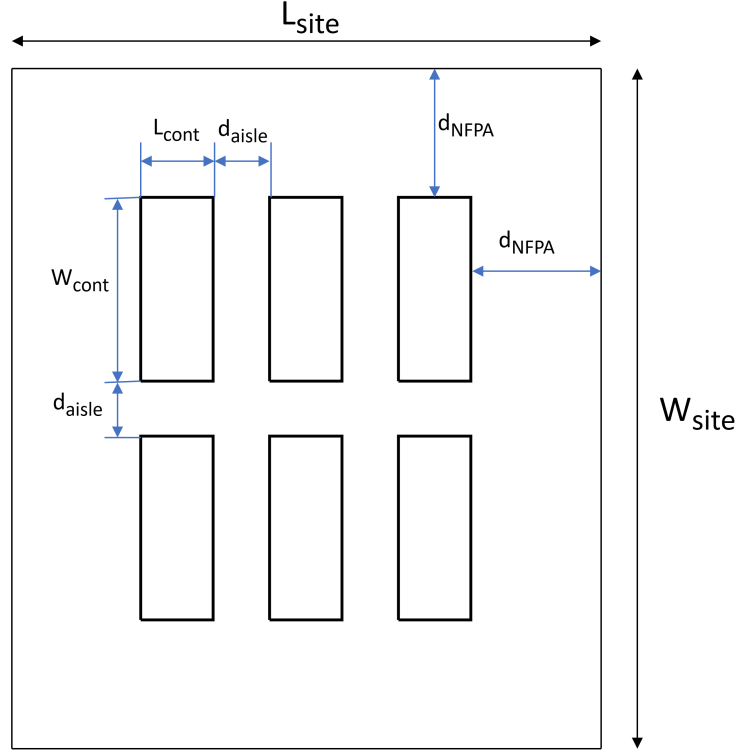
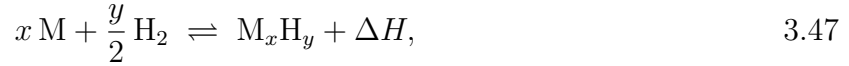


Figure 3.5: Schematic of the CGH₂ container layout and site footprint used in Eq. 3.46: container length L_{cont} and width W_{cont} , number of rows N_{row} and columns N_{col} , service-aisle spacing d_{aisle} , and perimeter clearance d_{NFPA} required by NFPA 2.

(PCM) heat availability at T_{des} for desorption). f_{σ} advances the level LOH_t and thermal states (bed/PCM). y_{σ} reports hydrogen throughput and the electric-heater power p_t^{EH} .

The reversible reaction is written, as shown in Eq. 3.47:



where x and y are the stoichiometric coefficients of the host metal M and hydrogen, respectively [-]; M_xH_y is the formed hydride phase; and ΔH is the reaction enthalpy.

The plateau (equilibrium) pressure is set by the van't Hoff relation, as shown in Eq. 3.48:

$$\ln \mathcal{P}^{\text{eq,MH}}(T) = \frac{\Delta H}{R_{\text{univ}} T} - \frac{\Delta S}{R_{\text{univ}}}, \quad 3.48$$

where $\mathcal{P}^{\text{eq,MH}}(T)$ is the equilibrium (plateau) pressure [bar]; R_{univ} is the universal gas constant [J/(mol K)]; ΔS is the entropy change [J/(mol K)]; and ΔH is as defined above [J/mol] [207, 208].

Desorption requires thermal energy q_{des} [kW h/kg] denoting the total thermal energy per kilogram of released hydrogen required to desorb at T_{des} .

If a PCM buffers absorption heat, the external duty becomes, as shown in Eq. 3.49:

$$q_{\text{des,PCM}} = (1 - \eta^{\text{PCM}}) q_{\text{des}}, \quad 3.49$$

where $q_{\text{des,PCM}}$ is the external thermal energy per kilogram of hydrogen when PCM heat recovery is employed [kW h/kg], and $\eta^{\text{PCM}} \in [0, 1]$ is the fraction of q_{des} recovered by the PCM [-] (a reasonable value according to the literature is 0.7) [209, 210].

Two representative classes under identical boundary conditions are considered: a high-temperature light-metal hydride (e.g., MgH₂) and a low-temperature intermetallic (e.g.,

LaNi₅). This choice spans the main solid-state storage design space: light-metal hydrides offer higher gravimetric capacity at the cost of higher desorption temperatures and larger thermal duties, whereas intermetallics operate near ambient with lower q_{des} but require a larger bed mass per unit hydrogen. To keep the model representative and traceable, the operating/desorption temperatures used later in the case studies are set to $T_{\text{des}} \approx 280^\circ\text{C}$ for MgH₂ and $T_{\text{des}} \approx 45^\circ\text{C}$ for LaNi₅, consistent with typical plateau-pressure windows and with published MH reactor integration studies [207, 208]. The bed and PCM inventories follow, as shown in Eq. 3.50:

$$\frac{m^{\text{MH}}}{m_{\text{bed}}^{\text{H}_2}} = \frac{100}{\text{wt}\%\text{H}}, \quad \frac{m_{\text{PCM}}}{m_{\text{bed}}^{\text{H}_2}} = \frac{q_{\text{des}}}{q_{\text{PCM}}}, \quad 3.50$$

where m^{MH} is the hydride-bed mass [kg]; $m_{\text{bed}}^{\text{H}_2}$ is the stored hydrogen mass associated with the bed [kg]; wt%H is the hydrogen weight percentage at the operating plateau [%]; m_{PCM} is the PCM mass [kg]; and q_{PCM} is the PCM latent heat at $T_{\text{PCM}} \approx T_{\text{des}}$ [kW h/kg] [208, 211, 212].

Heat-supply pathways and mapping to electricity. Usable industrial waste-heat rate from a sensible stream s (inlet temperature $T_{s,\text{in}}$) is computed, as shown in Eq. 3.51:

$$p_{s,t}^{\text{th}} = \frac{\dot{m}_{s,t} c p_s [T_{s,\text{in}} - (T_{\text{des}} + \Delta T_{\text{pp}})]}{3600}, \quad 3.51$$

where $p_{s,t}^{\text{th}}$ is the recoverable sensible-heat power [kW]; $\dot{m}_{s,t}$ is the mass flow rate of stream s [kg/h]; $c p_s$ is its specific heat capacity [kJ/(kg K)]; $T_{s,\text{in}}$ is the stream inlet temperature [K]; T_{des} is the desorption temperature [K]; and ΔT_{pp} is the heat-exchanger pinch temperature difference [K] [42, 207]. In implementation, $p_{s,t}^{\text{th}}$ is clipped to zero if $T_{s,\text{in}} \leq T_{\text{des}} + \Delta T_{\text{pp}}$.

Residual (uncovered) desorption duty is supplied by an electric resistance heater (EH) with efficiency η^{EH} . This choice is made for methodological clarity and minimum complexity: it provides a technology-agnostic and conservative mapping from thermal duty to electrical demand ($\text{COP} \approx 1$), and it preserves linearity in the subsequent MILP formulations; alternative heat supplies (e.g. dedicated burners or heat pumps) could be introduced if the site has a defined thermal network, but are out of scope here. The required electric powers are, as shown in Eq. 3.52:

$$p_t^{\text{EH}} = \frac{q_{\text{des}} \dot{m}_t^{\text{MH,des}} - p_{s,t}^{\text{th}}}{\eta^{\text{EH}}}, \quad p_t^{\text{EH,PCM}} = \frac{q_{\text{des,PCM}} \dot{m}_t^{\text{MH,des}} - p_{s,t}^{\text{th}}}{\eta^{\text{EH}}}, \quad 3.52$$

where q_{des} and $q_{\text{des,PCM}}$ are thermal energies per unit hydrogen mass [kW h/kg] and $\dot{m}_t^{\text{MH,des}}$ is the hydrogen desorption mass flow [kg/h], yielding p_t^{EH} and $p_t^{\text{EH,PCM}}$ in [kW]. In implementation, the arguments of Eq. 3.52 are clipped at zero so that the EH is idle whenever available waste heat covers the full desorption duty. In industrial settings such as hydrogen-based Direct Reduced Iron (DRI) and Electric Arc Furnace (EAF), realistic mass flows and temperatures often cover only a fraction of q_{des} , making EH the marginal provider in many locations (as quantified in Section 4.3).

Interface distinctions. Unlike CGH₂, both MgH₂ and LaNi₅ can be charged directly at typical electrolyser outlet pressure, avoiding a compressor on the charging path; discharge is pressure-at-temperature limited by the van't Hoff relation $\mathcal{P}^{\text{eq,MH}}(T)$, so post-compression may or may not be required depending on end-use pressure. Because MH modules operate at low pressure, their site footprint is compact and NFPA CGH₂ standoffs do not apply [213, 214].

Battery energy storage (BESS)

The BESS is a bounded electrical inventory block. The selector $\Gamma(\cdot)$ and policy $\mu_\sigma(\cdot)$ read the instantaneous electrical surplus/deficit and dispatch a mutually exclusive charge/discharge command with power setpoints $p_t^{\text{BESS,ch}}$ and $p_t^{\text{BESS,dis}}$. The device map $f_\sigma(\cdot)$ advances the internal state SOC_t (State of Charge) and, if enabled, updates the State of Health (SOH_t). The output map $y_\sigma(\cdot)$ exposes absorbed/delivered electric energy for KPI accounting. This follows common practice for Li-ion stationary systems [215].

Common inventory logic. Let $\text{SOC}_t \in [0, 1]$ be the State of Charge at time step t and Δt the simulator step in hours [h]. With self-discharge rate $\text{SDR} [\text{h}^{-1}]$, charging/discharging efficiencies $\eta^{\text{BESS,ch}}, \eta^{\text{BESS,dis}} \in (0, 1]$, and effective capacity E_t^{BESS} [kWh] (possibly degraded by SOH), the raw SOC update is shown in Eq. 3.53:

$$\text{SOC}_{t+1} = \text{SOC}_t (1 - \text{SDR} \Delta t) + \frac{p_t^{\text{BESS,ch}} \Delta t \eta^{\text{BESS,ch}}}{E_t^{\text{BESS}}} - \frac{p_t^{\text{BESS,dis}} \Delta t}{E_t^{\text{BESS}} \eta^{\text{BESS,dis}}}. \quad 3.53$$

Operational bounds are expressed via minimum and maximum admissible State of Charge, $\text{SOC}_{\min}$ and $\text{SOC}_{\max}$ (dimensionless):

$$\text{SOC}_{\min} \leq \text{SOC}_t \leq \text{SOC}_{\max}, \quad 0 \leq \text{SOC}_{\min} < \text{SOC}_{\max} \leq 1. \quad 3.54$$

Typical lithium-ion systems operate with $\text{SOC}_{\min} > 0$ and $\text{SOC}_{\max} < 1$ to limit degradation, so the usable energy window is $E_t^{\text{BESS}}(\text{SOC}_{\max} - \text{SOC}_{\min})$. Eq. 3.53 thus captures first-order inventory effects: (i) parasitic losses via the factor $(1 - \text{SDR} \Delta t)$, where SDR is obtained from a monthly value by conversion to the simulator time base; (ii) asymmetric charge/discharge pathways through $\eta^{\text{BESS,ch}}$ and $\eta^{\text{BESS,dis}}$ and (iii) the dependence on effective capacity E_t^{BESS} so that any SOH fade tightens the usable window.

Let $E_{\text{nom}}^{\text{BESS}}$ be the nameplate capacity [kWh] and $\text{SOH}_t \in (0, 1]$ the State of Health; the effective capacity is given by Eq. 3.55:

$$E_t^{\text{BESS}} = \text{SOH}_t E_{\text{nom}}^{\text{BESS}}. \quad 3.55$$

With C-rate $\mathcal{C} [\text{h}^{-1}]$, the admissible power region is shown in Eq. 3.56:

$$0 \leq p_t^{\text{BESS,ch}} \leq \mathcal{C} E_t^{\text{BESS}}, \quad 0 \leq p_t^{\text{BESS,dis}} \leq \mathcal{C} E_t^{\text{BESS}}. \quad 3.56$$

These limits reflect pack- and converter-level constraints: at any SOH, the maximum admissible charge/discharge power scales with E_t^{BESS} , meaning that ageing not only reduces stored energy but also derates peak power for a given $\mathcal{C}$.

Ageing model (weekly update). Ageing is represented via SOH_t and updated on a coarser (weekly) grid by accumulating (a) cyclic damage from rain-flow cycle counting and (b) calendar damage (SOC/temperature dependent). Cyclic damage per week is computed as shown in Eq. 3.57:

$$\mathcal{D}_{\text{cyc}} = \frac{N_{\text{cyc}}^{\text{eq}}}{\text{LC}}, \quad 3.57$$

where $N_{\text{cyc}}^{\text{eq}}$ is the equivalent number of full cycles from rain-flow counting over the week and $\text{LC} = 7000$ [216, 217]. Calendar damage per week is represented as shown in Eq. 3.58:

$$\mathcal{D}_{\text{cal}} = \chi(T, \text{SOC}) (2 - \text{SOH}) - \alpha(T), \quad 3.58$$

with the empirical polynomial given as shown in Eq. 3.59:

$$\begin{aligned} \chi(T, \text{SOC}) = & 3.274 \times 10^{-3} + 1.555 \times 10^{-3} \frac{T - 52.5}{7.5} + 6.40 \times 10^{-5} \left(\frac{T - 52.5}{7.5} \right)^2 \\ & + 1.416 \times 10^{-3} \frac{\text{SOC} - 0.6}{0.2} + 1.63 \times 10^{-4} \left(\frac{\text{SOC} - 0.6}{0.2} \right)^2 + 6.87 \times 10^{-4} \frac{T - 52.5}{7.5} \frac{\text{SOC} - 0.6}{0.2} \end{aligned} \quad 3.59$$

In our studies we hold $T = 52.5^\circ\text{C}$ (fixed thermal setting), yielding $\alpha(T) = 19.59$ [218, 219]. Total weekly damage and SOH are represented as shown in Eq. 3.60:

$$\mathcal{D}_{\text{tot}} = \mathcal{D}_{\text{cyc}} + \mathcal{D}_{\text{cal}}, \quad \text{SOH}(\text{week } n) = \text{SOH}(\text{week } n - 1) - \mathcal{D}_{\text{tot}} (1 - \text{EOL}), \quad 3.60$$

and the pack is scheduled for replacement upon reaching $\text{EOL} = 0.70$.

Figure 3.6 illustrates a representative 25-year trajectory obtained with this ageing model, showing the evolution of the State of Charge and the decomposition of State of Health into calendar and cyclic components.

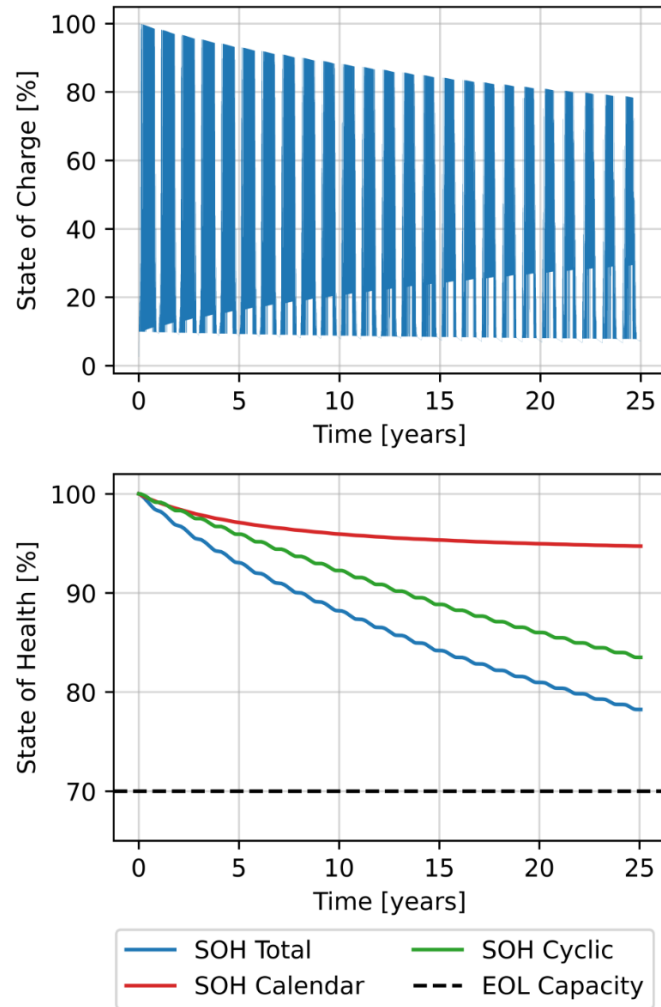


Figure 3.6: Example of battery ageing over a 25-year project horizon. Top: State of Charge (SOC) trajectory from the rule-based dispatcher. Bottom: decomposition of State of Health (SOH) into total, calendar and cyclic contributions with the end-of-life (EOL) capacity threshold at 70%.

The end-of-life threshold $\text{SOH} = 0.7$ and the nominal cyclic life $LC = 7000$ are aligned with values commonly assumed for stationary Li-ion systems (EoL at 70–80% of initial capacity

and cycle life of a few thousand up to $\sim 10\,000$ cycles depending on depth-of-discharge and temperature) [216, 217]. Figure 3.6 therefore illustrates a degradation magnitude and split (calendar vs cycling) consistent with this literature-based range.

The rain-flow step extracts half-cycles from the SOC trajectory and aggregates them into an equivalent number of full cycles $N_{\text{cyc}}^{\text{eq}}$, implicitly capturing the effect of cycle depth on wear (deeper swings contribute more to $\mathcal{D}_{\text{cyc}}$). This weekly aggregation substantially reduces runtime while preserving ageing trends over long horizons. Calendar ageing $\mathcal{D}_{\text{cal}}$ grows with higher resting SOC and temperature through $\chi(T, \text{SOC})$, whereas $\alpha(T)$ provides a diffusion-related offset calibrated at 52.5°C . The update in Eq. 3.60 modifies E_t^{BESS} (and therefore the feasible region in Eq. 3.56) directly, so dispatch decisions endogenously respond to degradation without extra constraints. The 70% EoL capacity threshold is a conventional criterion for stationary Li-ion systems; upon reaching it, replacement is triggered and the SOC window and power limits revert to nameplate values for the new pack. Eqs. 3.57–3.60 follow the approach applied in [220].

All parameters used to model the BESS are represented in Table 3.4. The defaults (charging/discharging efficiencies of 0.95) imply a round-trip efficiency close to 90%, and the monthly self-discharge (5 %) is translated into the hourly rate SDR so that parasitic losses scale consistently with the chosen Δt via the factor $(1 - \text{SDR} \Delta t)$.

Table 3.4: BESS parameters and default values used in the rule-based simulator (Li-ion).

Symbol	Name	Units	Value	Source
$\eta^{\text{BESS, ch}}$	Charging efficiency	—	0.95	[215, 221]
$\eta^{\text{BESS, dis}}$	Discharging efficiency	—	0.95	[215, 221]
SDR	Self-discharge rate (hourly)	h^{-1}	$0.05/(30 \times 24)$	[215]
$\text{SOC}_{\min}$	Minimum state of charge	—	0.10	[221, 222]
$\text{SOC}_{\max}$	Maximum state of charge	—	0.90	[221, 222]
$\mathcal{C}$	C-rate	h^{-1}	0.9	[222]
EOL	End-of-life capacity	—	0.70	[215, 222]
LC	Life cycles to EoL	—	7000	[217]
$\alpha(T)$	Diffusion-related term	—	19.59 (at 52.5°C)	[218]

Hydrogen conversion

Each hydrogen converter turns stored H_2 into electricity and, when enabled, useful heat. The controller enforces guards (minimum load, inventory threshold) and dispatches either a power setpoint or a hydrogen-consumption request; the device maps return time-indexed electric/thermal powers and hydrogen flows, and efficiencies are reported on a LHV basis.

Gas turbine (GT)

A simple-cycle gas turbine (GT) converts hydrogen to shaft power; a downstream HRSG recovers exhaust heat for steam. The controller dispatches either an electric-power setpoint p_t^{GT} or a steam-following request $\dot{m}_{\text{st},t}^*$. The output map $y_\sigma(\cdot)$ returns p_t^{GT} , $\dot{m}_{\text{st},t}$, and $\dot{m}_t^{\text{H}_2, \text{GT}}$.

A commercial aero-derivative such as the Siemens SGT-100 (see Table 3.5 for numerical figures) provides a reference geometry and baseline performance; vendor data and readiness for hydrogen co-firing guide the design point [99]. The plant model is assembled from modular components (compressor, combustor, turbine, HRSG) and solved simultaneously with a fully

implicit linearised scheme as in [223]. Off-design maps parameterise performance, as shown in Eq. 3.61:

$$(\eta_t^{\text{GT}}, p_t^{\text{GT}}, \dot{m}_{\text{exh},t}^{\text{GT}}, T_{\text{exh},t}) = \Phi(\text{load}_t, T_{\text{amb},t}), \quad 3.61$$

where η_t^{GT} is the (turbomachinery) efficiency $[-]$; p_t^{GT} the electric power at generator terminals [kW]; $\dot{m}_{\text{exh},t}^{\text{GT}}$ and $T_{\text{exh},t}$ the exhaust mass flow [kg/h] and temperature [K]; load_t the fractional load $[-]$; and $T_{\text{amb},t}$ the ambient temperature [K]. Operational guards act on load range and exhaust constraints (guardposts in Table 3.5). Hydrogen firing eliminates acid-dew concerns and carbon species in flue gas; thus, the lower stack-temperature bound used for fossil fuels can be relaxed, subject to plume buoyancy and local regulations [224, 225].

The hydrogen mass flow for a given electric power is shown in Eq. 3.62:

$$\dot{m}_t^{\text{H}_2,\text{GT}} = \frac{p_t^{\text{GT}}}{\eta_t^{\text{GT}} \eta^{\text{gen}} \text{LHV}_{\text{H}_2}}, \quad 3.62$$

where η^{gen} is the generator efficiency $[-]$. With $\text{H}_2 + \frac{1}{2}\text{O}_2 \rightarrow \text{H}_2\text{O}$ and dry air oxygen molar fraction x_{O_2} , the required (dry) stoichiometric air flow is scaled by an excess-air ratio Λ_{air} , as shown in Eq. 3.63:

$$\dot{m}_{\text{air},\text{in},t} = \Lambda_{\text{air}} \frac{0.5}{x_{\text{O}_2}} \frac{M_{\text{air}}}{M_{\text{H}_2}} \dot{m}_t^{\text{H}_2,\text{GT}}, \quad 3.63$$

and the hot-gas mass flow is (neglecting dilution or bleed), as shown in Eq. 3.64:

$$\dot{m}_{\text{exh},t}^{\text{GT}} = \dot{m}_{\text{air},\text{in},t} + \dot{m}_t^{\text{H}_2,\text{GT}}. \quad 3.64$$

Eqs. 3.63–3.64 anchor $\dot{m}_{\text{exh},t}^{\text{GT}}$ to fuel and air settings when the map in Eq. 3.61 is unavailable; otherwise, the map prevails and Λ_{air} is inferred.

GT–HRSG coupling. The HRSG recovers exhaust heat to generate saturated steam at $\mathcal{P}_{\text{st}}$. A bypass fraction $b_t \in [0, 1]$ allows part of the exhaust to skip the HRSG. The minimum feasible stack temperature consistent with a single-pressure HRSG and a pinch ΔT_{pp} is shown in Eq. 3.65:

$$T_{\text{stack},\text{min}} = T_{\text{sat}}(\mathcal{P}_{\text{st}}) + \Delta T_{\text{pp}}, \quad 3.65$$

while the economiser outlet (feedwater to drum) is subcooled below saturation by ΔT_{sub} , as shown in Eq. 3.66:

$$T_{\text{fw},\text{in}} = T_{\text{sat}}(\mathcal{P}_{\text{st}}) - \Delta T_{\text{sub}}. \quad 3.66$$

The sensible-heat rate available to the HRSG is then obtained as shown in Eq. 3.67:

$$p_t^{\text{HRSG,th,avail}} = (1 - b_t) \frac{\dot{m}_{\text{exh},t}^{\text{GT}} c_{p_{\text{exh}}} [T_{\text{exh},t} - T_{\text{stack},\text{min}}]}{3600}, \quad 3.67$$

where $p_t^{\text{HRSG,th,avail}}$ is the sensible-heat power available to the HRSG [kW]; $c_{p_{\text{exh}}}$ is the effective specific heat of the exhaust gas [kJ/(kg K)]; and $T_{\text{stack},\text{min}}$ is the minimum allowed stack temperature after heat recovery, accounting for the pinch temperature difference ΔT_{pp} [K] (a steam-side approach ΔT_{app} is enforced in HRSG design).

The steam production is obtained, as shown in Eq. 3.68:

$$\dot{m}_{\text{st},t} = \frac{3600 p_t^{\text{HRSG,th,avail}}}{[h_g(\mathcal{P}_{\text{st}}) - h_f(\mathcal{P}_{\text{st}})] + [h_f(\mathcal{P}_{\text{st}}) - h_f(\mathcal{P}_{\text{st}}, T_{\text{fw},\text{in}})]}, \quad 3.68$$

where $\dot{m}_{\text{st},t}$ is the saturated-steam mass flow [kg/h]; and $h_g(\mathcal{P}_{\text{st}})$ and $h_f(\mathcal{P}_{\text{st}})$ are the saturated-vapour and saturated-liquid specific enthalpies at $\mathcal{P}_{\text{st}}$ [kJ/kg].

The net CHP outputs are p_t^{GT} and $\dot{m}_{\text{st},t}$. The overall CHP efficiency on an LHV basis is, as shown in Eq. 3.69:

$$\eta_{\text{CHP}}^{\text{GT}} = \frac{p_t^{\text{GT}} + \phi_{\text{st}} \frac{\dot{m}_{\text{st},t} [h_g(\mathcal{P}_{\text{st}}) - h_f(\mathcal{P}_{\text{st}})]}{3600}}{\dot{m}_t^{\text{H}_2, \text{GT}} \text{LHV}_{\text{H}_2}}, \quad 3.69$$

where $\phi_{\text{st}} \in [0, 1]$ is the useful-steam utilisation factor $[-]$.

Design follows ISO conditions ($\mathcal{P}_{\text{ISO}}, T_{\text{ISO}}, \text{RH}_{\text{ISO}}$); the SGT-100 baseline is matched at the datasheet point; the resulting geometry feeds the HRSG design via ΔT_{pp} , ΔT_{sub} and $\mathcal{P}_{\text{st}}$. Off-design maps are then generated over load $\in [30, 120]\%$ and $T_{\text{amb}} \in [-10^\circ\text{C}, 40^\circ\text{C}]$, subject to inlet turbine temperature lower than 1530 K, and queried hourly (steam-following or power-following). Hydrogen operation is obtained by re-running the same geometry with 100% H_2 fuel; Table 3.5 reports baseline and hydrogen figures aligned with [99, 223].

Table 3.5: GT–HRSG modelling constants, guards and reference SGT-100 figures (ISO design).

Quantity	Description	Value / Source
$P_{\text{nom}}^{\text{GT}}$	SGT-100 rated shaft power	5.4 MW [99]
η^{GT}	Gross GT efficiency at ISO point	0.3 [99, 223]
$\dot{m}_{\text{exh}}^{\text{GT}}$ (ISO)	Exhaust mass flow (baseline NG)	21 kg/s [99]
T_{exh} (ISO)	Exhaust temperature (baseline NG)	549 °C [99]
$\mathcal{P}_{\text{ISO}}$	ISO ambient pressure	101 325 Pa [223]
T_{ISO}	ISO ambient temperature	15 °C [223]
RH_{ISO}	ISO relative humidity	60 % [223]
T_{amb} range	Off-design ambient span in Φ	-10°C to 40°C [223]
load range	Off-design load window in Φ	30–120% of rated [223]
TIT_{max}	Guard in dispatch (map constraint)	1530 K [223]
η^{gen}	Generator efficiency	0.98 (assumed)
$\mathcal{P}_{\text{st}}$	Steam pressure (paper-mill use case)	20 bar [223]
ΔT_{pp}	HRSG pinch-point (evaporator outlet)	10 K [223]
ΔT_{sub}	Economiser subcooling to drum	10 K [223]
$T_{\text{fw,ret}}$	Return condensate temperature (to pump)	30 °C [223]
$\mathcal{P}_{\text{fw,ret}}$	Return condensate pressure (pump inlet)	1 bar [223]
x_{O_2}	Air oxygen molar fraction	0.21 (dry air)
Λ_{air}	Excess-air ratio in combustor	1.6–2.6
$c_{p,\text{exh}}$	Exhaust c_p (effective, hot section)	1.10 kJ/(kg K)
$T_{\text{stack,min}}$	Lower stack temperature	363 K [224]

Solid-oxide fuel cell (SOFC) model

Scope note. Whereas the literature distinguishes low-temperature fuel cells (e.g., PEMFC, PAFC) and high-temperature fuel cells (e.g., SOFC, MCFC), the detailed electrochemical model developed in this thesis is specific to the SOFC case study. When other chapters refer generically to an FC within MILP scheduling, the FC is represented through a technology-agnostic (parameterised) conversion model; the economic and environmental KPI framework is the same, but the underlying device model differs by case study.

A solid-oxide fuel cell (SOFC) stack converts the chemical energy of hydrogen and oxygen into electricity and high-grade heat through ionic conduction of O^{2-} across a ceramic

electrolyte. Typical materials include a nickel/yttria-stabilised zirconia (Ni/YSZ) anode, a YSZ electrolyte, and a lanthanum strontium manganite-based cathode. Owing to electrolyte conductivity and cathode kinetics, operation at high temperature is standard (see Table 3.6), enabling internal reforming and direct sensible heating of reactants in the channels [226]. The selector $\Gamma(\cdot)$ enables the converter when hydrogen inventory and plant conditions warrant it; the policy $\mu_\sigma(\cdot)$ dispatches either an electric-power setpoint p_t^{FC} or a hydrogen-consumption request $\dot{m}_t^{\text{H}_2, \text{FC}}$, enforcing minimum load. The output map $y_\sigma(\cdot)$ exposes net electric power p_t^{FC} [kW], hydrogen consumption $\dot{m}_t^{\text{H}_2, \text{FC}}$ [kg/h], thermal output $p_t^{\text{FC, th}}$ [kW], and efficiencies.

Unless otherwise noted, all equations in this subsection refer to a single SOFC module ($P_{\text{nom, mod}}^{\text{FC}} = 100 \text{ kW}$ stack). Let $N_{\text{mod}, t}$ be the number of identical modules operating at time t (integer), and assume homogeneous dispatch so each active module follows the same setpoint. Then plant-level quantities are obtained by aggregation as shown in Eq. 3.70:

$$p_t^{\text{FC}} = N_{\text{mod}, t} p_t^{\text{FC, mod}}, \quad \dot{m}_t^{\text{H}_2, \text{FC}} = N_{\text{mod}, t} \dot{m}_t^{\text{H}_2, \text{FC, mod}}, \quad p_t^{\text{FC, th, net}} = N_{\text{mod}, t} p_t^{\text{FC, th, net, mod}}, \quad 3.70$$

and similarly for all other per-module mass/energy flows entering the HRSG.

As for all fuel cell types, the stack voltage is written as shown in Eq. 3.71:

$$V_{\text{stack}} = N_{\text{cell}} (V_{\text{rev}} - V_{\text{act}} - V_{\text{ohm}} - V_{\text{conc}}), \quad 3.71$$

where V_{stack} is the stack voltage [V], N_{cell} the number of series cells $[-]$, V_{rev} the reversible voltage [V], V_{act} the activation overpotential [V], V_{ohm} the ohmic overpotential [V], and V_{conc} the concentration overpotential [V]. At SOFC temperatures we set $V_{\text{act}} = 0$ (absorbed in $i_{0, \text{ca}}$ and ASR calibration for $T \geq 800 \text{ }^\circ\text{C}$) [226].

The reversible voltage follows the Nernst relation, as shown in Eq. 3.72:

$$V_{\text{rev}}(T, \mathcal{P}) = V^0(T) - \frac{R_{\text{univ}} T}{2F} \ln \left(\frac{\mathcal{P}_{\text{H}_2\text{O}}}{\mathcal{P}_{\text{H}_2} \mathcal{P}_{\text{O}_2}^{1/2}} \right), \quad 3.72$$

where $V^0(T)$ is the standard reversible potential [V] and $\mathcal{P}_{\text{H}_2}$, $\mathcal{P}_{\text{O}_2}$, $\mathcal{P}_{\text{H}_2\text{O}}$ are partial pressures [bar] so the logarithm is dimensionless. For air, set $\mathcal{P}_{\text{O}_2} = x_{\text{O}_2} \mathcal{P}_{\text{ca}}$; on the anode, compute $\mathcal{P}_{\text{H}_2}$ and $\mathcal{P}_{\text{H}_2\text{O}}$ from inlet composition.

Ohmic losses use an area-specific resistance (ASR), as shown in Eq. 3.73:

$$V_{\text{ohm}} = i \text{ ASR}, \quad \text{ASR} = \frac{\ell_{\text{elec}}}{\kappa_m(T)}, \quad \kappa_m(T) = \frac{K_{\text{ion}}}{T} \exp \left(- \frac{E_{\text{a, ion}}}{R_{\text{univ}} T} \right), \quad 3.73$$

where ASR is the area-specific resistance [$\Omega \text{ m}^2$], ℓ_{elec} is the electrolyte thickness [m], and $\kappa_m(T)$ is the ionic conductivity [S/m] with prefactor K_{ion} [K/($\Omega \text{ m}$)] and activation energy $E_{\text{a, ion}}$ [J/mol].

Concentration losses reflect diffusion-limited transport in porous electrodes. Neglecting anode-side concentration overpotential and using a cathode-side diffusion expression, we obtain Eq. 3.74:

$$V_{\text{conc}} = \frac{R_{\text{univ}} T}{4F \alpha_{\text{ct}}} \ln \left[\frac{i}{i_{0, \text{ca}} \left(x_{\text{O}_2} - \frac{\ell_{\text{ca}} i R_{\text{univ}} T}{4F \mathcal{P}_{\text{ca}} \text{Diff}_{\text{O}_2, \text{N}_2}^{\text{eff}}} \right)} \right], \quad 3.74$$

where α_{ct} is the (cathode) charge-transfer coefficient $[-]$; $i_{0, \text{ca}} = i_{0, \text{ca}}(T)$ is the cathode exchange current density [A/m^2]; x_{O_2} is the oxygen molar fraction in air $[-]$; ℓ_{ca} is the

cathode thickness [m]; $\mathcal{P}_{\text{ca}}$ is the cathode-side total pressure [bar]; and $\text{Diff}_{\text{O}_2, \text{N}_2}^{\text{eff}}$ is the effective oxygen diffusivity in the cathode gas mixture [m^2/s]. The temperature law for the exchange current is shown in Eq. 3.75:

$$i_{0,\text{ca}}(T) = i_{0,\text{ca},\text{ref}} \exp\left(\frac{b_{\text{act}} E_{\text{a,ca}}}{R_{\text{univ}}} \left[\frac{1}{T_{\text{ref}}} - \frac{1}{T}\right]\right), \quad 3.75$$

and the limiting current (domain guard) is shown in Eq. 3.76:

$$i_{\text{lim}} = \frac{4F x_{\text{O}_2} \mathcal{P}_{\text{ca}} \text{Diff}_{\text{O}_2, \text{N}_2}^{\text{eff}}}{\ell_{\text{ca}} R_{\text{univ}} T}, \quad 0 < i < i_{\text{lim}} \quad 3.76$$

When the active area is unknown, a practical sizing relation consistent with electrolysis is adopted, as shown in Eq. 3.77:

$$A_{\text{cell}} = \frac{P_{\text{nom,mod}}^{\text{FC}} 1000}{V_{\text{cell,min}} N_{\text{cell}} i_{\text{max}}}, \quad 3.77$$

where A_{cell} is the single-cell active area [m^2]; $P_{\text{nom,mod}}^{\text{FC}}$ is the module nameplate electrical power [kW]; $V_{\text{cell,min}}$ is the minimum admissible cell voltage at i_{max} [V]; N_{cell} is the number of series cells [-]; and i_{max} is the maximum operating current density used for sizing [A/m^2].

Hydrogen consumption follows Faraday's law (reported in kg/h), as shown in Eq. 3.78:

$$\dot{m}_t^{\text{H}_2, \text{FC,mod}} = \frac{I_{\text{cell}} N_{\text{cell}}}{2F} M_{\text{H}_2} \times 3600, \quad 3.78$$

where $I_{\text{cell}} = i A_{\text{cell}}$ is the cell current [A]; M_{H_2} is the molar mass of hydrogen [kg/mol]; and F is the Faraday constant [C/mol]. The corresponding molar oxygen flow is shown in Eq. 3.79:

$$\dot{n}_{\text{O}_2} = \frac{I_{\text{cell}} N_{\text{cell}}}{4F} \times 3600 \quad [\text{mol/h}]. \quad 3.79$$

An air feed with excess ratio Λ is then given by Eq. 3.80:

$$\dot{m}_{\text{air,in},t} = \Lambda \frac{\dot{n}_{\text{O}_2}}{x_{\text{O}_2}} M_{\text{air}}, \quad 3.80$$

where M_{air} is the average molar mass of air [kg/mol]. Faradaic outlet flows for the mass balance are represented in Eqs. 3.81 and 3.82:

$$\dot{n}_{\text{H}_2\text{O,out}} = \frac{I_{\text{cell}} N_{\text{cell}}}{2F} \times 3600, \quad \dot{n}_{\text{O}_2,\text{cons}} = \frac{I_{\text{cell}} N_{\text{cell}}}{4F} \times 3600, \quad 3.81$$

$$\dot{m}_{\text{H}_2\text{O,out}} = \dot{n}_{\text{H}_2\text{O,out}} M_{\text{H}_2\text{O}}, \quad \dot{m}_{\text{air,out},t} = \dot{m}_{\text{air,in},t} - \dot{n}_{\text{O}_2,\text{cons}} M_{\text{O}_2}, \quad 3.82$$

where $M_{\text{H}_2\text{O}}$ and M_{O_2} are the molar masses of water and oxygen [kg/mol], respectively.

The recoverable thermal power on an LHV basis is shown in Eq. 3.83:

$$p_t^{\text{FC,th,mod}} = \frac{I_{\text{cell}}}{1000} (N_{\text{cell}} V_{\text{LHV}} - V_{\text{stack}}), \quad 3.83$$

where $V_{\text{LHV}} = \text{LHV}_{\text{H}_2}/(2F)$ is the LHV-equivalent voltage [V]. The net high-grade heat for cogeneration subtracts reactant preheating (mass flows in kg/h, cp in kJ/(kg K)), as shown in Eq. 3.84:

$$p_t^{\text{FC,th,net,mod}} = \eta_{\text{HX}} p_t^{\text{FC,th,mod}} - \frac{\dot{m}_{\text{air,in},t} cp_{\text{air}} (T_{\text{air,out}} - T_{\text{air,in}})}{3600} - \frac{\dot{m}_t^{\text{H}_2, \text{FC,mod}} cp_{\text{H}_2} (T_{\text{H}_2,\text{out}} - T_{\text{H}_2,\text{in}})}{3600}, \quad 3.84$$

where η_{HX} is the heat-recovery efficiency [-]; cp_{air} and cp_{H_2} are the specific heats of air and hydrogen [kJ/(kg K)]; and $T_{\text{air,out}}$, $T_{\text{air,in}}$, $T_{\text{H}_2,\text{out}}$, $T_{\text{H}_2,\text{in}}$ are inlet/outlet temperatures [K]. Unless otherwise stated, we take $T_{\text{air,out}} = T_{\text{H}_2,\text{out}} = T_{\text{op}}$ and $T_{\text{air,in}} = T_{\text{H}_2,\text{in}} = 298.15$ K.

Instantaneous electrical and cogeneration efficiencies on an LHV basis are, respectively, as shown in Eq. 3.85:

$$\eta^{\text{el,FC}} = \frac{p_t^{\text{FC}}}{\dot{m}_t^{\text{H}_2,\text{FC}} \text{LHV}_{\text{H}_2}}, \quad \eta^{\text{tot,FC}} = \frac{p_t^{\text{FC}} + \eta_{\text{HX}} p_t^{\text{FC,th}}}{\dot{m}_t^{\text{H}_2,\text{FC}} \text{LHV}_{\text{H}_2}}. \quad 3.85$$

Figure 3.7 illustrates the resulting single-module performance, showing the dependence of global efficiency and hydrogen consumption on current density according to Eqs. 3.71–3.85 under nominal operating conditions from Table 3.6.

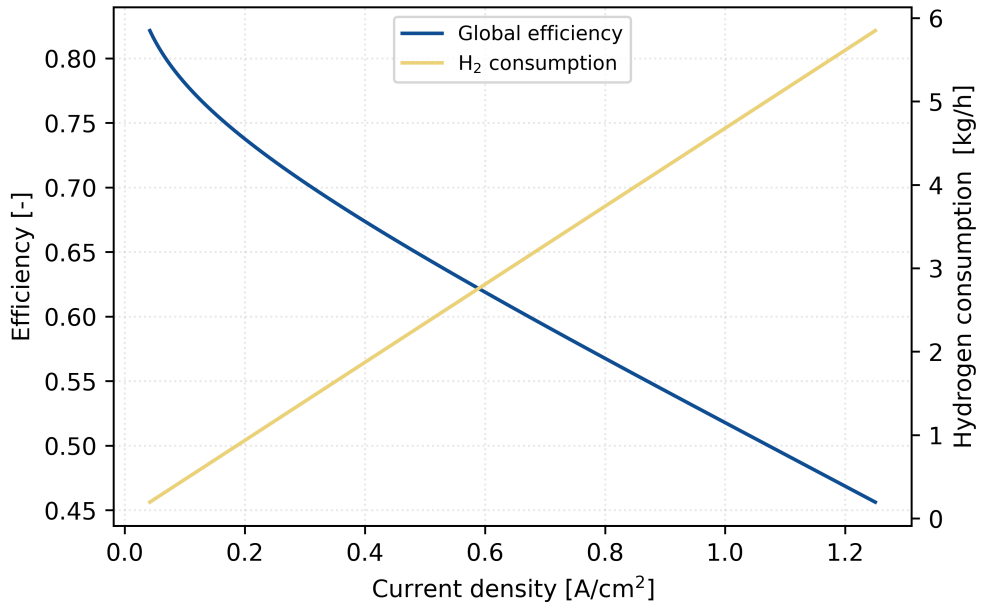


Figure 3.7: Resulting performance of a single SOFC module under nominal conditions: module-level (stack-based) global (electrical + thermal) efficiency (left axis) and hydrogen consumption (right axis) as functions of current density. Thermal integration is accounted for through heat recovery (η_{HX}) and explicit subtraction of reactant pre-heating duties (Eq. 3.84).

Modelling boundary (BoP and thermal integration). The curve in Figure 3.7 is reported at the module boundary, i.e., it reflects the electrochemical conversion and the recoverable thermal power as modelled by Eqs. 3.71–3.84. Balance-of-plant electrical auxiliaries (e.g., air handling, pumps, power electronics) are not modelled as separate power sinks in this thesis; hence, system-level net electrical efficiency would be slightly lower, with the deviation typically becoming more relevant at low-load operation. Thermal integration effects are explicitly represented by (i) a heat-recovery factor η_{HX} and (ii) subtraction of reactant pre-heating duties to the operating temperature (Eq. 3.84), and by the subsequent SOFC–HRSG sensible-heat coupling and pinch constraints (Section ?? and equations below).

SOFC–HRSG coupling. The SOFC exhaust consists of two streams per module that mix before the HRSG: the cathode gas (mostly N_2 , essentially dry) and the anode exhaust (mostly H_2O). Let $\dot{m}_{\text{ca,out},t}$ and $\dot{m}_{\text{an,out},t}$ be their mass flows [kg/h], with temperatures $T_{\text{ca,out}}$ and $T_{\text{an,out}}$ [K] (typically $T_{\text{ca,out}} \approx T_{\text{an,out}} \approx T_{\text{op}}$). The mixture entering the HRSG is shown

in Eq. 3.86:

$$\dot{m}_{\text{exh},t}^{\text{FC}} = \dot{m}_{\text{ca,out},t} + \dot{m}_{\text{an,out},t}, \quad h_{\text{mix},t} = \frac{\dot{m}_{\text{ca,out},t} h(T_{\text{ca,out}}, \mathbf{y}_{\text{ca}}) + \dot{m}_{\text{an,out},t} h(T_{\text{an,out}}, \mathbf{y}_{\text{an}})}{\dot{m}_{\text{exh},t}^{\text{FC}}}, \quad 3.86$$

where $h(\cdot)$ is the specific enthalpy [kJ/kg] and $\mathbf{y}_{\text{ca}}, \mathbf{y}_{\text{an}}$ are gas mass (or molar) fractions. The inlet gas temperature $T_{\text{exh,in},t}$ to the HRSG follows from $h_{\text{mix},t}$ via the effective heat capacity $cp_{\text{exh}}(\mathbf{y}_{\text{mix}}, T)$.

The same stack-floor relation as the GT section is used here, as shown in Eq. 3.87:

$$T_{\text{stack,min}} = T_{\text{sat}}(\mathcal{P}_{\text{st}}) + \Delta T_{\text{pp}}, \quad 3.87$$

and, as for the GT case, the economiser subcooling is set as shown in Eq. 3.88:

$$T_{\text{fw,in}} = T_{\text{sat}}(\mathcal{P}_{\text{st}}) - \Delta T_{\text{sub}}. \quad 3.88$$

The sensible-heat rate available to the HRSG is then shown in Eq. 3.89:

$$p_t^{\text{HRSG,th,avail}} = (1 - b_t) \frac{\dot{m}_{\text{exh},t}^{\text{FC}} cp_{\text{exh}}(T_{\text{exh,in},t} - T_{\text{stack,min}})}{3600}, \quad 3.89$$

where $p_t^{\text{HRSG,th,avail}}$ is the sensible-heat power available to the HRSG [kW]; cp_{exh} is evaluated on the exhaust mixture at an appropriate mean temperature [kJ/(kg K)]; and b_t is the exhaust bypass fraction [–].

The saturated-steam generation rate at $\mathcal{P}_{\text{st}}$ is then, as in the GT case, represented in Eq. 3.90:

$$\dot{m}_{\text{st},t} = \frac{3600 p_t^{\text{HRSG,th,avail}}}{[h_{\text{g}}(\mathcal{P}_{\text{st}}) - h_{\text{f}}(\mathcal{P}_{\text{st}})] + [h_{\text{f}}(\mathcal{P}_{\text{st}}) - h_{\text{f}}(\mathcal{P}_{\text{st}}, T_{\text{fw,in}})]}, \quad 3.90$$

where $\dot{m}_{\text{st},t}$ is the saturated-steam mass flow [kg/h]; and $h_{\text{g}}(\mathcal{P}_{\text{st}})$ and $h_{\text{f}}(\mathcal{P}_{\text{st}})$ are the saturated-vapour and saturated-liquid specific enthalpies at $\mathcal{P}_{\text{st}}$ [kJ/kg].

3.1.2 Key performance indicators (KPIs)

This section introduces the time index, the simulator channels exposed by the output map $y_t = y_{\sigma_t}(x_t, u_t, \xi_t)$ in Eq. 3.1, the price signals carried by ξ_t , and the annual aggregators used later to build economic metrics.

Time index and annual partition. Timesteps are $t = 1, \dots, N_T$ with constant step Δt [h]. The horizon spans N calendar years. For each year $y \in \{1, \dots, N\}$, let $\mathcal{T}_y \subset \{1, \dots, N_T\}$ be the set of timesteps that fall in year y .

Simulator channels used for KPIs (outputs of y_{σ_t}). The following powers and mass/volumetric

Table 3.6: SOFC stack parameters and HRSG constants used in Section 3.1.1.

Quantity	Description	Value
$P_{\text{nom,mod}}^{\text{FC}}$	Module nominal power	100 kW
T_{op}	Nominal SOFC operating temperature	800 °C
V^0	Open-circuit potential at SOFC conditions	1.16 V
x_{O_2}	Oxygen molar fraction in air	0.21
$\mathcal{P}_{\text{ca}}$	Cathode total pressure	1.013 bar
$\mathcal{P}_{\text{H}_2,\text{in}}$	Anode inlet H ₂ pressure	1.16 bar
α_{ct}	Charge-transfer coefficient (cathode)	0.5
ℓ_{ca}	Cathode thickness (in V_{conc})	0.8 mm
$\text{Diff}_{\text{O}_2,\text{N}_2}^{\text{eff}}$	Effective O ₂ diffusivity (cathode gas)	0.2 cm ² /s
$i_{0,\text{ca,ref}}$	Cathode exchange current density at T_{ref}	0.2 A/cm ²
$E_{\text{a,ca}}$	Cathode activation energy (for $i_{0,\text{ca}}$)	160 kJ/mol
b_{act}	Activation coefficient	10
T_{ref}	Reference temperature for $i_{0,\text{ca}}$	750 °C
ℓ_{elec}	Electrolyte thickness	0.03 mm
K_{ion}	Prefactor in $\kappa_m(T)$	9000 K/(Ω m)
$E_{\text{a,ion}}$	Ionic-conduction activation energy	100 kJ/mol
Λ	Air excess ratio (cathode path)	1.2
i_{max}	Max. operating current density (sizing)	1.25 A/cm ²
$V_{\text{cell,min}}$	Design cell voltage at i_{max}	0.633 V
A_{cell}	Single-cell active area (per module)	0.1292 m ²
N_{cell}	Cells per stack	97
cp_{air}	Specific heat of air	1.04 kJ/(kg K)
cp_{H_2}	Specific heat of hydrogen	14.3 kJ/(kg K)
$\mathcal{P}_{\text{st}}$	HRSG steam pressure	20 bar
ΔT_{pp}	HRSG pinch-point (evaporator outlet)	10 K
ΔT_{sub}	Economiser subcooling to drum	75 K

flows are computed by closing the site balances at each step:

$p_t^{\text{grid,imp}}$ [kW]	grid-import active power;
$p_t^{\text{grid,exp}}$ [kW]	grid-export active power;
p_t^{EL} [kW]	electrolyser electrical demand (sum of active modules);
p_t^{COMP} [kW]	compressor electrical demand;
p_t^{EH} [kW]	electric-heater demand for MH desorption (if employed);
$p_t^{\text{FC}}, p_t^{\text{GT}}$ [kW]	net electrical production (by technology);
$\dot{m}_t^{\text{H}_2}$ [kg/h]	net hydrogen production rate at the facility boundary;
$\dot{m}_t^{\text{HS,ch}}$ [kg/h]	hydrogen charge flow at storage interfaces;
$\dot{m}_t^{\text{HS,dis}}$ [kg/h]	hydrogen discharge flow at storage interfaces;
$\dot{m}_t^{\text{O}_2,\text{EL}}$ [kg/h]	oxygen co-product rate (from electrolysis);
$p_t^{\text{th,net}}$ [kW]	net useful heat;
$\dot{m}_{\text{st},t}$ [kg/h]	steam mass flow (at the specified steam pressure $\mathcal{P}_{\text{st}}$) from HRSG/CHP;
$\dot{V}_t^{\text{H}_2\text{O,EL}}$ [m ³ /h]	process-water volumetric flow to electrolyzers.

Price signals (components of ξ_t). Unit prices used to value the corresponding simulator channels are represented below:

$c_t^{\text{el,imp}}$ [€/kWh]	price for imported electricity at time t ;
$c_t^{\text{el,exp}}$ [€/kWh]	remuneration for exported electricity at time t ;
$c_y^{\text{H}_2\text{O}}$ [€/m ³]	unit cost of process water including treatment (year-indexed);
c_y^{NG} [€/kWh]	reference price of natural-gas energy (LHV basis);
$c_y^{\text{H}_2,\text{grey}}$ [€/kg]	reference cost of grey hydrogen;
c_y^{cert} [€/kg]	unit premium per certified kilogram of H ₂ under RED III.

Import/export electricity prices are time-varying to capture hourly/tariff structures, while the others are constant throughout the year. The natural-gas price is expressed on an LHV basis to align with CHP references. The certification premium c_y^{cert} is a year-indexed exogenous incentive per certified kilogram, consistent with the provenance ledger described later in Section 3.1.2 [10].

Annual aggregators. For any power time series p_t [kW], the undiscounted annual energy is shown in Eq. 3.91:

$$E_y\{p_t\} = \sum_{t \in \mathcal{T}_y} p_t \Delta t \quad [\text{kW h}], \quad 3.91$$

with Δt in h. For any mass-flow series $\dot{m}_t$ [kg/h], the annual mass is shown in Eq. 3.92:

$$m_y\{\dot{m}_t\} = \sum_{t \in \mathcal{T}_y} \dot{m}_t \Delta t \quad [\text{kg}], \quad 3.92$$

and for any volumetric-flow series $\dot{V}_t$ [m³/h], the annual volume is shown in Eq. 3.93:

$$V_y\{\dot{V}_t\} = \sum_{t \in \mathcal{T}_y} \dot{V}_t \Delta t \quad [\text{m}^3], \quad 3.93$$

so that flows are consistently in 1/h and aggregation uses Δt in h.

Derived yearly energies and masses. Applying Eqs. 3.91–3.93 to the simulator channels yields the yearly totals used later in the economic KPIs:

$$\begin{aligned}
E_y^{\text{grid,imp}} &= E_y\{p_t^{\text{grid,imp}}\} \text{ [kW h]} && \text{annual imported electrical energy;} \\
E_y^{\text{grid,exp}} &= E_y\{p_t^{\text{grid,exp}}\} \text{ [kW h]} && \text{annual exported electrical energy;} \\
m_y^{\text{H}_2} &= m_y\{\dot{m}_t^{\text{H}_2}\} \text{ [kg]} && \text{annual net hydrogen production;} \\
E_y^{\text{FC}} &= E_y\{p_t^{\text{FC}}\}, \quad E_y^{\text{GT}} = E_y\{p_t^{\text{GT}}\} \text{ [kW h]} && \text{annual production by H}_2\text{-to-power converters;} \\
E_y^{\text{th,net}} &= E_y\{p_t^{\text{th,net}}\} \text{ [kW h]} && \text{annual net useful heat;} \\
V_y^{\text{EL}} &= V_y\{\dot{V}_t^{\text{H}_2\text{O,EL}}\} \text{ [m}^3\text{]} && \text{annual process-water volume to electrolyzers.}
\end{aligned}$$

PV and wind generation are tracked separately as p_t^{PV} and p_t^{WT} (see Section 3.1.1); their yearly energies are $E_y^{\text{PV}} = E_y\{p_t^{\text{PV}}\}$ and $E_y^{\text{WT}} = E_y\{p_t^{\text{WT}}\}$. The converter-specific totals E_y^{FC} , and E_y^{GT} ensure no double-counting with RES.

Cash flows composition

Simulator outputs are translated into yearly monetary terms by pairing each physical driver with the corresponding tariff and integrating over time (“quantity $\times$ price”). Replacements are treated as time-stamped capital outlays occurring in the year in which they take place (e.g., stack replacements). Accordingly, we distinguish the upfront investment C_0 (year $y=0$) from replacement outflows $\text{CAPEX}_y^{\text{repr}}$ (years $y > 0$), which are discounted at the year of occurrence in the economic KPIs (see Eq. 3.107). Energies come from Eq. 3.91, masses from Eq. 3.92, and volumes from Eq. 3.93.

Revenues. These are positive cash inflows associated with external sales or avoided purchases.

Whenever the site is a net exporter, the exported electrical energy is remunerated at the export tariff $c_t^{\text{el,exp}}$; the yearly revenue is, as shown in Eq. 3.94:

$$\text{REV}_y^{\text{el,exp}} = \sum_{t \in \mathcal{T}_y} c_t^{\text{el,exp}} p_t^{\text{grid,exp}} \Delta t, \quad 3.94$$

which values only the surplus injected to the grid. Self-consumed on-site generation is monetised implicitly by lower imports (see $\text{OPEX}_y^{\text{el}}$ below) and is not double-counted here.

When on-site H_2 covers a hydrogen demand that would otherwise be met with grey hydrogen, the avoided purchase is valued, as shown in Eq. 3.95:

$$\text{REV}_y^{\text{H}_2,\text{sav}} = c_y^{\text{H}_2,\text{grey}} m_y^{\text{H}_2,\text{cov}}, \quad 3.95$$

where $c_y^{\text{H}_2,\text{grey}}$ [€/kg] is the reference cost of grey hydrogen and $m_y^{\text{H}_2,\text{cov}}$ [kg] is the portion of the site hydrogen demand actually supplied by the project in year y .

When the project covers electric and/or thermal loads that, in a baseline, were provided by another device, the savings equal the baseline NG energy that would have been burnt to deliver the same services, as shown in Eq. 3.96:

$$\text{REV}_y^{\text{NG,sav}} = c_y^{\text{NG}} E_y^{\text{NG,ref}}, \quad 3.96$$

where $E_y^{\text{NG,ref}}$ [kW h] is the baseline natural-gas energy (LHV basis) that would have been used to supply the displaced services in year y .

When quantities of hydrogen are certified by the provenance ledger, an incentive is recognised per certified kilogram, as shown in Eq. 3.97:

$$\text{REV}_y^{\text{cert}} = c_y^{\text{cert}} m_y^{\text{H}_2,\text{cert}}, \quad 3.97$$

where $m_y^{\text{H}_2, \text{cert}}$ [kg] is the certified hydrogen mass in year y (defined in Eq. 3.121) under the adopted annual RED III correlation and threshold [10].

The total revenue is, as shown in Eq. 3.98:

$$\text{REV}_y = \text{REV}_y^{\text{el,exp}} + \text{REV}_y^{\text{H}_2, \text{sav}} + \text{REV}_y^{\text{NG, sav}} + \text{REV}_y^{\text{cert}}. \quad 3.98$$

Operating expenditures (OPEX). These are cash outflows required to operate the plant.

Imported electricity is valued at the time-varying import tariff $c_t^{\text{el,imp}}$ and integrated over the year, as shown in Eq. 3.99:

$$\text{OPEX}_y^{\text{el}} = \sum_{t \in \mathcal{T}_y} c_t^{\text{el,imp}} p_t^{\text{grid,imp}} \Delta t, \quad 3.99$$

Demineralised water sent to electrolyzers is charged at the water price, as shown in Eq. 3.100:

$$\text{OPEX}_y^{\text{H}_2\text{O}} = c_y^{\text{H}_2\text{O}} V_y^{\text{EL}}, \quad 3.100$$

Fixed O&M covers annualised service contracts, scheduled maintenance, and overheads modelled as a fraction of installed capital by asset, as shown in Eq. 3.101:

$$\text{OPEX}_y^{\text{O\&M, fix}} = \sum_{a \in \mathcal{A}} \text{frac}_a^{\text{O\&M}} \text{CAPEX}_a, \quad 3.101$$

where $\text{frac}_a^{\text{O\&M}} \in [0, 1]$ is the annual O&M fraction (e.g., 0.03 for 3% /yr) and CAPEX_a is the installed capital cost of asset a [€]. Short-lifetime replacements are excluded here and treated as CAPEX in the investment metrics.

Summing the operating costs, as shown in Eq. 3.102:

$$\text{OPEX}_y = \text{OPEX}_y^{\text{el}} + \text{OPEX}_y^{\text{H}_2\text{O}} + \text{OPEX}_y^{\text{O\&M, fix}}. \quad 3.102$$

Cash flows. Year- y operating cash flow is revenue minus operating costs, as shown in Eq. 3.103:

$$CF_y = \text{REV}_y - \text{OPEX}_y. \quad 3.103$$

CF_y [€] feeds the investment metrics (NPV, payback). It excludes upfront investment C_0 and any replacements $\text{CAPEX}_y^{\text{repr}}$, which are handled explicitly later together with the investment metrics.

Investment metrics

This part upgrades the operating picture into standard investment indicators by discounting yearly operating cash flows CF_y from Eq. 3.103 and combining them with capital outlays. Unless stated otherwise, DR denotes the real discount rate. Short-lifetime replacements are treated explicitly as capital expenditures $\text{CAPEX}_y^{\text{repr}}$ and excluded from OPEX_y , in line with common practice [227, 228]. The upfront investment is defined from installed asset costs and standard adders, as shown in Eqs. 3.104–3.106:

$$\text{CAPEX}_{\text{tot}} = \sum_{a \in \mathcal{A}} \text{CAPEX}_a \quad [\text{€}], \quad 3.104$$

where CAPEX_a for each asset a is expressed as:

$$\text{CAPEX}_a = \text{CAPEX}_a^{\text{unit}} \cdot P_{\text{nom}}^a \quad [\text{€}], \quad 3.105$$

with $\text{CAPEX}_a^{\text{unit}}$ being the cost per unit of nominal power for asset a [€/kW], and P_{nom}^a the nominal power of asset a [kW].

$$C_0 = (1 + \text{frac}^{\text{inst}} + \text{frac}^{\text{eng}}) \text{CAPEX}_{\text{tot}} \quad [\text{€}], \quad 3.106$$

where $\text{CAPEX}_{\text{tot}}$ is the sum of installed capital costs by asset [€]; and $\text{frac}^{\text{inst}}, \text{frac}^{\text{eng}} \in [0, 1]$ are the installation/BOP and engineering fractions, respectively.

Net present value (NPV). NPV aggregates all discounted operating cash flows and subtracts both the upfront investment C_0 and the discounted replacements $\text{CAPEX}_y^{\text{repr}}$, as shown in Eq. 3.107:

$$\text{NPV} = \sum_{y=1}^N \frac{CF_y - \text{CAPEX}_y^{\text{repr}}}{(1 + \text{DR})^y} - C_0. \quad 3.107$$

A positive NPV indicates value creation at the chosen DR. In practice, if a component is replaced in year $\bar{y}$, the associated cost enters as $\text{CAPEX}_{\bar{y}}^{\text{repr}}/(1 + \text{DR})^{\bar{y}}$, i.e., it is discounted at the year in which the replacement occurs (it is not lumped into C_0).

Net present cost (NPC). NPC is the present value of all project costs over the analysis horizon; it excludes any revenues or incentives, as represented in Eq. 3.108:

$$\text{NPC} = C_0 + \sum_{y=1}^N \frac{\text{CAPEX}_y^{\text{repr}} + \text{OPEX}_y}{(1 + \text{DR})^y}. \quad 3.108$$

Here we deliberately exclude revenues so as not to conflate NPC with NPV.

Discounted payback period. The discounted payback Y^* is the smallest year for which the cumulative discounted cash flow becomes nonnegative (i.e., the investment is recovered in present-value terms), as shown in Eq. 3.109:

$$Y^* = \min \left\{ Y \in \{1, \dots, N\} : \sum_{y=1}^Y \frac{CF_y}{(1 + \text{DR})^y} \geq C_0 \right\}. \quad 3.109$$

This metric is informative about recovery time but ignores post-payback benefits and should be read alongside NPV.

Levelised cost of hydrogen (LCOH). LCOH reports the discounted average cost per kilogram of H_2 at the facility boundary, using the same accounting boundary as in Section 3.1.2. The numerator contains all capital items (upfront and replacements) and operating costs; the denominator is the discounted hydrogen output. Using discounted sums keeps LCOH consistent with NPV-style evaluation [229]. The definition is given in Eq. 3.110:

$$\text{LCOH} = \frac{C_0 + \sum_{y=1}^N \frac{\text{CAPEX}_y^{\text{repr}} + \text{OPEX}_y}{(1 + \text{DR})^y}}{\sum_{y=1}^N \frac{m_y^{\text{H}_2}}{(1 + \text{DR})^y}} \quad [\text{€/kg}]. \quad 3.110$$

In a PtH configuration focused on supplying H_2 , revenues from selling electricity or other energy carriers that are not fed to the electrolyzers are excluded from the LCOH numerator. The LCOH boundary here reflects the cost of producing hydrogen rather than monetising surplus energy.

Levelised cost of electricity (LCOE). When hydrogen is reconverted to electricity (SOFC/GT), an electrical-only boundary is used in the denominator, i.e., the net on-site electric energy produced by those converters. This keeps LCOE comparable to electric-only benchmarks. Discounting mirrors the LCOH convention [230]. The definition is given in Eq. 3.111:

$$\text{LCOE} = \frac{C_0 + \sum_{y=1}^N \frac{\text{CAPEX}_y^{\text{repr}} + \text{OPEX}_y}{(1 + \text{DR})^y}}{\sum_{y=1}^N \frac{E_y^{\text{FC}} + E_y^{\text{GT}}}{(1 + \text{DR})^y}} \quad [\text{€/kWh}], \quad 3.111$$

where the denominator counts only electricity from H₂-to-power converters (SOFC/GT), consistent with Section 3.1.2.

Environmental KPIs

Environmental KPIs are computed at the simulator timestep and aggregated yearly.

Annual carbon intensity of produced hydrogen. Let the total electric demand of the hydrogen chain at time t be, as shown in Eq. 3.112:

$$p_t^{\text{H}_2, \text{tot}} = p_t^{\text{EL}} + p_t^{\text{COMP}} + p_t^{\text{EH}}, \quad 3.112$$

where $p_t^{\text{H}_2, \text{tot}}$ is the total electric demand attributable to the H₂ chain [kW]. After closing the electrical balance, each load is tagged with a grid vs. on-site supply share; denote by $\text{share}_t^{\text{grid}, \text{H}_2} \in [0, 1]$ the fraction of $p_t^{\text{H}_2, \text{tot}}$ supplied by the grid. The grid-attributed electric power used by the H₂ chain and its annual energy are, as shown in Eq. 3.113:

$$p_t^{\text{H}_2, \text{imp}} = \text{share}_t^{\text{grid}, \text{H}_2} p_t^{\text{H}_2, \text{tot}}, \quad E_y^{\text{H}_2, \text{imp}} = E_y \left\{ p_t^{\text{H}_2, \text{imp}} \right\}. \quad 3.113$$

Let CI_t^{grid} be the grid carbon-intensity time series [kg_{CO2eq}/kWh] provided via ξ_t (e.g., Electricity Maps) [231]. The annual, electricity-attributed carbon intensity of hydrogen is then, as shown in Eq. 3.114:

$$CI_y^{\text{H}_2} = \frac{\sum_{t \in \mathcal{T}_y} p_t^{\text{H}_2, \text{imp}} CI_t^{\text{grid}} \Delta t}{m_y^{\text{H}_2}} \quad [\text{kg}_{\text{CO2eq}}/\text{kg}_{\text{H}_2}]. \quad 3.114$$

If additional non-electric emissions are modelled (e.g., backup NG boilers), their contributions are added to the numerator with the appropriate factors and listed explicitly in the inventory.

Certification scheme. Certification is computed in post-processing from the hourly trajectories generated by the rule-based simulator. A subset of the yearly hydrogen production is selected that can be backed by eligible electricity while meeting the RFNBO (RED III delegated acts) GHG-savings requirement, expressed here as an equivalent carbon-intensity limit. The threshold is shown in Eq. 3.115:

$$CI_{\text{max}}^{\text{RFNBO}} = 3.38 \quad [\text{kg}_{\text{CO2eq}}/\text{kg}_{\text{H}_2}], \quad 3.115$$

consistent with [11]. In addition to the GHG-savings requirement, RFNBO eligibility depends on electricity sourcing conditions (additionality, temporal correlation and geographical correlation / bidding zone) set by the complementary delegated act [10]. In this thesis, these aspects are operationalised as follows: (i) geographical correlation is enforced by modelling

production and grid attributes within a single Italian bidding zone; (ii) temporal correlation is tested through alternative matching windows implemented via the annual aggregators used in the certification post-processing; (iii) additionality is approximated by treating on-site renewable generation as the certifiable supply, while residual grid imports remain non-eligible unless covered by the selected matching rule.

The total electric demand of the hydrogen chain $p_t^{\text{H}_2, \text{tot}}$ and its grid-attributed share $p_t^{\text{H}_2, \text{imp}}$ are defined in Eqs. 3.112–3.113. The non-grid (eligible) electric power that may support certification is then computed as shown in Eq. 3.116:

$$p_t^{\text{elig}} = \max \{0, p_t^{\text{H}_2, \text{tot}} - p_t^{\text{H}_2, \text{imp}}\} \quad [\text{kW}]. \quad 3.116$$

The corresponding fraction of the hydrogen-chain demand that can be backed by eligible electricity is given in Eq. 3.117:

$$\alpha_t^{\text{elig}} = \begin{cases} \frac{p_t^{\text{elig}}}{p_t^{\text{H}_2, \text{tot}}}, & p_t^{\text{H}_2, \text{tot}} > 0, \\ 0, & p_t^{\text{H}_2, \text{tot}} = 0, \end{cases} \quad 3.117$$

so that $0 \leq \alpha_t^{\text{elig}} \leq 1$ at all times. Hourly emissions attributable to the hydrogen chain (from grid power only) are computed as shown in Eq. 3.118:

$$e_t^{\text{H}_2} = p_t^{\text{H}_2, \text{imp}} C I_t^{\text{grid}} \Delta t \quad [\text{kgCO}_{2\text{eq}}], \quad 3.118$$

and the corresponding instantaneous carbon intensity of produced hydrogen is given in Eq. 3.119:

$$C I_t^{\text{H}_2} = \begin{cases} \frac{e_t^{\text{H}_2}}{\dot{m}_t^{\text{H}_2} \Delta t}, & \dot{m}_t^{\text{H}_2} > 0, \\ 0, & \dot{m}_t^{\text{H}_2} = 0, \end{cases} \quad [\text{kgCO}_{2\text{eq}}/\text{kgH}_2]. \quad 3.119$$

We adopt a simple ex-post allocation rule: in any hour where the hydrogen-chain intensity respects the RED-III limit, only the fraction of produced hydrogen backed by eligible electricity is assigned to the certified pool; otherwise, no mass from that hour is certified. The certified hydrogen mass-flow rate is therefore given in Eq. 3.120:

$$\dot{m}_t^{\text{H}_2, \text{cert}} = \begin{cases} \alpha_t^{\text{elig}} \dot{m}_t^{\text{H}_2}, & C I_t^{\text{H}_2} \leq C I_{\text{max}}^{\text{REDIII}}, \\ 0, & C I_t^{\text{H}_2} > C I_{\text{max}}^{\text{REDIII}}. \end{cases} \quad 3.120$$

Using the mass aggregator in Eq. 3.92, the certified hydrogen mass in year y is then obtained as shown in Eq. 3.121:

$$m_y^{\text{H}_2, \text{cert}} = m_y \{ \dot{m}_t^{\text{H}_2, \text{cert}} \} = \sum_{t \in \mathcal{T}_y} \dot{m}_t^{\text{H}_2, \text{cert}} \Delta t \quad [\text{kg}]. \quad 3.121$$

Each certified kilogram is therefore (i) produced at the facility boundary in an hour whose electricity-attributed intensity is below $C I_{\text{max}}^{\text{REDIII}}$ and (ii) backed, in energy terms, by eligible non-grid electricity.

Incentive revenue is then obtained by applying Eq. 3.97 from Section 3.1.2, with the certified mass $m_y^{\text{H}_2, \text{cert}}$ computed from Eq. 3.121.

3.1.3 Genetic Algorithm sizing for rule-based simulators

Sizing is posed as a simulation–optimisation loop: a genetic algorithm (GA) proposes a candidate design s (time-invariant sizing vector); the rule-based simulator MESS (Section 3.1) evaluates multi-year techno–economic performance; the GA updates the population accordingly. Small-population, steady-state, real-coded GAs with high crossover and low mutation are suitable for continuous engineering design as represented in the following workflow [232].

- (a) *Population initialization.* Create an initial set of candidate designs.
- (b) *Evaluation by simulation.* For each $s^{(j)}$, run MESS over N years with the fixed rule-based dispatch. Aggregate energies and masses, compute yearly cash flows, and compute LCOH as shown in Eq. 3.110. Extract constraint summaries such as Unmet Demand UD (annual unmet hydrogen mass), end-of-horizon hydrogen level LOH_{NT} , and battery level SOC_{NT} .
- (c) *Fitness assignment.* The GA needs a single scalar to rank designs. Define the fitness $\mathcal{F}(s)$ so that it equals the economic objective on feasible designs and adds penalties on infeasible ones, as shown in Eq. 3.125.
- (d) *Selection.* Choose parent designs from the current population using a probabilistic rule (e.g., tournament or rank selection). Designs with lower fitness are more likely to be chosen. In a steady-state scheme, only a few parents are selected each generation because only a few offspring will replace incumbents.
- (e) *Crossover.* Form one or two offspring from a pair of parents by recombining their genes (decision variables). With simulated-binary crossover (SBX), each offspring gene is a controlled blend of the corresponding parent genes. Crossover is applied with probability Pr_{cx} ; otherwise one parent is copied forward unchanged.
- (f) *Mutation.* After crossover, perturb each offspring gene with a small random change to maintain variability and escape local traps. Polynomial mutation is applied with probability Pr_{mut} per gene.
- (g) *Repair, replacement, elitism.* Enforce admissibility by clipping to bounds and rounding discrete items to module multiples. Insert the repaired offspring by steady-state replacement, removing a few of the worst individuals. Apply elitism: copy the best two designs into the next generation unchanged.
- (h) *Stopping.* Repeat steps (b)–(g) until convergence of the best fitness over several generations or until a preset generation cap is reached. Record the best feasible design s^* and its KPIs.

The typical decision variables are component sizes. A general vector is adopted, as shown in Eq. 3.122:

$$s = [P_{\text{nom}}^{\text{PV}}, P_{\text{nom}}^{\text{WT}}, P_{\text{nom}}^{\text{EL}}, E_{\text{nom}}^{\text{BESS}}, m_{\text{nom}}^{\text{HS}}, P_{\text{nom}}^{\text{COMP}}, P_{\text{nom}}^{\text{FC}}, \dots], \quad 3.122$$

Box bounds $s_i^{\min} \leq s_i \leq s_i^{\max}$ are applied (e.g., on electrolyser size) to guarantee feasibility targets such as meeting the annual hydrogen demand at nominal continuous operation.

The objective is to minimise LCOH, as shown in Eq. 3.123:

$$\min_s \text{LCOH}(s) \quad \text{with LCOH as shown in Eq. 3.110.} \quad 3.123$$

Annual adequacy is imposed as hard constraints, as shown in Eq. 3.124:

$$\begin{aligned} \text{UD}(s) &= 0, & \text{no hydrogen unmet demand over the year,} \\ \text{LOH}_{\text{NT}}(s) &\geq \text{LOH}_0, & \text{hydrogen inventory not depleted at horizon end,} \\ \text{SOC}_{\text{NT}}(s) &\geq \text{SOC}_0, & \text{battery inventory not depleted at horizon end.} \end{aligned} \quad 3.124$$

The fitness $\mathcal{F}(s)$ guides selection and equals the economic objective on the feasible set; outside it, a scale-aware penalty ranks designs by severity of violation while keeping pressure toward feasibility, as shown in Eq. 3.125:

$$\mathcal{F}(s) = \text{LCOH}(s) + \text{wgt}_1 \left[\frac{\text{UD}(s)}{m_y^{\text{H}_2, \text{dem}}} \right]_+ + \text{wgt}_2 [\text{LOH}_0 - \text{LOH}_{\text{NT}}(s)]_+ + \text{wgt}_3 [\text{SOC}_0 - \text{SOC}_{\text{NT}}(s)]_+, \quad 3.125$$

with $[x]_+ = \max\{x, 0\}$. Here $m_y^{\text{H}_2, \text{dem}}$ is the annual hydrogen demand [kg] computed from $\dot{m}_t^{\text{H}_2, \text{dem}}$ using the yearly aggregator defined earlier; the normalisation ensures all bracketed penalty terms are dimensionless, so that the weights wgt_k carry units consistent with LCOH [€/kg]. The weights wgt_k are set each generation to a multiple of the population's median LCOH.

Simulation kernel. Given s , the kernel: (i) instantiates the component models with those sizes under the fixed rule-based policy (Section 3.1); (ii) advances the system at each timestep by selecting the operating mode, issuing device set-points and closing balances through y_{σ_t} ; (iii) updates degradation and triggers replacements on the configured schedules; (iv) aggregates yearly KPIs and computes LCOH via Eq. 3.110; (v) extracts UD, LOH_{NT} , SOC_{NT} and returns $\mathcal{F}(s)$ as shown in Eq. 3.125. Individuals are evaluated in parallel.

The population size is 40, crossover probability $\text{Pr}_{\text{cx}}=0.7$, mutation probability $\text{Pr}_{\text{mut}}=0.3$, SBX index =10, polynomial-mutation index =15, steady-state replacement, and a fixed random seed for reproducibility.

This metaheuristic layer cleanly decouples operations (fixed by the rule-based policy) from design (searched by GA), while keeping all device physics, ageing and economics consistent with the rest of the framework [232].

3.2 Optimisation-based methods

The rule-based layer in Section 3.1 provides a fast, fully transparent way to propagate plant physics forward in time. At each step t , the selector $\Gamma(\cdot)$ chooses an operating mode σ_t , the control map $\mu_{\sigma_t}(\cdot)$ proposes feasible set-points u_t , and the device/state map $f_{\sigma_t}(\cdot)$ updates the internal memories x_{t+1} such as SOC_t and LOH_t . This architecture is excellent for *what-if* studies, feasibility screening, and techno-economic accounting under a given policy. However, it is still a policy: priorities, minimum loads, import/export choices, and charge/discharge decisions are imposed heuristically and applied myopically at each t .

Two problems follow. First, nothing guarantees that the realised trajectory is economically optimal (or even “good”) once all couplings are enforced simultaneously: PV/Wind curtailment competes with electrolyser loading; the battery competes with grid import and the fuel cell; hydrogen storage competes with direct demand fulfilment and fuel-cell back-conversion. Second, when capacities are being sized, the rule set itself can bias the answer: e.g. an aggressive “keep the electrolyser always on” heuristic may force oversizing of PV or of hydrogen storage, not because those assets are intrinsically required by the physics, but because the policy never allows flexible turn-down.

To remove that bias, the second half of this chapter formulates a single optimisation baseline that uses the same device semantics, state variables, and balance equations introduced for the rule-based simulator, but no longer fixes the policy. Instead, dispatch decisions (and, if enabled, nameplate sizes) are obtained by solving a MILP. All physical balances and equipment limits are written explicitly as linear equalities/inequalities. Binary variables are introduced only where logically necessary (on/off, minimum stable load, mutually exclusive charge vs. discharge). The objective aggregates operating costs, revenues, and penalty terms; if sizing is enabled, it also adds the investment cost $J(s)$ consistently with the KPIs (e.g. LCOH) defined earlier.

This unified MILP “plant model” is written once, with every time-varying variable indexed by both time and an uncertainty scenario. Then three shells are obtained as thin overlays:

1. **Deterministic MILP** (perfect foresight): all exogenous series are assumed known, so the scenario index is dropped.
2. **Two-stage stochastic MILP**: the here-and-now design s (capacities, configuration choices) is chosen before uncertainty is revealed; operations $v_{t,\omega}$ adapt per-scenario $\omega \in \Omega$. Non-anticipativity is enforced on s .
3. **Multi-stage stochastic MILP**: decisions are distributed over a scenario tree. Early-stage bids/commitments are coupled across branches that share the same information history; later corrective recourse can diverge. Non-anticipativity is imposed stage by stage using the pairing sets Π_k already introduced in the State of the Art.

In what follows, a single scenario-ready MILP is introduced. Every time-varying signal or decision will carry two subscripts (t, ω) : $t = 1, \dots, N_T$ is the discrete time index with step Δt , and $\omega \in \Omega$ indexes a realisation of uncertain inputs (renewables, prices, demands). Dropping ω recovers the deterministic (perfect-foresight) formulation. In the multi-stage stochastic shell, the scenario index ω is later replaced by a scenario-tree node index $n \in \mathcal{N}_k$, but the plant physics and constraints remain identical. The idea is that one common MILP plant model is written once, and deterministic, two-stage, and multi-stage variants differ only in how information is revealed and which decisions must be identical across scenarios.

Decision structure and notation. A finite horizon of length N_T time steps is considered. Let Δt be the step duration, consistent with the simulation step used in Section 3.1 (typically 1 h for dispatch studies; sub-hourly refinements are possible without changing the algebra).

Uncertain exogenous data at step t are collected in $\xi_{t,\omega}$. Typical entries of $\xi_{t,\omega}$ are: (i) renewable availability, namely PV/WT production $p_{t,\omega}^{\text{PV}}, p_{t,\omega}^{\text{WT}}$, (ii) electricity import/export prices $c_{t,\omega}^{\text{el,imp}}, c_{t,\omega}^{\text{el,exp}}$ and (iii) site electrical demand $p_{t,\omega}^{\text{el,dem}}$ and hydrogen demand $\dot{m}_{t,\omega}^{\text{H}_2,\text{dem}}$.

For two-stage stochastic optimisation a finite scenario set Ω with probabilities π_ω such that $\sum_{\omega \in \Omega} \pi_\omega = 1$ is employed. Each scenario ω spans the full horizon $t = 1, \dots, N_T$. For multi-stage stochastic optimisation, Ω is replaced by a scenario tree with node sets $\mathcal{N}_k$ at each stage k , children sets $\mathcal{C}(\langle n \rangle)$, and node-wise information ζ_n ; the mapping between “global” time indices t and a node n is given by $\mathcal{T}(n)$.

The optimisation problem uses three classes of decision variables:

- **Sizing / design**: the here-and-now vector $s \in \mathcal{Z}$. Its entries are plant-wide nameplate values, e.g. $P_{\text{nom}}^{\text{PV}}, P_{\text{nom}}^{\text{WT}}, E_{\text{nom}}^{\text{BESS}}, P_{\text{nom}}^{\text{EL}}, P_{\text{nom}}^{\text{COMP}}, m_{\text{nom}}^{\text{HS}}, P_{\text{nom}}^{\text{FC}}$. This is exactly the design vector s already introduced in the GA sizing loop. An additional Diesel Generator (DG) of nominal power $P_{\text{nom}}^{\text{DG}}$ can be included to help satisfy the electrical demand in off-grid conditions.

- **Operational continuous decisions:** $v_{t,\omega} \in \mathbb{R}^{n_t}$. These are the per-step schedules:

$$v_{t,\omega} \supset (p_{t,\omega}^{\text{EL}}, p_{t,\omega}^{\text{BESS,ch}}, p_{t,\omega}^{\text{FC}}, p_{t,\omega}^{\text{grid,imp}}, p_{t,\omega}^{\text{grid,exp}}, p_{t,\omega}^{\text{DG}}, \dot{m}_{t,\omega}^{\text{H}_2,\text{EL}}, \dot{m}_{t,\omega}^{\text{H}_2,\text{FC}}, \dot{m}_{t,\omega}^{\text{HS,dis}}, \dots).$$

As in Section 3.1 $p^{(\cdot)}$ are electrical powers [kW], $\dot{m}^{(\cdot)}$ are hydrogen mass-flow rates [kg/h].

- **Operational binary / integer decisions:** $\delta_{t,\omega} \in \{0,1\}^{n^{(\delta)}}$. These encode on/off states, minimum-load commitments and mutually exclusive modes. Examples: $\delta_{t,\omega}^{\text{EL,on}}$ (electrolyser on mode), $\delta_{t,\omega}^{\text{FC,sb}}$ (fuel-cell stand-by mode), $\delta_{t,\omega}^{\text{BESS}}$ (BESS discharge vs. charge), $\delta_{t,\omega}^{\text{HS}}$ (hydrogen storage discharge vs. charge).

Plant memory states $x_{t,\omega}$ (battery SOC _{t,ω} , hydrogen level LOH _{t,ω} , etc.) are propagated explicitly by linear inventory equations identical to those in Section 3.1, now indexed by ω .

By construction, all $v_{t,\omega}$ and $\delta_{t,\omega}$ are dispatch variables to be optimised, not dictated by a heuristic rule priority. They replace the rule-based maps $\mu_{\sigma_t}(\cdot)$ and $\Gamma(\cdot)$, but keep the same physical meanings and units.

3.2.1 System balances and state recursions

Two coupled resource loops must hold at every step (t, ω) : an electrical balance and a hydrogen balance. In addition, the inventories SOC and LOH must evolve according to physically correct storage dynamics.

Electrical balance. Let $p_{t,\omega}^{\text{el,dem}}$ be the exogenous site electrical demand, i.e. the AC load that must be served at each step (t, ω) . The optimisation can satisfy this demand using on-site renewables, storage discharge, the fuel cell, the diesel generator, and/or grid imports.

We define: $p_{t,\omega}^{\text{grid,imp}} \geq 0$ as power imported from the grid, $p_{t,\omega}^{\text{grid,exp}} \geq 0$ as power exported to the grid, $p_{t,\omega}^{\text{PV}}$ and $p_{t,\omega}^{\text{WT}}$ as PV and wind electrical power actually injected at the AC node, $p_{t,\omega}^{\text{PV,curt}} \geq 0$ and $p_{t,\omega}^{\text{WT,curt}} \geq 0$ as PV and wind curtailment (spilled renewable power that is available but not injected), $p_{t,\omega}^{\text{FC,on}}$ as fuel-cell electrical production, $p_{t,\omega}^{\text{DG}}$ as diesel-generator electrical production, and $p_{t,\omega}^{\text{BESS,dis}}$ as BESS discharge power. Electrical consumptions are: the in-plant demand $p_{t,\omega}^{\text{el,dem}}$, the electrolyser $p_{t,\omega}^{\text{EL}}$, the compressor $p_{t,\omega}^{\text{COMP}}$, any electric heater $p_{t,\omega}^{\text{EH}}$ (e.g. MH desorption), the FC standby draw $p_{t,\omega}^{\text{FC,sb}}$, and the BESS charging power $p_{t,\omega}^{\text{BESS,ch}}$.

Because curtailed power is not injected into the AC node, $p_{t,\omega}^{\text{PV,curt}}$ and $p_{t,\omega}^{\text{WT,curt}}$ do not appear in the nodal balance; they only ensure feasibility in surplus situations (in particular in islanded cases where $p_{t,\omega}^{\text{grid,exp}} = 0$ and storage is full). The nodal AC power balance is therefore represented in Eq. 3.126

$$p_{t,\omega}^{\text{PV}} + p_{t,\omega}^{\text{WT}} + p_{t,\omega}^{\text{FC,on}} + p_{t,\omega}^{\text{DG}} + p_{t,\omega}^{\text{BESS,dis}} + p_{t,\omega}^{\text{grid,imp}} = p_{t,\omega}^{\text{el,dem}} + p_{t,\omega}^{\text{EL}} + p_{t,\omega}^{\text{COMP}} + p_{t,\omega}^{\text{EH}} + p_{t,\omega}^{\text{BESS,ch}} + p_{t,\omega}^{\text{FC,sb}} + p_{t,\omega}^{\text{grid,exp}}, \quad 3.126$$

The diesel generator $p_{t,\omega}^{\text{DG}}$ only needs to run (and thus incur cost/emissions in the objective) when renewables, storage and (if available) the grid cannot alone cover $p_{t,\omega}^{\text{el,dem}}$. In a strict islanded study, $p_{t,\omega}^{\text{grid,imp}} = p_{t,\omega}^{\text{grid,exp}} = 0$ feasibility is then maintained in two complementary ways: (i) any renewable surplus must be either stored or curtailed via $p_{t,\omega}^{\text{PV,curt}}$ and $p_{t,\omega}^{\text{WT,curt}}$ when there is nowhere to send it, and (ii) any residual deficit is covered by dispatching $p_{t,\omega}^{\text{DG}}$ (up to $P_{\text{nom}}^{\text{DG}}$), together with BESS discharge $p_{t,\omega}^{\text{BESS,dis}}$ and fuel-cell output $p_{t,\omega}^{\text{FC,on}}$.

Hydrogen balance. Hydrogen is produced by the electrolyser, can be sent directly to the external offtaker (the site's hydrogen demand), can be compressed into storage, can

be withdrawn from storage, and can be consumed by the fuel cell. We denote by $\dot{m}_{t,\omega}^{\text{H}_2,\text{EL}}$ [kg/h] the hydrogen production rate from electrolysis, $\dot{m}_{t,\omega}^{\text{HS,ch}}$ and $\dot{m}_{t,\omega}^{\text{HS,dis}}$ [kg/h] the hydrogen charge/discharge mass flows at the storage interface, $\dot{m}_{t,\omega}^{\text{H}_2,\text{dem}}$ [kg/h] the hydrogen mass flow delivered to the offtaker at the facility boundary, and $\dot{m}_{t,\omega}^{\text{H}_2,\text{FC}}$ [kg/h] the hydrogen consumption rate of the fuel cell when generating electric power.

At every time step (t, ω) the site-wide hydrogen routing must satisfy:

$$\dot{m}_{t,\omega}^{\text{H}_2,\text{EL}} + \dot{m}_{t,\omega}^{\text{HS,dis}} = \dot{m}_{t,\omega}^{\text{H}_2,\text{dem}} + \dot{m}_{t,\omega}^{\text{H}_2,\text{FC}} + \dot{m}_{t,\omega}^{\text{HS,ch}}, \quad \forall t, \forall \omega. \quad 3.127$$

Eq. 3.127 enforces (i) full satisfaction of the hydrogen demand $\dot{m}_{t,\omega}^{\text{H}_2,\text{dem}}$ at the boundary and (ii) conservation of mass between production, storage, on-site conversion (fuel cell), and export to the offtaker. No slack variable for unmet $\dot{m}_{t,\omega}^{\text{H}_2,\text{dem}}$ is allowed: feasibility requires that demand is always covered by some combination of fresh production $\dot{m}_{t,\omega}^{\text{H}_2,\text{EL}}$ and withdrawals $\dot{m}_{t,\omega}^{\text{HS,dis}}$.

Pressure levels enter implicitly through $\dot{m}_{t,\omega}^{\text{HS,ch}}$ and $\dot{m}_{t,\omega}^{\text{HS,dis}}$. Charging $\dot{m}_{t,\omega}^{\text{HS,ch}}$ represents hydrogen that has been raised (via the compressor) from the electrolyser outlet pressure $\mathcal{P}^{\text{EL}}$ to the storage set-point. For compressed-gas or underground storage this target pressure is $\mathcal{P}^{\text{HS}}$; for metal hydrides it is the plateau pressure $\mathcal{P}^{\text{eq,MH}}(T)$ at desorption/absorption temperature.

3.2.2 Components modelling

The following device models are linear and therefore directly admissible in a MILP. All variables carry (t, ω) and slots in $v_{t,\omega}$ or $\delta_{t,\omega}$, unless stated otherwise. Where a binary is introduced (on/off or mutual exclusivity) it becomes one entry of $\delta_{t,\omega}$.

Photovoltaics (PV)

Design parameter: $P_{\text{nom}}^{\text{PV}}$ [kW] is the installed PV nameplate power (entry of s).

Inputs (exogenous data): $\bar{p}_{t,\omega}^{\text{PV,1kW}}$ [kW/kW] is the specific PV production profile obtained from PVGIS for 1 kW of installed PV under the assumed mounting configuration for the irradiance/ambient conditions associated with (t, ω) . This profile is not a decision variable.

For any installed capacity $P_{\text{nom}}^{\text{PV}}$, the available PV electrical power before curtailment is computed as in Eq. 3.128

$$\bar{p}_{t,\omega}^{\text{PV}} = \bar{p}_{t,\omega}^{\text{PV,1kW}} P_{\text{nom}}^{\text{PV}} \quad [\text{kW}], \quad 3.128$$

which directly scales the PVGIS-derived specific production by the installed nameplate.

Decision variables: $p_{t,\omega}^{\text{PV}} \geq 0$ is the PV power actually injected into the AC node (this is what appears in the electrical balance in Eq. 3.126); $p_{t,\omega}^{\text{PV,curt}} \geq 0$ is curtailed PV power (spilled locally, not injected).

Curtailment is modelled explicitly by splitting the available PV power between injected and curtailed fractions, as shown in Eq. 3.129:

$$p_{t,\omega}^{\text{PV}} + p_{t,\omega}^{\text{PV,curt}} = \bar{p}_{t,\omega}^{\text{PV}}, \quad \forall t, \forall \omega. \quad 3.129$$

Both $p_{t,\omega}^{\text{PV}}$ and $p_{t,\omega}^{\text{PV,curt}}$ are individually bounded by the same available limit, as represented in Eq. 3.130:

$$0 \leq p_{t,\omega}^{\text{PV}} \leq \bar{p}_{t,\omega}^{\text{PV}}, \quad 0 \leq p_{t,\omega}^{\text{PV,curt}} \leq \bar{p}_{t,\omega}^{\text{PV}}, \quad \forall t, \forall \omega. \quad 3.130$$

In grid-connected cases, large instantaneous availability $\bar{p}_{t,\omega}^{\text{PV}}$ can be routed to $p_{t,\omega}^{\text{grid,exp}}$ via Eq. 3.126. In strictly islanded cases where $p_{t,\omega}^{\text{grid,exp}} = 0$, any surplus beyond local demand, BESS charging, and electrolyser loading is forced into $p_{t,\omega}^{\text{PV,curt}}$, which is why curtailment must be explicitly modelled.

Wind turbine (WT)

Design parameter: $P_{\text{nom}}^{\text{WT}}$ [kW] is the installed wind-turbine nameplate power (entry of s).

Inputs (exogenous data): PVGIS provides the wind speed time series at a reference height z_{ref} , denoted $w_{\text{ref},t,\omega}$ [m/s], for each (t, ω) . This reference wind speed is extrapolated to the turbine hub height z_{hub} using the standard power-law shear model, as represented in Eq. 3.7 of the rule-based section and extended scenario-wise in Eq. 3.131:

$$w_{h,t,\omega} = w_{\text{ref},t,\omega} \left(\frac{z_{\text{hub}}}{z_{\text{ref}}} \right)^{\alpha_{\text{shear}}}, \quad \forall t, \forall \omega, \quad 3.131$$

where $w_{h,t,\omega}$ is the hub-height wind speed [m/s] at (t, ω) , and α_{shear} is the site-specific or assumed shear exponent $[-]$. This is the same transformation described earlier for $w_{h,t}$ in Eq. 3.7, now indexed by scenario ω .

Given $w_{h,t,\omega}$, the available wind electrical power follows the three-region characteristic curve, as shown in Eq. 3.6 in the rule-based formulation and reproduced with explicit (t, ω) in Eq. 3.132:

$$\bar{p}_{t,\omega}^{\text{WT}} = \begin{cases} 0, & w_{h,t,\omega} \leq w_{\text{ci}}, \\ P_{\text{nom}}^{\text{WT}} \frac{w_{h,t,\omega}^3 - w_{\text{ci}}^3}{w_{\text{rat}}^3 - w_{\text{ci}}^3}, & w_{\text{ci}} < w_{h,t,\omega} < w_{\text{rat}}, \\ P_{\text{nom}}^{\text{WT}}, & w_{\text{rat}} \leq w_{h,t,\omega} \leq w_{\text{co}}, \\ 0, & w_{h,t,\omega} \geq w_{\text{co}}, \end{cases} \quad \forall t, \forall \omega, \quad 3.132$$

where w_{ci} [m/s] is cut-in speed, w_{rat} [m/s] the rated speed, w_{co} [m/s] the cut-out speed, and $P_{\text{nom}}^{\text{WT}}$ [kW] the WT nameplate power. Eq. 3.132 is exactly the deterministic three-zone law in Eq. 3.6, just applied to each scenario ω .

To make the MILP linear, $\bar{p}_{t,\omega}^{\text{WT}}$ in Eq. 3.132 is treated as an input parameter. Dispatch then decides how much of that available power is actually injected and how much is curtailed.

Decision variables: $p_{t,\omega}^{\text{WT}} \geq 0$ is WT power injected into the AC node; $p_{t,\omega}^{\text{WT,curt}} \geq 0$ is WT curtailment (spilled wind power, not injected).

The available wind power $\bar{p}_{t,\omega}^{\text{WT}}$ from Eq. 3.132 is split linearly between injected and curtailed parts, as shown in Eq. 3.133:

$$p_{t,\omega}^{\text{WT}} + p_{t,\omega}^{\text{WT,curt}} = \bar{p}_{t,\omega}^{\text{WT}}, \quad \forall t, \forall \omega. \quad 3.133$$

Both contributions are individually upper-bounded by the same availability, as represented in Eq. 3.134:

$$0 \leq p_{t,\omega}^{\text{WT}} \leq \bar{p}_{t,\omega}^{\text{WT}}, \quad 0 \leq p_{t,\omega}^{\text{WT,curt}} \leq \bar{p}_{t,\omega}^{\text{WT}}, \quad \forall t, \forall \omega. \quad 3.134$$

As in the PV case, in grid-connected operation a surplus $\bar{p}_{t,\omega}^{\text{WT}}$ can be exported via $p_{t,\omega}^{\text{grid,exp}}$. In islanded operation where $p_{t,\omega}^{\text{grid,exp}} = 0$, any residual surplus after covering $p_{t,\omega}^{\text{el,dem}}$, charging the BESS, and loading the electrolyser is forced into $p_{t,\omega}^{\text{WT,curt}}$.

Electrolyser (EL)

Design parameters: The electrolyser is characterised by its nameplate electrical input power $P_{\text{nom}}^{\text{EL}}$ [kW], the minimum stable load fraction $u_{\text{min}}^{\text{EL}} \in (0, 1]$ (the stack cannot operate below $u_{\text{min}}^{\text{EL}} P_{\text{nom}}^{\text{EL}}$ when producing hydrogen), a standby fraction $u_{\text{sb}}^{\text{EL}} \in [0, 1]$ that represents the parasitic draw needed to keep the stack hot and pressurised, and the specific electric consumption SEC^{EL} [kWh/kg], defined as the electrical energy required to produce one kilogram of hydrogen. In the rule-based simulator this SEC^{EL} was not constant: the stack voltage was computed from the polarisation curve as a function of current density and temperature. In the optimisation-based formulation SEC^{EL} is treated as constant so that electrical power and hydrogen production remain linearly linked, as shown in Eq. 3.140.

Inputs (exogenous data): The electrolyser has no weather-driven availability profile. Any time-varying energy tariff, water cost or certification penalty is handled in the objective and is not shown here.

Decision variables: The model distinguishes three mutually exclusive operating modes: *ON* (actively producing hydrogen), *STANDBY* (hot/pressurised but not producing), and *OFF*. We introduce: $p_{t,\omega}^{\text{EL,on}}$ [kW] for EL electrical power when producing hydrogen, $p_{t,\omega}^{\text{EL,sb}}$ [kW] for standby electrical power, $p_{t,\omega}^{\text{EL}}$ [kW] for total EL electrical consumption, which appears in the AC balance of Eq. 3.126, $\dot{m}_{t,\omega}^{\text{H}_2,\text{EL}}$ [kg/h] for hydrogen production rate, and three binary mode indicators $\delta_{t,\omega}^{\text{EL,on}}, \delta_{t,\omega}^{\text{EL,sb}}, \delta_{t,\omega}^{\text{EL,off}} \in \{0, 1\}$.

In addition, two extra binary variables are defined to distinguish how the stack was started: $\delta_{t,\omega}^{\text{EL,warm}}$ and $\delta_{t,\omega}^{\text{EL,cold}} \in \{0, 1\}$. These are used later in the cost function to price thermal stress and stack degradation differently for a warm start (from *STANDBY*) and a cold start (from *OFF*).

Exactly one operating mode is active at each (t, ω) , as shown in Eq. 3.135:

$$\delta_{t,\omega}^{\text{EL,on}} + \delta_{t,\omega}^{\text{EL,sb}} + \delta_{t,\omega}^{\text{EL,off}} = 1, \quad \forall t, \forall \omega. \quad 3.135$$

When the electrolyser is producing hydrogen (*ON* state), its load must remain between the minimum stable load and the nameplate rating, as represented in Eq. 3.136 and Eq. 3.137:

$$p_{t,\omega}^{\text{EL,on}} \geq u_{\text{min}}^{\text{EL}} P_{\text{nom}}^{\text{EL}} \delta_{t,\omega}^{\text{EL,on}}, \quad \forall t, \forall \omega, \quad 3.136$$

$$p_{t,\omega}^{\text{EL,on}} \leq P_{\text{nom}}^{\text{EL}} \delta_{t,\omega}^{\text{EL,on}}, \quad \forall t, \forall \omega. \quad 3.137$$

When the electrolyser is in *STANDBY*, it draws a parasitic fraction of nominal power to remain hot and pressurised, but it does not produce hydrogen. This standby draw is written in Eq. 3.138:

$$p_{t,\omega}^{\text{EL,sb}} = u_{\text{sb}}^{\text{EL}} P_{\text{nom}}^{\text{EL}} \delta_{t,\omega}^{\text{EL,sb}}, \quad \forall t, \forall \omega. \quad 3.138$$

When the electrolyser is *OFF* ($\delta_{t,\omega}^{\text{EL,off}} = 1$) both $p_{t,\omega}^{\text{EL,on}}$ and $p_{t,\omega}^{\text{EL,sb}}$ are zero as a consequence of Eq. 3.135–3.138.

The net electrical draw that enters the AC balance Eq. 3.126 is the sum of production load and standby load, as shown in Eq. 3.139:

$$p_{t,\omega}^{\text{EL}} = p_{t,\omega}^{\text{EL,on}} + p_{t,\omega}^{\text{EL,sb}}, \quad \forall t, \forall \omega. \quad 3.139$$

Hydrogen production is proportional to the electrical power in the *ON* state through the specific electric consumption SEC^{EL} , which is assumed constant in the MILP. This linear relation is shown in Eq. 3.140:

$$p_{t,\omega}^{\text{EL,on}} = \text{SEC}^{\text{EL}} \dot{m}_{t,\omega}^{\text{H}_2,\text{EL}}, \quad \forall t, \forall \omega. \quad 3.140$$

Eq. 3.140 replaces the full stack voltage/current model of the rule-based simulator with a single affine conversion, and makes the EL block MILP-compatible.

In addition to electric power, the electrolyser consumes process water. Let $\dot{V}_{t,\omega}^{\text{H}_2\text{O},\text{EL}}$ [m³/h] be the volumetric flow of demineralized water into the stacks. This is proportional to the hydrogen production rate as shown in Eq. 3.141:

$$\dot{V}_{t,\omega}^{\text{H}_2\text{O},\text{EL}} = s_{\text{CH}_2\text{O}} \dot{m}_{t,\omega}^{\text{H}_2,\text{EL}}, \quad \forall t, \forall \omega, \quad 3.141$$

where $s_{\text{CH}_2\text{O}}$ [m³/kg] is the specific water-use parameter (volume of purified water per kilogram of H₂ produced).

To maintain physical plausibility of operation across time steps, two additional ingredients are introduced: (i) forbidden “jump” transitions between certain modes, and (ii) warm vs. cold start identification. These constraints couple step t to step $t-1$ and are enforced for $t > 1$ (the $t=1$ state is given as initial condition).

Direct transitions between *OFF* and *STANDBY* are disallowed. In words: the stack cannot suddenly appear hot/pressurised after being *OFF*, and it cannot instantly drop from *STANDBY* to fully *OFF* without first going through an *ON*/offline ramp that is modelled as a start/stop event. This is enforced as shown in Eq. 3.142 and Eq. 3.143:

$$\delta_{t,\omega}^{\text{EL},\text{sb}} + \delta_{t-1,\omega}^{\text{EL},\text{off}} \leq 1, \quad t > 1, \forall \omega, \quad 3.142$$

$$\delta_{t,\omega}^{\text{EL},\text{off}} + \delta_{t-1,\omega}^{\text{EL},\text{sb}} \leq 1, \quad t > 1, \forall \omega. \quad 3.143$$

Eq. 3.142 prevents an *OFF*→*STANDBY* jump, and Eq. 3.143 prevents a *STANDBY*→*OFF* jump. Together with Eq. 3.135, they force changes in thermal state to pass through appropriate activation / cooldown behaviour rather than teleporting.

Warm and cold starts are then identified for costing purposes. A “warm start” means the EL is switched to *ON* after being in *STANDBY* in the previous step; a “cold start” means the EL is switched to *ON* after being *OFF* in the previous step. We detect these by introducing $\delta_{t,\omega}^{\text{EL},\text{warm}}$ and $\delta_{t,\omega}^{\text{EL},\text{cold}}$ and enforcing Eq. 3.144 and Eq. 3.145:

$$\delta_{t,\omega}^{\text{EL},\text{warm}} \geq \delta_{t,\omega}^{\text{EL},\text{on}} + \delta_{t-1,\omega}^{\text{EL},\text{sb}} - 1, \quad \delta_{t,\omega}^{\text{EL},\text{warm}} \in \{0, 1\}, \quad t > 1, \forall \omega, \quad 3.144$$

$$\delta_{t,\omega}^{\text{EL},\text{cold}} \geq \delta_{t,\omega}^{\text{EL},\text{on}} + \delta_{t-1,\omega}^{\text{EL},\text{off}} - 1, \quad \delta_{t,\omega}^{\text{EL},\text{cold}} \in \{0, 1\}, \quad t > 1, \forall \omega. \quad 3.145$$

As shown in Eq. 3.144, if the stack is *ON* at time t but was *STANDBY* at $t-1$, then $\delta_{t,\omega}^{\text{EL},\text{warm}}$ must be 1; similarly, Eq. 3.145 activates $\delta_{t,\omega}^{\text{EL},\text{cold}}$ for an *OFF*→*ON* transition. These binaries do not affect feasibility directly, but they enter the cost function so that warm and cold starts can be penalised differently.

All constraints above (*ON*/*STANDBY*/*OFF* admissible regions, minimum load, standby draw, total power, linear hydrogen conversion, forbidden transitions and warm/cold start logic) are kept identical in the deterministic, two-stage, and multi-stage stochastic MILP shells. This guarantees that start-up costs, parasitic standby consumption, and stack degradation are accounted for consistently across all optimisation-based methods.

Compressor (COMP)

Design parameters: The compressor is characterised by its nameplate electrical input power $P_{\text{nom}}^{\text{COMP}}$ [kW] and by a specific electric consumption SEC^{COMP} [kW h/kg], defined as the electrical energy required to raise one kilogram of hydrogen from electrolyser outlet pressure to the storage (or delivery) pressure. In the rule-based formulation this dependence was represented via a pressure-span-dependent SEC^{COMP} (Eq. 3.41) and here as well it is

considered as a constant SEC^{COMP} so that the compressor remains linear in the MILP, as shown in Eq. 3.148.

Inputs (exogenous data): No stochastic availability input is needed. The pressure regime (low-pressure buffer plus high-pressure tank, or directly high-pressure storage) is treated as a configuration choice and affects SEC^{COMP} , but it does not introduce new decision variables.

Decision variables: The compressor draws electrical power $p_{t,\omega}^{\text{COMP}}$ [kW] and processes a hydrogen mass flow $\dot{m}_{t,\omega}^{\text{H}_2,\text{COMP}}$ [kg/h]. When the compressor is dedicated to charging the storage, this flow coincides with the hydrogen charging term at the storage interface, $\dot{m}_{t,\omega}^{\text{HS,ch}}$ [kg/h], already used in the hydrogen balance (Eq. 3.127) and in the storage-state update of Section 3.2.2. This link is enforced explicitly in Eq. 3.146:

$$\dot{m}_{t,\omega}^{\text{H}_2,\text{COMP}} = \dot{m}_{t,\omega}^{\text{HS,ch}}, \quad \forall t, \forall \omega. \quad 3.146$$

The compressor cannot exceed its nameplate electrical power, as represented in Eq. 3.147:

$$0 \leq p_{t,\omega}^{\text{COMP}} \leq P_{\text{nom}}^{\text{COMP}}, \quad \forall t, \forall \omega. \quad 3.147$$

Electrical consumption is proportional to the hydrogen flow through the compressor via SEC^{COMP} , as shown in Eq. 3.148:

$$p_{t,\omega}^{\text{COMP}} = \text{SEC}^{\text{COMP}} \dot{m}_{t,\omega}^{\text{H}_2,\text{COMP}}, \quad \forall t, \forall \omega. \quad 3.148$$

In the AC balance Eq. 3.126, $p_{t,\omega}^{\text{COMP}}$ appears on the consumption side together with the electrolyser. In the hydrogen balance Eq. 3.127, $\dot{m}_{t,\omega}^{\text{HS,ch}}$ appears as storage charging; through Eq. 3.146 this is consistently tied to the compressor throughput. This means that in an islanded case, excess renewable generation can be diverted into $p_{t,\omega}^{\text{COMP}}$ in order to build up inventory in the hydrogen storage rather than being curtailed, and this decision is captured directly by Eqs. 3.147–3.148.

Hydrogen storage (HS)

Design parameters: Hydrogen storage is represented as a buffer tank with nominal usable mass $m_{\text{nom}}^{\text{HS}}$ [kg]. The model uses the normalised inventory variable $\text{LOH}_{t,\omega} \in [0, 1]$ to indicate the fraction of $m_{\text{nom}}^{\text{HS}}$ present in the tank at the start of time step t . Charging and discharging are limited by a maximum interface throughput $\dot{m}^{\text{HS,max}}$ [kg/h], and can incur different efficiencies $\eta^{\text{HS,ch}}$ and $\eta^{\text{HS,dis}}$.

Inputs (exogenous data): No weather-driven availability is associated with HS. Whether the tank is high-pressure, whether it is metal hydride plus heater, etc., affects parameters like $\eta^{\text{HS,ch}}$, $\eta^{\text{HS,dis}}$, and $\dot{m}^{\text{HS,max}}$, but does not introduce additional state variables at MILP level.

Decision variables: The storage can be charged at a rate $\dot{m}_{t,\omega}^{\text{HS,ch}}$ [kg/h] (hydrogen flowing into the tank) and discharged at a rate $\dot{m}_{t,\omega}^{\text{HS,dis}}$ [kg/h] (hydrogen flowing out of the tank). Only one direction is allowed per time step, enforced by a binary $\delta_{t,\omega}^{\text{HS}} \in \{0, 1\}$ that selects charging vs. discharging.

Physical limits on these charge and discharge rates and the mutual exclusivity of the two directions are enforced as shown in Eq. 3.149 and Eq. 3.150:

$$0 \leq \dot{m}_{t,\omega}^{\text{HS,ch}} \leq \dot{m}^{\text{HS,max}} (1 - \delta_{t,\omega}^{\text{HS}}), \quad \forall t, \forall \omega, \quad 3.149$$

$$0 \leq \dot{m}_{t,\omega}^{\text{HS,dis}} \leq \dot{m}^{\text{HS,max}} \delta_{t,\omega}^{\text{HS}}, \quad \forall t, \forall \omega. \quad 3.150$$

When HS is a metal-hydride (MH) system, discharging (desorption) requires low-grade heat. In the MILP this thermal duty is represented as an electric load $p_{t,\omega}^{\text{EH}}$ [kW] supplied by an electric heater (Section 3.1.1), and it is proportional to the hydrogen discharge mass flow:

$$p_{t,\omega}^{\text{EH}} = \frac{q_{\text{des,PCM}}}{\eta^{\text{EH}}} \dot{m}_{t,\omega}^{\text{HS,dis}}, \quad \forall t, \forall \omega. \quad 3.151$$

Here $q_{\text{des,PCM}}$ [kW h/kg] is the external thermal energy per kilogram of released H_2 after any PCM heat recovery, and η^{EH} is the electric-heater efficiency. For compressed-gas or underground storage, where no desorption heater is needed, $q_{\text{des,PCM}}$ is set to zero, so $p_{t,\omega}^{\text{EH}} = 0$. The variable $p_{t,\omega}^{\text{EH}}$ then appears explicitly in the electrical balance Eq. 3.126 as part of the site's electric demand.

The storage state update is written as a linear inventory recursion on $\text{LOH}_{t,\omega}$, as shown in Eq. 3.152:

$$\text{LOH}_{t+1,\omega} = \text{LOH}_{t,\omega} + \frac{\Delta t}{m_{\text{nom}}^{\text{HS}}} \left(\eta^{\text{HS,ch}} \dot{m}_{t,\omega}^{\text{HS,ch}} - \frac{\dot{m}_{t,\omega}^{\text{HS,dis}}}{\eta^{\text{HS,dis}}} \right), \quad \forall t = 1, \dots, N_T - 1, \forall \omega. \quad 3.152$$

Admissible bounds on the storage fill level are enforced at every time step, as shown in Eq. 3.153:

$$\text{LOH}_{\min} \leq \text{LOH}_{t,\omega} \leq \text{LOH}_{\max}, \quad \forall t, \forall \omega. \quad 3.153$$

To avoid end-of-horizon depletion, the initial and terminal inventories are fixed, as represented in Eq. 3.154:

$$\text{LOH}_{1,\omega} = \text{LOH}_0, \quad \text{LOH}_{N_T,\omega} = \text{LOH}_T, \quad \forall \omega. \quad 3.154$$

Eq. 3.153 and Eq. 3.154 ensure that hydrogen in storage stays between $\text{LOH}_{\min}$ and $\text{LOH}_{\max}$ at all intermediate steps, and that the optimiser cannot “cheat” by emptying the tank at the last period to satisfy demand.

Fuel cell (FC)

Design parameters: The fuel cell is characterised by its nameplate electrical output $P_{\text{nom}}^{\text{FC}}$ [kW], the minimum stable load fraction $u_{\min}^{\text{FC}} \in (0, 1]$, the standby fraction $u_{\text{sb}}^{\text{FC}} \in [0, 1]$, and a specific fuel consumption coefficient SFC^{FC} [kg/kWh], defined as the hydrogen mass flow rate required to sustain 1 kW of electrical output in the producing state. In the rule-based formulation this conversion depended on the FC polarisation curve and stack efficiency; the MILP replaces that nonlinear map with a constant SFC^{FC} , so that hydrogen draw and electrical power remain linearly related, as shown in Eq. 3.159.

Inputs (exogenous data): The FC has no exogenous availability profile; it is dispatchable subject to its technical limits. Fuel availability is enforced indirectly via storage and the hydrogen balance Eq. 3.127.

Decision variables: Three mutually exclusive operating modes are considered: *ON* (producing electrical power from hydrogen), *STANDBY* (hot/ready but not producing), and *OFF*. The decision variables are: $p_{t,\omega}^{\text{FC,on}}$ [kW] for FC electrical output in the producing state, $p_{t,\omega}^{\text{FC,sb}}$ [kW] for standby parasitic draw, $\dot{m}_{t,\omega}^{\text{H}_2,\text{FC}}$ [kg/h] for the hydrogen consumption rate when producing, and the binary mode indicators $\delta_{t,\omega}^{\text{FC,on}}, \delta_{t,\omega}^{\text{FC,sb}}, \delta_{t,\omega}^{\text{FC,off}} \in \{0, 1\}$.

Two additional binary variables are introduced for start characterisation: $\delta_{t,\omega}^{\text{FC,warm}}$ and $\delta_{t,\omega}^{\text{FC,cold}} \in \{0, 1\}$ distinguish a warm start (from *STANDBY*) from a cold start (from *OFF*). These are used later in the cost function to penalise thermal stress and degradation differently.

Exactly one FC mode is allowed at each (t, ω) , as shown in Eq. 3.155:

$$\delta_{t,\omega}^{\text{FC,on}} + \delta_{t,\omega}^{\text{FC,sb}} + \delta_{t,\omega}^{\text{FC,off}} = 1, \quad \forall t, \forall \omega. \quad 3.155$$

When the FC is producing (*ON*), its electrical output must respect the minimum load fraction and cannot exceed its nameplate, as shown in Eq. 3.156 and Eq. 3.157:

$$p_{t,\omega}^{\text{FC,on}} \geq u_{\min}^{\text{FC}} P_{\text{nom}}^{\text{FC}} \delta_{t,\omega}^{\text{FC,on}}, \quad \forall t, \forall \omega, \quad 3.156$$

$$p_{t,\omega}^{\text{FC,on}} \leq P_{\text{nom}}^{\text{FC}} \delta_{t,\omega}^{\text{FC,on}}, \quad \forall t, \forall \omega. \quad 3.157$$

When the FC is in *STANDBY*, it does not export power; instead it draws a parasitic fraction of nominal to stay hot and ready. This standby consumption is written in Eq. 3.158:

$$p_{t,\omega}^{\text{FC,sb}} = u_{\text{sb}}^{\text{FC}} P_{\text{nom}}^{\text{FC}} \delta_{t,\omega}^{\text{FC,sb}}, \quad \forall t, \forall \omega. \quad 3.158$$

When the FC is *OFF* ($\delta_{t,\omega}^{\text{FC,off}} = 1$), both $p_{t,\omega}^{\text{FC,on}}$ and $p_{t,\omega}^{\text{FC,sb}}$ are zero as a consequence of Eq. 3.155–3.158.

Hydrogen consumption is proportional to the produced electrical power through SFC^{FC} , as shown in Eq. 3.159:

$$\dot{m}_{t,\omega}^{\text{H}_2,\text{FC}} = \text{SFC}^{\text{FC}} p_{t,\omega}^{\text{FC,on}}, \quad \forall t, \forall \omega. \quad 3.159$$

The term $\dot{m}_{t,\omega}^{\text{H}_2,\text{FC}}$ appears in the hydrogen balance Eq. 3.127 together with electrolyser production $\dot{m}_{t,\omega}^{\text{H}_2,\text{EL}}$ and storage flows $\dot{m}_{t,\omega}^{\text{HS,ch}} / \dot{m}_{t,\omega}^{\text{HS,dis}}$, so that the optimiser must decide whether hydrogen is used immediately in the FC for power, sent to storage, or used to satisfy external demand.

To preserve physically meaningful thermal behaviour and to track degradation cost, two families of additional constraints are adopted. First, direct *OFF*→*STANDBY* and *STANDBY*→*OFF* jumps are forbidden, in analogy with the electrolyser. This prevents the FC from “teleporting” into a hot standby state or dropping instantly to cold. The linear constraints are shown in Eq. 3.160 and Eq. 3.161 and apply for $t > 1$:

$$\delta_{t,\omega}^{\text{FC,sb}} + \delta_{t-1,\omega}^{\text{FC,off}} \leq 1, \quad t > 1, \forall \omega, \quad 3.160$$

$$\delta_{t,\omega}^{\text{FC,off}} + \delta_{t-1,\omega}^{\text{FC,sb}} \leq 1, \quad t > 1, \forall \omega. \quad 3.161$$

Second, warm and cold starts are identified for costing purposes. A warm start means the FC is switched *ON* after being in *STANDBY* at the previous time step; a cold start means the FC is switched *ON* after being *OFF*. This is enforced by introducing $\delta_{t,\omega}^{\text{FC,warm}}$ and $\delta_{t,\omega}^{\text{FC,cold}}$ and constraining them as shown in Eq. 3.162 and Eq. 3.163:

$$\delta_{t,\omega}^{\text{FC,warm}} \geq \delta_{t,\omega}^{\text{FC,on}} + \delta_{t-1,\omega}^{\text{FC,sb}} - 1, \quad \delta_{t,\omega}^{\text{FC,warm}} \in \{0, 1\}, \quad t > 1, \forall \omega, \quad 3.162$$

$$\delta_{t,\omega}^{\text{FC,cold}} \geq \delta_{t,\omega}^{\text{FC,on}} + \delta_{t-1,\omega}^{\text{FC,off}} - 1, \quad \delta_{t,\omega}^{\text{FC,cold}} \in \{0, 1\}, \quad t > 1, \forall \omega. \quad 3.163$$

As shown in Eq. 3.162 and Eq. 3.163, these binaries become active whenever the FC enters the ON state at t from *STANDBY* or *OFF* at $t-1$. They do not change feasibility, but they enter the cost function so that warm starts and cold starts can be penalised differently. All constraints in this FC card (state exclusivity, minimum load, standby draw, net power injection, linear hydrogen consumption, forbidden *OFF*↔*STANDBY* transitions, and warm/cold start tracking) are kept identical across the deterministic, two-stage and multi-stage formulations, so that the FC behaves consistently in every optimisation shell.

Battery energy storage system (BESS)

Design parameters: The battery energy storage system is characterised by its usable energy capacity $E_{\text{nom}}^{\text{BESS}}$ [kW h], the charge and discharge efficiencies $\eta^{\text{BESS, ch}}$ and $\eta^{\text{BESS, dis}} \in (0, 1]$, and a per-step self-discharge rate $\text{SDR} \in [0, 1]$, which represents standing losses between consecutive time steps. The admissible state-of-charge range is defined by $\text{SOC}_{\min}$ and $\text{SOC}_{\max}$, expressed in per unit of $E_{\text{nom}}^{\text{BESS}}$. The C-rate coefficient $\mathcal{C}$ [1/h] links instantaneous charging and discharging power limits to the installed energy capacity. Initial and terminal SoC targets SOC_0 and SOC_T specify how full the battery must be at the first and last step of the optimisation horizon.

Inputs (exogenous data): The BESS has no weather-dependent availability.

Decision variables: Battery operation is described by the charging power $p_{t,\omega}^{\text{BESS, ch}}$ [kW] and discharging power $p_{t,\omega}^{\text{BESS, dis}}$ [kW]. The stored energy is tracked by $\text{SOC}_{t,\omega} \in [0, 1]$, which is the state of charge at the start of period t , normalised by $E_{\text{nom}}^{\text{BESS}}$. A binary $\delta_{t,\omega}^{\text{BESS}} \in \{0, 1\}$ enforces mutually exclusive behaviour: $\delta_{t,\omega}^{\text{BESS}} = 1$ allows discharging and blocks charging, and $\delta_{t,\omega}^{\text{BESS}} = 0$ allows charging and blocks discharging.

The instantaneous charge and discharge limits, and the no-simultaneous-charge/discharge condition, are enforced through the C-rate as shown in Eq. 3.164 and Eq. 3.165:

$$0 \leq p_{t,\omega}^{\text{BESS, dis}} \leq \mathcal{C} E_{\text{nom}}^{\text{BESS}} \delta_{t,\omega}^{\text{BESS}}, \quad \forall t, \forall \omega, \quad 3.164$$

$$0 \leq p_{t,\omega}^{\text{BESS, ch}} \leq \mathcal{C} E_{\text{nom}}^{\text{BESS}} (1 - \delta_{t,\omega}^{\text{BESS}}), \quad \forall t, \forall \omega. \quad 3.165$$

As shown in Eq. 3.164 and Eq. 3.165, the BESS cannot charge and discharge in the same time step, and the admissible power in each mode scales linearly with the chosen energy capacity $E_{\text{nom}}^{\text{BESS}}$.

The SOC dynamics follows the same structure used in Section 3.1, including the self-discharge rate SDR. The update from t to $t+1$ is written in Eq. 3.166:

$$\text{SOC}_{t+1,\omega} = \text{SOC}_{t,\omega} (1 - \text{SDR}) + \frac{p_{t,\omega}^{\text{BESS, ch}} \Delta t \eta^{\text{BESS, ch}}}{E_{\text{nom}}^{\text{BESS}}} - \frac{p_{t,\omega}^{\text{BESS, dis}} \Delta t}{E_{\text{nom}}^{\text{BESS}} \eta^{\text{BESS, dis}}}, \quad \forall t, \forall \omega. \quad 3.166$$

As shown in Eq. 3.166, charging increases $\text{SOC}_{t,\omega}$ with efficiency $\eta^{\text{BESS, ch}}$, discharging reduces $\text{SOC}_{t,\omega}$ accounting for $\eta^{\text{BESS, dis}}$, and SDR accounts for idle losses between steps even if $p_{t,\omega}^{\text{BESS, ch}} = p_{t,\omega}^{\text{BESS, dis}} = 0$.

Admissible SoC bounds are imposed at every time step, as shown in Eq. 3.167:

$$\text{SOC}_{\min} \leq \text{SOC}_{t,\omega} \leq \text{SOC}_{\max}, \quad \forall t, \forall \omega. \quad 3.167$$

Terminal feasibility is enforced in complete analogy with hydrogen storage. The initial SoC at $t=0$ and the end-of-horizon SoC at $t=N_T$ are fixed (or kept within tight bands) so that the optimiser cannot “borrow” net energy from or “dump” net energy into the battery over the horizon, as shown in Eq. 3.168:

$$\text{SOC}_{1,\omega} = \text{SOC}_0, \quad \text{SOC}_{N_T,\omega} = \text{SOC}_T, \quad \forall \omega. \quad 3.168$$

In the AC power balance of Eq. 3.126, $p_{t,\omega}^{\text{BESS, dis}}$ appears on the supply side together with $p_{t,\omega}^{\text{PV}}$, $p_{t,\omega}^{\text{WT}}$, $p_{t,\omega}^{\text{FC}}$ and $p_{t,\omega}^{\text{DG}}$, while $p_{t,\omega}^{\text{BESS, ch}}$ appears on the demand side together with $p_{t,\omega}^{\text{EL}}$, $p_{t,\omega}^{\text{COMP}}$, $p_{t,\omega}^{\text{EH}}$ and $p_{t,\omega}^{\text{FC, sb}}$. Eqs. 3.164–3.168 therefore ensure that (i) the BESS does not violate its charge/discharge power capability; (ii) the BESS never charges and discharges simultaneously and (iii) the BESS cannot be artificially emptied or overfilled at the horizon boundaries just to satisfy demand or reduce cost.

Diesel generator (DG)

Design parameter: $P_{\text{nom}}^{\text{DG}}$ [kW] is the DG nameplate electrical power. Including a DG allows islanded operation and provides a controllable (but carbon-intensive) fallback to satisfy $p_{t,\omega}^{\text{el,dem}}$ and to support the hydrogen chain when renewables, storage and grid imports are insufficient.

Inputs (exogenous data): The DG has no stochastic availability profile.

Decision variables: $p_{t,\omega}^{\text{DG}} \geq 0$ [kW] is the DG electrical output injected into the AC node in Eq. 3.126. $\dot{V}_{t,\omega}^{\text{DG}} \geq 0$ [m³/h] is the volumetric diesel fuel flow.

The DG cannot exceed its nameplate as in Eq. 3.169:

$$0 \leq p_{t,\omega}^{\text{DG}} \leq P_{\text{nom}}^{\text{DG}}, \quad \forall t, \forall \omega. \quad 3.169$$

Electrical output is proportional to the volumetric fuel draw as shown in Eq. 3.170:

$$p_{t,\omega}^{\text{DG}} = \eta^{\text{DG}} \text{LHV}_{\text{vol}}^{\text{DG}} \dot{V}_{t,\omega}^{\text{DG}}, \quad \forall t, \forall \omega, \quad 3.170$$

where $\eta^{\text{DG}} \in (0, 1]$ is the DG electrical efficiency and $\text{LHV}_{\text{vol}}^{\text{DG}}$ [kW h/m³] is the diesel lower heating value per unit volume. Given CI^{DG} [kg_{CO2eq}/kWh] the carbon intensity of the DG, per-step DG equivalent emissions can be written as $CI^{\text{DG}} p_{t,\omega}^{\text{DG}} \Delta t$.

Grid interface

Design parameter: No fixed nameplate limit is enforced here. The point of common coupling is treated as an unlimited sink/source for active power exchanges.

Inputs (exogenous data): $c_{t,\omega}^{\text{el,imp}}$ and $c_{t,\omega}^{\text{el,exp}}$ are the time-varying import tariff and export remuneration [€/kWh]. These can be part of the scenario data $\xi_{t,\omega}$.

Decision variables: $p_{t,\omega}^{\text{grid,imp}} \geq 0$ [kW] is active power imported from the grid; $p_{t,\omega}^{\text{grid,exp}} \geq 0$ [kW] is active power exported to the grid; $\delta_{t,\omega}^{\text{grid}} \in \{0, 1\}$ enforces mutual exclusivity.

Mutual exclusivity between import and export is imposed using a big- M linearisation as represented in Eq. 3.171 and 3.172:

$$0 \leq p_{t,\omega}^{\text{grid,imp}} \leq \bar{P}^{\text{grid}} \delta_{t,\omega}^{\text{grid}}, \quad \forall t, \forall \omega, \quad 3.171$$

$$0 \leq p_{t,\omega}^{\text{grid,exp}} \leq \bar{P}^{\text{grid}} (1 - \delta_{t,\omega}^{\text{grid}}), \quad \forall t, \forall \omega, \quad 3.172$$

where $\bar{P}^{\text{grid}}$ [kW] is chosen large enough that it never binds in practice. Eqs. 3.171–3.172 guarantee that in each (t, ω) the plant is either importing or exporting, but not both. The resulting $p_{t,\omega}^{\text{grid,imp}}$ and $p_{t,\omega}^{\text{grid,exp}}$ then appear in the nodal AC balance Eq. 3.126.

Certification cap

To embed the RED III-style green-hydrogen requirement of Section 3.1.2 directly in the MILP, we mirror the electric-demand and carbon-intensity definitions with an added scenario index $\omega \in \Omega$. The instantaneous electrical demand of the hydrogen chain in each scenario is defined as shown in Eq. 3.173:

$$p_{t,\omega}^{\text{H}_2,\text{tot}} = p_{t,\omega}^{\text{EL}} + p_{t,\omega}^{\text{COMP}} + p_{t,\omega}^{\text{EH}}, \quad \forall t, \forall \omega, \quad 3.173$$

which is the stochastic counterpart of Eq. 3.112. In the optimisation layers, all electrical demand modelled in Eq. 3.173 is attributable to the hydrogen chain, so the grid-import power $p_{t,\omega}^{\text{grid,imp}}$ coincides with the grid-attributed hydrogen-chain power used in the KPI definition of

Section 3.1.2. The scenario-weighted produced hydrogen mass over the certification window (here, the optimisation horizon of N_T timesteps) is then computed as shown in Eq. 3.174:

$$m_y^{\text{H}_2} = \sum_{\omega \in \Omega} \pi_\omega \sum_{t=1}^{N_T} \dot{m}_{t,\omega}^{\text{H}_2} \Delta t \quad [\text{kg}], \quad 3.174$$

With $CI_{t,\omega}^{\text{grid}}$ the (given) grid carbon intensity $[\text{kg}_{\text{CO}_2\text{eq}}/\text{kWh}]$ in scenario ω , the scenario-weighted carbon intensity of produced hydrogen is defined as shown in Eq. 3.175:

$$CI_y^{\text{H}_2} = \frac{\sum_{\omega \in \Omega} \pi_\omega \sum_{t=1}^{N_T} p_{t,\omega}^{\text{grid,imp}} CI_{t,\omega}^{\text{grid}} \Delta t}{m_y^{\text{H}_2}} \quad \left[\text{kg}_{\text{CO}_2\text{eq}}/\text{kg}_{\text{H}_2} \right], \quad 3.175$$

the stochastic analogue of Eq. 3.114. The RED III limit is enforced by cross-multiplying the linear-fractional expression in Eq. 3.175, yielding the linear constraint shown in Eq. 3.176:

$$\sum_{\omega \in \Omega} \pi_\omega \sum_{t=1}^{N_T} p_{t,\omega}^{\text{grid,imp}} CI_{t,\omega}^{\text{grid}} \Delta t \leq CI_{\max}^{\text{REDIII}} \sum_{\omega \in \Omega} \pi_\omega \sum_{t=1}^{N_T} \dot{m}_{t,\omega}^{\text{H}_2} \Delta t. \quad 3.176$$

Eqs. 3.173–3.176 are therefore the optimisation-ready equivalent of the rule-based environmental KPI formulation in Section 3.1.2: the MILP is only allowed to dispatch and import electricity such that the aggregate CO_2 -equivalent per kilogram of hydrogen produced at the facility boundary stays below the RED III threshold $CI_{\max}^{\text{REDIII}}$.

3.2.3 Deterministic MILP shell

The deterministic shell is the first concrete implementation of the optimisation framework introduced in Section 3.2. It assumes perfect foresight of all exogenous trajectories over a representative operating year: renewable availability, electricity prices, and hydrogen demand are all treated as known inputs. The scenario index ω is therefore dropped, so that any $v_{t,\omega}$ and $x_{t,\omega}$ become v_t and x_t . The timestep is $\Delta t = 1$ h, and the index $t = 1, \dots, N_T$ spans one full calendar year ($N_T=8760$).

Within this horizon the model co-optimises design and operation: the nominal sizes of PV, WT, EL, COMP, and HS are chosen together with their hourly dispatch schedules. Consequently the problem is a single-stage MILP. This deterministic MILP underpins the techno-economic comparison of hydrogen storage technologies presented in Section 4.3 and in [233], where a hybrid PtH plant is sized and dispatched to supply a continuous hydrogen offtake.

Economic objective and KPI definition. All techno-economic results are reported in terms of the LCOH, consistent with the KPI definitions of Section 3.1.2.

The design vector s contains the nameplate capacities that are optimised in this study,

$$s = \left(P_{\text{nom}}^{\text{PV}}, P_{\text{nom}}^{\text{WT}}, P_{\text{nom}}^{\text{EL}}, P_{\text{nom}}^{\text{COMP}}, m_{\text{nom}}^{\text{HS}} \right),$$

Let $\mathcal{A} = \{\text{PV}, \text{WT}, \text{EL}, \text{COMP}, \text{HS}\}$ collect these assets.

For each $a \in \mathcal{A}$, $\text{CAPEX}_a(s)$ [€] denotes the installation cost of asset a , and $\text{CAPEX}_{\text{tot}} = \sum_{a \in \mathcal{A}} \text{CAPEX}_a(s)$ is the sum of all such asset-level costs. The upfront investment (including installation and engineering adders) is then C_0 [€], defined in Eq. 3.106. Short-lifetime replacements appear explicitly as $\text{CAPEX}_y^{\text{repl}}$ in the LCOH estimation.

Operating expenditure also follows the structure of Section 3.1.2. The hourly simulator channels $p_t^{\text{grid,imp}}$, p_t^{EL} , p_t^{COMP} , p_t^{EH} , and $\dot{V}_t^{\text{H}_2\text{O,EL}}$ are defined by the plant balances; the corresponding price signals $c_t^{\text{el,imp}}$ [€/kWh] and $c_y^{\text{H}_2\text{O}}$ [€/m³] are part of ξ_t . Let V_y^{EL} [m³] be the annual deionised-water volume sent to the stacks. Fixed O&M is represented as an annual fraction $\text{frac}_a^{\text{O\&M}}$ of the installed cost of each asset. The yearly operating expenditure $\text{OPEX}_y(s, \{v_t\})$ is defined in Eq. 3.177:

$$\text{OPEX}_y(s, \{v_t\}) = \underbrace{\sum_{t \in \mathcal{T}_y} c_t^{\text{el,imp}} p_t^{\text{grid,imp}} \Delta t}_{\text{OPEX}_y^{\text{el}}} + \underbrace{c_y^{\text{H}_2\text{O}} V_y^{\text{EL}}}_{\text{OPEX}_y^{\text{H}_2\text{O}}} + \underbrace{\sum_{a \in \mathcal{A}} \text{frac}_a^{\text{O\&M}} \text{CAPEX}_a(s)}_{\text{OPEX}_y^{\text{O\&M,fix}}} \quad [\text{€}]. \quad 3.177$$

Only the cost of imported electricity appears here; any revenue from exported electricity is deliberately excluded from the numerator of LCOH, as accounted in Eq. 3.178:

$$\text{LCOH} = \frac{C_0 + \sum_{y=1}^N \frac{\text{CAPEX}_y^{\text{repr}} + \text{OPEX}_y(s, \{v_t\})}{(1 + \text{DR})^y}}{\sum_{y=1}^N \frac{m_y^{\text{H}_2}}{(1 + \text{DR})^y}} \quad [\text{€/kg}]. \quad 3.178$$

Where DR is the real discount rate. One representative operating year is optimised and assumed to be repeated identically over the project lifetime.

In the considered study the PtH plant consists only of PV, WT, EL, COMP and HS as represented in Figure 4.19. FC, BESS, and DG introduced in Secs. 3.2.2–3.2.2 are thus disabled.

RES available power is given by Eq. 3.128 for PV and by the wind profile construction in Eq. 3.132 for WT. Curtailment is not modelled in this shell: we set $p_t^{\text{PV}} = \bar{p}_t^{\text{PV}}$ and $p_t^{\text{WT}} = \bar{p}_t^{\text{WT}}$ (with $p_t^{\text{PV,curt}} = p_t^{\text{WT,curt}} = 0$), and any surplus is routed to $p_t^{\text{grid,exp}}$. The EL is modelled with a deliberate simplification: in this deterministic perfect-foresight shell the stack is treated as continuously variable between zero and its nameplate $P_{\text{nom}}^{\text{EL}}$, with no binary on/off commitment, no minimum stable load, no standby mode, and no warm/cold start tracking. We identify p_t^{EL} with the producing power in Eq. 3.140, so that $p_t^{\text{EL}} = \text{SEC}^{\text{EL}} \dot{m}_t^{\text{H}_2, \text{EL}}$, and we retain the proportional water-consumption law of Eq. 3.141. This keeps hydrogen production $\dot{m}_t^{\text{H}_2, \text{EL}}$, electrolyser power p_t^{EL} , and stack water use $\dot{V}_t^{\text{H}_2\text{O,EL}}$ coupled in a physically meaningful but MILP-friendly way, while intentionally ignoring start-up penalties and minimum-load logic. Those integer details are reintroduced later in the multi-stage scheduling shell, where bidding into electricity markets and stack degradation costs become important. The COMP is enforced exactly as in Section 3.2.2. HS (Section 3.2.2) is always active. The usable inventory LOH_t evolves according to the linear recursion in Eq. 3.152, is kept within bounds by Eq. 3.153, and must satisfy the cyclic boundary condition of Eq. 3.154 so that the HS cannot be emptied at the end of the horizon to artificially improve cost. Charging and discharging flows, $\dot{m}_t^{\text{HS, ch}}$ and $\dot{m}_t^{\text{HS, dis}}$, are limited and made mutually exclusive by the binary δ_t^{HS} through Eqs. 3.149–3.150; this binary is retained because it encodes a real physical exclusivity (no simultaneous charge and discharge). When the storage technology is a MH, hydrogen withdrawal requires desorption heat. This is modelled as an EH load p_t^{EH} proportional to $\dot{m}_t^{\text{HS, dis}}$ via Eq. 3.151, and p_t^{EH} then appears explicitly in the plant's AC power balance. For CGH₂ or UHS, $q_{\text{des, PCM}} = 0$. The grid interface is included. Grid import $p_t^{\text{grid,imp}}$ and grid export $p_t^{\text{grid,exp}}$ are both decision variables; exclusivity of import vs. export in a given hour is imposed by the binary δ_t^{grid} and the big- M constraints in Eqs. 3.171–3.172. Imported electricity is billed at $c_t^{\text{el,imp}}$ and enters the certification logic; exported electricity,

by construction of the LCOH, is not accounted for. The GHG / certification cap is enforced through Eqs. 3.173–3.176. Finally, there is no exogenous on-site electric demand $p_t^{\text{el,dem}}$ beyond the hydrogen chain itself. In other words, the only electrical consumers that matter for feasibility and cost are the EL, the COMP, and (for MH) the desorption heater.

Deterministic MILP formulation. After dropping the scenario index ω (perfect foresight) and restricting the device set as just described, the problem is a MILP in the sizing vector s , the hourly dispatch trajectories $\{v_t\}_{t=1}^{N_T}$, the binary operating flags $\{\delta_t\}_{t=1}^{N_T}$, and the states $\{x_t\}_{t=1}^{N_T}$. The complete deterministic MILP, with the assumptions stated above, can therefore be summarised in Eq. 3.179:

$$\begin{aligned}
 & \min_{s, \{v_t, \delta_t, x_t\}_{t=1}^{N_T}} \quad \text{LCOH}(s, \{v_t\}) \\
 & \text{s.t.} \quad \text{AC-node electrical power balance (Eq. 3.126)} \\
 & \quad \text{Hydrogen mass balance and routing (Eq. 3.127)} \\
 & \quad \text{PV/WT availability and bounds (Eqs. 3.128–3.130 and 3.131–3.134)} \\
 & \quad \text{EL conversion and water use (Eqs. 3.140, 3.141)} \\
 & \quad \text{COMP rating and linear electric load (Eqs. 3.147–3.148)} \\
 & \quad \text{HS dynamics and bounds (Eqs. 3.149–3.154)} \\
 & \quad \text{Grid import/export exclusivity (Eqs. 3.171–3.172)} \\
 & \quad \text{GHG-intensity cap (Eqs. 3.173–3.176)}
 \end{aligned} \tag{3.179}$$

3.2.4 Two-stage stochastic MILP shell

The two-stage stochastic shell is the second concrete implementation of the optimisation framework introduced in Section 3.2, and it mirrors the generic two-stage stochastic programming structure presented in Section 2.3.1: a single here-and-now design is chosen before uncertainty is revealed, and then scenario-dependent operating schedules adapt after the uncertainty is realised. Unlike the deterministic shell of Section 3.2.3, which assumes perfect foresight and optimises one nominal trajectory over a representative year, this shell acknowledges that future renewable availability is uncertain. The design s (PV size, WT size etc.) is therefore selected to perform well in expectation (risk-neutral) across a set of plausible scenarios $\omega \in \Omega$; the operating schedules $\{v_{t,\omega}, \delta_{t,\omega}, x_{t,\omega}\}_{t=1}^{N_T}$ are allowed to adapt to each ω independently. Non-anticipativity is enforced by construction: s has no ω index, so the same capacities must serve all scenarios.

This two-stage stochastic MILP shell is used for joint sizing and dispatch of a full PtH off-grid plant under uncertainty, presented in Section 4.4 (Figure 4.27) and in [234]. Compared with the hydrogen-only deterministic study in Section 3.2.3, the active plant now includes the entire energy hub, in fact the design vector s contains:

$$s = \left(P_{\text{nom}}^{\text{PV}}, P_{\text{nom}}^{\text{WT}}, P_{\text{nom}}^{\text{EL}}, P_{\text{nom}}^{\text{COMP}}, m_{\text{nom}}^{\text{HS}}, P_{\text{nom}}^{\text{FC}}, E_{\text{nom}}^{\text{BESS}}, P_{\text{nom}}^{\text{DG}} \right),$$

In the case study analysed the hybrid RES–storage system supplies an islanded microgrid that is treated as fully off-grid. No connection to an external transmission grid is available; consequently, no grid import/export variables are included and the green hydrogen certification constraints are not enforced. The only exogenous service obligation is the satisfaction of the island electrical demand $p_{t,\omega}^{\text{el,dem}}$ at all times. Hydrogen is not exported as a commercial product, and there is no external H_2 offtake: hydrogen acts purely as an intermediate energy

carrier that can be produced (via the EL), buffered in HS, and later reconverted to electricity in the FC.

Objective function and ϵ -constraint on diesel emissions. The optimisation target is the minimisation of the expected Total Annualised Cost (TAC), defined as an equivalent yearly cost of owning and operating the plant, so that different layouts s can be compared on a per-year basis even if they have very different capital intensities. It is written as in Eq. 3.180:

$$\text{TAC}(s, \{v_{t,\omega}, \delta_{t,\omega}\}) = \text{CAPEX}^{\text{ann}}(s) + \sum_{\omega \in \Omega} \pi_{\omega} \text{OPEX}_{\omega}(s, \{v_{t,\omega}, \delta_{t,\omega}\}) \quad [\text{€/year}]. \quad 3.180$$

Let DR be the real discount rate and N the project lifetime in years (consistent with Section 3.1.2). All capital outlays are first expressed as an equivalent present-value lump sum C_0^{eq} , which aggregates the upfront investment C_0 (including installation and engineering fractions) and all discounted replacements as shown in Eq. 3.181:

$$C_0^{\text{eq}} = C_0 + \sum_{y=1}^N \frac{\text{CAPEX}_y^{\text{repr}}}{(1 + \text{DR})^y} \quad [\text{€}]. \quad 3.181$$

C_0^{eq} is then converted into an equivalent uniform yearly payment over the same lifetime N using the standard capital-recovery (annuity) factor $\text{CRF}(\text{DR}, N) = \frac{\text{DR}(1 + \text{DR})^N}{(1 + \text{DR})^N - 1}$, yielding the annualised capital cost in Eq. 3.182:

$$\text{CAPEX}^{\text{ann}}(s) = \text{CRF}(\text{DR}, N) C_0^{\text{eq}} \quad [\text{€/year}]. \quad 3.182$$

$\text{CAPEX}^{\text{ann}}(s)$ is in fact the single yearly payment that would recover both the initial investment C_0 and all discounted replacements $\text{CAPEX}_y^{\text{repr}}$ over N years at discount rate DR.

$\text{OPEX}_{\omega}(s, \{v_{t,\omega}, \delta_{t,\omega}\})$ [€/year] is the operating expenditure for one representative operating year under scenario ω as shown in Eq. 3.183:

$$\text{OPEX}_{\omega}(s, \{v_{t,\omega}, \delta_{t,\omega}\}) = \underbrace{\sum_{t=1}^{N_T} \left(c^{\text{DG}} \dot{V}_{t,\omega}^{\text{DG}} + c^{\text{H}_2\text{O}} \dot{V}_{t,\omega}^{\text{H}_2\text{O},\text{EL}} \right) \Delta t}_{\text{OPEX}_{\omega}^{\text{var}}} + \underbrace{\sum_{a \in \mathcal{A}} \text{frac}_a^{\text{O\&M}} \text{CAPEX}_a(s)}_{\text{OPEX}^{\text{O\&M,fix}}}. \quad 3.183$$

The variable annual costs are due to diesel and water supply, respectively for DG and EL, while the fixed annual costs are attributed to O&M for all the installed assets,

$$\mathcal{A} = \{\text{PV}, \text{WT}, \text{BESS}, \text{EL}, \text{COMP}, \text{HS}, \text{FC}, \text{DG}\},$$

Because OPEX_{ω} is computed over one “representative operating year”, there is no further discounting inside TAC: the expectation $\sum_{\omega \in \Omega} \pi_{\omega}(\cdot)$ is simply the scenario-weighted average annual OPEX of that representative year.

The DG is the only fossil source in the island and thus the only direct driver of CO₂ emissions. Let CI^{DG} [kg_{CO₂}/kWh] be the DG specific carbon intensity and $p_{t,\omega}^{\text{DG}}$ [kW] the DG electrical output (Section 3.2.2). The expected annual CO₂ emissions from diesel usage are then shown in Eq. 3.184

$$E^{\text{DG}}(\{v_{t,\omega}\}) = \sum_{\omega \in \Omega} \pi_{\omega} \sum_{t=1}^{N_T} CI^{\text{DG}} p_{t,\omega}^{\text{DG}} \Delta t \quad [\text{kg}_{\text{CO}_2}/\text{year}]. \quad 3.184$$

An explicit cap is imposed on these emissions following the ϵ -constraint formulation:

$$E^{\text{DG}}(\{v_{t,\omega}\}) \leq \epsilon^{\text{CO}_2}, \quad 3.185$$

where ϵ^{CO_2} [kg_{CO₂}/year] is a prescribed yearly emissions budget. Tightening ϵ^{CO_2} reduces admissible diesel usage and typically forces higher renewable penetration and/or larger storage capacity, which increases CAPEX^{ann}(s) and can increase OPEX _{ω} ; relaxing ϵ^{CO_2} allows more DG dispatch, usually lowering TAC but increasing E^{DG} .

In summary, the stochastic two-stage problem minimises $\text{TAC}(s, \{v_{t,\omega}, \delta_{t,\omega}\})$ subject to plant physics, island security of supply, and the diesel-emissions cap 3.185.

Active components and constraint set. The system activates all physical blocks introduced in Section 3.2.2 except the grid interface and the certification cap. The system consists of PV, WT, an EL with COMP feeding HS, a FC that reconverts stored hydrogen to electricity, a BESS, and a DG as represented in Figure 4.27. All of these contribute to balancing the island electrical demand $p_{t,\omega}^{\text{el,dem}}$ at each time step.

PV and WT are modelled as in Secs. 3.2.2–3.2.2. Because the system is off-grid and $p_{t,\omega}^{\text{grid,exp}}$ is not allowed, curtailment is the only admissible sink for any instantaneous RES surplus that cannot be absorbed by storage or by flexible conversion into hydrogen. The EL block of Section 3.2.2 is retained in linear form but without the integer operating-state logic. The EL is modelled as continuously variable between zero and its nameplate $P_{\text{nom}}^{\text{EL}}$, with a single linear conversion between electrical power draw and hydrogen production rate via Eq. 3.140, plus proportional water use via Eq. 3.141. This relaxation avoids replicating EL start-up binaries for every time t and scenario ω , which would otherwise cause a combinatorial explosion for hourly simulations for a year (the same rationale applies below to the FC). The COMP model of Section 3.2.2 is used unchanged. HS is modelled exactly as in Section 3.2.2. No MH storage is considered; instead, Type I CGH₂ tanks at high pressure are used, thus the electric-heater load $p_{t,\omega}^{\text{EH}}$ is not present. Similarly to the EL, the FC block of Section 3.2.2 is simplified by excluding all binary variables indicating different operating states. The BESS model of Section 3.2.2 is retained in full, as well as the DG block of Section 3.2.2. The DG is the last-resort supplier during extended low-wind / low-solar periods when both BESS and HS+FC are depleted.

Two coupled balances close the loop for every (t, ω) . (i) The AC-node electrical balance of Section 3.2.1 reduces to an off-grid form with no grid import/export. (ii) Since there is no hydrogen demand, the hydrogen mass balance of Section 3.2.1 simplifies to an internal loop: hydrogen produced by the EL either (i) charges HS (after compression) or (ii) is later withdrawn from HS to feed the FC.

Two-stage stochastic MILP formulation. The two-stage problem is a stochastic MILP with non-anticipativity on the design vector s and scenario-dependent recourse on the operating schedules $\{v_{t,\omega}, \delta_{t,\omega}, x_{t,\omega}\}$. After specialising the plant physics to the off-grid setting and applying the modelling simplifications for EL and FC, the complete formulation can be summarised as Eq. 3.186, in direct analogy with the deterministic MILP summary in Eq. 3.179.

$$\begin{aligned}
 & \min_{s, \{v_{t,\omega}, \delta_{t,\omega}, x_{t,\omega}\}_{t=1}^{N_T}, \omega \in \Omega} \text{TAC}(s, \{v_{t,\omega}, \delta_{t,\omega}\}) \\
 & \text{s.t.} \quad \text{Off-grid AC-node power balance – no grid import/export (Eq. 3.126)} \\
 & \quad \text{Hydrogen mass balance and routing (Eq. 3.127)} \\
 & \quad \text{PV/WT availability (Eqs. 3.128–3.130 and 3.131–3.134)} \\
 & \quad \text{EL conversion and water use (Eqs. 3.140, 3.141)} \\
 & \quad \text{COMP rating and linear electric load (Eqs. 3.147–3.148)} \\
 & \quad \text{HS dynamics and bounds (Eqs. 3.149–3.154)} \\
 & \quad \text{BESS dynamics and bounds (Eqs. 3.164–3.168)} \\
 & \quad \text{DG balance (Eqs. 3.169–3.170)} \\
 & \quad \text{DG emissions cap (Eq. 3.185)}
 \end{aligned} \tag{3.186}$$

Scenario construction (generation and reduction) Each scenario $\omega \in \Omega$ carries a full-year hourly realisation of the exogenous signals $\xi_{t,\omega}$. In the off-grid two-stage shell considered here, uncertainty is placed on renewable availability only (PV and WT), while the site electrical demand $p_t^{\text{el,dem}}$ is taken as a fixed profile common to all scenarios. Accordingly, we construct scenario-wise specific PV production $\bar{p}_{t,\omega}^{\text{PV,1kW}}$ and available wind electrical power $\bar{p}_{t,\omega}^{\text{WT}}$ (or, equivalently, wind hub-height speed $w_{h,t,\omega}$ mapped through the WT curve), and set

$$\xi_{t,\omega} = \left(\bar{p}_{t,\omega}^{\text{PV,1kW}}, \bar{p}_{t,\omega}^{\text{WT}} \right), \quad t = 1, \dots, N_T, \omega \in \Omega.$$

Monte Carlo + Bootstrap daily recombination [235, 236]. To preserve realistic intra-day correlation and seasonality, scenarios are generated by sampling and concatenating whole daily historical profiles within each month. Let $m = 1, \dots, 12$ index calendar months and $n_{d,m}$ be the number of days in month m . From the historical archive, form sets of daily 24-hour vectors

$$\mathcal{X}_m^{\text{PV}} = \{\mathbf{x}_{m,d}^{\text{PV}} \in \mathbb{R}^{24}\}, \quad \mathcal{X}_m^{\text{WT}} = \{\mathbf{x}_{m,d}^{\text{WT}} \in \mathbb{R}^{24}\},$$

where $\mathbf{x}_{m,d}^{\text{PV}}$ are specific PV outputs for 1 kW and $\mathbf{x}_{m,d}^{\text{WT}}$ are available WT powers obtained after applying the shear law and the three-region WT map of Section 3.2.2 to the historical wind speeds. For each resource $r \in \{\text{PV}, \text{WT}\}$ and for each Monte Carlo sample index κ , draw with replacement $n_{d,m}$ daily vectors from $\mathcal{X}_m^r$, and build the annual hourly vector by month-wise concatenation as shown in Eq. 3.187:

$$\mathbf{X}_\kappa^r = \bigoplus_{m=1}^{12} \bigoplus_{j=1}^{n_{d,m}} \mathbf{x}_{m,d^*(m,j)}^r \tag{3.187}$$

where $d^*(m, j)$ are independent identically distributed bootstrap indices on $\mathcal{X}_m^r$, and $\oplus$ denotes concatenation (thus $\mathbf{X}_\kappa^r \in \mathbb{R}^{N_T}$) [237]. This Monte Carlo–Bootstrap construction preserves realistic hourly structure and seasonal variability without requiring parametric time-series models. A large pool (e.g. $S_{\text{MC}}^{\text{PV}} = S_{\text{MC}}^{\text{WT}} = 10\,000$) is generated independently for PV and WT.

Scenario reduction via k-means on annual profiles. For tractability, each Monte Carlo pool is reduced to a small set of representative annual profiles by k -means clustering on $\mathbb{R}^{N_T}$. For resource r , let $\mathcal{S}_{\text{MC}}^r = \{\mathbf{X}_\kappa^r\}$ be the Monte Carlo set and partition it into S_{CL}^r clusters

$\{\mathcal{S}_i^r\}_{i=1}^{S_{\text{CL}}^r}$. Centroids $\{\boldsymbol{\mu}_i^r \in \mathbb{R}^{N_T}\}$ are obtained by solving Eq. 3.188:

$$\min_{\{\boldsymbol{\mu}_i^r\}} \sum_{i=1}^{S_{\text{CL}}^r} \sum_{\mathbf{x}_\kappa^r \in \mathcal{S}_i^r} \|\mathbf{x}_\kappa^r - \boldsymbol{\mu}_i^r\|_2^2, \quad r \in \{\text{PV}, \text{WT}\}. \quad 3.188$$

Each centroid $\boldsymbol{\mu}_i^r$ is adopted as one reduced scenario profile; its probability is the cluster mass as represented in Eq. 3.189:

$$\pi_i^r = \frac{|\mathcal{S}_i^r|}{|\mathcal{S}_{\text{MC}}^r|}, \quad i = 1, \dots, S_{\text{CL}}^r. \quad 3.189$$

In the case study that inspired this thesis, $S_{\text{CL}}^{\text{PV}} = S_{\text{CL}}^{\text{WT}} = 10$, obtained from 10,000 Monte Carlo realisations per resource; probabilities are the empirical cluster frequencies.

Cartesian product and scenario probabilities. Assuming independence between PV and WT generation after reduction, the global scenario set is the Cartesian product

$$\Omega = \Omega^{\text{PV}} \times \Omega^{\text{WT}} = \{(i, j) : i = 1, \dots, S_{\text{CL}}^{\text{PV}}, j = 1, \dots, S_{\text{CL}}^{\text{WT}}\},$$

with $|\Omega| = S_{\text{CL}}^{\text{PV}} S_{\text{CL}}^{\text{WT}}$. For $\omega \equiv (i, j)$, the exogenous profiles are

$$\bar{p}_{t,\omega}^{\text{PV},1\text{kW}} = \boldsymbol{\mu}_i^{\text{PV}}[t], \quad \bar{p}_{t,\omega}^{\text{WT}} = \boldsymbol{\mu}_j^{\text{WT}}[t], \quad t = 1, \dots, N_T,$$

and the scenario probability factorises as in Eq. 3.190

$$\pi_\omega = \pi_i^{\text{PV}} \pi_j^{\text{WT}}, \quad \sum_{\omega \in \Omega} \pi_\omega = 1. \quad 3.190$$

This is exactly the “outer-product” rule used in the reference study to combine PV and wind scenario weights.

Use in the plant model. Given a design s , the available PV power before curtailment in scenario ω is $\bar{p}_{t,\omega}^{\text{PV}} = \bar{p}_{t,\omega}^{\text{PV},1\text{kW}} P_{\text{nom}}^{\text{PV}}$ (Eq. 3.128); the available WT power $\bar{p}_{t,\omega}^{\text{WT}}$ is taken directly from the centroid time series (or equivalently reconstructed from $w_{h,t,\omega}$ via Eq. 3.132) and then split between injection and curtailment by Eqs. 3.133–3.134. The AC and hydrogen balances are then enforced at every (t, ω) as in Section 3.2.1. All scenario-dependent operating variables $\{v_{t,\omega}, \delta_{t,\omega}, x_{t,\omega}\}$ adapt to $\xi_{t,\omega}$, whereas the here-and-now design s is common to all ω (non-anticipativity by construction).

3.2.5 Multi-stage stochastic MILP shell

Once the plant is commissioned, economic value is created—or eroded—hour by hour through scheduling and marketing decisions. As discussed in Section 2.3, electricity–hydrogen systems operated against markets face sequential uncertainty in prices and renewable generation; over- or under-committing at early gates (e.g., day-ahead) can necessitate costly recourse at intraday or real-time stages. To address this, a multi-stage stochastic MILP that co-optimises, over a single daily horizon of $N_T = 24$ hourly intervals with $\Delta t = 1$ h, all market positions and physical set-points has been developed. The formulation enforces intertemporal feasibility so that earlier bids/awards remain deliverable under uncertainty, while mitigating myopic behaviour. This multi-stage shell underpins the stochastic optimisation of day-ahead, intraday, and real-time scheduling and offers for a full PtH plant supplying a hydrogen refueling station (HRS) under uncertainty, presented in Section 4.5 and in [238]. In this study the asset portfolio comprises PV, BESS, PEMEL, COMP, HS, and FC as

shown in Figure 4.37. Device physics and inter-hour state recursions follow Secs. 3.2.1–3.2.2. Unlike the joint sizing-scheduling variant—in which explicit enumeration of EL/FC operating states (*ON/STANDBY/OFF*) is computationally prohibitive—the present scheduling model includes binary commitment variables to capture start-up, shut-down, and standby behavior.

Relative to the joint sizing-scheduling setting, only three differences apply: (i) PV curtailment is disabled; (ii) there is no explicit net grid-exchange variable—transactions with the system operator occur exclusively through market positions, which are the sole buy/sell channels; (iii) hydrogen routing is extended to permit optional external sales, implemented via the mass balance shown in Eq. 3.191.

$$\dot{m}_{t,\omega}^{\text{H}_2,\text{EL}} + \dot{m}_{t,\omega}^{\text{H}_2,\text{dis}} = \dot{m}_{t,\omega}^{\text{H}_2,\text{dem}} + \dot{m}_{t,\omega}^{\text{H}_2,\text{sold}} + \dot{m}_{t,\omega}^{\text{H}_2,\text{FC}} + \dot{m}_{t,\omega}^{\text{H}_2,\text{ch}}, \quad \forall t, \forall \omega. \quad 3.191$$

A configuration flag $\phi \in \{0, 1\}$ enables or disables sales. With an optional throughput cap $\bar{m}^{\text{H}_2,\text{sold}}$ (set large if unused), by imposing Eq. 3.192:

$$0 \leq \dot{m}_{t,\omega}^{\text{H}_2,\text{sold}} \leq \phi \bar{m}^{\text{H}_2,\text{sold}}, \quad \forall t, \forall \omega. \quad 3.192$$

When $\phi = 0$, the model reduces to pure internal use ($\dot{m}_{t,\omega}^{\text{H}_2,\text{sold}} = 0$); when $\phi = 1$, the optimiser may export hydrogen at price c^{H_2} [€/kg], with the revenue included in the objective.

Market structure (Spain, pre-June 2024). The HRS participates sequentially in the day-ahead market (DA), the secondary reserve market (RM), six auction-based intraday markets (IM1–IM6), a seventh block (IM7) representing the first four hours of the second intraday auction of day $D+1$, and the imbalance settlement (IB). This mirrors the organisation and timelines of liberalised European power systems and the Spanish implementation we follow in the case studies, as represented in Figure 3.8 [239, 240].

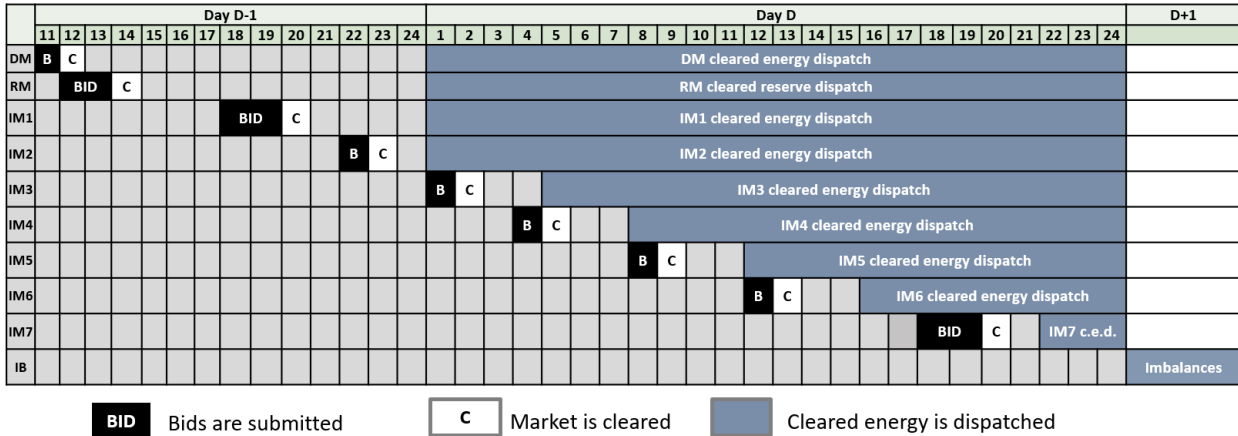


Figure 3.8: Timeline of bid submissions and market clearings (Spain, pre-June 2024), including DA, RM, six IM auctions, and IB; IM7 represents the first four hours of the second intraday market of day $D+1$.

For each delivery hour $t = 1, \dots, N_T$ (day D) and scenario ω , the optimisation carries: day-ahead sell/buy powers $p_{t,\omega}^{\text{DA}+}$, $p_{t,\omega}^{\text{DA}-}$ [kW], reserve capacities $p_{t,\omega}^{\text{RU}}$, $p_{t,\omega}^{\text{RD}}$ [kW], intraday corrections $p_{t,\omega}^{\text{IM}_i}$ [kW] (signed: >0 sell, <0 buy) for $i \in \{1, \dots, 6, 7\}$, and imbalance volumes $p_{t,\omega}^{\text{IB}+}$, $p_{t,\omega}^{\text{IB}-}$ [kW]. The corresponding prices are $c_{t,\omega}^{\text{DA}}$ [€/kWh], $c_{t,\omega}^{\text{RM}}$ [€/kW] for capacity, $c_{t,\omega}^{\text{IM}_i}$ [€/kWh], and $c_{t,\omega}^{\text{IB}\pm}$ [€/kWh], respectively [241].

The timeline in Figure 3.8 matches Table 3.7: DA clears at 12:00 on day $D-1$ and fixes a 24-hour schedule for day D ; RM clears at 14:00 with capacity payments for the whole day; IM1 and IM2 still cover all N_T hours; IM3–IM6 re-open trading only for the yet-to-start

Table 3.7: Sequence of markets, clearing times, and delivery coverage (day D).

Market	Clearing time (day $D-1/D$)	Delivery hours covered
Day-Ahead (DA)	12:00 (day $D-1$)	$t = 1, \dots, 24$ of day D
Reserve Market (RM, aFRR)	14:00 (day $D-1$)	$t = 1, \dots, 24$ of day D
Intraday 1 (IM1)	20:00 (day $D-1$)	$t = 1, \dots, 24$ of day D
Intraday 2 (IM2)	24:00 (midnight $D-1 \rightarrow D$)	$t = 1, \dots, 24$ of day D
Intraday 3 (IM3)	04:00 (day D)	$t = 4, \dots, 24$
Intraday 4 (IM4)	07:00 (day D)	$t = 7, \dots, 24$
Intraday 5 (IM5)	10:00 (day D)	$t = 10, \dots, 24$
Intraday 6 (IM6)	13:00 (day D)	$t = 13, \dots, 24$
Intraday 7 (IM7)	21:00 (day D)	first four hours of 2 nd IM of $D+1$
Imbalance (IB)	after delivery	per-hour settlement ex post

hours (from their clearing time onward); IM7 captures the first four hours of the second intraday auction of day $D+1$, a standard modelling device to hedge the early next-day block within the same optimisation [242].

At each market layer, the net power to be physically delivered in hour t is the cleared DA posture adjusted by the signed intraday corrections up to the last auction that still covered hour t , plus any activated reserve energy (modelled later), with residual deviations settled at IB prices. Casting this as a multi-stage stochastic program lets the scheduler shape early commitments (DA, RM) while reserving recourse at IM1–IM6 and, ultimately, at IB, exactly reflecting how economic exposure and deliverability evolve along the day.

Market constraints. All market variables are powers [kW]; prices are [€/kWh]. Settlements in the objective are obtained by multiplying powers by Δt . Figure 4.37 gives a visual representation of all market variables employed in the system. For each delivery hour $t = 1, \dots, N_T$ and scenario $\omega \in \Omega$ the following feasibility relations are imposed.

Day-Ahead (DA). For each (t, ω) the DA position is represented by nonnegative sell and buy powers $p_{t,\omega}^{\text{DA}+} \geq 0$ and $p_{t,\omega}^{\text{DA}-} \geq 0$, activated by binaries $\delta_{t,\omega}^{\text{DA}+}, \delta_{t,\omega}^{\text{DA}-} \in \{0, 1\}$. A minimum bid-block E^{DA} [kWh] is mapped to a per-hour minimum power $P^{\text{DA},\min} = E^{\text{DA}}/\Delta t$ [kW]. Upper bounds reflect the HRS's technical capability in either selling or buying direction as in Eqs. 3.193–3.194:

$$P^{\text{DA},\min} \delta_{t,\omega}^{\text{DA}+} \leq p_{t,\omega}^{\text{DA}+} \leq (P_{\text{nom}}^{\text{PV}} + \mathcal{C}E_{\text{nom}}^{\text{BESS}} + P_{\text{nom}}^{\text{FC}}) \delta_{t,\omega}^{\text{DA}+}, \quad \forall t, \forall \omega, \quad 3.193$$

$$P^{\text{DA},\min} \delta_{t,\omega}^{\text{DA}-} \leq p_{t,\omega}^{\text{DA}-} \leq (\mathcal{C}E_{\text{nom}}^{\text{BESS}} + P_{\text{nom}}^{\text{EL}} + P_{\text{nom}}^{\text{COMP}} + u_{\text{sb}}^{\text{FC}} P_{\text{nom}}^{\text{FC}}) \delta_{t,\omega}^{\text{DA}-}, \quad \forall t, \forall \omega. \quad 3.194$$

Only one direction can be active in a given hour as shown in Eq. 3.195:

$$\delta_{t,\omega}^{\text{DA}+} + \delta_{t,\omega}^{\text{DA}-} \leq 1, \quad \forall t, \forall \omega. \quad 3.195$$

The offers in DA market are represented as bidding curves. Let $\Omega^{\text{DA}} = \{\omega_1^{\text{DA}}, \dots, \omega_{|\Omega|}^{\text{DA}}\}$ be the scenario list sorted by increasing DA price for hour t , i.e. $c_{t,\omega_1^{\text{DA}}}^{\text{DA}} \leq \dots \leq c_{t,\omega_{|\Omega|}^{\text{DA}}}^{\text{DA}}$. The sequences $\{p_{t,\omega_i^{\text{DA}}}^{\text{DA}+}\}_i$ and $\{p_{t,\omega_i^{\text{DA}}}^{\text{DA}-}\}_i$ are then forced to be nondecreasing as shown in Eq. 3.196:

$$p_{t,\omega_i^{\text{DA}}}^{\text{DA}+} \leq p_{t,\omega_{i+1}^{\text{DA}}}^{\text{DA}+}, \quad p_{t,\omega_i^{\text{DA}}}^{\text{DA}-} \leq p_{t,\omega_{i+1}^{\text{DA}}}^{\text{DA}-}, \quad \forall i, \forall t. \quad 3.196$$

This construction yields valid, monotone step-wise supply (sell) and demand (buy) curves for each hour t : for any realised clearing price, the matched DA volume is the value that

corresponds to the price's rank in Ω^{DA} . Constraints 3.193–3.196 therefore encode minimum bid size, directional exclusivity, technical headroom/footroom and the monotonicity required by market rules.

Secondary Reserve Market (RM). Upward and downward reserve capacities are denoted $p_{t,\omega}^{\text{RU}} \geq 0$ and $p_{t,\omega}^{\text{RD}} \geq 0$ and are the sum of component contributions from BESS, EL, and FC (PV does not provide reserve) as represented in Eqs. 3.197–3.198:

$$p_{t,\omega}^{\text{RU}} = p_{t,\omega}^{\text{RU,BESS}} + p_{t,\omega}^{\text{RU,EL}} + p_{t,\omega}^{\text{RU,FC}}, \quad \forall t, \forall \omega, \quad 3.197$$

$$p_{t,\omega}^{\text{RD}} = p_{t,\omega}^{\text{RD,BESS}} + p_{t,\omega}^{\text{RD,EL}} + p_{t,\omega}^{\text{RD,FC}}, \quad \forall t, \forall \omega. \quad 3.198$$

The market operator requires that any awarded reserve can be sustained for a continuous activation window T^{RM} [h]; in this study $T^{\text{RM}} = 0.25$ (15 minutes). The following constraints guarantee both instantaneous power headroom/footroom and energy feasibility over T^{RM} .

For the BESS rate headroom/footroom with respect to current charging/discharging set-points, and SOC margins to sustain a T^{RM} -long activation as represented in Eqs. 3.199–3.202:

$$p_{t,\omega}^{\text{RU,BESS}} - p_{t,\omega}^{\text{BESS,ch}} + p_{t,\omega}^{\text{BESS,dis}} \leq \mathcal{C}E_{\text{nom}}^{\text{BESS}}, \quad \forall t, \forall \omega, \quad 3.199$$

$$p_{t,\omega}^{\text{RD,BESS}} + p_{t,\omega}^{\text{BESS,ch}} - p_{t,\omega}^{\text{BESS,dis}} \leq \mathcal{C}E_{\text{nom}}^{\text{BESS}}, \quad \forall t, \forall \omega, \quad 3.200$$

$$\text{SOC}_{t,\omega} \geq \text{SOC}_{\min} + \frac{T^{\text{RM}}}{E_{\text{nom}}^{\text{BESS}} \eta^{\text{BESS,dis}}} p_{t,\omega}^{\text{RU,BESS}}, \quad \forall t, \forall \omega, \quad 3.201$$

$$\text{SOC}_{t,\omega} \leq \text{SOC}_{\max} - \frac{T^{\text{RM}} \eta^{\text{BESS,ch}}}{E_{\text{nom}}^{\text{BESS}}} p_{t,\omega}^{\text{RD,BESS}}, \quad \forall t, \forall \omega. \quad 3.202$$

Inequalities 3.199–3.200 ensure the BESS can shift power by the offered amount without exceeding its C-rate in either direction; 3.201–3.202 guarantee sufficient energy margin to deliver the activation for T^{RM} .

For the EL upward reserve corresponds to the ability to reduce EL consumption (thus increasing net injection) and it can be provided only in *ON* state, while downward reserve corresponds to increasing consumption, thus it can be provided both in *ON* and in *STANDBY* states. Feasible operating region and storage impact are enforced as represented in Eqs. 3.203–3.206:

$$p_{t,\omega}^{\text{EL,on}} - p_{t,\omega}^{\text{RU,EL}} \geq u_{\min}^{\text{EL}} P_{\text{nom}}^{\text{EL}} \delta_{t,\omega}^{\text{EL,on}}, \quad \forall t, \forall \omega, \quad 3.203$$

$$p_{t,\omega}^{\text{EL}} + p_{t,\omega}^{\text{RD,EL}} \leq P_{\text{nom}}^{\text{EL}} (1 - \delta_{t,\omega}^{\text{EL,off}}), \quad \forall t, \forall \omega, \quad 3.204$$

$$\text{LOH}_{t,\omega} + \frac{T^{\text{RM}} \eta^{\text{HS,ch}}}{m_{\text{nom}}^{\text{HS}} \text{SEC}^{\text{EL}}} p_{t,\omega}^{\text{RD,EL}} \leq \text{LOH}_{\max}, \quad \forall t, \forall \omega, \quad 3.205$$

$$\text{LOH}_{t,\omega} - \frac{T^{\text{RM}}}{m_{\text{nom}}^{\text{HS}} \text{SEC}^{\text{EL}}} p_{t,\omega}^{\text{RU,EL}} \geq \text{LOH}_{\min}, \quad \forall t, \forall \omega. \quad 3.206$$

Constraints 3.203–3.204 keep the EL inside *ON*/nameplate bounds after the reserve shift; 3.205–3.206 ensure that the induced change in hydrogen flows remains compatible with the HS inventory over T^{RM} .

For the FC, upward reserve means increasing FC output (so it can be provided in both *ON* and *STANDBY* states), while downward reserve means reducing it, so it can be provided only in *ON* state. Operating-region and HS feasibility are enforced as represented

in Eqs. 3.207–3.210:

$$p_{t,\omega}^{\text{FC,on}} - p_{t,\omega}^{\text{FC,sb}} + p_{t,\omega}^{\text{RU,FC}} \leq P_{\text{nom}}^{\text{FC}} (1 - \delta_{t,\omega}^{\text{FC,off}}), \quad \forall t, \forall \omega, \quad 3.207$$

$$p_{t,\omega}^{\text{FC,on}} - p_{t,\omega}^{\text{RD,FC}} \geq u_{\min}^{\text{FC}} P_{\text{nom}}^{\text{FC}} \delta_{t,\omega}^{\text{FC,on}}, \quad \forall t, \forall \omega, \quad 3.208$$

$$\text{LOH}_{t,\omega} - \frac{T^{\text{RM}} \text{SFC}^{\text{FC}}}{m_{\text{nom}}^{\text{HS}} \eta^{\text{HS,dis}}} p_{t,\omega}^{\text{RU,FC}} \geq \text{LOH}_{\min}, \quad \forall t, \forall \omega, \quad 3.209$$

$$\text{LOH}_{t,\omega} + \frac{T^{\text{RM}} \text{SFC}^{\text{FC}}}{m_{\text{nom}}^{\text{HS}}} p_{t,\omega}^{\text{RD,FC}} \leq \text{LOH}_{\max}, \quad \forall t, \forall \omega. \quad 3.210$$

Inequalities 3.207–3.208 preserve minimum-load and nameplate limits after the reserve shift; 3.209–3.210 ensure that the hydrogen inventory can support T^{RM} -long activation in either direction.

Intraday markets (IM). Let $\mathcal{I} = \{1, \dots, 7\}$ be the set of intraday sessions and let $\mathcal{T}_i \subseteq \{1, \dots, N_T\}$ denote the delivery hours tradable in session i . For each hour t , define the set of sessions that still cover t as $\mathcal{I}_t := \{i \in \mathcal{I} : t \in \mathcal{T}_i\}$.

For each $i \in \mathcal{I}$ and $t \in \mathcal{T}_i$, let $p_{t,\omega}^{\text{IM}_i} \in \mathbb{R}$ [kW] be the signed position (positive = sell, negative = buy); enforce zero outside tradable hours as represented in Eq. 3.211:

$$p_{t,\omega}^{\text{IM}_i} = 0, \quad \forall i \in \mathcal{I}, \forall t \notin \mathcal{T}_i, \forall \omega. \quad 3.211$$

To limit speculative reshaping, cap (i) the net intraday correction per hour and (ii) the per-session volume by a factor $R^{\text{IM/DA}} \geq 0$ relative to the DA activity as shown in Eqs. 3.212–3.213:

$$-R^{\text{IM/DA}} (p_{t,\omega}^{\text{DA}+} + p_{t,\omega}^{\text{DA}-}) \leq \sum_{i \in \mathcal{I}_t} p_{t,\omega}^{\text{IM}_i} \leq R^{\text{IM/DA}} (p_{t,\omega}^{\text{DA}+} + p_{t,\omega}^{\text{DA}-}), \quad \forall t, \forall \omega, \quad 3.212$$

$$-R^{\text{IM/DA}} (p_{t,\omega}^{\text{DA}+} + p_{t,\omega}^{\text{DA}-}) \leq p_{t,\omega}^{\text{IM}_i} \leq R^{\text{IM/DA}} (p_{t,\omega}^{\text{DA}+} + p_{t,\omega}^{\text{DA}-}), \quad \forall i \in \mathcal{I}, \forall t \in \mathcal{T}_i, \forall \omega. \quad 3.213$$

Inequality 3.212 limits the *net* intraday reshaping of the DA posture for each hour, while 3.213 applies the same cap to each individual session covering that hour.

Imbalance settlement (IB). Positive and negative imbalances are represented by nonnegative powers $p_{t,\omega}^{\text{IB}+} \geq 0$ and $p_{t,\omega}^{\text{IB}-} \geq 0$ (optionally capped by $P_{t,\omega}^{\text{IB}+}$, $P_{t,\omega}^{\text{IB}-}$). Imbalance equals the realised net injection minus the scheduled net position (DA $\pm$ IM) as shown in Eq. 3.214:

$$p_{t,\omega}^{\text{IB}+} - p_{t,\omega}^{\text{IB}-} = \underbrace{p_{t,\omega}^{\text{DA}-} + p_{t,\omega}^{\text{PV}} + p_{t,\omega}^{\text{BESS,dis}} + p_{t,\omega}^{\text{FC,on}}}_{\text{realised injections and scheduled purchases}} - \underbrace{\left(p_{t,\omega}^{\text{DA}+} + \sum_{i \in \mathcal{I}_t} p_{t,\omega}^{\text{IM}_i} + p_{t,\omega}^{\text{BESS,ch}} + p_{t,\omega}^{\text{EL}} + p_{t,\omega}^{\text{COMP}} + p_{t,\omega}^{\text{FC,sb}} \right)}_{\text{realised withdrawals and scheduled sales}}, \quad \forall t, \forall \omega, \quad 3.214$$

$$0 \leq p_{t,\omega}^{\text{IB}+} \leq P_{t,\omega}^{\text{IB}+}, \quad 0 \leq p_{t,\omega}^{\text{IB}-} \leq P_{t,\omega}^{\text{IB}-}, \quad \forall t, \forall \omega. \quad 3.215$$

Eq. 3.214 measures the ex-post deviation from the market schedule; 3.215 bounds the magnitude of upward and downward imbalances in order to avoid too much speculation on a risky aspect like imbalances.

Constraints 3.193–3.215 complete the market-side feasibility relations used later by the multi-stage shell; non-anticipativity, stage coupling and the economic objective (revenues, penalties, ageing) are introduced in the following subsections.

Non-anticipativity constraints Let Ω be the scenario set. At each gate, Ω is partitioned into blocks (also called clusters) that collect scenarios indistinguishable under the information available at that gate; blocks are pairwise disjoint and their union equals Ω . Denote: (i) C_1 the DA partition at 12:00 of day $D-1$; (ii) C_R the RM partition at 14:00 of day $D-1$; (iii) CS_{i-1}^I the partition just before IM session $i \in \{1, \dots, 7\}$ clears; (iv) CSR_{t-1} the partition just before hour t starts (delivery-stage set-points); (v) CSR_t the partition at IB settlement of hour t . Inside any block c , list its $|\cdot|$ children (scenarios) in an arbitrary but fixed order as $\{\omega_1, \dots, \omega_{|c|}\}$. Non-anticipativity is enforced by equating, within each block, the decisions that must be fixed at that gate [152–154].

Non-anticipativity for DA offers. DA sell/buy powers and direction flags must be identical across scenarios within the same DA block. This is represented in Eq. 3.216:

$$\begin{cases} p_{t,\omega_j}^{\text{DA}+} = p_{t,\omega_{j+1}}^{\text{DA}+} & p_{t,\omega_j}^{\text{DA}-} = p_{t,\omega_{j+1}}^{\text{DA}-} \\ \delta_{t,\omega_j}^{\text{DA}+} = \delta_{t,\omega_{j+1}}^{\text{DA}+} & \delta_{t,\omega_j}^{\text{DA}-} = \delta_{t,\omega_{j+1}}^{\text{DA}-} \end{cases} \quad \forall j = 1, \dots, |c|-1, \forall c \in C_1, \forall t = 1, \dots, N_T. \quad 3.216$$

Non-anticipativity for RM capacities. Upward/downward capacities and their technology splits must coincide within each RM block. This is shown in Eq. 3.217:

$$\begin{cases} p_{t,\omega_j}^{\text{RU}} = p_{t,\omega_{j+1}}^{\text{RU}} & p_{t,\omega_j}^{\text{RD}} = p_{t,\omega_{j+1}}^{\text{RD}} \\ p_{t,\omega_j}^{\text{RU,BESS}} = p_{t,\omega_{j+1}}^{\text{RU,BESS}} & p_{t,\omega_j}^{\text{RD,BESS}} = p_{t,\omega_{j+1}}^{\text{RD,BESS}} \\ p_{t,\omega_j}^{\text{RU,EL}} = p_{t,\omega_{j+1}}^{\text{RU,EL}} & p_{t,\omega_j}^{\text{RD,EL}} = p_{t,\omega_{j+1}}^{\text{RD,EL}} \\ p_{t,\omega_j}^{\text{RU,FC}} = p_{t,\omega_{j+1}}^{\text{RU,FC}} & p_{t,\omega_j}^{\text{RD,FC}} = p_{t,\omega_{j+1}}^{\text{RD,FC}} \end{cases} \quad \forall j = 1, \dots, |c|-1, \forall c \in C_R, \forall t = 1, \dots, N_T. \quad 3.217$$

Non-anticipativity for IM redispatch. For each session i and tradable hour $t \in \mathcal{T}_i$, the intraday correction must be identical within the pre-session block. This is represented in Eq. 3.218:

$$p_{t,\omega_j}^{\text{IM}_i} = p_{t,\omega_{j+1}}^{\text{IM}_i}, \quad \forall j = 1, \dots, |c|-1, \forall c \in CS_{i-1}^I, \forall t \in \mathcal{T}_i, \forall i \in \{1, \dots, 7\}. \quad 3.218$$

Non-anticipativity for IB settlement. Positive/negative imbalances for hour t are fixed at its settlement and must be equal within the settlement block, as shown in Eq. 3.219:

$$\begin{cases} p_{t,\omega_j}^{\text{IB}+} = p_{t,\omega_{j+1}}^{\text{IB}+} \\ p_{t,\omega_j}^{\text{IB}-} = p_{t,\omega_{j+1}}^{\text{IB}-} \end{cases} \quad \forall j = 1, \dots, |c|-1, \forall c \in CSR_t, \forall t = 1, \dots, N_T. \quad 3.219$$

Non-anticipativity for hourly operating set-points (delivery stage). All physical set-points and logical modes used to deliver hour t are chosen just before t starts; they must therefore

be identical within the pre-delivery block CSR_{t-1} . This is represented in Eq. 3.220:

$$\left\{ \begin{array}{ll} p_{t,\omega_j}^{\text{BESS,ch}} = p_{t,\omega_{j+1}}^{\text{BESS,ch}} & p_{t,\omega_j}^{\text{BESS,dis}} = p_{t,\omega_{j+1}}^{\text{BESS,dis}} \\ \delta_{t,\omega_j}^{\text{BESS}} = \delta_{t,\omega_{j+1}}^{\text{BESS}} & \text{SOC}_{t,\omega_j} = \text{SOC}_{t,\omega_{j+1}} \\ p_{t,\omega_j}^{\text{EL}} = p_{t,\omega_{j+1}}^{\text{EL}} & p_{t,\omega_j}^{\text{EL,on}} = p_{t,\omega_{j+1}}^{\text{EL,on}} \\ p_{t,\omega_j}^{\text{EL,sb}} = p_{t,\omega_{j+1}}^{\text{EL,sb}} & \dot{m}_{t,\omega_j}^{\text{H}_2,\text{EL}} = \dot{m}_{t,\omega_{j+1}}^{\text{H}_2,\text{EL}} \\ \delta_{t,\omega_j}^{\text{EL,on}} = \delta_{t,\omega_{j+1}}^{\text{EL,on}} & \delta_{t,\omega_j}^{\text{EL,sb}} = \delta_{t,\omega_{j+1}}^{\text{EL,sb}} \\ \delta_{t,\omega_j}^{\text{EL,off}} = \delta_{t,\omega_{j+1}}^{\text{EL,off}} & \delta_{t,\omega_j}^{\text{EL,warm}} = \delta_{t,\omega_{j+1}}^{\text{EL,warm}} \\ \delta_{t,\omega_j}^{\text{EL,cold}} = \delta_{t,\omega_{j+1}}^{\text{EL,cold}} & p_{t,\omega_j}^{\text{COMP}} = p_{t,\omega_{j+1}}^{\text{COMP}} \\ \dot{m}_{t,\omega_j}^{\text{HS,ch}} = \dot{m}_{t,\omega_{j+1}}^{\text{HS,ch}} & \dot{m}_{t,\omega_j}^{\text{HS,dis}} = \dot{m}_{t,\omega_{j+1}}^{\text{HS,dis}} \\ \delta_{t,\omega_j}^{\text{HS}} = \delta_{t,\omega_{j+1}}^{\text{HS}} & \text{LOH}_{t,\omega_j} = \text{LOH}_{t,\omega_{j+1}} \\ p_{t,\omega_j}^{\text{FC,on}} = p_{t,\omega_{j+1}}^{\text{FC,on}} & p_{t,\omega_j}^{\text{FC,sb}} = p_{t,\omega_{j+1}}^{\text{FC,sb}} \\ \dot{m}_{t,\omega_j}^{\text{H}_2,\text{FC}} = \dot{m}_{t,\omega_{j+1}}^{\text{H}_2,\text{FC}} & \delta_{t,\omega_j}^{\text{FC,on}} = \delta_{t,\omega_{j+1}}^{\text{FC,on}} \\ \delta_{t,\omega_j}^{\text{FC,sb}} = \delta_{t,\omega_{j+1}}^{\text{FC,sb}} & \delta_{t,\omega_j}^{\text{FC,off}} = \delta_{t,\omega_{j+1}}^{\text{FC,off}} \\ \delta_{t,\omega_j}^{\text{FC,warm}} = \delta_{t,\omega_{j+1}}^{\text{FC,warm}} & \delta_{t,\omega_j}^{\text{FC,cold}} = \delta_{t,\omega_{j+1}}^{\text{FC,cold}} \\ \dot{m}_{t,\omega_j}^{\text{H}_2,\text{sold}} = \dot{m}_{t,\omega_{j+1}}^{\text{H}_2,\text{sold}} & \end{array} \right. \quad \forall j = 1, \dots, |c|-1, \forall c \in CSR_{t-1}, \forall t = 1, \dots, T$$

3.220

The NAC equalities in Eqs. 3.216–3.220 yield a multi-stage MILP consistent with risk-neutral multi-stage programming principles [152–154].

Stages overview. The NAC equalities in Eqs. 3.216–3.220 determine, gate by gate, which variables must coincide across scenarios that are indistinguishable at that point in time. This yields a time-consistent, DA→RM→IM→IB multi-stage MILP where decisions fixed earlier (e.g., DA bids, RM capacities) become the baseline against which later recourse acts (IM redispatch, delivery set-points, imbalances). The table below enumerates the stages in chronological order, indicating for each one the decision packages, the exogenous information revealed, and the recourse variables that are committed at that stage (and that function as decisions for the subsequent stage).

For each delivery hour $k = 1, \dots, N_T$, let

$$X_k = \{ p_{k,\omega}^{\text{BESS,ch}}, p_{k,\omega}^{\text{BESS,dis}}, \delta_{k,\omega}^{\text{BESS}}, \text{SOC}_{k,\omega}, p_{k,\omega}^{\text{EL}}, p_{k,\omega}^{\text{EL,on}}, p_{k,\omega}^{\text{EL,sb}}, \dot{m}_{k,\omega}^{\text{H}_2,\text{EL}}, \delta_{k,\omega}^{\text{EL,on}}, \delta_{k,\omega}^{\text{EL,sb}}, \delta_{k,\omega}^{\text{EL,off}}, \delta_{k,\omega}^{\text{EL,warm}}, \delta_{k,\omega}^{\text{EL,cold}}, p_{k,\omega}^{\text{COMP}}, \dot{m}_{k,\omega}^{\text{HS,ch}}, \dot{m}_{k,\omega}^{\text{HS,dis}}, \dot{m}_{k,\omega}^{\text{H}_2,\text{sold}}, \delta_{k,\omega}^{\text{HS}}, \text{LOH}_{k,\omega}, p_{k,\omega}^{\text{FC,on}}, p_{k,\omega}^{\text{FC,sb}}, \dot{m}_{k,\omega}^{\text{H}_2,\text{FC}}, \delta_{k,\omega}^{\text{FC,on}}, \delta_{k,\omega}^{\text{FC,sb}}, \delta_{k,\omega}^{\text{FC,off}}, \delta_{k,\omega}^{\text{FC,warm}}, \delta_{k,\omega}^{\text{FC,cold}} \},$$

and collect all reserve-capacity variables as

$$R_k = \{ p_{k,\omega}^{\text{RU}}, p_{k,\omega}^{\text{RU,BESS}}, p_{k,\omega}^{\text{RU,EL}}, p_{k,\omega}^{\text{RU,FC}}, p_{k,\omega}^{\text{RD}}, p_{k,\omega}^{\text{RD,BESS}}, p_{k,\omega}^{\text{RD,EL}}, p_{k,\omega}^{\text{RD,FC}} \}.$$

The summary of stages is thus represented in Table 3.8:

Objective function. The scheduler maximises expected profit over the daily horizon and all scenarios represented in Eq. 3.221:

$$\mathbb{E}\Pi = \sum_{\omega \in \Omega} \pi_{\omega} \sum_{t=1}^{N_T} \left(\text{REV}_{t,\omega} - \text{OPEX}_{t,\omega} \right) \quad 3.221$$

Table 3.8: Summary of stages, decision variables, observations, and recourse variables (day D).

Stage	Decision variables	Observations at stage	Recourse variables
1	—	$c_{\cdot,\omega}^{\text{DA}} \in \mathbb{R}^{N_T}$	$p_{t,\omega}^{\text{DA}+}, p_{t,\omega}^{\text{DA}-}, \delta_{t,\omega}^{\text{DA}+}, \delta_{t,\omega}^{\text{DA}-}$
2	$R_k, k=1:N_T$	$c_{\cdot,\omega}^{\text{RM}} \in \mathbb{R}^{N_T}$	—
3	$p_{t,\omega}^{\text{IM}_1}, t \in \mathcal{T}_1$	$c_{\cdot,\omega}^{\text{IM}_1} \in \mathbb{R}^{ \mathcal{T}_1 }$	—
4	$p_{t,\omega}^{\text{IM}_2}, t \in \mathcal{T}_2$	$c_{\cdot,\omega}^{\text{IM}_2} \in \mathbb{R}^{ \mathcal{T}_2 }$	—
5	X_1	$\bar{p}_{1,\omega}^{\text{PV}}, c_{1,\omega}^{\text{IB}\pm}$	$p_{1,\omega}^{\text{IB}+}, p_{1,\omega}^{\text{IB}-}$
6	X_2	$\bar{p}_{2,\omega}^{\text{PV}}, c_{2,\omega}^{\text{IB}\pm}$	$p_{2,\omega}^{\text{IB}+}, p_{2,\omega}^{\text{IB}-}$
7	$p_{t,\omega}^{\text{IM}_3}, t \in \mathcal{T}_3$	$c_{\cdot,\omega}^{\text{IM}_3} \in \mathbb{R}^{ \mathcal{T}_3 }$	—
8	X_3	$\bar{p}_{3,\omega}^{\text{PV}}, c_{3,\omega}^{\text{IB}\pm}$	$p_{3,\omega}^{\text{IB}+}, p_{3,\omega}^{\text{IB}-}$
9	X_4	$\bar{p}_{4,\omega}^{\text{PV}}, c_{4,\omega}^{\text{IB}\pm}$	$p_{4,\omega}^{\text{IB}+}, p_{4,\omega}^{\text{IB}-}$
10	X_5	$\bar{p}_{5,\omega}^{\text{PV}}, c_{5,\omega}^{\text{IB}\pm}$	$p_{5,\omega}^{\text{IB}+}, p_{5,\omega}^{\text{IB}-}$
11	$p_{t,\omega}^{\text{IM}_4}, t \in \mathcal{T}_4$	$c_{\cdot,\omega}^{\text{IM}_4} \in \mathbb{R}^{ \mathcal{T}_4 }$	—
12	X_6	$\bar{p}_{6,\omega}^{\text{PV}}, c_{6,\omega}^{\text{IB}\pm}$	$p_{6,\omega}^{\text{IB}+}, p_{6,\omega}^{\text{IB}-}$
13	X_7	$\bar{p}_{7,\omega}^{\text{PV}}, c_{7,\omega}^{\text{IB}\pm}$	$p_{7,\omega}^{\text{IB}+}, p_{7,\omega}^{\text{IB}-}$
14	X_8	$\bar{p}_{8,\omega}^{\text{PV}}, c_{8,\omega}^{\text{IB}\pm}$	$p_{8,\omega}^{\text{IB}+}, p_{8,\omega}^{\text{IB}-}$
15	X_9	$\bar{p}_{9,\omega}^{\text{PV}}, c_{9,\omega}^{\text{IB}\pm}$	$p_{9,\omega}^{\text{IB}+}, p_{9,\omega}^{\text{IB}-}$
16	$p_{t,\omega}^{\text{IM}_5}, t \in \mathcal{T}_5$	$c_{\cdot,\omega}^{\text{IM}_5} \in \mathbb{R}^{ \mathcal{T}_5 }$	—
17	X_{10}	$\bar{p}_{10,\omega}^{\text{PV}}, c_{10,\omega}^{\text{IB}\pm}$	$p_{10,\omega}^{\text{IB}+}, p_{10,\omega}^{\text{IB}-}$
18	X_{11}	$\bar{p}_{11,\omega}^{\text{PV}}, c_{11,\omega}^{\text{IB}\pm}$	$p_{11,\omega}^{\text{IB}+}, p_{11,\omega}^{\text{IB}-}$
19	X_{12}	$\bar{p}_{12,\omega}^{\text{PV}}, c_{12,\omega}^{\text{IB}\pm}$	$p_{12,\omega}^{\text{IB}+}, p_{12,\omega}^{\text{IB}-}$
20	X_{13}	$\bar{p}_{13,\omega}^{\text{PV}}, c_{13,\omega}^{\text{IB}\pm}$	$p_{13,\omega}^{\text{IB}+}, p_{13,\omega}^{\text{IB}-}$
21	$p_{t,\omega}^{\text{IM}_6}, t \in \mathcal{T}_6$	$c_{\cdot,\omega}^{\text{IM}_6} \in \mathbb{R}^{ \mathcal{T}_6 }$	—
22	X_{14}	$\bar{p}_{14,\omega}^{\text{PV}}, c_{14,\omega}^{\text{IB}\pm}$	$p_{14,\omega}^{\text{IB}+}, p_{14,\omega}^{\text{IB}-}$
23	X_{15}	$\bar{p}_{15,\omega}^{\text{PV}}, c_{15,\omega}^{\text{IB}\pm}$	$p_{15,\omega}^{\text{IB}+}, p_{15,\omega}^{\text{IB}-}$
24	X_{16}	$\bar{p}_{16,\omega}^{\text{PV}}, c_{16,\omega}^{\text{IB}\pm}$	$p_{16,\omega}^{\text{IB}+}, p_{16,\omega}^{\text{IB}-}$
25	X_{17}	$\bar{p}_{17,\omega}^{\text{PV}}, c_{17,\omega}^{\text{IB}\pm}$	$p_{17,\omega}^{\text{IB}+}, p_{17,\omega}^{\text{IB}-}$
26	X_{18}	$\bar{p}_{18,\omega}^{\text{PV}}, c_{18,\omega}^{\text{IB}\pm}$	$p_{18,\omega}^{\text{IB}+}, p_{18,\omega}^{\text{IB}-}$
27	X_{19}	$\bar{p}_{19,\omega}^{\text{PV}}, c_{19,\omega}^{\text{IB}\pm}$	$p_{19,\omega}^{\text{IB}+}, p_{19,\omega}^{\text{IB}-}$
28	$p_{t,\omega}^{\text{IM}_7}, t \in \mathcal{T}_7$	$c_{\cdot,\omega}^{\text{IM}_7} \in \mathbb{R}^{ \mathcal{T}_7 }$	—
29	X_{20}	$\bar{p}_{20,\omega}^{\text{PV}}, c_{20,\omega}^{\text{IB}\pm}$	$p_{20,\omega}^{\text{IB}+}, p_{20,\omega}^{\text{IB}-}$
30	X_{21}	$\bar{p}_{21,\omega}^{\text{PV}}, c_{21,\omega}^{\text{IB}\pm}$	$p_{21,\omega}^{\text{IB}+}, p_{21,\omega}^{\text{IB}-}$
31	X_{22}	$\bar{p}_{22,\omega}^{\text{PV}}, c_{22,\omega}^{\text{IB}\pm}$	$p_{22,\omega}^{\text{IB}+}, p_{22,\omega}^{\text{IB}-}$
32	X_{23}	$\bar{p}_{23,\omega}^{\text{PV}}, c_{23,\omega}^{\text{IB}\pm}$	$p_{23,\omega}^{\text{IB}+}, p_{23,\omega}^{\text{IB}-}$
33	X_{24}	$\bar{p}_{24,\omega}^{\text{PV}}, c_{24,\omega}^{\text{IB}\pm}$	$p_{24,\omega}^{\text{IB}+}, p_{24,\omega}^{\text{IB}-}$

Revenues.

$$\begin{aligned}
\text{REV}_{t,\omega} = & \underbrace{c_{t,\omega}^{\text{DA}} (p_{t,\omega}^{\text{DA}+} - p_{t,\omega}^{\text{DA}-}) \Delta t}_{\text{DA revenues}} + \underbrace{c_{t,\omega}^{\text{RM}} (p_{t,\omega}^{\text{RU}} + p_{t,\omega}^{\text{RD}})}_{\text{Reserve capacity payment}} \\
& + \underbrace{\sum_{i \in \mathcal{I}_t} c_{t,\omega}^{\text{IM}_i} p_{t,\omega}^{\text{IM}_i} \Delta t}_{\text{Intraday redispatch}} + \underbrace{c_{t,\omega}^{\text{IB}+} p_{t,\omega}^{\text{IB}+} \Delta t}_{\text{Positive imbalance credit}} \\
& + \underbrace{c^{\text{H}_2} \dot{m}_{t,\omega}^{\text{H}_2, \text{sold}} \Delta t}_{\text{Hydrogen sales (if } \phi=1)} .
\end{aligned} \tag{3.222}$$

Operating expenditure.

$$\begin{aligned}
 \text{OPEX}_{t,\omega} = & \underbrace{c_{t,\omega}^{\text{IB-}} p_{t,\omega}^{\text{IB-}} \Delta t}_{\text{Negative imbalance payment}} + \underbrace{c^{\text{H}_2\text{O}} \dot{V}_{t,\omega}^{\text{H}_2\text{O,EL}} \Delta t}_{\text{Electrolyser water consumption}} \\
 & + \underbrace{c^{\text{EL,warm}} P_{\text{nom}}^{\text{EL}} \delta_{t,\omega}^{\text{EL,warm}} + c^{\text{EL,cold}} P_{\text{nom}}^{\text{EL}} \delta_{t,\omega}^{\text{EL,cold}}}_{\text{Electrolyser start-up}} \\
 & + \underbrace{c^{\text{FC,warm}} P_{\text{nom}}^{\text{FC}} \delta_{t,\omega}^{\text{FC,warm}} + c^{\text{FC,cold}} P_{\text{nom}}^{\text{FC}} \delta_{t,\omega}^{\text{FC,cold}}}_{\text{Fuel cell start-up}} \\
 & + \underbrace{c^{\text{age,BESS}} \frac{p_{t,\omega}^{\text{BESS,dis}} + p_{t,\omega}^{\text{BESS,ch}}}{2 E_{\text{nom}}^{\text{BESS}}} \Delta t}_{\text{BESS ageing (cycle-throughput proxy)}} \\
 & + \underbrace{c^{\text{age,EL}} \delta_{t,\omega}^{\text{EL,on}} \Delta t}_{\text{Electrolyser ageing (ON-hours)}} + \underbrace{c^{\text{age,FC}} \delta_{t,\omega}^{\text{FC,on}} \Delta t}_{\text{Fuel-cell ageing (ON-hours)}}.
 \end{aligned} \tag{3.223}$$

Ageing coefficients.

$$c^{\text{age,BESS}} = \frac{\text{SRC}^{\text{BESS}} E_{\text{nom}}^{\text{BESS}}}{\text{cyc}_{\text{max}}}, \quad c^{\text{age,EL}} = \frac{\text{SRC}^{\text{EL}} P_{\text{nom}}^{\text{EL}}}{\text{LT}^{\text{EL}}}, \quad c^{\text{age,FC}} = \frac{\text{SRC}^{\text{FC}} P_{\text{nom}}^{\text{FC}}}{\text{LT}^{\text{FC}}}, \tag{3.224}$$

with SRC^{BESS} [€/kWh], SRC^{EL} [€/kW], and SRC^{FC} [€/kW] being the specific replacement costs of BESS, EL, and FC respectively. Here cyc_{max} [cycles] is the number of equivalent full cycles over the BESS lifetime, while LT^{EL} [h] and LT^{FC} [h] are the operating lifetimes of EL and FC.

Interpretation of the revenue terms.

DA revenues. The DA posture provides the baseline energy schedule. A positive $p_{t,\omega}^{\text{DA+}}$ is a sale that earns the DA price $c_{t,\omega}^{\text{DA}}$, whereas a positive $p_{t,\omega}^{\text{DA-}}$ is a purchase that reduces the net DA revenue. The factor Δt converts the cleared powers into settled energy.

Reserve capacity payment. Upward and downward secondary reserve capacities, $p_{t,\omega}^{\text{RU}}$ and $p_{t,\omega}^{\text{RD}}$, receive a capacity fee $c_{t,\omega}^{\text{RM}}$ in €/kW for the delivery hour. The reserve-feasibility constraints (rate headroom/footroom and energy margins) ensure that the offered capacities can be sustained for the activation window without violating device limits (BESS C-rate and SOC margins, EL/FC operating regions, HS inventory bounds).

Intraday redispatch. Intraday sessions allow for sequential corrections of the DA posture as new prices and forecasts arrive. Each signed position $p_{t,\omega}^{\text{IM}_i}$ settles at its session price $c_{t,\omega}^{\text{IM}_i}$. Positive values represent additional sales; negative values represent purchases. Session- and hour-wise caps relative to DA curb excessive reshuffling and speculation.

Positive imbalance credit. If the realised net injection exceeds the scheduled posture after DA and IM trades, the surplus $p_{t,\omega}^{\text{IB+}}$ is credited at $c_{t,\omega}^{\text{IB+}}$. The realised injection is determined by the delivery-stage AC balance coupled with the hydrogen routing, while the scheduled posture is the sum of DA and intraday positions.

Hydrogen sales. When the sale flag ϕ is active, exported hydrogen $\dot{m}_{t,\omega}^{\text{H}_2,\text{sold}}$ earns c^{H_2} [€/kg]. This term monetises hydrogen as a product and competes with either storing it in HS for later use or reconvertng it to electricity in the FC at high-value hours. When $\phi=0$, the sale variable is forced to zero and the term vanishes.

Interpretation of the OPEX terms.

Negative imbalance payment. If the realised net injection is short of the scheduled posture, the shortfall $p_{t,\omega}^{\text{IB-}}$ is settled at $c_{t,\omega}^{\text{IB-}}$ (always higher than $c_{t,\omega}^{\text{IB+}}$ for definition). Together, the

positive and negative imbalance settlements create a strong incentive to maintain feasible delivery-stage set-points and to use intraday markets and reserves prudently.

Electrolyser water consumption. Hydrogen production consumes demineralised water which is priced at $c^{\text{H}_2\text{O}}$.

Electrolyser and fuel-cell start-up costs ($\text{€}/\text{kW}\cdot\text{event}$). Warm and cold starts are priced per event using nameplate powers and coefficients $c^{\text{EL,warm}}, c^{\text{EL,cold}}, c^{\text{FC,warm}}, c^{\text{FC,cold}}$ in $\text{€}/\text{kW}$. Multiplying by $P_{\text{nom}}^{\text{EL}}$ or $P_{\text{nom}}^{\text{FC}}$ scales the event cost to the installed capacity. Distinguishing warm/cold captures different thermal stress, consumables, and degradation impacts, and discourages gratuitous cycling among OFF/STANDBY/ON.

BESS ageing (cycle-throughput proxy). The BESS ageing term estimates the rate of equivalent full cycles in the hour as the total power throughput divided by energy capacity, then prices it at $c^{\text{age,BESS}}$ [$\text{€}/\text{cycle}$]. This linear proxy is a MILP-friendly surrogate for rainflow counting: shallow opportunistic adjustments cost little, while sustained high-depth cycling accumulates larger ageing expenditure and is thus optimised only when economically justified.

Electrolyser and fuel-cell ageing (ON-hours). Producing hours are priced by $c^{\text{age,EL}}$ and $c^{\text{age,FC}}$ [$\text{€}/\text{h}$] through the mode indicators $\delta_{t,\omega}^{\text{EL,on}}$ and $\delta_{t,\omega}^{\text{FC,on}}$. These terms capture the progressive wear associated with time-at-load (stack degradation), while the start-up costs capture the concentrated damage due to thermal and electrochemical transients. The combination avoids unnecessary runtime and unnecessary starts without introducing nonlinearities beyond the already present commitment binaries.

Multi-stage stochastic MILP formulation (market-coupled scheduling). Dropping sizing (pure scheduling) and enforcing gate-wise non-anticipativity, the complete multi-stage stochastic MILP is summarised in Eq. 3.225. Let $\{v_{t,\omega}\}$ collect continuous operating set-points and market powers, $\{\delta_{t,\omega}\}$ all binary mode/commitment and direction flags, and $\{x_{t,\omega}\}$ the intertemporal states (e.g., SOC, LOH).

$$\begin{aligned}
 & \max_{\{v_{t,\omega}, \delta_{t,\omega}, x_{t,\omega}\}_{t=1}^{N_T}, \omega \in \Omega} && \mathbb{EP} \text{ as in Eqs. 3.221–3.223} \\
 & \text{s.t.} && \text{Hydrogen mass balance and sale switch (Eqs. 3.191–3.192)} \\
 & && \text{PV availability (no curtailment) (Eqs. 3.128–3.130)} \\
 & && \text{EL conversion and operating states (Eqs. 3.135–3.145)} \\
 & && \text{COMP rating and linear electric load (Eqs. 3.147–3.148)} \\
 & && \text{HS dynamics and bounds (Eqs. 3.149–3.154)} \\
 & && \text{FC conversion and operating states (Eqs. 3.155–3.163)} \\
 & && \text{BESS dynamics and bounds (Eqs. 3.164–3.168)} \\
 & && \text{DA: bounds and monotone bidding curves (Eqs. 3.193–3.196)} \\
 & && \text{RM: tech splits and feasibility over } T^{\text{RM}} \text{ (Eqs. 3.197–3.210)} \\
 & && \text{IM redispatch (Eqs. 3.212–3.213)} \\
 & && \text{IB settlement: ex-post deviation and bounds (Eqs. 3.214–3.215)} \\
 & && \text{Gate-wise NAC (Eqs. 3.216–3.220)}
 \end{aligned} \tag{3.225}$$

Scenario generation and reduction. The stochastic drivers entering the multi-stage MILP are the PV availability and the market prices at the information times defined by the DA→RM→IM→delivery→IB sequence. For each delivery hour $t = 1, \dots, N_T$ and scenario

$\omega \in \Omega$, the model consumes the paths

$$\bar{p}_{t,\omega}^{\text{PV}}, \quad c_{t,\omega}^{\text{DA}}, \quad c_{t,\omega}^{\text{RM}}, \quad \{c_{t,\omega}^{\text{IM}_i}\}_{i \in \mathcal{I}_t}, \quad c_{t,\omega}^{\text{IB}^+}, \quad c_{t,\omega}^{\text{IB}^-},$$

with probabilities π_ω satisfying $\pi_\omega \geq 0$ and $\sum_{\omega \in \Omega} \pi_\omega = 1$. The joint stochastic process is approximated by a discrete-time scenario tree that preserves the sequential information structure of the decision problem [243]. Historical series for DA, RM, IM, and IB are sourced from OMIE, and PV generation at the HRS site from PVGIS. All prices are converted to the units used in the formulation (energy prices in €/kWh, capacity prices in €/kW); missing values are imputed conservatively and time-stamps are aligned to the Spanish market calendar. To build the scenario tree a two-phase pipeline is adopted, as it has been done in [244].

- (i) **Phase I: statistical generation of a scenario fan.** A Time Series Factor Analysis (TSFA) is first used to reduce dimensionality of the stacked vector of PV and prices while retaining the dominant comovements [245]. On the latent factors, a vector autoregressive model $\text{VAR}(p)$ is fitted to capture temporal and cross-variable dependence [246]. Future factor paths are generated by bootstrap of the fitted VAR innovations [247]; reconstruction through the TSFA loadings yields a large Monte Carlo fan of joint trajectories for $(\bar{p}_t^{\text{PV}}, c_t^{\text{DA}}, c_t^{\text{RM}}, \{c_t^{\text{IM}_i}\}_i, c_t^{\text{IB}^+}, c_t^{\text{IB}^-})_{t=1}^{N_T}$. This phase preserves: (a) marginal distributions of each series; (b) serial correlation; (c) cross-market and PV–price dependencies.
- (ii) **Phase II: forward tree construction (scenario reduction).** The fan is compressed into a tractable, recombining scenario tree by a forward selection algorithm in the sense of Dupačová–Gröwe-Kuska–Römisch [158]. The reduction minimises a transportation (Wasserstein/Kantorovich) distance between the empirical distribution of the fan and the reduced tree, computed on standardized variables so that PV and the various price series contribute comparably. Branching points are aligned with observation times (DA, RM, each IM session, and the pre-delivery/IB updates), i.e., with the partitions $C_1, C_R, CS_{i-1}^I, CSR_{t-1}$, and CSR_t introduced in the non-anticipativity constraints. In this way, each node aggregates fan paths that are indistinguishable at that gate, and children represent the admissible information reveals at the next gate. Leaf nodes correspond to full-day trajectories; their probabilities π_ω are the reduced (reweighted) masses inherited from the selected fan members.

Interface with the MILP. The reduced tree provides, for every node/gate and delivery hour t , the scenario-indexed inputs $\bar{p}_{t,\omega}^{\text{PV}}$ and market prices $c_{t,\omega}^{\text{DA}}, c_{t,\omega}^{\text{RM}}, \{c_{t,\omega}^{\text{IM}_i}\}_{i \in \mathcal{I}_t}, c_{t,\omega}^{\text{IB}^\pm}$. Because branching times coincide with the gates used to define non-anticipativity, the equality constraints in Eqs. 3.216–3.220 are satisfied by construction: decisions fixed at a node are common to all its children, while recourse at later gates can adapt to the branch taken. This ensures time-consistent, gate-wise feasible scheduling while keeping the number of scenarios $|\Omega|$ computationally tractable.

Calibration and checks. Prior to reduction, all series are standardized (zero-mean, unit-variance) within each delivery hour to respect intraday seasonality; after reduction, the selected tree is de-standardized and re-scaled to physical units. Basic diagnostics verify that (i) hourly marginals are reproduced (quantiles and means), (ii) key cross-correlations (PV–price, DA–IM–IB) are retained, and (iii) the reduced tree yields DA-to-IM price spreads and IB premia consistent with historical evidence.

This compact description follows the scenario-tree methodology of [244] (see also [243]). For complete modelling details, statistical options, and algorithmic parameters (TSFA specification, VAR order selection, bootstrap settings, and the specific distance used in the forward selection), the reader is referred to the Ph.D. thesis of Cuadrado Guevara [244].

4. RESULTS AND DISCUSSION

This chapter reports five independent studies. Each has its own section, with methods referenced to the relevant chapters: the rule-based Multi-Energy System Simulator in Section 3.1, deterministic mixed-integer linear programming in Section 3.2.3, two-stage stochastic mixed-integer linear programming in Section 3.2.4, and multi-stage stochastic mixed-integer linear programming in Section 3.2.5. In brief:

- **Rule-based: Case I — SOFC-based CHP for a paper mill** (Section 4.1). A like-for-like benchmark of a solid-oxide fuel cell with a heat-recovery steam generator against a natural-gas-fired gas turbine with a heat-recovery steam generator under real paper-mill loads (electricity plus 20 bar saturated steam), using hourly rule-based simulations with the Multi-Energy System Simulator; the techno-economic analysis reports the levelised cost of hydrogen (LCOH) for grey and green hydrogen and the system-level net present cost (NPC) [248].
- **Rule-based: Case II — Optimal grid-connected PV-PtH plant** (Section 4.2). Nation-wide sizing of a grid-connected PV-based power-to-hydrogen plant to serve a constant industrial hydrogen demand; a genetic algorithm coupled to the Multi-Energy System Simulator searches designs across the Italian bidding zones, with degradation of the photovoltaic system, battery and the electrolyser reflected in the LCOH [249].
- **Deterministic MILP — Hydrogen storage technologies** (Section 4.3). A perfect-foresight joint sizing-scheduling baseline that embeds storage inside the plant optimisation; compares compressed gaseous hydrogen tanks, underground hydrogen storage, and metal-hydride storage on a common LCOH basis under a certification cap consistent with the European Union Renewable Energy Directive III [233].
- **Two-stage stochastic MILP — Island decarbonisation** (Section 4.4). A stand-alone hybrid renewable energy system for a real Mediterranean island (Pantelleria): a single design is chosen before uncertainty is realised, while hourly operations adapt scenario-by-scenario; the system includes photovoltaic generation, wind turbines, an electrolyser, a compressor, hydrogen storage, a fuel cell, a battery energy storage system, and a diesel generator; the study quantifies the premium for reliability and emissions compliance relative to the deterministic baseline [234].

- **Multi-stage stochastic MILP — Market-coupled scheduling** (Section 4.5). Operating-phase scheduling for a hydrogen refuelling station treated as a hydrogen-enabled virtual power plant: the formulation co-optimises day-ahead bidding, secondary-reserve capacity, all intraday redispatches, and ex-post imbalance settlement along the Iberian market sequence to reduce the LCOH in the operative phase [238].

4.1 Rule-based: Case I — SOFC-based CHP for a paper mill

4.1.1 Motivation, scope and contributions

Industry remains one of the most energy- and carbon-intensive sectors, with many processes requiring the simultaneous supply of electricity and high-temperature heat. The pulp-and-paper sector is emblematic: it exhibits relatively flat electric loads alongside a persistent demand for saturated steam at medium pressure, making it a natural candidate for cogeneration yet a difficult target for full electrification of heat. Hydrogen has emerged as a promising cross-vector for decarbonisation, enabling both short-term storage and fuel substitution. Within this context, SOFCs offer high electrical efficiency and high-grade thermal by-product, potentially suitable for steam generation when appropriately integrated with a HRSG.

Despite growing attention to hydrogen in multi-energy systems, the use of SOFC cogeneration to deliver pressurised process steam for industrial users remains comparatively underexplored. This case study examines whether an SOFC-based CHP layout—embedded in a hydrogen-centred, renewable-integrated system—can meet the stringent steam and electricity needs of a real paper mill while improving environmental and techno-economic performance versus a conventional GT–HRSG benchmark.

Contributions. Building on the case and methods of Section 3.1.1 and [248], this study: (i) benchmarks SOFC+HRSG against a proven GT+HRSG baseline under identical industrial loads; (ii) embeds SOFC cogeneration within a multi-energy framework with on-site green-H₂ production, compression and daily storage; (iii) quantifies techno-economics via LCOH for the PtH chain and net present cost (NPC) at system level. Hourly simulations are conducted with the rule-based MESS framework to capture load variability and part-load behaviour of components. The application is a paper mill in Tuscany (Italy) with hourly electric demand $p_t^{\text{el,dem}}$ and thermal demand $p_t^{\text{th,dem}}$ in the form of saturated steam at $\mathcal{P}_{\text{st}} = 20$ bar (Figure 4.1). The demand time series are treated as exogenous inputs to MESS.

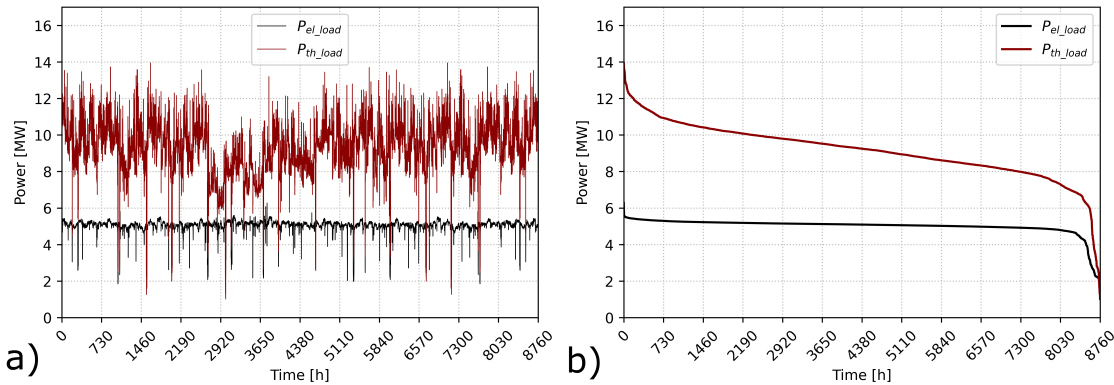


Figure 4.1: a) Electric and thermal load profiles. b) Electric and thermal load curve.

4.1.2 Configurations

GT and SOFC modelling—including electrochemistry/thermodynamics, off-design, and HRSG couplings—follow the dedicated component sections (GT: Section 3.1.1; SOFC: Section 3.1.1). To ensure a like-for-like comparison, the nominal electrical powers are matched:

$$P_{\text{nom}}^{\text{GT}} = P_{\text{nom}}^{\text{FC}} = 5.4 \text{ MW}_{\text{el}},$$

implemented on the SOFC side as $N_{\text{mod}} = 54$ identical modules of 100 kW each.

Three cogeneration alternatives are compared to satisfy the demands:

1. *GT configuration (baseline)*. Figure 4.2. A hydrogen-fired GT supplies electric power; its hot exhaust drives a single-pressure HRSG delivering saturated steam to the mill header at $\mathcal{P}_{\text{st}} = 20$ bar. An auxiliary steam generator (SG) covers residual thermal deficits.

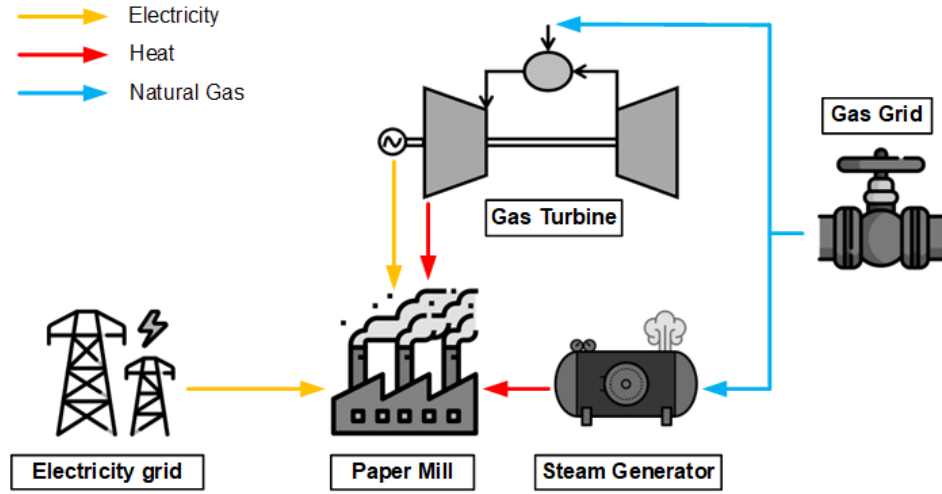


Figure 4.2: Baseline GT+HRSG configuration (schematic).

2. *S1 configuration (SOFC on grey H_2)*. Figure 4.3. An SOFC-based CHP plant provides electricity and high-grade heat; the mixed SOFC exhaust drives a single-pressure HRSG to the same header. Hydrogen is supplied from an on-site steam-methane reformer (SMR) and an auxiliary SG covers residual thermal deficits.
3. *S2 configuration (SOFC on green H_2)*. Figure 4.4. On-site green hydrogen is produced via a PV field (Section 3.1.1) driving a PEM electrolyser (Section 3.1.1); hydrogen is compressed (Section 3.1.1) and stored as CGH_2 at $\mathcal{P}^{\text{HS}} = 300$ bar (Section 3.1.1). The SOFC+HRSG supply electricity and steam as in S1; an SMR provides grey- H_2 back-up and an auxiliary SG covers residual thermal deficits.

Unlike the other components, the SMR and auxiliary SG are not detailed in Section 3.1.1; their simplified models are summarised here. A conventional SMR mixes pressurised CH_4 with steam to produce H_2 . Following He and Li [250], an overall SMR efficiency $\eta^{\text{SMR}} = 68.7\%$ (LHV basis) is adopted. In S2, the SMR is enabled only as a back-up to keep the SOFC operating overnight when the green- H_2 inventory in the CGH_2 tank would otherwise drop below its lower bound; in S1 it acts as the primary hydrogen source. The SG is modelled at fixed efficiency $\eta^{\text{SG}} = 90\%$ (LHV) [251], converting NG to saturated steam at $\mathcal{P}_{\text{st}} = 20$ bar.

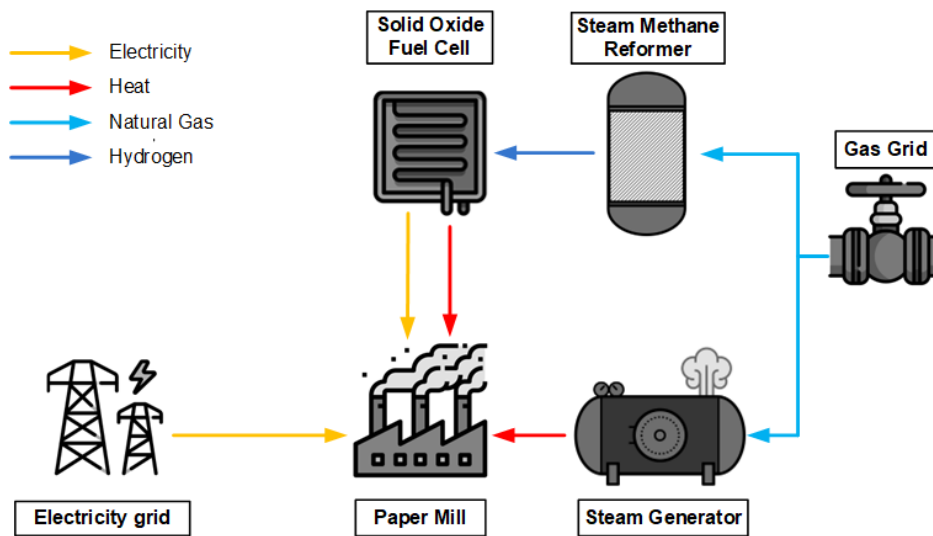


Figure 4.3: S1 configuration: SOFC+HRSG on grey H₂ supplied by a SMR. SG back-up.

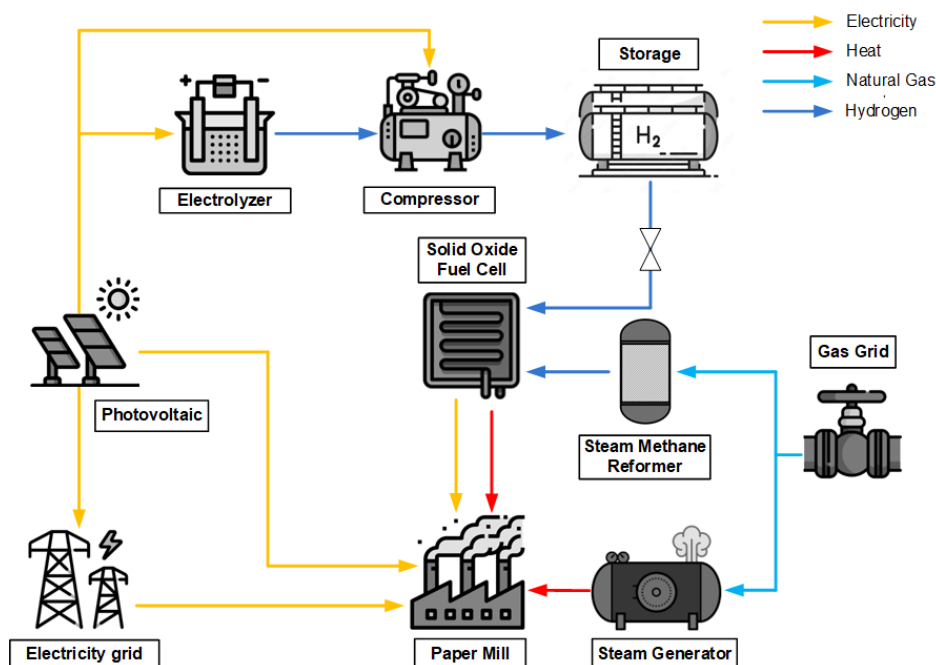


Figure 4.4: S2 configuration: SOFC+HRSG on green H₂ (PV→EL→COMP→CGH₂, SMR and SG back-up).

4.1.3 Rule-based workflow

For conciseness, the following dispatch sequence refers to the S2 (green-H₂) layout; the GT baseline and S1 are recovered by disabling the PV–EL–COMP–HS chain and/or replacing the prime mover as described above. At each step of the loop in Section 3.1: (i) PV generation first serves $p_t^{\text{el,dem}}$; (ii) any PV surplus drives the electrolyser, subject to device guards and available storage headroom; (iii) produced H₂ is compressed to $\mathcal{P}^{\text{HS}}$ and updates the tank LOH; (iv) when PV is insufficient, the SOFC is dispatched within its part-load envelope to supply electricity and, via the HRSG mapping, steam; (v) if LOH hits its lower bound, the SMR supplies H₂ (primary in S1, back-up in S2); (vi) the HRSG-derived steam is compared against $p_t^{\text{th,dem}}$; any residual is met by the SG; (vii) the residual electric load is covered by the grid; (viii) inventories and device states are updated.

Figure 4.5 illustrates the hourly dispatch produced by the rule-based simulator for the S2 layout over representative two-week windows in February, July and December. Photovoltaic surplus is converted to hydrogen and stored during daytime; the tank discharges overnight to sustain solid-oxide fuel cell operation, while the steam–methane reformer provides back-up only when the storage inventory reaches its lower bound.

4.1.4 Technical and economic inputs

The techno-economic assessment adopts two main metrics defined in Section 3.1.2: (i) LCOH for the PtH chain (PV, EL, COMP, CGH₂) defined in Eq. 3.110 and (ii) NPC for the whole system (including SOFC/GT, SG, SMR) defined in Eq. 3.108. Following common practice, LCOH excludes revenues from electricity exported to the grid to avoid biasing plant sizing; NPC is also reported without remuneration, while sensitivity including remuneration is discussed separately. The discount rate and project lifetime are set to $\text{DR} = 5\%$ and $N = 30$ years, respectively.

Table 4.1: Asset-specific economic inputs.

Asset a	$\text{CAPEX}_a^{\text{unit}}$	$\text{frac}_a^{\text{O\&M}}$	LT_a	$\text{frac}_a^{\text{repr}}$	Reference
PV	690 [€/kW]	0.0129	25	0.80	[252]
EL	See Eq. 4.1	See Eq. 4.2	15	0.30	
HS (CGH ₂ , 300 bar)	463 [€/kg]	0.02	30	0.80	[253]
SOFC	3000 [€/kW]	0.02	15	0.80	[94]
COMP	See Eq. 4.3	0.02	20	0.80	
SG	308 [€/kW]	0.01	30	0.80	[254]
SMR	280 [€/kW]	0.02	30	0.80	[250, 255, 256]

Table 4.1 reports the asset inputs, in particular $\text{CAPEX}_a^{\text{unit}}$, fixed O&M fractions $\text{frac}_a^{\text{O\&M}}$, lifetimes, and replacement fractions $\text{frac}_a^{\text{repr}}$.

The EL capital cost CAPEX_{EL} [€] is evaluated according to industrial stakeholder data via the correlation in Eq. 4.1:

$$\text{CAPEX}_{\text{EL}} = 1185 (P_{\text{nom}}^{\text{EL}})^{0.925}, \quad 4.1$$

with $P_{\text{nom}}^{\text{EL}}$ [kW]. The EL fixed O&M cost $\text{O\&M}_{\text{EL}}$ [€/year] is not treated as a simple fraction of the capital investment, but is computed from the correlation in Eq. 4.2:

$$\text{O\&M}_{\text{EL}} = (349.8 (P_{\text{nom}}^{\text{EL}})^{-0.305}) P_{\text{nom}}^{\text{EL}}. \quad 4.2$$

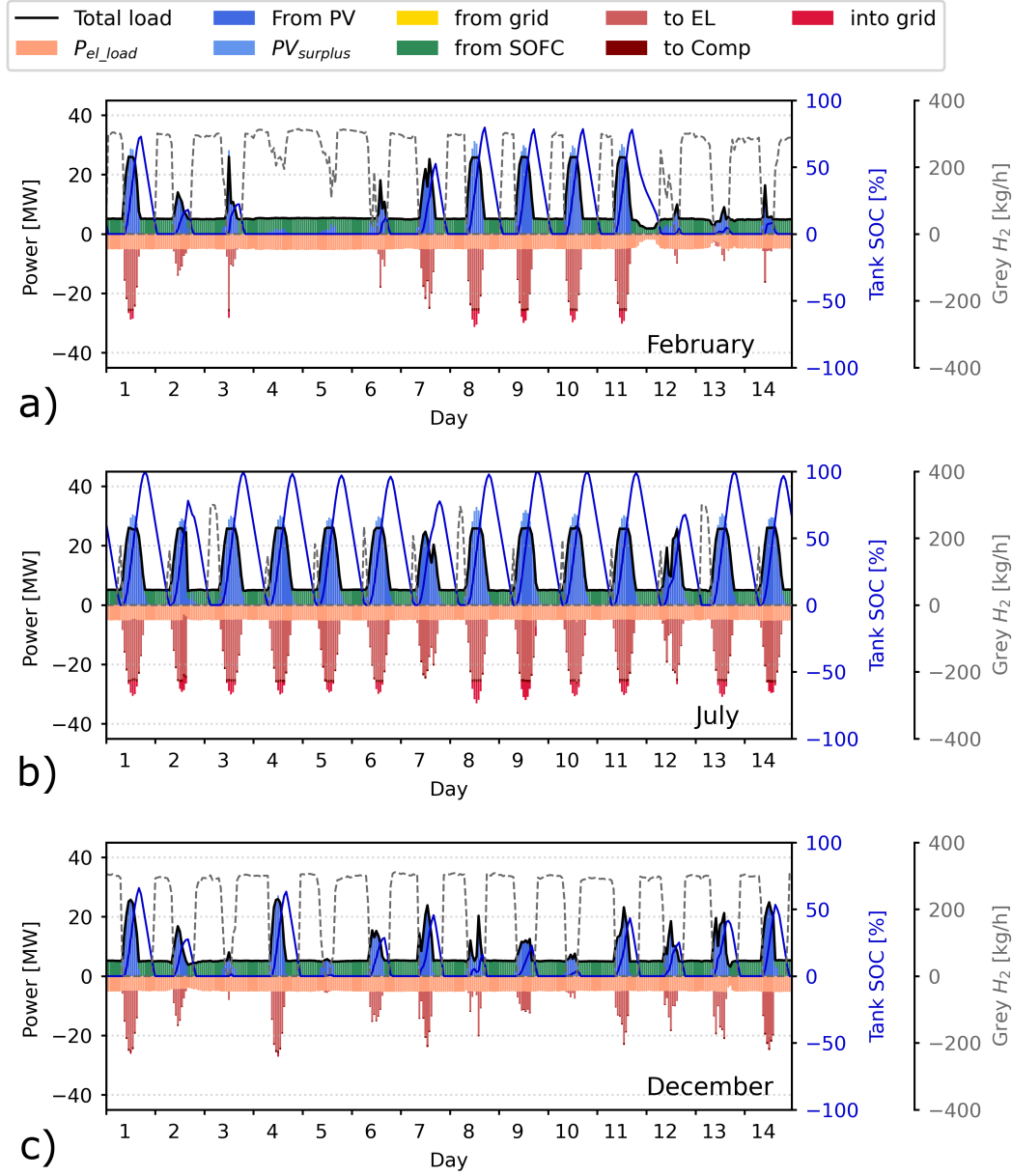


Figure 4.5: Hourly electric balances, hydrogen storage inventory (LOH), and steam-methane reformer back-up over representative two-week windows in February (a), July (b), and December (c). Layout: 40 MW_{el} PV, 20 MW_{el} electrolyser, 1.1 MW_{el} compressor, 3.2 t compressed-gaseous-hydrogen storage at 300 bar, 5.4 MW_{el} solid-oxide fuel cell, 10.8 MW_{th} steam-methane reformer, 15.5 MW_{th} auxiliary steam generator.

The COMP capital cost $\text{CAPEX}_{\text{COMP}}$ [€] is evaluated by the correlation in Eq. 4.3:

$$\text{CAPEX}_{\text{COMP}} = 0.91 \times 51901 \times (\dot{m}_{\text{max}}^{\text{H}_2, \text{EL}})^{0.65}, \quad 4.3$$

where $\dot{m}_{\text{max}}^{\text{H}_2, \text{EL}}$ [kg/h] is the maximum hydrogen production rate of the EL.

Table 4.2 lists the baseline values used in the revenue and cost KPIs.

Table 4.2: Baseline price signals used in the KPIs.

Stream	Symbol	Baseline value	Reference
Electricity imported from grid	$c_t^{\text{el,imp}}$	200 [€/MWh]	[257]
Electricity exported to grid	$c_t^{\text{el,exp}}$	65 [€/MWh]	[258]
Process water purchased	$c_y^{\text{H}_2\text{O}}$	4 [€/m ³]	[259]
Natural gas purchased (LHV)	c_y^{NG}	40.9 [€/MWh]	[260]

4.1.5 Results and discussion

GT vs SOFC cogeneration result. Consistently with the reference SGT-100 (Section 3.1.1), the GT prime mover is set to $P_{\text{nom}}^{\text{GT}} = 5.4 \text{ MW}_{\text{el}}$. For a fair benchmark, the SOFC stack is sized identically, $P_{\text{nom}}^{\text{FC}} = 5.4 \text{ MW}_{\text{el}}$ (Section 3.1.1). Although P_{nom} is matched, the technologies differ markedly in electric/thermal performance and in how their exhaust couples to a single-pressure HRSG delivering saturated steam at 20 bar ($T_{\text{sat}} \approx 212^\circ\text{C}$). The HRSG guards specified in the component sections are adopted: $\Delta T_{\text{pp}} = 10 \text{ K}$ for both GT and SOFC; economiser subcooling $\Delta T_{\text{sub}} = 10 \text{ K}$ for the GT (Table 3.5) and $\Delta T_{\text{sub}} = 75 \text{ K}$ for the SOFC (Table 3.6); minimum stack temperature $T_{\text{stack,min}} = 105^\circ\text{C}$ applied to both cases to enforce a common floor. Table 4.3 summarises nominal figures at ISO design. With $\eta^{\text{el,GT}} = 30.2\%$ and $\eta^{\text{el,FC}} = 50.5\%$, the corresponding LHV input powers are $P_{\text{th,in}}^{\text{GT}} = 17.8 \text{ MW}_{\text{th}}$ and $P_{\text{th,in}}^{\text{FC}} = 10.8 \text{ MW}_{\text{th}}$.

Table 4.3: Nominal GT vs SOFC characteristics and HRSG guards at $\mathcal{P}_{\text{st}} = 20 \text{ bar}$.

Parameter	Units	GT	SOFC
Output electric power	[MW]	5.4	5.4
Electric efficiency	[%]	30.2	50.5
Input thermal power	[MW]	17.8	10.8
Exhaust temperature	[°C]	549	800
Exhaust mass flow	[kg/s]	21	2.6
Pinch point ΔT_{pp}	[K]	10	10
Subcooling ΔT_{sub}	[K]	10	75
Stack temperature floor $T_{\text{stack,min}}$	[°C]	105	105
Steam generated to 20 bar	[kg/s]	3.97	0.98

For a hydrogen-fired GT, the exhaust is mainly N_2 and H_2O with residual O_2 . The SOFC, by contrast, mixes a dry cathode stream (mostly N_2 , little/no O_2) with a wet anode stream

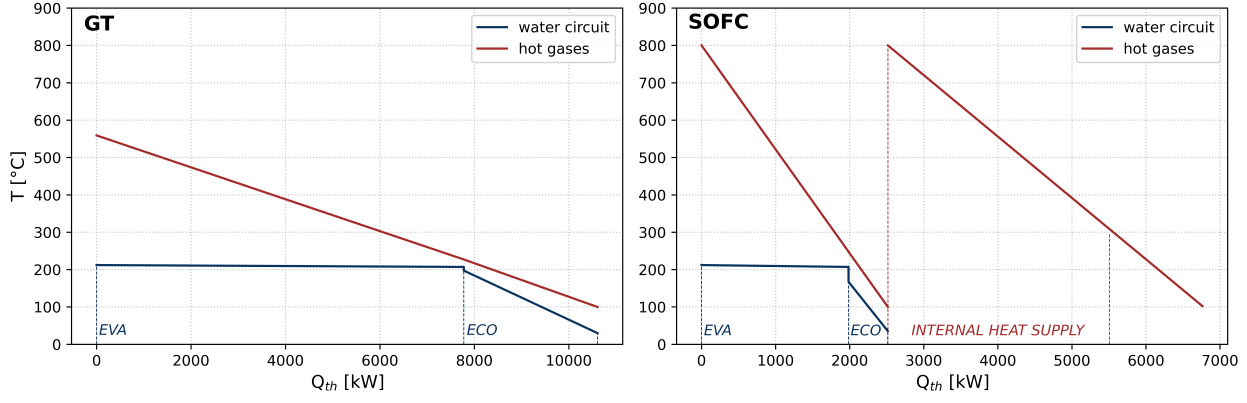


Figure 4.6: HRSG temperature–heat (T–Q) diagram for GT+HRSG and SOFC+HRSG.

rich in H_2O . Figure 4.6 depicts the HRSG temperature–heat (T–Q) diagram for GT+HRSG and SOFC+HRSG.

Figure 4.6 shows that the SOFC exhaust carries substantial latent heat at near-atmospheric pressure that cannot be converted to 20 bar saturated steam while honouring $T_{\text{stack,min}} > 105^\circ\text{C}$ and the ΔT guards (Eqs. 3.87–3.90). Combined with $\dot{m}_{\text{exh}}^{\text{FC}} \ll \dot{m}_{\text{exh}}^{\text{GT}}$ (partly offset by the higher T_{exh}), this limits convertible sensible heat: with the guards above, $\dot{m}_{\text{st}}^{\text{FC}} = 0.98 \text{ kg s}^{-1}$ versus $\dot{m}_{\text{st}}^{\text{GT}} = 3.97 \text{ kg s}^{-1}$. The SOFC steam is $\sim 25\%$ of the GT case at the same header conditions. As a result, the SOFC branch attains an effective thermal utilisation of $\eta^{\text{th,FC}} \approx 25\%$, for $\eta^{\text{tot,FC}} \approx 75.5\%$ (definitions in Eq. 3.85). These values are consistent with literature ranges for SOFC-CHP and, crucially here, rationalise dispatch choices and the SG sizing to cover the remaining steam load.

GT, S1 and S2 configuration comparison. For the reasons explained in the previous paragraph, the auxiliary SG capacities differ across configurations: in the GT baseline the SG is sized at $P_{\text{nom}}^{\text{SG}} = 3.5 \text{ MW}_{\text{th}}$ (header guarantee at peak), in S1 at $12.7 \text{ MW}_{\text{th}}$ (to compensate the limited SOFC-derived steam), and in S2 at $15.2 \text{ MW}_{\text{th}}$ (SOFC often idles during sunny hours due to PV priority on the electric load). Where present, the SMR is sized on the SOFC fuel input to ensure continuity when green H_2 is unavailable: $P_{\text{out}}^{\text{SMR}} = 10.8 \text{ MW}_{\text{th}}$. In S2, the PtH chain adopts the reference pair $(P_{\text{nom}}^{\text{PV}}, P_{\text{nom}}^{\text{EL}}) = (40 \text{ MW}_{\text{el}}, 20 \text{ MW}_{\text{el}})$; the compressor is sized on the EL’s $\dot{m}_{\text{max}}^{\text{H}_2, \text{EL}}$ ($P_{\text{nom}}^{\text{COMP}} = 1.1 \text{ MW}_{\text{el}}$), and CGH_2 storage is set to $m_{\text{nom}}^{\text{HS}} = 3.2 \text{ t}$ at $P^{\text{HS}} = 300 \text{ bar}$, targeting $\sim 8 \text{ h}$ daily cycling rather than seasonal storage.

Annual energetic outcomes. In the GT configuration, the GT+HRSG cogeneration block satisfies 93% of the steam demand and 85% of the electricity. The residual 7% of steam is supplied by the SG and 15% of electricity by the grid. In fuel terms this corresponds to an annual NG consumption of 10915 t in total (about 10452 t in the GT and 463 t in the SG). With the SOFC in S1 (electric-follow), the picture flips: the SOFC covers essentially all electricity (99.9%) but, due to the HRSG convertibility limit discussed in the previous paragraph, delivers only 26% of the steam. Consequently the SG must supply the remaining 74%, raising site fuel consumption. Producing the SOFC fuel via the on-site SMR entails 2561 t H_2 (grey) over the year, which requires 9424 t NG. The SG adds a further 4992 t NG, so total NG rises to 14416 t y^{-1} , i.e. about +32% vs GT. This outcome is structural at $P_{\text{st}} = 20 \text{ bar}$: matching P_{nom} maximises fairness on the electric side, but the lower steam deliverability of SOFC+HRSG compels sustained SG operation.

Introducing the PtH plant (S2 configuration) shifts the balance. PV generation directly serves the electric load first and drives the EL with any surplus, enabling 701 t H_2 (green) over the year. Because winter and night-time PV are limited, the SOFC still relies on the

SMR in continuity mode (853 t H₂ grey), concentrated in low-irradiance periods. Electrically, PV supplies 39% and the SOFC the remaining 61%, leaving a negligible grid share (0.02%). Thermally, the HRSG on the SOFC exhaust contributes 16% of steam and the SG the remaining 84%—higher than in S1 because PV often meets the electric load at mid-day, idling the SOFC and shifting the entire steam duty to the SG. In fuel terms, S2 uses 3137 t NG in the SMR and 5675 t NG in the SG, totalling 8812 t y⁻¹, i.e. only about -20% versus the GT baseline while meeting the same loads. Thus, without optimising the sizes in the S2 configuration, the gain in terms of reduced emissions is limited.

S2 configuration optimisation. A simulation-based optimisation is performed for the S2 layout with the LCOH as objective and NPC and annual NG use as additional indicators. The sizing vector is $s = P_{\text{nom}}^{\text{PV}}, P_{\text{nom}}^{\text{EL}}$. The compressor is still rated on the EL maximum hydrogen flow $\dot{m}_{\text{max}}^{\text{H}_2, \text{EL}}$ and the CGH₂ tank capacity $m_{\text{nom}}^{\text{HS}}$ provides 8 h of continuous EL output (daily storage). Two S2 economic cases are considered for LCOH: *Case A* (no remuneration for PV exports) and *Case B* (PV exports remunerated at $c_t^{\text{el,exp}} = 65 \text{ €/MWh}$ [258]). Points with $P_{\text{nom}}^{\text{PV}} = 0$ correspond to S1 configuration (SOFC relying only on grey H₂), but export remuneration is not applied to S1. Figure 4.7 shows contour maps for capacity factors (CFs), annual H₂ production, and LCOH over the design plane $P_{\text{nom}}^{\text{PV}} \in [0, 200] \text{ MW}_{\text{el}}$ and $P_{\text{nom}}^{\text{EL}} \in [0, 175] \text{ MW}_{\text{el}}$. In Figure 4.7a, the SOFC CF decreases as $P_{\text{nom}}^{\text{PV}}$ increases (PV priority on the electric load); the SOFC CF reduces from 92% (S1) to about 50% at high PV, with the covered electric load falling from 99% to 55% and the HRSG-derived steam share from 26% to 14%. The EL CF remains bounded below 30% because the EL operates only on PV surplus. In Figure 4.7b, green H₂ for SOFC feedstock rises from 0 t (S1) up to 1400 t by increasing PV and EL, while grey H₂ falls from 2561 t to 5 t. The non-zero grey requirement at large sizes is a direct consequence of adopting daily—not seasonal—storage. Figure 4.7c shows cost maps: grey LCOH increases when PV/EL displace SMR throughput (lower cost recovery), whereas green LCOH attains a minimum in a band $P_{\text{nom}}^{\text{PV}} = 38\text{--}60 \text{ MW}_{\text{el}}$, $P_{\text{nom}}^{\text{EL}} = 18\text{--}30 \text{ MW}_{\text{el}}$. Beyond this band, the incremental capex of PV/EL exceeds the benefit from higher EL utilisation.

For each value of the annual grey-H₂ share used by the SOFC, the configuration achieving the minimum green LCOH is selected and plotted. Figure 4.8a reports the NPC breakdown by asset (stacked bars, left axis) and the NG use relative to the GT baseline (points, right axis). At 100% grey (S1 configuration), NPC is lowest and dominated by the SMR, but the total NG use is 14416 t y⁻¹, which is 32% higher than in the GT configuration. As the grey share decreases, the cost centre shifts from SMR/SG to PV and EL; the “Grid export” bar grows because larger PV plants export surplus electricity. Near-zero grey share requires significant storage investment (e.g., 28 t CGH₂, about 7% of NPC), in line with [261]. Complete decarbonisation is precluded by the 20 bar steam requirement: even with negligible grey H₂, NG can only be reduced by about 50% because the SG remains essential.

Figure 4.8b shows the green and grey LCOH for *Case A* and *Case B*. For 0% grey, the green LCOH is 14.2 €/kg in Case A and 8.5 €/kg in Case B. The minimum green LCOH is reached at about 40% grey share, equal to 5.81 €/kg (Case A) and 5.26 €/kg (Case B). These values fall within the upper portion of the ranges reported for PV-based PtH systems [262, 263].

The minimum-LCOH configuration occurs at a grey share of 40% with

$$P_{\text{nom}}^{\text{PV}} = 50.6 \text{ MW}_{\text{el}}, \quad P_{\text{nom}}^{\text{EL}} = 25.2 \text{ MW}_{\text{el}}, \quad P_{\text{nom}}^{\text{comp}} = 1.4 \text{ MW}_{\text{el}}, \quad m_{\text{nom}}^{\text{HS}} = 3.9 \text{ t}.$$

A 25% reduction in NG relative to GT is obtained, and the green LCOH equals 5.81 €/kg in Case A (5.26 €/kg in Case B). The PV/EL capacity ratio equals 2, consistent with [264,

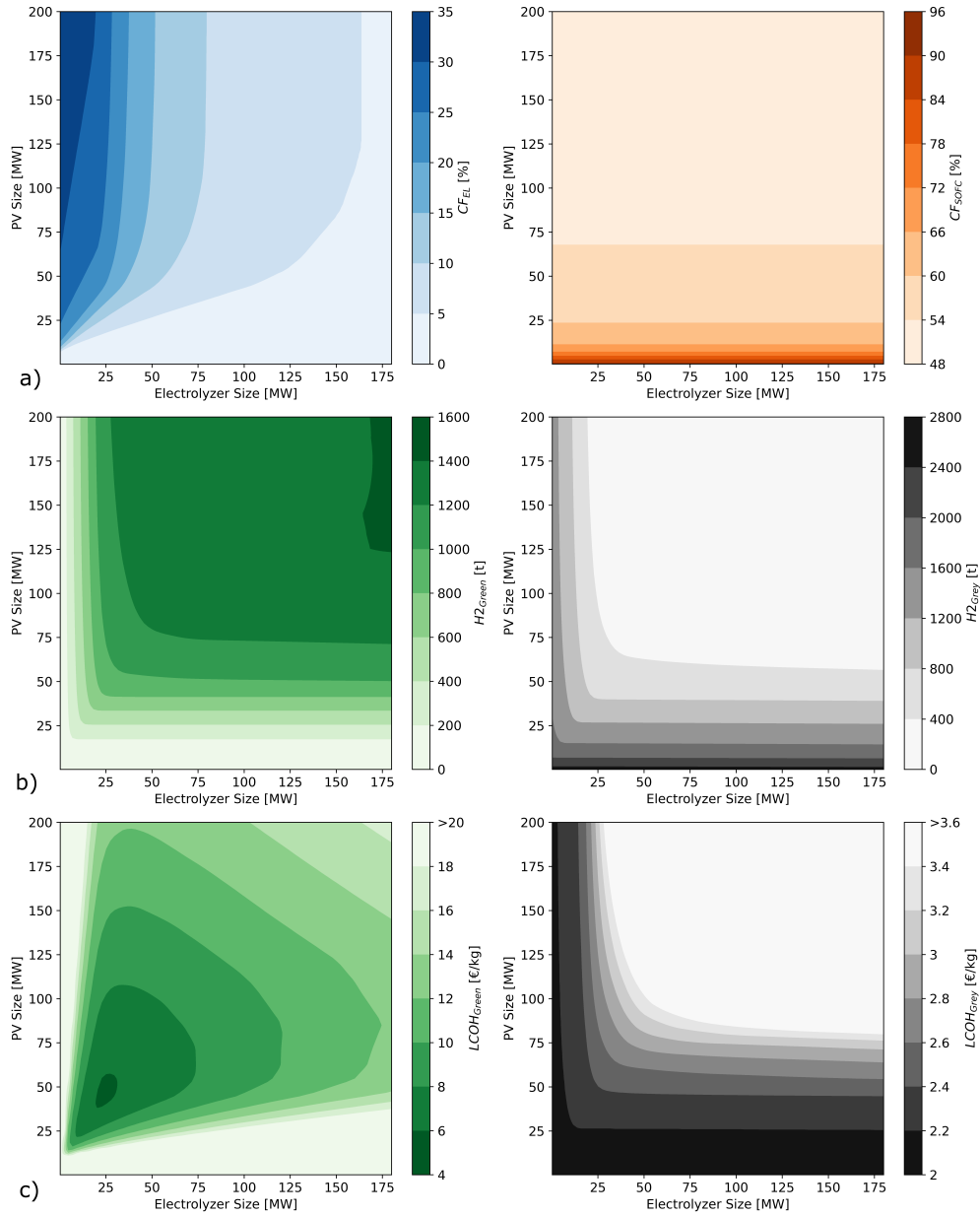


Figure 4.7: S2 configuration. a) EL and SOFC capacity factor, b) total green and grey- H_2 produced, c) green and grey LCOH varying PV and EL capacity. The line with $P_{nom}^{PV} = 0$ reduces to S1.

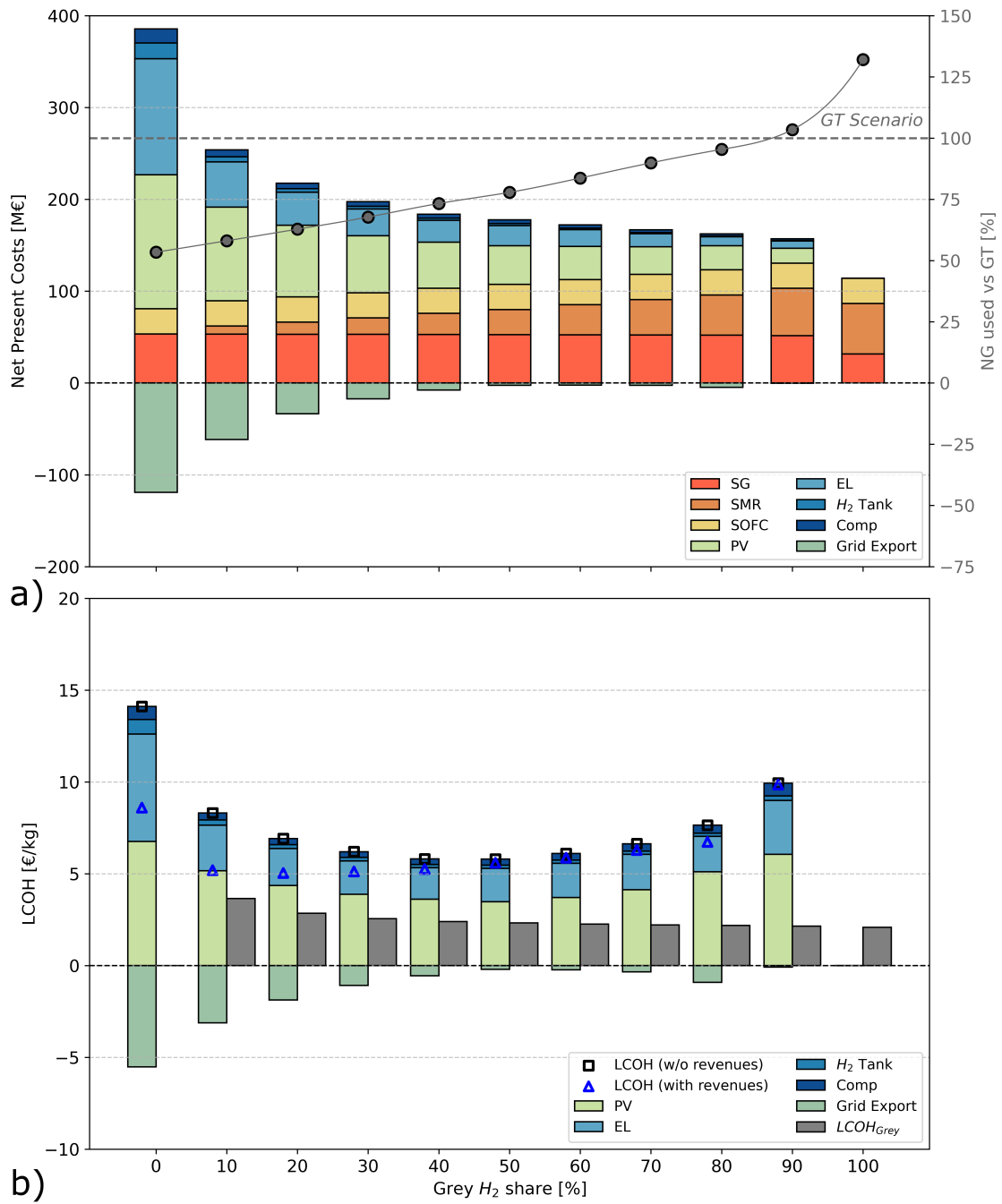


Figure 4.8: a) NPC and NG consumption breakdown, and b) grey LCOH and the green LCOH trend for different values of grey hydrogen share. Two main scenarios are analyzed: 1) no remuneration for the excess PV electricity (black-edge squares), and 2) the electricity sale price is set equal to 65 €/MWh (blue-edge triangles)

265]. On an annual basis, PV production is allocated as follows: 17.65 GWh (24%) to the site electric load, 46.21 GWh (63%) to the EL, 1.82 GWh (2.5%) to the compressor, and 7.64 GWh (10%) exported. The SOFC supplies about 60% of the site electricity using 59% green and 41% grey H_2 , whereas the SOFC+HRSG provides 15% of the steam; the remainder is supplied by the SG, which limits the achievable CO_2 reduction to about 25% with the given header pressure.

Figure 4.9a reports the LCOH percentage contributions at the optimum: PV exceeds 50% of total, namely 3.62 €/kg. Accounting for the 24% share of PV used directly by the site reduces the PV-attributed LCOH to 2.75 €/kg and the adjusted total to 4.95 €/kg (4.4 €/kg in Case B). Figure 4.9b shows the NPC percentage contributions: SG 28.7%, PV 27.3%, SOFC 14.9%, EL 12.9%, SMR 12.5%, compressor 2.3%, CGH_2 tank 1.3%. Including PV export remuneration lowers the total NPC by about 4% (from 183.8 M€ to 176.2 M€).

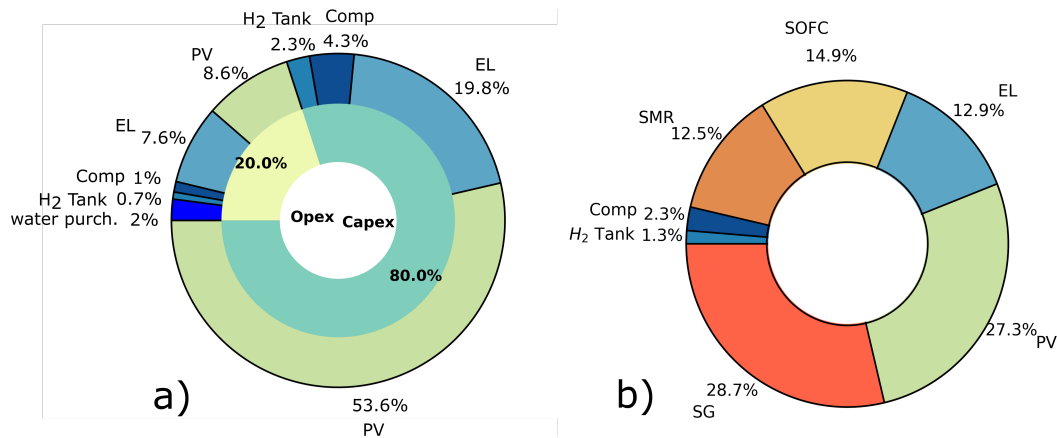


Figure 4.9: LCOH (a) and NPC (b) percentage contributions in the optimal S2 configuration.

4.1.6 Main findings and methodological reflections

Main findings. Within the rule-based MESS framework of Section 3.1, the case confirms that SOFC-CHP can be integrated effectively in an industrial multi-energy setting, but its coupling to a single-pressure HRSG at $P_{st} = 20$ bar structurally limits steam deliverability compared with a like-for-like GT. Under the common guards, the GT exhaust maps to $\dot{m}^{st} = 3.97 \text{ kg s}^{-1}$ while the SOFC exhaust maps to 0.98 kg s^{-1} (Figure 4.6); hence the SOFC branch retains its electrical advantage but yields modest thermal recovery. Annual balances reflect this: the GT covers 85% of electricity and 93% of steam with 10 915 t NG; S1 (SOFC on grey H_2) covers 99.9% of electricity but only 26% of steam, requiring 2 561 t H_2 from SMR and 14 416 t NG; S2 (PV+PtH+SOFC) shifts a large share of electricity to PV (about 39%) and reduces NG to 8 812 t, but the SG remains the thermal closer when PV idles the SOFC at mid-day (Figs. 4.7–4.8). The S2 optimisation identifies a clear LCOH minimum at $P_{nom}^{PV} = 50.6 \text{ MW}_{el}$, $P_{nom}^{EL} = 25.2 \text{ MW}_{el}$, $P_{nom}^{comp} = 1.4 \text{ MW}_{el}$, $m_{nom}^{HS} = 3.9 \text{ t}$, with green LCOH = 5.81 €/kg (dropping to 5.26 €/kg with export remuneration) and a 25% reduction in NG versus GT (Figs. 4.7, 4.9). Full site decarbonisation is not achieved because the SG structurally supplies most steam.

From an industrial perspective, these results suggest that SOFC-CHP at equal P_{nom} is best aligned with sites whose electric demand dominates the thermal duty, or with steam conditions and heat-recovery schemes less restrictive than a single-pressure HRSG at 20 bar. In paper mills with steam-heavy profiles, SOFCs still play a valuable role as high-efficiency

electric anchors within PV–PtH systems, but achieving deep decarbonisation of the steam duty requires decarbonising even the SG fuel.

Methodological reflections. Methodologically, the rule-based approach used throughout the thesis behaves as intended: it encodes physical guards and operational priorities transparently, reproduces plant-like behaviour without perfect-foresight dispatch, and scales to parametric mapping with modest computational burden. At the same time, it does not guarantee global optimality and its outcomes depend on the rule stack (e.g., PV priority idling the SOFC at mid-day). This coherence between method and outcomes reinforces the thesis claim that rule-based simulation is a practical decision aid for early-stage sizing and benchmarking of multi-energy industrial systems.

4.2 Rule-based: Case 2 — Optimal grid-connected PV-based PtH plant

4.2.1 Motivation, scope and contributions

Building on the previously analysed case, this section extends the analysis from a single industrial site (the paper mill in Tuscany) to a nation-wide perspective. In the previous case, component sizes were explored via multiple rule-based simulations without an explicit optimiser, and the plant served combined electrical and thermal demands via CHP logic. Here, the focus shifts to a grid-connected PV-based PtH plant dedicated to a constant industrial H_2 demand; component sizes are optimised with a Genetic Algorithm (GA) embedded in MESS to minimise the LCOH. While green H_2 costs remain higher than fossil-derived alternatives, the study quantifies how location (Italian bidding zones), hourly resource availability and price signals, and rule-based operating constraints shape cost-optimal designs under grid-connected operation. Dispatch is done using MESS (Section 3.1).

Contributions. Building on the components and methods of Section 3.1.1 and [249], this study: (i) integrates ageing of PV, EL and BESS (with replacements where due) directly into the techno-economic model so that LCOH reflects lifetime performance drift rather than nominal points; (ii) clarifies the role of short-term H_2 storage versus a battery, showing that daily H_2 storage is typically the primary flexibility lever, with batteries only attractive under specific market/regulatory conditions; (iii) delivers GA-based, zone-specific sizing that links hourly PV producibility and zonal prices to LCOH and grid exchanges under the adopted rule-based dispatch.

4.2.2 Configurations

All technologies involved in the PtH plant adopt the physics-faithful rule-based blocks in Section 3.1.1: PV (Section 3.1.1), AEL (Section 3.1.1), COMP (Section 3.1.1), CGH_2 storage (Section 3.1.1), and (optionally) BESS (Section 3.1.1). A constant industrial hydrogen demand $\dot{m}_t^{\text{H}_2, \text{dem}} = 500 \text{ kg h}^{-1}$ typical of HTA sectors is imposed at the simulator timestep (hourly). At nominal conditions this requires a continuous electrical input of about $27.1 \text{ MW}_{\text{el}}$ to the AEL; due to PV intermittency, the installed AEL capacity is oversized relative to this nominal requirement so that short-term H_2 buffers can be built and later dispatched. Two grid-connected alternatives are assessed:

1. *S1 (baseline PtH).* Figure 4.10a. PV drives the AEL; produced H_2 is compressed and stored in CGH_2 vessels; the grid is used for residual import/export.

2. $S2$ ($PtH + BESS$). Figure 4.10b. Same as $S1$ with the addition of a grid-coupled Li-ion BESS integrated on the AC bus for hour-scale reshaping of PV usage.

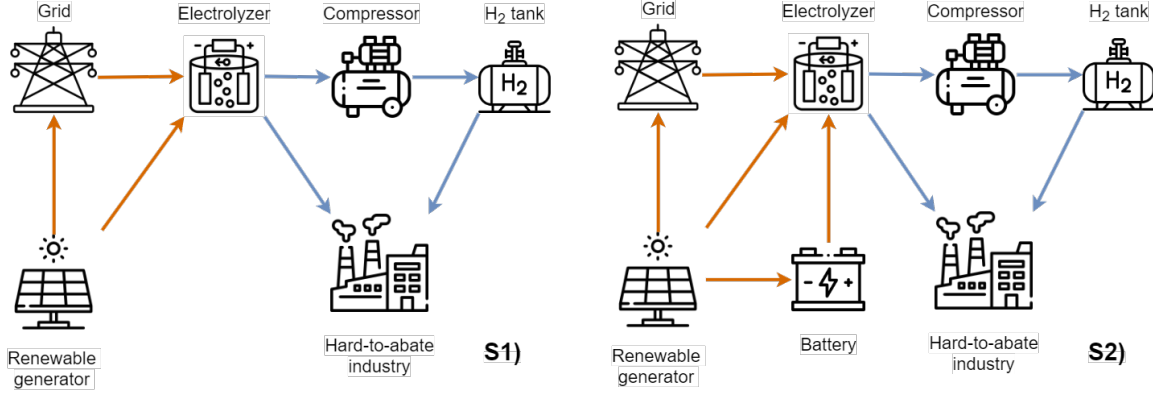


Figure 4.10: PtH plant configurations: a) S1; b) S2.

PV production p_t^{PV} is obtained from PVGIS TMY series and scaled via Eq. 3.2; geometry is single horizontal-axis tracking (N–S), with a site-dependent tilt and azimuth fixed due south. Annual module ageing of 1% and system losses of 9% are applied to find $\bar{p}_t^{PV, 1kW}$, consistently with Section 3.1.1. The AEL block is instantiated as a bank of identical 500 kW commercial modules operated in parallel with sequential commitment; a per-module minimum input power guard of 10% is enforced. Using the numerical values summarised in Table 3.3 the nominal specific electricity consumption is $SEC^{EL} = 54.1 \text{ kWh kg}^{-1}$ (about 61% on an LHV basis). Ageing follows Eq. 3.31; modules start at $V_{op} = 100 \text{ V}$ and are replaced upon reaching $V_{op} = 115 \text{ V}$. Hydrogen compression power is computed from the pressure-span-dependent specific consumption in Eq. 3.41; this corresponds to a specific electricity consumption of 2.21 kWh kg^{-1} for the chosen pressure span. CGH_2 storage provides daily balancing, with the inventory state LOH_t advanced by Eq. 3.42. The operating pressure band is set at 300 bar. In S2 only, a Li-ion BESS is included. Its SOC_t evolves according to Eq. 3.53 under the bounds in Eq. 3.54; numerical BESS parameters are reported in Table 3.4. SOH updates follow Eq. 3.60 on a weekly grid.

4.2.3 Rule-based workflow

At each hour, MESS applies the same policy structure as in Case 1 (Section 4.1), adapted to a pure H_2 service: (i) acquire p_t^{PV} (after PVGIS losses and ageing) and set a provisional EL request; (ii) determine the admissible EL window from the multi-module guards—if the available power permits at least 10% of nominal power per active module, share uniformly; otherwise reduce the active count so that each module meets the guard—then map p_t^{EL} to $\dot{m}_t^{H_2, EL}$ via Eq. 3.36 and advance ageing via Eq. 3.31; (iii) route $\dot{m}_t^{H_2, EL}$ through COMP and update LOH_t using Eq. 3.42, enforcing storage bounds; (iv) meet $\dot{m}_t^{H_2, dem} = 500 \text{ kg h}^{-1}$ from instantaneous EL output and, when insufficient, discharge CGH_2 ; any residual electric surplus/deficit is settled with the grid; (v) BESS intervention (S2 only): if p_t^{PV} exceeds the instantaneous EL+COMP electric demand, charge the BESS; on deficit, discharge the BESS to sustain EL above module thresholds before drawing H_2 from tanks or importing from the grid—BESS discharge is not used to overproduce H_2 for storage; SOC_t /SOH evolve via Eqs. 3.53 and 3.60; (vi) update LOH_t , SOC_t and component internal states, and apply replacement when EL modules reach $V_{op} = 115 \text{ V}$ (EoL).

Figure 4.11 illustrates the hourly balances for a representative week using the following illustrative sizes: $P_{\text{nom}}^{\text{PV}} = 100$ MW, $P_{\text{nom}}^{\text{EL}} = 50$ MW, a daily CGH_2 buffer of 8 t, and (for S2) a 90 MWh BESS. The stacked bars report electric powers (PV, BESS charge/discharge, grid exchange; EL and COMP on the demand side), while the blue dashed line tracks LOH_t . The black line marks the total electric load (EL+COMP). In low-PV periods (e.g., March) the CGH_2 storage tends to deplete overnight; in high-PV periods (e.g., July) PV covers most of the duty; with S2, the BESS shifts part of the midday surplus to evening hours, reducing grid reliance and moderating CGH_2 storage swings.

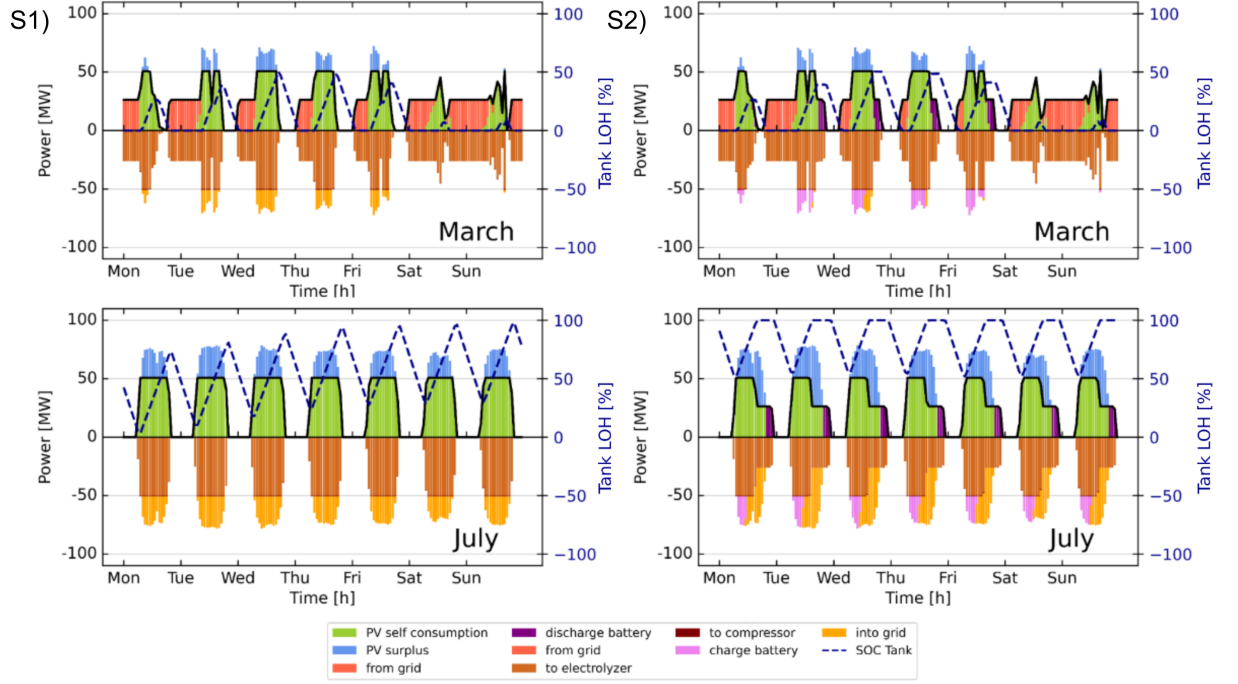


Figure 4.11: Hourly power balances and CGH_2 storage LOH_t over one week in two different months: March and July. S1 vs. S2.

4.2.4 Sizing approach

Following Section 3.1.3, sizing is cast as a simulation–optimisation loop driven by a GA. The decision vector is restricted to the present PtH scope, $s = [P_{\text{nom}}^{\text{PV}}, P_{\text{nom}}^{\text{EL}}, E_{\text{nom}}^{\text{BESS}}, m_{\text{nom}}^{\text{HS}}]$. For any s , MESS evaluates multi-year techno–economics under the fixed rule-based dispatch explained before, including ageing and replacements, and returns KPIs and LCOH from Eq. 3.110. The optimisation objective is to minimise $\text{LCOH}(s)$ (Eq. 3.123) subject to the annual-adequacy constraints in Eq. 3.124, with feasibility enforced by the penalty fitness in Eq. 3.125. Box bounds are applied component-wise; in particular, (i) the lower bounds are 0 for $P_{\text{nom}}^{\text{PV}}$, $E_{\text{nom}}^{\text{BESS}}$ and $m_{\text{nom}}^{\text{HS}}$, and 27.1 MW for $P_{\text{nom}}^{\text{EL}}$ so that the constant $\dot{m}_t^{\text{H}_2, \text{dem}} = 500 \text{ kg h}^{-1}$ can be met in continuous nominal operation; (ii) the upper bounds are set sufficiently loose not to bind the optimum. GA settings follow the values in Section 3.1.3: population 40, $\text{Pr}_{\text{cx}} = 0.7$, $\text{Pr}_{\text{mut}} = 0.3$, SBX index 10, polynomial-mutation index 15, and steady-state replacement with 2-elite carryover; offspring are repaired to bounds and discrete items rounded to module multiples. The evaluation horizon is $N = 25$ years so that ageing and replacements are reflected in LCOH; the stopping rule halts when the best-fitness improvement between generations drops below 10^{-4} . This setup preserves the decoupling between fixed rule-based operations

and design search while ensuring physics, ageing and economics remain consistent with the rest of the framework.

4.2.5 Technical and economic inputs

The economic metrics used in this study are LCOH and NPV. Consistently with Section 3.1.2, the cost boundary includes the upfront investment C_0 , discounted replacements and operating costs. Although Section 3.1.2 defines LCOH without crediting revenues, here we intentionally include the hydrogen-certification incentive as a negative cost in the numerator so that LCOH reflects the policy's effect on the final cost of hydrogen. PV CAPEX is excluded because PV energy is procured via a pay-as-produced PPA; all PV energy costs therefore enter OPEX.

The incentive-inclusive definition is adopted as in Eq. 4.4:

$$\text{LCOH} = \frac{C_0 + \sum_{y=1}^N \frac{\text{CAPEX}_y^{\text{repr}} + \text{OPEX}_y}{(1 + \text{DR})^y} - \sum_{y=1}^N \frac{\text{REV}_y^{\text{cert}}}{(1 + \text{DR})^y}}{\sum_{y=1}^N \frac{m_y^{\text{H}_2}}{(1 + \text{DR})^y}} \quad [\text{€}/\text{kg}], \quad 4.4$$

with $\text{REV}_y^{\text{cert}}$ defined in Eq. 3.97 and certification decided per Section 3.1.2, using the $3.38 \text{ kg}_{\text{CO}_2\text{eq}}/\text{kg}_{\text{H}_2}$ limit in Eq. 3.115. Even when annual output is the main KPI, computing $CI_y^{\text{H}_2}$ in Eq. 3.114 requires an hourly grid-intensity series CI_t^{grid} , which materially affects whether hydrogen qualifies for certification [231].

Yearly operating costs OPEX_y follow Eqs. 3.99–3.102: PV purchases via PPA, grid purchases via corrected PUN, water purchases, fixed O&M by asset, personnel, and land rent; replacements are handled outside OPEX as $\text{CAPEX}_y^{\text{repr}}$. NPV is evaluated with Eq. 3.107 using the operating cash flows CF_y from Section 3.1.2. Here remuneration for electricity exports is included and valued at the zonal price (ZP) $c_t^{\text{el,exp}}$, which changes for each Italian bidding zone, i.e., North (NO), Central-North (CNO), Central-South (CSO), South (SO), Sicily (SIC), and Sardinia (SAR). All asset-specific economic inputs are reported in Table 4.4 while price and financial inputs are reported in Table 4.5.

Table 4.4: Asset-specific economic inputs.

Asset a	$\text{CAPEX}_a^{\text{unit}}$	$\text{frac}_a^{\text{O\&M}}$	LT_a	$\text{frac}_a^{\text{repr}}$	Ref.
Electrolyser (AEL)	1094 [€/kW]	0.04	ageing-driven	0.80	[266]
BESS (Li-ion)	250 [€/kWh]	0.04	ageing-driven	0.80	[215]
CGH ₂ storage	450 [€/kg]	0.01	30 y	0.80	[253]
Compressor	see Eq. 4.3	0.02	20 y	0.80	

Engineering and installation adders follow Eq. 3.106 with $\text{frac}^{\text{eng}}=15\%$ and $\text{frac}^{\text{inst}}=18\%$. Civil works are added and charged as 370 €/m^2 over a specific footprint of $500 \text{ m}^2/\text{MW}$ for EL, BESS and CGH₂ storage (compressor area neglected). Personnel costs are 200 k€/y , and land rent is $2 \text{ €/m}^2 \text{ y}$. All as in [267].

Notes. (i) PV investment costs are excluded from C_0 ; all PV electricity is purchased under the PPA and valued in OPEX. (ii) For LCOH, export remuneration is not credited; only certification revenues $\text{REV}_y^{\text{cert}}$ reduce the numerator per Eq. 4.4. The term c^{cert} represents

Table 4.5: Price and financial inputs; export remuneration follows the bidding-zone price.

Item	Symbol	Value	Ref.
PV PPA (pay-as-produced)	c^{PPA}	80 €/MWh	[268–270]
Import electricity price	$c_t^{\text{el,imp}}$	hourly series (2023)	[271–273]
Export electricity price	$c_t^{\text{el,exp}}$	hourly ZP series (2023)	[271]
Demineralised water price	$c^{\text{H}_2\text{O}}$	2.5 €/m ³	[259]
H ₂ -certification incentive	c^{cert}	2.25 €/kg (10 years)	[274]
RFNBO GHG-savings requirement (equiv. CI limit)	$CI_{\text{max}}^{\text{RFNBO}}$	3.38 kg _{CO2eq} /kg _{H₂}	[11]
Grid emission factor	CI_t^{grid}	hourly series (2023)	[231]
Discount rate	DR	7.4%	
Project lifetime	N	25 years	

an output-based premium paid per kilogram of *certified* RFNBO hydrogen during an initial support window (here 10 years), consistent with the “fixed premium” logic adopted in the EU Hydrogen Bank / Innovation Fund pilot auction design [274]. Given that the auction framework discloses an explicit ceiling price (maximum bid) of 4.5 €/kg_{H₂} for the fixed premium [275], we treat c^{cert} as an uncertain policy driver and explicitly include it in the sensitivity analysis (from 0 to 4.5 €/kg) to quantify how results and optimal designs change under weaker/stronger support. (iii) AEL and BESS replacements are triggered by the ageing models of Secs. 3.1.1 and 3.1.1; CGH₂ storage and compressor replacements follow Table 4.4. (iv) The corrected PUN series $c_t^{\text{el,imp}}$ is obtained by applying a constant markup mk so that its annual average equals the industrial gross average of 193 €/MWh [273]:

$$c_t^{\text{el,imp}} = \text{PUN}_t(1+mk), \quad \text{s.t. the yearly mean of } c_t^{\text{el,imp}} \text{ is } 193 \text{ €/MWh,}$$

(v) Even with annual correlation for incentives (Section 3.1.2), an hourly database for CI_t^{grid} is essential to evaluate $CI_y^{\text{H}_2}$ in Eq. 3.114 and to determine which hours qualify for certification.

Linking bidding zones to geographical inputs. For the bidding-zone comparison (NO, CNO, CSO, SO, SIC, SAR), the electricity-price series $c_t^{\text{el,imp}}$ and $c_t^{\text{el,exp}}$ are taken from the corresponding *zonal* hourly series (GME, year 2023), and the grid emission factor CI_t^{grid} is taken from the corresponding *zonal/regional* hourly series (year 2023). PV producibility, instead, is inherently site-dependent; therefore, for each bidding zone we retrieve the PVGIS TMY at a representative location within that zone (Table 4.6). The same PVGIS assumptions (tracking, losses, ageing) described above are used for all zones, so differences across zones reflect location-specific irradiance and weather.

4.2.6 Results and discussion

A representative hard-to-abate site in Puglia, in the South (SO) Italian bidding zone, with a constant demand $\dot{m}_t^{\text{H}_2,\text{dem}}=500 \text{ kg h}^{-1}$ is analysed over $N=25$ years at hourly resolution. Puglia is selected as a representative Southern Italian location because it combines (i) high solar resource (favourable PV yield for PtH designs) and (ii) a relevant presence of hard-to-abate industrial demand in the South bidding zone, making it a meaningful stress-test for certification and cost sensitivity under Southern price/emission profiles. Hourly price and grid-intensity series correspond to the South zone; incentives adopt the annual correlation used in Section 3.1.2. The GA minimises LCOH (Eq. 4.4) under the rule-based dispatch previously discussed.

Table 4.6: Representative locations used to retrieve PVGIS producibility for the Italian bidding-zone analysis (PV), and linkage of zonal inputs (prices and grid EF) to the same bidding-zone definition.

Bidding zone	Representative PVGIS location	Lat [°]	Lon [°]
NO (North)	Milan	45.46	9.19
CNO (Central-North)	Florence	43.77	11.25
CSO (Central-South)	Rome	41.90	12.50
SO (South)	Bari	41.12	16.87
SIC (Sicily)	Palermo	38.12	13.36
SAR (Sardinia)	Cagliari	39.22	9.12

Sizing outcomes (S1 vs. S2). For the baseline PtH configuration (S1), the GA returns a PV-to-AEL ratio of about 1.9:1 (PV =112 MW, AEL=58.5 MW) and a daily CGH₂ buffer of 7.6 t (roughly 12 h at the nominal surplus AEL rate). This falls within ranges reported for PV-driven, grid-connected PtH plants, where the economically favourable PV:AEL ratio increases with electricity price [276]. Hub-level studies likewise indicate that storage needs are predominantly intra-day to stabilise a constant 500 kg h⁻¹ delivery; seasonal tanks would dominate costs without improving adequacy in the present rule-based setting [277, 278]. In S2 configuration the GA returns $E_{\text{nom}}^{\text{BESS}}=0$ with the adopted costs, because BESS CAPEX and fixed O&M outweigh the value of short-term reshaping when the objective is LCOH minimisation without an explicit constraint on maximum $CI_y^{\text{H}_2}$. To compare emissions and incentives, a 100 MWh BESS layered onto the S1 optimum (same PV/AEL/CGH₂) is therefore tested.

Multi-year operation with ageing. Figure 4.12 compacts the 25-year trajectories. PV production declines linearly at 1%/y; the AEL nominal specific consumption worsens from 54.1 kWh kg⁻¹ to 61 kWh kg⁻¹ by the EoL, with replacements triggered at $V_{\text{op}}=115$ V. In S1, EoL occurs after 132 500 h (15.2 yr); in S2 after 129 000 h (14.8 yr), because the BESS shifts demand and keeps the AEL operating more hours each year. The CGH₂ inventory LOH_t exhibits the intended diurnal cycling; the annual peak LOH drifts downward with ageing (lower PV yield, lower AEL efficiency), then partially rebounds after AEL stack replacement but never returns to year-1 levels because PV modules are not replaced.

In S2, the BESS undergoes calendar and cyclic ageing but remains above the EoL threshold (70% of nominal) over the horizon; limited PV surplus restricts full-cycle equivalents to 3650 over 25 years. Detailed ageing curves are reported in Figure 4.13 which shows AEL efficiency and polarisation curves at selected years together with BESS SOC/SOH for S2. As the stack voltage increases, module efficiency declines; the module hits the 115 V threshold in the fifteenth year and is replaced. For the BESS, SOH remains above the 70% EoL threshold over 25 years. Despite a relatively low utilisation, cyclic ageing dominates SOH loss, while calendar ageing is minor given the observed operating profile.

Energy balances, certification and incentives. Although annual hydrogen output is fixed by design, energy splits evolve with ageing. In S1 year 1, PV covers 77% of electrolysis and compression energy and the grid 23%, giving $CI_y^{\text{H}_2} = 3.59 \text{ kg}_{\text{CO}_2\text{eq}} \text{ kg}_{\text{H}_2}^{-1}$. By year 14 the PV share falls (lower PV yield, lower AEL efficiency), grid share rises, and $CI_y^{\text{H}_2}$ climbs to $5.54 \text{ kg}_{\text{CO}_2\text{eq}} \text{ kg}_{\text{H}_2}^{-1}$, which tightens eligibility. Importantly, certification is not decided on the year-average intensity of the entire output, but on a certified subset selected in post-processing via Eq. 3.121: the algorithm allocates α_t to the lowest-emissions hours first, subject to eligible

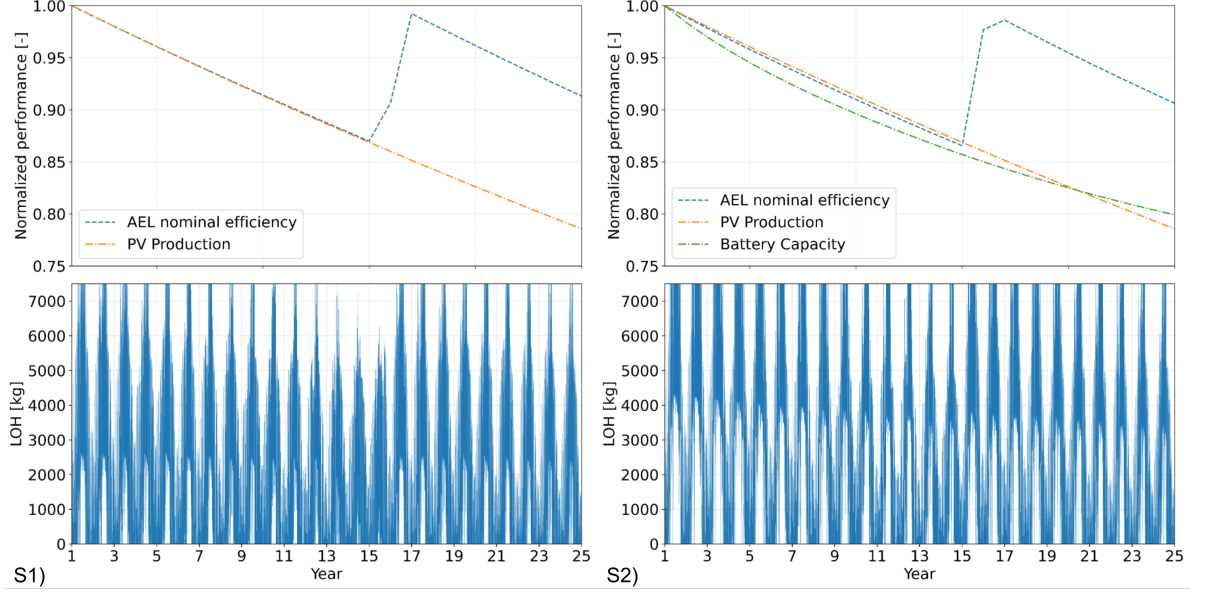


Figure 4.12: Normalised performance and LOH_t over 25 years for S1 (left) and S2 (right).

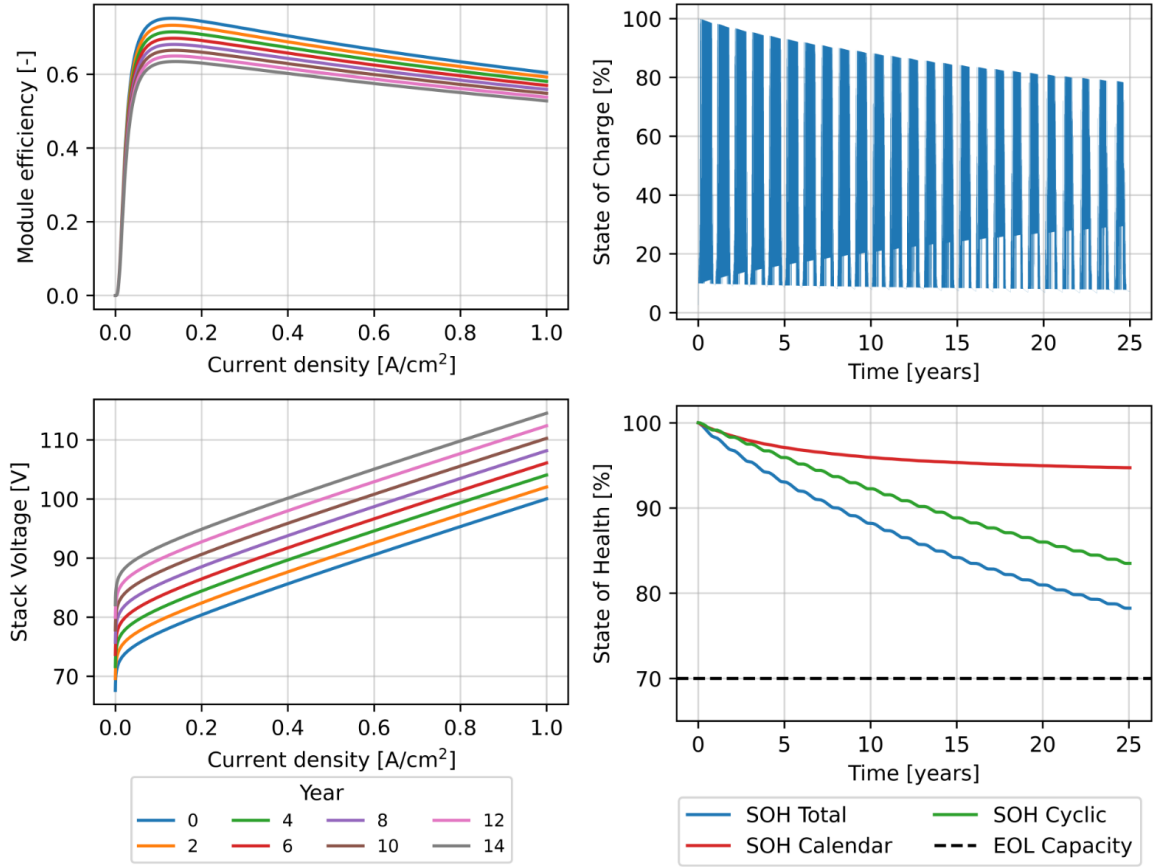


Figure 4.13: Aging effects in S2 configuration. a) AEL efficiency curve and AEL polarization curve. b) BESS SOC and BESS SOH.

energy and the RFNBO GHG-savings bound. Hence a nonzero $m_y^{\text{H}_2, \text{cert}}$ (and incentive credit) can arise even when $CI_y^{\text{H}_2} > CI_{\text{max}}^{\text{RFNBO}}$. In S2, shifting PV energy to evening hours with the BESS lowers the early-year intensity (e.g., $3.01 \text{ kg}_{\text{CO}_2\text{eq}} \text{ kg}_{\text{H}_2}^{-1}$ in year 1) and increases the certified fraction under the same annual rule; the advantage erodes with AEL and BESS ageing (e.g., $4.85 \text{ kg}_{\text{CO}_2\text{eq}} \text{ kg}_{\text{H}_2}^{-1}$ by year 14).

Economic outcomes and cost composition. Figure 4.14 decomposes LCOH and shows how ageing shifts contributions. In both S1 and S2, OPEX dominates (80% of total), with PV electricity (pay-as-produced PPA) and grid electricity the two largest items. For S1, an illustrative breakdown attributes roughly 41% of LCOH to PV electricity and 33% to grid purchases; AEL CAPEX contributes about 17%, fixed O&M 6%, and civil works+engineering+installation around 7.5%. Adding a 100 MWh BESS (S2) decreases the grid-electricity slice but raises total LCOH by 5%. Certification revenues reduce LCOH by 10% when the intensity threshold is met. Ageing magnifies grid-electricity exposure more than it reduces certified mass: in S1 the ageing uplift attributable to higher grid use is 0.50 €/kg , while the loss of incentives adds 0.03 €/kg ; S2 shows similar but smaller effects (0.40 €/kg and 0.04 €/kg). Accurate ageing modelling is therefore necessary to avoid underestimating LCOH by several percent over long horizons.

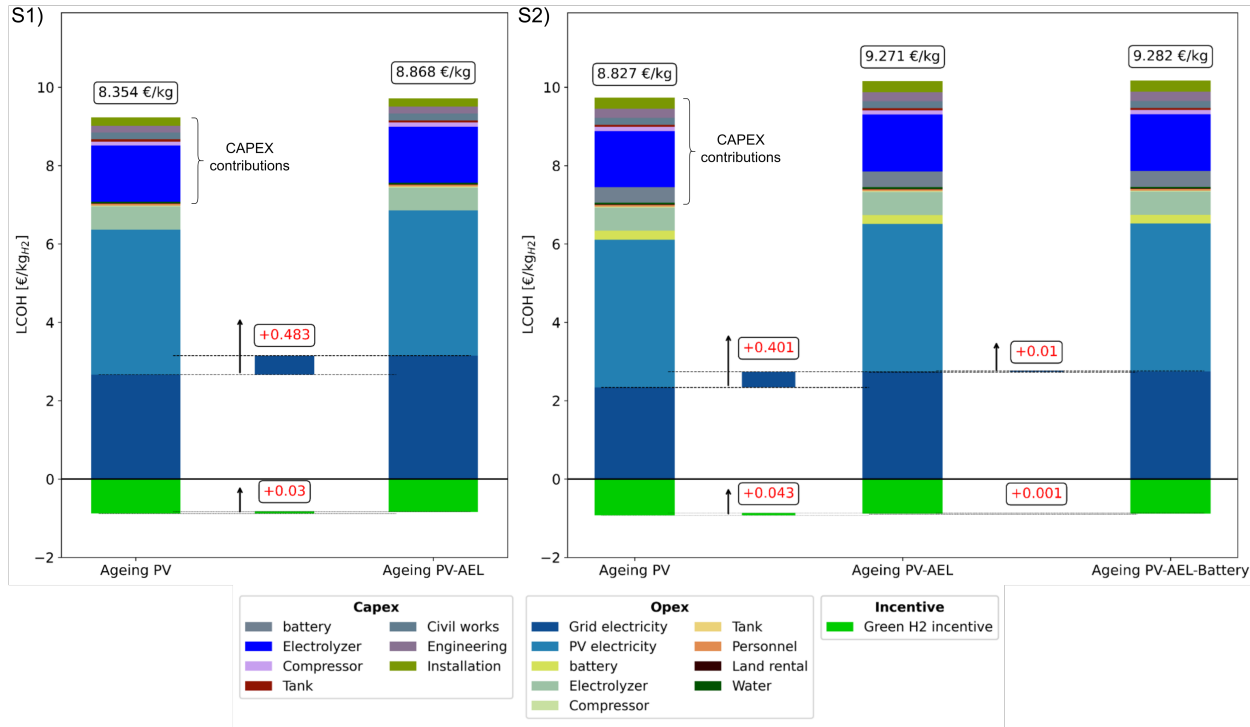


Figure 4.14: Decomposition of LCOH and ageing effects: S1 (left) and S2 (right). Stacks group CAPEX items (top), OPEX items (centre) and incentive credit (green, bottom). Callouts show incremental ΔLCOH due to ageing of the indicated components.

Optimal sizing across Italian bidding zones. A systematic application of the workflow is carried out across all Italian bidding zones — North (NO), Central–North (CNO), Central–South (CSO), South (SO), Sicily (SIC), and Sardinia (SAR) — using 2023 hourly series for zonal prices, grid emission factors and PV producibility. Figure 4.15 summarises, for each zone, the operating-hour averages of the grid emission factor and the zonal price (i.e., averages computed over the hours when the plant is actually drawing from or injecting to the grid), with the percentage deviation from the annual mean shown in parentheses.

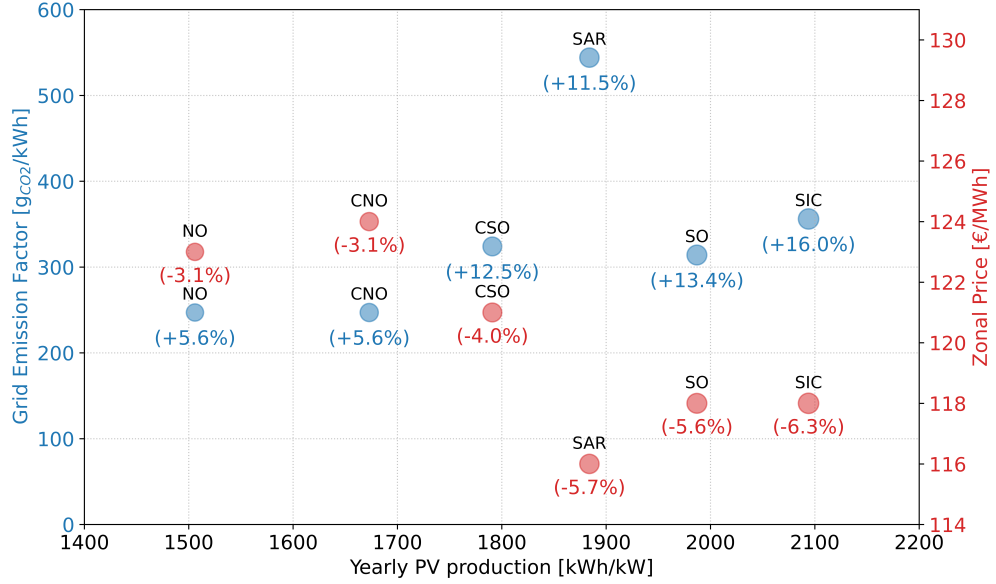


Figure 4.15: Average grid emission factor (EF) and zonal price (ZP) during plant operating hours across Italian bidding zones; percentage deviation from the respective annual averages is shown in parentheses.

Three robust signatures emerge from Figure 4.15. Firstly, (i) a timing penalty arises: exports occur predominantly at midday, when ZP sits below its annual mean due to PV abundance, whereas imports concentrate in off-sun hours, when EF lies above its annual mean. This worsens both the revenue side (low selling price) and the environmental side (high importing EF). The penalty is strongest in southern zones where the PV share is higher. Second (ii), a north–south asymmetry persists: northern zones combine lower EF and relatively lower ZP despite poorer PV yield, reflecting a more diversified mix (notably hydro), while SAR exhibits the highest EF due to carbon-intensive generation. Third, (iii) the operating-hour EF and ZP are jointly unfavourable across all zones compared to annual means, which reinforces the need to model hourly coupling rather than adopt annual averages.

Optimal S1 configurations by zone. Table 4.7 reports the GA outputs for S1 in each bidding zone (component sizes and first-year certified mass under the annual rule applied in post-processing). Two design levers reappear zone-wide: (i) oversizing PV versus AEL to lift PV self-coverage of electrolysis in sunny hours while avoiding chronic curtailment, and (ii) daily H₂ storage to bridge the diurnal mismatch and protect the minimum per-module guard on the AEL stack. The PV–to–AEL ratio declines as PV yield improves (e.g., SIC), which allows the same annual H₂ duty with less PV oversizing; conversely, in NO the ratio increases toward 2.1:1 to compensate weaker insolation.

Table 4.7: Optimal S1 sizes and first-year certified hydrogen by bidding zone.

	SO	SAR	SIC	CSO	CNO	NO
$P_{\text{nom}}^{\text{PV}}$ [MW]	112	113	110	114	115	117
$P_{\text{nom}}^{\text{EL}}$ [MW]	58.5	57.5	60.5	57.0	56.5	55.0
$P_{\text{nom}}^{\text{COMP}}$ [MW]	4.0	4.0	4.1	3.9	3.9	3.8
$m_{\text{nom}}^{\text{HS}}$ proxy [m ³]	460	451	479	449	447	439
$m_1^{\text{H}_2, \text{cert}}$ [t]	3120	3050	3305	2774	2674	2338

The row labelled $m_{\text{nom}}^{\text{HS}}$ proxy reports the equivalent CGH_2 vessel volume at 300 bar, which is proportional to the underlying mass capacity $m_{\text{nom}}^{\text{HS}}$ used in the MESS model. Beyond PV/AEL scaling, the compressor nominal power remains close to 3.8 MW to 4.1 MW everywhere, in line with a lower/higher AEL size. The daily tank proxy follows the same intra-day rationale and scales mildly with PV yield: higher PV output increases midday surplus, raising the value of a slightly larger buffer to maintain the AEL above the minimum guard while evening demand is met from storage.

Zone-wise cost and intensity (S1 vs. S2). Using the S1 optima in Table 4.7 and layering a 100 MWh BESS (S2), Figure 4.16 reports LCOH and the annual carbon intensity by zone; percentages in parentheses show the LCOH uplift when incentives are removed.

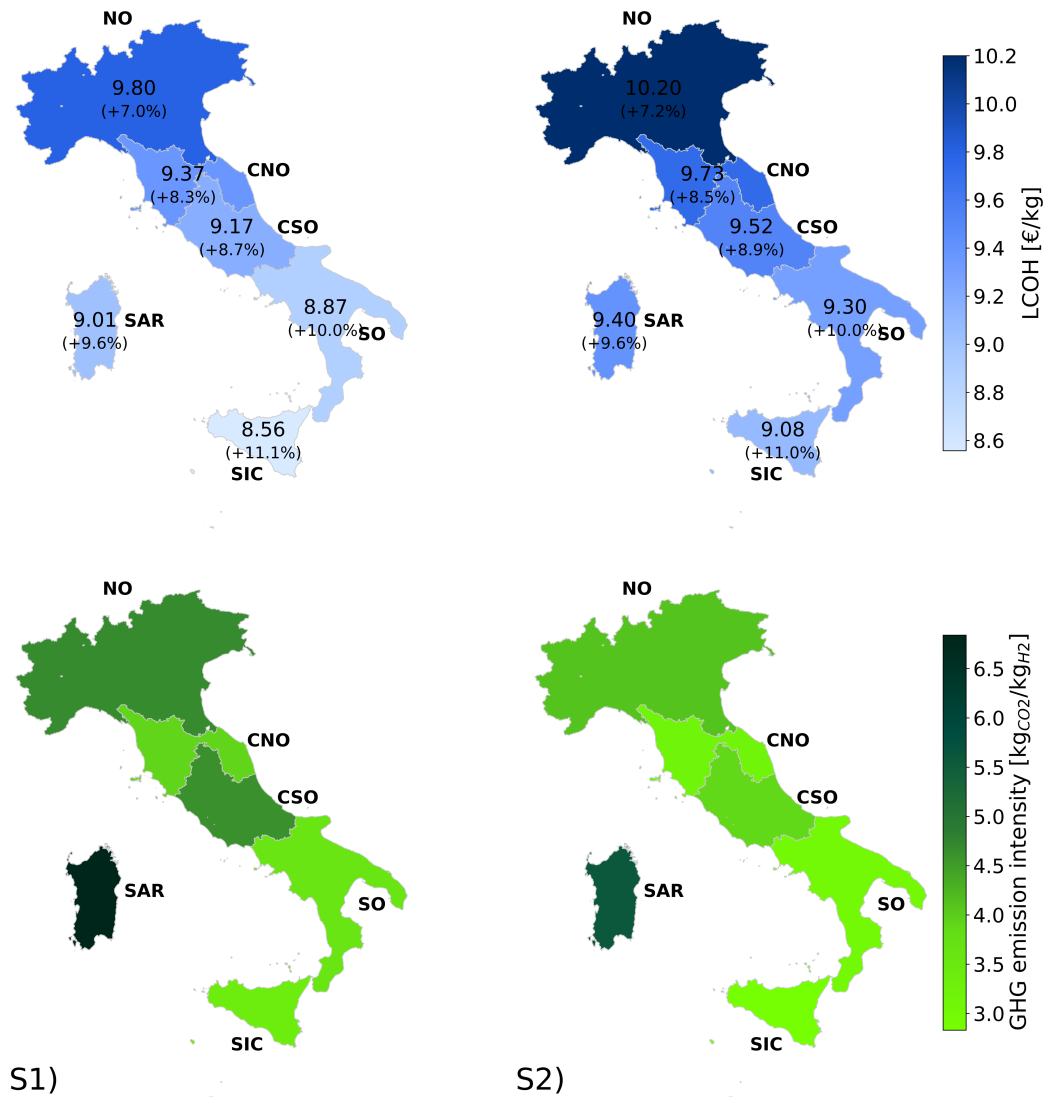


Figure 4.16: Zone-wise LCOH and emission intensity for S1 and S2. Percentages in parentheses indicate the LCOH uplift without incentives.

Three observations stand out. (i) LCOH systematically decreases moving southwards (about 9.8 €/kg in NO to 8.6 €/kg in SIC), dominated by higher PV yield and the associated incentive leverage, which is largest in SIC (double-digit percentage relief) and smallest in NO. (ii) the BESS raises LCOH by $\sim 5\%$ on average at today's costs with the rule-based approach stated above: it lowers grid purchases and increases the share of PV-backed operation but

does not cycle enough to pay back its CAPEX. (iii) the annual carbon intensity ranges from a minimum in SIC to a maximum in SAR, driven by the EF of imports and the diurnal composition of self-consumption; nonetheless, southern zones with better solar resource tend to secure larger certified fractions even when average EF is less favourable, because more hours sit in the low-intensity tail.

Is BESS ever cost-effective? Figure 4.17 explores LCOH in S2 versus BESS CAPEX for multiple battery sizes and incentive rates (south zone reference, S1 sizes for the rest). With today's large-scale CAPEX around 250 €/kWh, none of the capacities is cost-competitive: limited PV surplus, the pay-as-produced obligation and the availability of daily H₂ storage constrain useful cycling. Without incentives, breakeven appears only near 50 €/kWh for 120 MWh and around 120 €/kWh for 40 MWh. Higher incentive rates improve the economics of BESS because more hours become certifiable at lower intensity, yet the shift required remains substantial at current price levels.

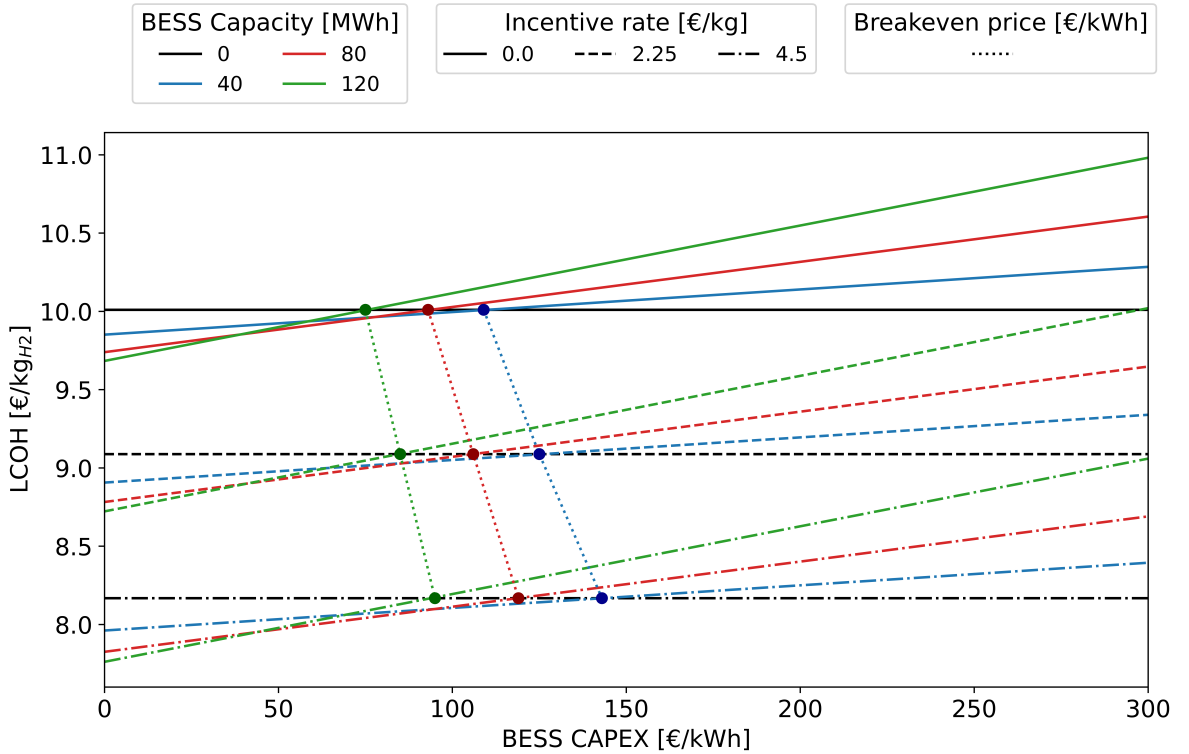


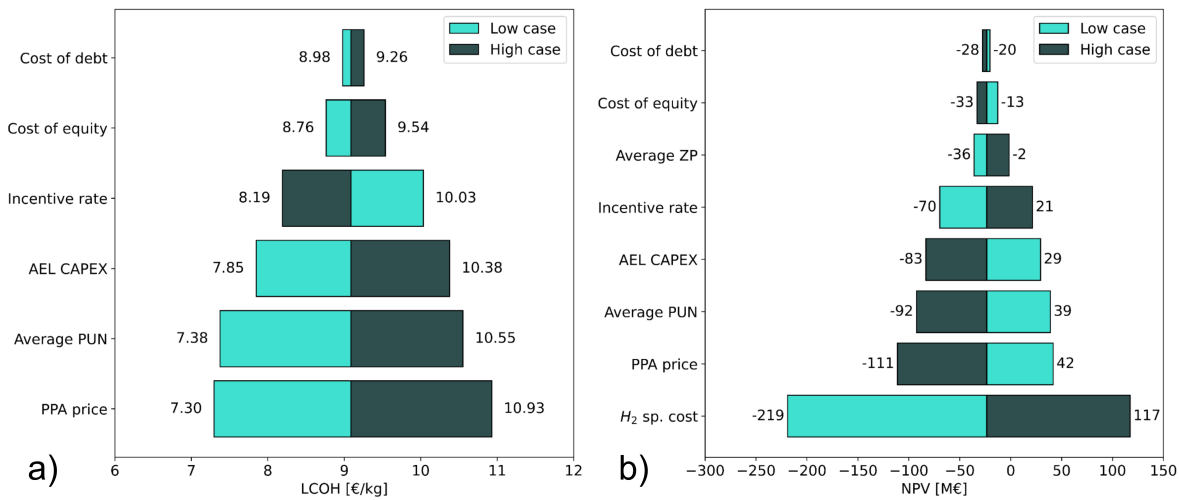
Figure 4.17: S2 LCOH vs. BESS CAPEX for different capacities and incentive rates (SO zone reference; S1 sizes). Black lines: S1 benchmarks.

Sensitivity to techno-economic and financial inputs. A one-at-a-time sensitivity around the south reference zone (S1 optimum) clarifies the dominant risk factors. Table 4.8 lists the ranges; Figure 4.18 shows tornado plots for LCOH and NPV.

Two price levers dominate LCOH: a $\pm 50\%$ variation in the PPA price produces a $\pm 20\%$ LCOH swing; a $\pm 50\%$ variation in the average PUN yields a nearly equal swing. Because the PPA applies to the full PV purchase stream, a given [€/MWh] reduction in PPA has more than double the leverage of the same reduction in PUN. A $\pm 50\%$ shift in AEL CAPEX translates to about $\pm 15\%$ on LCOH despite a $\sim 17\%$ baseline contribution, confirming that CAPEX still matters even in OPEX-heavy plants. Varying the incentive between 0 €/kg and 4.5 €/kg moves LCOH by roughly 2 €/kg due to the 10-year cap. On NPV, electricity selling price (ZP) and the benchmark cost of grey hydrogen $c^{\text{H}_2, \text{grey}}$ dominate; financial rates (debt/equity) have a secondary role because operating cash flows are small compared to C_0 .

Table 4.8: Ranges used in the one-at-a-time sensitivity for LCOH (and NPV where marked).

Parameter	Symbol	Nominal	Min	Max	Ref.
AEL CAPEX [€/kW]	CAPEX_{EL}	1094	547	1641	[266]
PPA price [€/MWh]	c^{PPA}	80	40	120	[268–270]
Avg. PUN [€/MWh]	—	193	96	290	[272, 273]
Avg. ZP [€/MWh] (NPV)	—	125	62	188	[271]
Incentive rate [€/kg]	c^{cert}	2.25	0	4.5	[274]
H ₂ specific cost [€/kg] (NPV)	$c^{\text{H}_2, \text{grey}}$	8	4	12	—
Cost of equity [%]	—	9	4	14	—
Cost of debt [%]	—	6	1	11	—

**Figure 4.18:** One-at-a-time sensitivity (SO zone, S1 optimum): (a) LCOH; (b) NPV. Central lines mark nominal values; bars rank parameters by impact.

Implications. Across zones, the combination of (i) pay-as-produced PV procurement, (ii) hourly EF/price timing, and (iii) daily—not seasonal—storage needs yields an LCOH in the 8.6 €/kg to 9.8 €/kg band under current signals, with batteries not yet cost-effective at prevailing CAPEX. Even with annual certification and a 2.25 €/kg premium over 10 years, the gap to typical grey hydrogen supply remains material. This points to two complementary levers: relieving the timing penalty (e.g., contracts that better align settlement to the PV profile or favourably price evening imports) and reducing the structural cost components that dominate OPEX (PPA/PUN) and the leading CAPEX driver (AEL). As signals evolve, the value of flexible assets (BESS and/or larger daily H₂ buffers) increases by enabling more low-intensity operating hours, but cost parity still hinges on electricity prices and electrolyser cost trajectories rather than storage alone.

4.2.7 Main findings and methodological reflections

Main findings. Across Italy, the GA sizing under rule-based dispatch yields a consistent design pattern: (i) PV is oversized versus AEL (typically $\sim 2:1$ in low-sun zones, declining where PV yield is higher) and (ii) daily CGH₂ storage is the primary flexibility lever. LCOH sits in the 8.6 €/kg to 9.8 €/kg band and is OPEX-dominated (PPA and corrected PUN); moving south lowers LCOH via higher PV yield but the timing penalty remains (exports at low ZP, imports at high EF). The 2.25 €/kg 10-year incentive gives only a modest LCOH relief (order ~ 1 €/kg); a 100 MWh BESS improves early-year carbon profile yet raises LCOH by $\sim 5\%$ at current CAPEX. Sensitivities confirm electricity prices as the dominant levers (PPA and average PUN), with AEL CAPEX the leading CAPEX driver.

Methodological reflections. Relative to the Case 1 study, the present PtH analysis replaces ad-hoc parametric exploration with an explicit GA search: sizes are now determined by an optimiser that delivers a reproducible minimum of LCOH (to numerical tolerance) for the chosen rule stack. This strengthens optimality on the design side while keeping a conscious limitation on the operations side: dispatch remains fixed (rule-based), and non-perfect-foresight of exogenous inputs. In other words, the GA provides an optimiser-backed optimum conditional on the policy; it does not co-optimize hourly actions against prices/EF or anticipate future states. This separation is deliberate because in this way components' physics and ageing are preserved without turning the problem into a full MILP. However, it also implies that any “global” optimum is bounded by the dispatch rules. Motivated by these findings, the remainder of the thesis will show results obtained with MILP algorithms moving to joint design-operation optimisation.

4.3 Deterministic MILP — Hydrogen storage technologies

4.3.1 Motivation, scope and contributions

The rule-based studies of Sections 4.1 and 4.2 established clear design signatures for PV→PtH plants (PV:AEL oversizing, daily CGH₂ buffers), but they remain policy-bound: priorities and exclusivities are imposed heuristically and applied myopically at each t . To remove that bias, this section implements the perfect-foresight joint sizing-scheduling MILP introduced in Section 3.2.3, solving one representative operating year ($\Delta t=1$ h, $N_T=8760$) with explicit AC and H₂ balances, storage inventories, and a RED III-style certification cap (Section 3.2.2). The plant serves a constant industrial hydrogen demand $\dot{m}_t^{\text{H}_2, \text{dem}}$ and co-optimises the design vector $s = (P_{\text{nom}}^{\text{PV}}, P_{\text{nom}}^{\text{WT}}, P_{\text{nom}}^{\text{EL}}, P_{\text{nom}}^{\text{COMP}}, m_{\text{nom}}^{\text{HS}})$ and the hourly dispatch $\{v_t, \delta_t\}$ to minimise LCOH (Eq. 3.178). FC, BESS and DG are disabled in this shell

by construction (Section 3.2.3); the grid interface is active with import/export exclusivity, imported energy is costed and enters certification accounting, and export is not credited in the LCOH numerator. Within this unified optimisation baseline, three hydrogen-storage families are compared on a whole-plant basis: compressed gas (CGH₂, Types I–IV), underground hydrogen storage (UHS), and metal hydrides (MH, e.g. MgH₂, LaNi₅) with desorption duty represented via an electric-heater load proportional to $\dot{m}_t^{\text{HS,dis}}$ (Eq. 3.151). The study follows the scope and dataset of [233], enabling a storage-aware benchmark of LCOH under identical signals and feasibility guards.

Contributions. Building on Secs. 2.2 and 3.2 and the storage study in [233], this section: (i) replaces rule priorities with a single perfect-foresight MILP that delivers reproducible optima for s and hourly routing under balances, exclusivities, and inventory dynamics; (ii) embeds CGH₂, UHS and MH inside the plant co-optimisation, quantifying system-level trade-offs (CAPEX, footprint, installed mass) on a common LCOH basis rather than via stand-alone LCOS; (iii) enforces a linearised RED III cap (Section 3.2.2) to expose when environmental compliance, rather than pure cost, binds the optimum; (iv) preserves linear physics for key devices (EL, COMP, HS) while retaining only physically necessary binaries (HS direction and grid import/export), keeping year-long horizons tractable; (v) reports decision-relevant metrics beyond LCOH (e.g. storage footprint, installed tank mass) to inform siting/permitting alongside economics.

4.3.2 Modelling inputs for storage technologies

The deterministic MILP instantiates hydrogen storage following the card of Section 3.2.2, as bounded inventories with charge/discharge decisions and state advance on LOH_t . All device-level maps and thermodynamics (CGH₂ geometry/footprint; MH equilibrium and heat duties; heat-to-electric mapping; siting clearances) are those already defined in Section 3.1.1. Technology-specific mappings (payloads, areas, masses, and auxiliary powers) reuse the device relations defined in Section 3.1.1: (i) CGH₂ geometry and footprint from Eqs. 3.44–3.46; (ii) heat-to-electric mapping for desorption by Eq. 3.52. This subsection specifies the technology datasets (geometry, pressures, masses, costs, areas; waste-heat figures) used by the optimisation without restating equations.

CGH₂ Type I–IV (pressure classes and site constraints). Vessels follow the standard taxonomy [198]. The adopted geometric envelope uses $D_{\text{ext}}=490$ mm and $L_{\text{tank}}=12$ m, which permits 5×5 stacking inside a 40-ft ISO container (internal envelope $12 \text{ m} \times 2.4 \text{ m} \times 2.4 \text{ m}$) and mirrors tube-trailer practice [200]. Wall thicknesses are taken from code and manufacturer practice: Type I (all-metal) via ISO 9809 design-stress rules [279]; Types II–IV (composites) via ISO 11119 compliance and certified datasheets, where admissible fibre-stress ratios and prototype testing govern the overwrap rather than a single closed-form stress expression [201, 202, 280, 281]. Operating gauge pressures reflect catalogue ratings for each type/pressure class. For mass and payload mapping, empty masses are read from product specifications (steel/aluminium tubes for Type I, hoop-wrapped for Type II, fully wrapped with metal or polymer liner for Types III/IV). Internal free volume Vol_{int} follows from the envelope and wall thickness (Eqs. 3.44–3.45); hydrogen density $\rho_{\text{H}_2}(\mathcal{P}^{\text{HS}}, T^{\text{HS}})$ is evaluated as real gas at the declared storage operating pressure and temperature. Site area is computed container-by-container by Eq. 3.46, with a uniform perimeter clearance d_{NFPA} set by NFPA 2 for outdoor compressed-hydrogen systems [199]. In practice, the increase of d_{NFPA} with pressure partly offsets the area benefit of higher ρ_{H_2} at 700 bar; this pattern is visible in the footprint-per-kg column of Table 4.9. Specific costs are assigned per type/pressure class following consolidated techno-economic ranges for CGH₂ vessels [282], with pressure adjustments according to the

correlations in [283].

Table 4.9 compiles the dataset used downstream (payloads, areas, masses and specific costs). From a design standpoint: (i) moving from Type I/II to Type III/IV sharply improves payload per area due to higher allowable pressure and lower structural mass; (ii) the marginal footprint gain above the 350 bar class is moderated by the larger d_{NFPA} ; (iii) composite vessels carry a clear cost premium per [€/kg_{H₂}] that will later reflect in the cost–area trade-offs.

Table 4.9: Reference parameters for CGH₂ storage. One container holds 25 vessels stacked 5×5.

Tank Type	$\mathcal{P}$ [bar]	Density [kg/m ³]	Wall [mm]	Empty mass [t]	Vol. [m ³]	Mass [kg]	Vessels/ container	container mass [kg]	NFPA2 [m]	Footprint* [m ²]	Footprint [m ² /kg]	Cost [€/kg]
I	30	2.45	8	2.30	2.1	5	25	125	5	273	2.18	200
I	200	14.71	26	2.40	1.8	26	25	650	6	346	0.532	222
II	350	23.65	56	2.15	1.3	31	25	775	4	208	0.268	333
II	700	39.69	84	2.40	1.0	40	25	1000	5	273	0.273	383
III	350	23.65	28	1.30	1.8	43	25	1075	4	208	0.193	650
III	700	39.69	42	1.40	1.5	60	25	1500	5	273	0.182	730
IV	350	23.65	28	1.20	1.8	43	25	1075	4	208	0.193	800
IV	700	39.69	42	1.40	1.5	60	25	1500	5	273	0.182	830

Notes. Geometry: $D_{\text{ext}}=490$ mm, $L_{\text{tank}}=12$ m [200]. * Footprints computed by Eq. 3.46 with a 1 m service aisle in both directions and the listed NFPA distances.

UHS (salt caverns). UHS is abstracted as a large compressed-gas inventory bounded by the host rock. In line with current practice at moderate depths, the pressure window is represented by $\mathcal{P}_{\text{max}}^{\text{UHS}} \approx 200$ bar with a cushion-gas fraction of $\sim 30\%$; the working inventory is thus the remaining fraction of the geometric capacity that can be cycled [205, 206]. Since the cavern provides the pressure boundary, the surface system only accounts for wellhead compression power during charge/discharge; no explicit area term is included because practical cavern capacities far exceed the daily/weekly buffers relevant here. For comparability with CGH₂, transport to/from the cavern is neglected (assumed proximity to the PtH site). The specific CAPEX enters the optimiser as 38 €/kg_{H₂} of working capacity, consistent with depth-resolved breakdowns and recent European hub announcements [206, 284, 285]. This choice makes UHS the low-OPEX, high-upfront option with very large working capacities when geology is available; feasibility is therefore constrained by siting rather than by thermodynamics.

Metal hydrides (MgH₂ and LaNi₅) with PCM heat recovery. MH blocks use the equilibrium mapping and thermal duties already defined in Section 3.1.1. Two representative material classes are considered under identical boundary conditions: a high-temperature light-metal hydride (MgH₂) and a low-temperature intermetallic (LaNi₅). The former offers high wt%H and compact bed mass at the cost of high T_{op} and higher desorption duty; the latter operates near ambient with a lower duty but requires a much larger bed mass per unit hydrogen. PCM recovery is sized at the desorption setpoint for each material; the residual duty maps to electric-heater power via the heat–to–electric conversion already defined. No additional compressor is required on charge, and post-compression on discharge is only needed if the end-use pressure exceeds $\mathcal{P}^{\text{eq,MH}}(T)$. The external desorption duty q_{des} [kWh_{th}/kg_{H₂}] combines (i) the reaction enthalpy associated with dehydrogenation and (ii) the sensible heat needed to bring the bed and embedded heat-exchanger structures from ambient to T_{op} [207]. The hydrogen content in Table 4.10 is reported as gravimetric density [wt%]; the corresponding MH-bed mass per unit hydrogen, [kg_{MH}/kg_{H₂}], follows directly from Eq. 3.50. For the adopted values (7.6 wt% for MgH₂, 1.36 wt% for LaNi₅), this yields 13 and 73 kg_{MH}/kg_{H₂}, respectively. Adding the rest-of-system (vessel, insulation, internal heat exchangers and auxiliaries) gives the total MH mass per kilogram of stored hydrogen, with rest-of-system terms recomputed

from prototype data for MgH_2 and LaNi_5 [286, 287]. The volumetric densities in Table 4.10 are consistent with typical ranges reported for stationary MH systems [83, 87].

Phase-change materials (PCMs) are integrated to buffer the thermal duty between absorption and desorption. A PCM with melting point $T_{\text{PCM}} \approx T_{\text{op}}$ absorbs heat during exothermic absorption and releases it during endothermic desorption [211]. The PCM effectiveness $\eta_{\text{PCM}} \in [0, 1]$ represents the fraction of q_{des} that can be supplied by the PCM around T_{PCM} , and the residual external heat requirement is represented in Eq. 3.49. The PCM latent heat q_{PCM} [$\text{kWh}/\text{kg}_{\text{PCM}}$] is taken at T_{PCM} , and the PCM mass per kilogram of hydrogen, $[\text{kg}_{\text{PCM}}/\text{kg}_{\text{H}_2}]$, follows from storing $q_{\text{des,PCM}}$ with latent heat at that temperature. The values of η_{PCM} , $q_{\text{des,PCM}}$, q_{PCM} and PCM mass in Table 4.10 are synthesised from detailed reactor and system studies of MH+PCM integration [209, 210, 288–290].

Containerised MH modules operate at relatively low pressures ($\lesssim 15$ bar), so no additional NFPA CGH_2 standoffs are required and a compact specific footprint is adopted. Site footprints and system-level masses are consistent with commercial MgH_2 and LaNi_5 modules [213, 214]. MH and PCM specific costs per kg_{H_2} are taken from techno-economic assessments of solid-state hydrogen and thermal storage [286] and are applied directly in the CAPEX accounting.

Table 4.10: Techno-economic inputs for MH storage (MgH_2 vs. LaNi_5).

Parameter	MgH_2	LaNi_5
Class	Light metal hydride	Intermetallic hydride
Desorption temperature T_{op} [$^{\circ}\text{C}$]	280	45
Plateau pressure at T_{op} [bar]	15	5
Hydrogen content [wt%]	7.6	1.36
MH mass per kg H_2 [$\text{kg}_{\text{MH}}/\text{kg}_{\text{H}_2}$]	13	73
Total MH (bed+RoS) mass [$\text{kg}/\text{kg}_{\text{H}_2}$]	116	107
Volumetric density [$\text{kg}_{\text{H}_2}/\text{m}^3$]	80	106
Desorption heat q_{des} [$\text{kWh}_{\text{th}}/\text{kg}_{\text{H}_2}$]	10.3	4.2
Site footprint [$\text{m}^2/\text{kg}_{\text{H}_2}$]	0.04	0.04
PCM type; T_{PCM} [$^{\circ}\text{C}$]	Salt eutectic; 282	Paraffin C22; 50
PCM effectiveness η_{PCM} [%]	70	70
$q_{\text{des,PCM}}$ [$\text{kWh}_{\text{th}}/\text{kg}_{\text{H}_2}$]	3.10	1.26
PCM latent heat q_{PCM} [$\text{kWh}/\text{kg}_{\text{PCM}}$]	0.088	0.053
PCM mass per kg H_2 [$\text{kg}_{\text{PCM}}/\text{kg}_{\text{H}_2}$]	117	79
Total MH+PCM mass [$\text{kg}/\text{kg}_{\text{H}_2}$]	233	186
MH specific cost [$\text{€}/\text{kg}_{\text{H}_2}$]	258	1460
PCM specific cost [$\text{€}/\text{kg}_{\text{H}_2}$]	350	350

Waste-heat pathways and mapping to electricity. Industrial waste-heat (WH) integration follows Eq. 3.51, with a water-coupled loop for LaNi_5 and a hot-air/flue-gas loop for MgH_2 . Representative streams and setpoints adopt steelmaking profiles (H_2 –DRI/EAF conversion context) [42, 52, 291, 292]. Table 4.11 reports, per kilogram of released hydrogen, the recoverable sensible heat from each stream and the fraction of q_{des} it covers. In both cases, WH alone provides only a minority share, so the residual desorption duty is supplied electrically (electric heater efficiency $\eta^{\text{EH}}=0.95$) using the mapping already defined in Section 3.1.1. These figures are used directly to compute the net electric load of MH discharge inside the optimiser.

Deterministic MILP instantiation. This study instantiates the perfect-foresight optimi-

Table 4.11: Specific industrial waste heat per kilogram of H₂ released and coverage of q_{des} (illustrative streams for steelmaking sites).

Material	Stream	$T_{s,\text{in}}$ [°C]	T_{op} [°C]	ΔT_{pp} [°C]	q_s [kWh _{th} /kgH ₂]	q_s/q_{des} [%]
MgH ₂	Flue gas (hot air loop)	350	280	20	0.184	1.8
LaNi ₅	Water loop	55	45	4	0.311	7.4

Notes. Stream mass flow proxies follow steel site benchmarks; parameters compiled from [42, 292] and mapped via Eq. 3.51. q_{des} as in Table 4.10.

sation shell of Section 3.2.3 as a single-year, hourly MILP that jointly sizes and schedules the PtH plant with explicit AC and H₂ balances, storage inventories, and a certification cap. The exogenous inputs ξ_t comprise the renewable-availability profiles, electricity prices, and (when the grid is enabled) grid emission intensity. The decision vector combines (i) the design variables

$$s = (P_{\text{nom}}^{\text{PV}}, P_{\text{nom}}^{\text{WT}}, P_{\text{nom}}^{\text{EL}}, P_{\text{nom}}^{\text{COMP}}, m_{\text{nom}}^{\text{HS}}),$$

and (ii) the hourly operating variables $\{v_t\}$ (power flows, hydrogen flows), binaries $\{\delta_t\}$ (exclusivities), and states $\{x_t\}$ (inventories). The complete constraint set is exactly the one already given in the model formulation of Eq. 3.179. A summary of the main techno-economic parameters adopted in the MILP is reported in Table 4.12.

Table 4.12: Summary of techno-economic parameters adopted in the MILP.

Parameter [unit]	Symbol	Value	Ref.
Reference wind height [m]	z_{ref}	10	[293]
Turbine hub height [m]	z_{hub}	100	–
Cut-in wind speed [m/s]	w_{ci}	3	[180]
Cut-out wind speed [m/s]	w_{co}	25	[180]
Rated wind speed [m/s]	w_{rat}	13	[180]
EL operating pressure [bar]	$\mathcal{P}^{\text{EL}}$	30	–
EL spec. cons. [kWh/kgH ₂]	SEC^{EL}	55.54	[294]
Water use factor [m ³ /kgH ₂]	$sc_{\text{H}_2\text{O}}$	0.015	[191]
Minimum storage fill [–]	LOH_{min}	0.10	–
Storage charge efficiency [–]	$\eta^{\text{HS, ch}}$	0.995	–
Storage discharge efficiency [–]	$\eta^{\text{HS, dis}}$	0.995	–
COMP cons. 30→200 bar [kWh/kgH ₂]	$\text{SEC}_{30 \rightarrow 200}^{\text{COMP}}$	1.70	[197]
COMP cons. 30→350 bar [kWh/kgH ₂]	$\text{SEC}_{30 \rightarrow 350}^{\text{COMP}}$	2.22	[197]
COMP cons. 30→700 bar [kWh/kgH ₂]	$\text{SEC}_{30 \rightarrow 700}^{\text{COMP}}$	3.35	[197]

An additional KPI is introduced, namely the Levelised Cost of Storage (LCOS), which isolates the unit cost of the storage function over lifetime, using only storage-related cash flows and the actual discharged hydrogen, as represented in Eq. 4.5:

$$\text{LCOS} = \frac{C_0^{\text{HS}} + \sum_{y=1}^N \frac{\text{CAPEX}_y^{\text{repr, HS}} + \text{OPEX}_y^{\text{HS}}}{(1 + \text{DR})^y}}{\sum_{y=1}^N \frac{m_y^{\text{HS, dis}}}{(1 + \text{DR})^y}} \quad [\text{€/kg}], \quad 4.5$$

where C_0^{HS} is the upfront storage investment and $\text{CAPEX}_y^{\text{repr,HS}}$ collects storage-only replacements. Eq. 4.5 is a post-processing KPI computed on the optimal schedules; it does not replace LCOH in the MILP objective, but it provides a clean apples-to-apples comparison of storage families by normalising their costs to the actually delivered hydrogen from storage.

4.3.3 Configurations

Two plant configurations are analysed to bracket how grid access and certification constraints shape optimal sizing and scheduling of a PtH plant supplying a constant industrial offtake $\dot{m}_t^{\text{H}_2, \text{dem}}$ equal to 38 kg/h (i.e., 333 t/y). This value is intended to represent a modular/pilot-scale industrial demand compatible with a partial deployment of an H₂-DRI/EAF pathway: using typical specific hydrogen needs of the order of $\sim 50 \text{ kg}_{\text{H}_2}$ per tonne of steel output, it corresponds to roughly 6–7 kt/y of steel production equivalent [52]. The hydrogen duty is kept fixed across locations (Hajira, Bari, Bremen, Houston) to isolate the impact of exogenous signals (RES profiles, electricity prices, grid EF and certification constraints) on optimal storage and scheduling choices. Schematic flow diagrams for the two storage interfaces are shown in Figure 4.19: the top panel depicts CGH₂/UHS, where a COMP raises the EL outlet to the HS pressure; the bottom panel depicts MH, where high-pressure compression is avoided but a dedicated desorption-heat path (waste heat and/or electric heater) is required.

(1) *Off-grid hybrid VRE.* PV and WT are the only electric sources; there is no grid interconnection. The AC balance must be met hour by hour using only renewable generation and storage auxiliaries. This setting reveals the intrinsic PV/WT-to-hydrogen coupling and the minimum storage needed to bridge diurnal/weekly mismatches without external energy.

(2) *Grid-connected hybrid VRE.* PV and WT are supported by a bidirectional grid interface with import/export exclusivity at each t . Imported electricity is billed at $c_t^{\text{el,imp}}$ and contributes to the GHG-intensity accounting; Exports are allowed but, by construction of LCOH in Eq. 3.178, they are not credited in the numerator. A site-specific annual GHG cap for certifying green hydrogen applies, using the grid emission factors and limits in Table 4.13. This configuration represents a realistic near-term deployment where the grid buffers renewable variability under an explicit certification constraint.

Technology scope. Three storage families are embedded in the MILP: (i) CGH₂ vessels Type I–IV at representative pressures (30/200/350/700 bar), (ii) UHS (salt cavern) operated around $\mathcal{P}_{\text{max}}^{\text{UHS}} \approx 200$ bar with cushion gas, and (iii) MH (MgH₂, LaNi₅) with three heat-supply variants for each material: 100% on-site waste heat (WH), 100% electric heater (EH), and EH with PCM buffering. The detailed technology parameters (pressures, masses, areas, costs, and heat duties) are those compiled in Tables 4.9 and 4.10.

Locations and motivation. Four sites—Hajira (India), Bari (Italy), Bremen (Germany), and Houston (USA)—are selected to span (i) contrasting renewable resource shapes and capacity factors, (ii) electricity price levels, (iii) grid carbon intensities relevant to certification, and (iv) different GHG caps for “green hydrogen”. The objective is to probe storage choices under markedly different exogenous signals while holding the hydrogen duty fixed. Table 4.13 summarises location inputs (PV/WT capacity factors and seasonal shares, electricity prices, grid EF, and annual GHG limits). Figure 4.20 shows the normalised hourly PV and WT production profiles used in the optimisation. From Figure 4.20 and Table 4.13, these main considerations arise:

- Hajira (India). High PV capacity factor with winter-leaning PV and strong monsoon-season winds. PV and WT exhibit partial seasonal complementarity (WT peak in

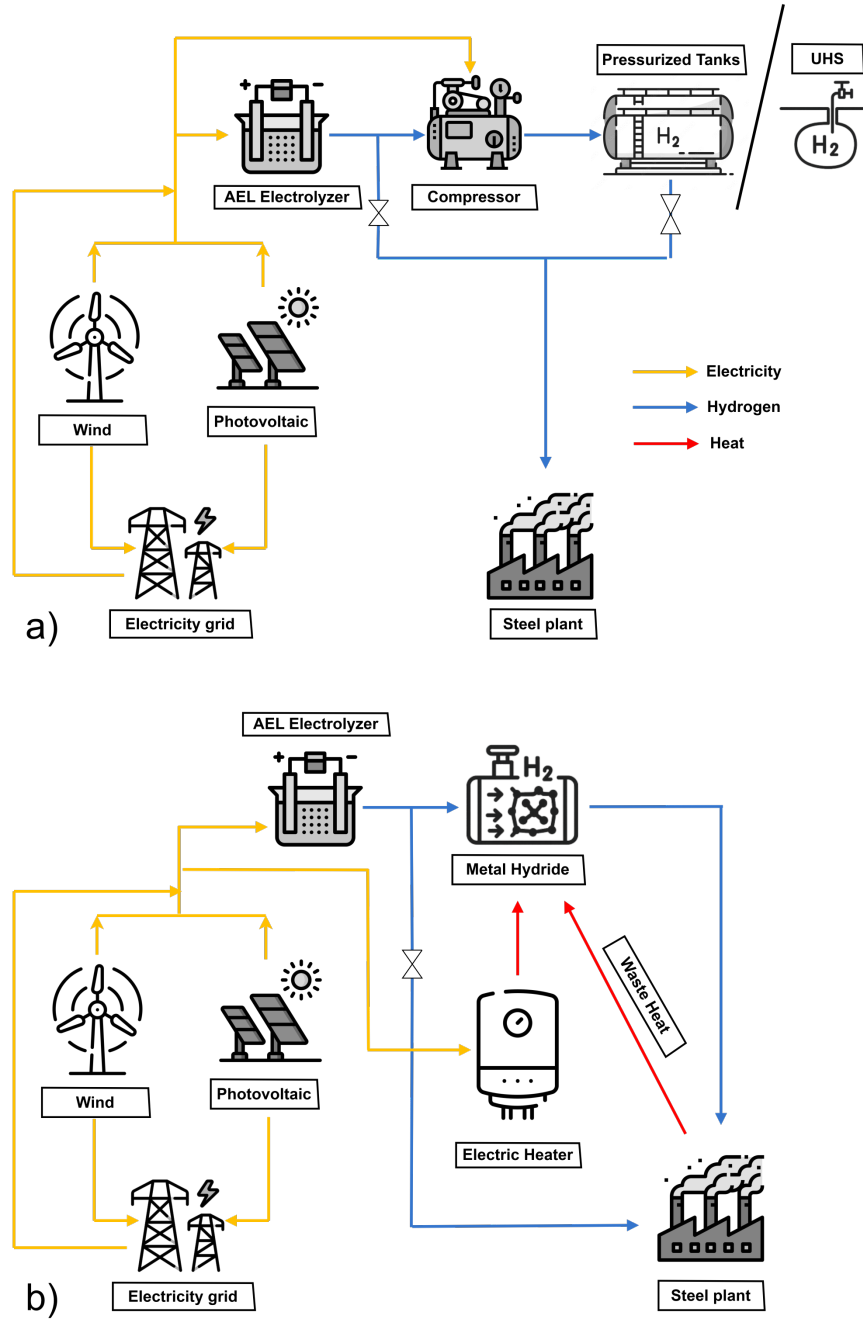


Figure 4.19: Grid-connected PtH schemes for the three storage families considered. (a) CGH_2/UHS : compressor upstream of storage; delivery throttled to ≈ 1 bar. (b) MH: direct charge at electrolyser outlet pressure; discharge requires heat (electric heater and/or waste heat with PCM buffering).

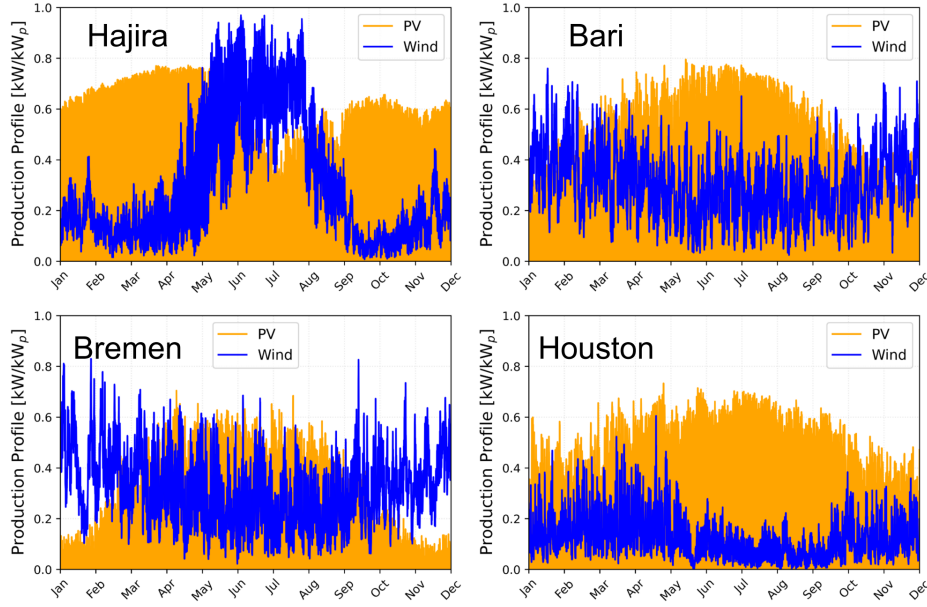


Figure 4.20: Hourly PV and WT production profiles at the four locations used as exogenous inputs in the MILP.

Table 4.13: Renewable and policy parameters per location. PV and WT seasonality are expressed so that seasonal shares (winter, spring, summer, autumn) sum to 100%.

Parameter	Hajira (IN)	Bari (IT)	Bremen (DE)	Houston (US)
WT exponent α [–]	0.23	0.33	0.37	0.20
WT capacity factor [%]	29.8	29.9	31.1	12.2
PV capacity factor [%]	24.1	21.6	13.9	20.7
WT seasonality [%]	15/21/52/12	32/25/20/23	33/25/18/24	29/35/17/19
PV seasonality [%]	26/31/19/23	14/29/37/20	7/36/41/16	18/27/32/23
Electricity price [€/kWh]	0.12 [295]	0.20 [296]	0.22 [296]	0.13 [297]
Grid EF [gCO ₂ /kWh]	750 [231]	350 [231]	380 [231]	300 [231]
Emission cap [kgCO ₂ eq/kgH ₂]	2.00 [298]	3.38 [11]	3.38 [11]	3.00 [299]

summer, PV stronger in winter), which tends to reduce short-term storage needs but leaves some inter-seasonal balancing to the grid or to larger inventories.

- Bari (Italy). Mid-range PV and WT; pronounced summer PV and spring/winter wind. Significant day-to-day variability favours flexible electrolyser utilisation and moderate CGH₂ buffers.
- Bremen (Germany). Highest WT capacity factor and the weakest PV among the four. Winter-biased wind smooths diurnal PV swings but calls for larger daily/weekly buffers when calm spells occur—making UHS or higher-pressure CGH₂ attractive for multi-day coverage.
- Houston (USA). Comparatively uniform PV and poor WT. The flatter PV profile reduces intraday swings but can increase reliance on grid imports during extended cloudy periods; policy levers (price, EF, cap) then become decisive for storage sizing.

Scenario matrix. A full-factorial matrix is solved: 4 locations $\times$ 2 configurations (off-grid, grid-connected) $\times$ 15 storage options (CGH₂ Types I–IV at four pressures, UHS, MgH₂ with three heat variants, LaNi₅ with three heat variants) for a total of $4 \times 2 \times 15 = 120$ MILP runs. Each run uses the technical set of Table 4.12, the financial inputs of Tables 4.14–4.15, the storage datasets compiled in the preceding subsections of Section 4.3, and the site parameters of Table 4.13. Figures 4.19 and 4.20 provide the visual context referenced throughout the results.

Table 4.14: Major equipment financial inputs.

Asset	Cost [€/kW]	O&M [%]	Lifetime [y]	Repl. [% CAPEX]	Ref.
PV	921	2	30	–	[248, 300]
WT	1779	4	30	–	[301, 302]
EL	1094	4	15	100	[266]
COMP	4577	4	15	100	[303, 304]

Table 4.15: Additional common financial inputs.

Item	Value	Notes	Ref.
Civil works [€/m ²]	370	Bare EL floor area	–
Electrolyser specific area [m ² /kW]	0.5	Used for civil works	–
Engineering add-on [%]	15	Applied to bare CAPEX	[249]
Installation add-on [%]	18	Applied to bare CAPEX	[249]
Personnel [€/y]	200,000	24 h supervision	–
Land rent [€/ (m ² y)]	2	–	–
Water cost [€/Sm ³]	2.38	Deionised water	[259]
Discount rate (DR) [%]	7	$N=30$ y analysis horizon	–

Note on supervision assumption. The 24 h supervision cost is included to represent continuous on-site staffing for safe operation of a hydrogen facility that includes high-pressure equipment (compression and storage) and associated auxiliaries. While modern electrolyzers

can be remotely monitored, in this work the same supervision assumption is applied to all configurations so that comparisons across storage technologies are not biased by different OPEX staffing choices.

4.3.4 Results and discussion

This section reports the optimisation outcomes for the four sites defined in Table 4.13. For Hajira with Type I tanks at 200 bar, it is firstly compared the off-grid and grid-connected configurations, while then, still for Hajira, all storage alternatives in the grid-connected configuration. After that a sensitivity analysis on the electricity price is carried out and finally a comparison of results obtained even for Bari, Bremen, and Houston under the same workflow.

Hajira — Type I tanks at 200 bar: off-grid vs. grid-connected. Figure 4.21 summarises the two configurations, and Table 4.16 lists the corresponding optima.

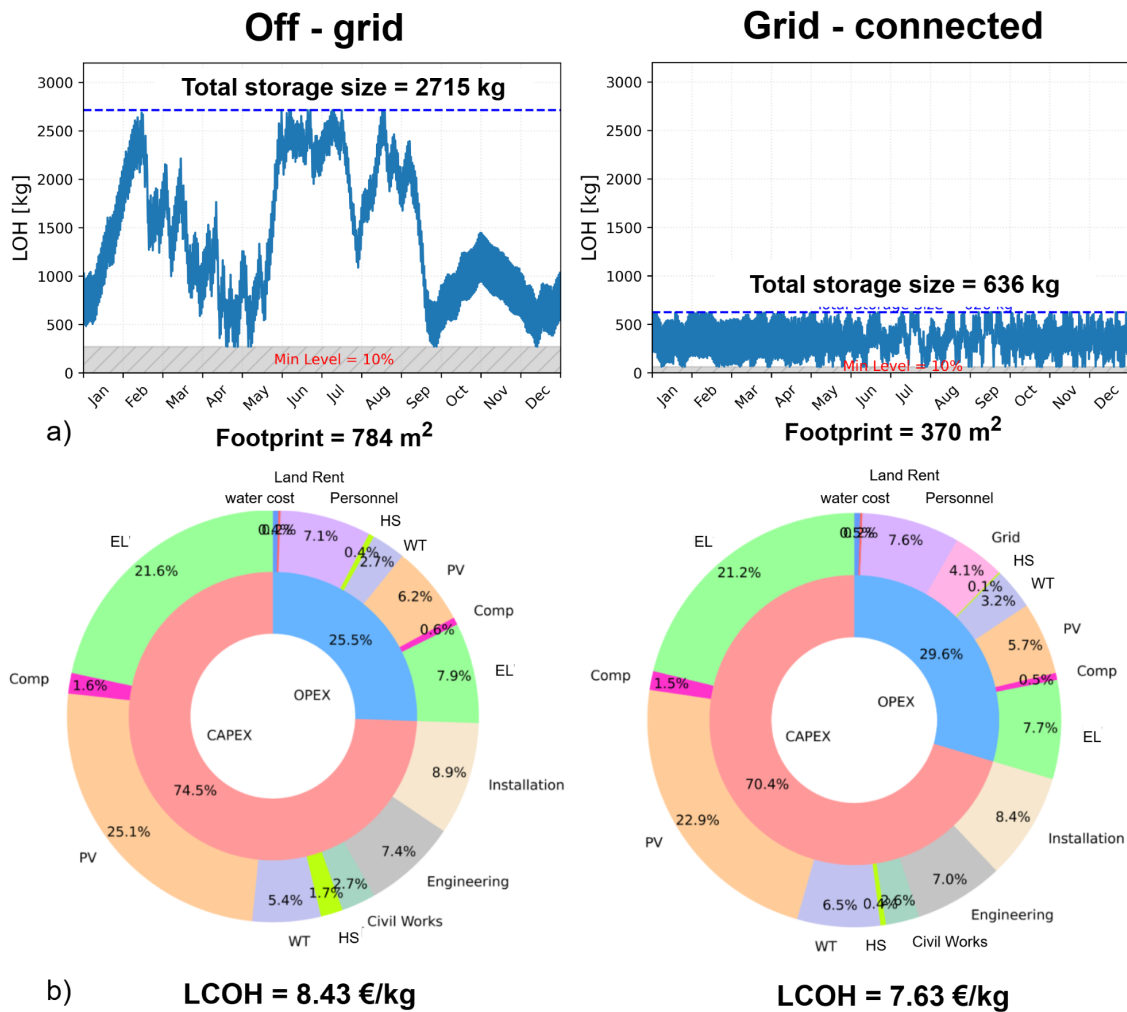


Figure 4.21: Hajira, Type I tanks at 200 bar: off-grid (left) vs. grid-connected under the 2 kgCO₂/kgH₂ cap (right). Hourly LOH and LCOH breakdown.

As visible in Figure 4.21a, the off-grid case requires multi-tonne seasonal buffering with extended charge/discharge periods. Under the grid-connected configuration constrained by the 2 kgCO₂/kgH₂ annual cap (Table 4.13), storage operates within a narrow band, which reduces the number of vessels from 105 to 24 (−77%) and the number of tube trailers from 5 to 1 (−80%). Footprint falls from 784 m² to 370 m² (−53%), a decrease smaller than the

Table 4.16: Hajira, Type I tanks at 200 bar: optimal system sizes.

Component [unit]	Symbol	Off-grid	Grid-connected
Photovoltaics [MW]	$P_{\text{nom}}^{\text{PV}}$	9.50	7.62
Wind turbine [MW]	$P_{\text{nom}}^{\text{WT}}$	1.05	1.26
Electrolyser [MW]	$P_{\text{nom}}^{\text{EL}}$	5.05	4.36
Compressor [MW]	$P_{\text{nom}}^{\text{COMP}}$	0.09	0.13
Storage capacity [t H ₂]	$m_{\text{nom}}^{\text{HS}}$	2.71	0.63
Vessels [–]	–	105	24
Tube trailers [–]	–	5	1
Footprint [m ²]	A_{site}	784	370

–76% size reduction ($2.71 \rightarrow 0.63$ t H₂) because footprint scales by container count and is subject to minimum NFPA separations and access clearances (Eq. 3.46).

The LCOH is lower in the grid-connected case (7.63 €/kg versus 8.4 €/kg off-grid). Grid electricity supplies 4.8% of the annual EL consumption; given India’s grid EF of 750 gCO₂/kWh, the certification cap is binding at the optimum. The small permitted grid share, however, meaningfully reduces the need for oversized PV/EL/HS, lowering total CAPEX, while OPEX rises modestly due to purchases. Net effect: lower LCOH and smaller footprint. The same ordering holds for the other storage families; therefore, subsequent comparisons focus on grid-connected scenarios.

Hajira — grid-connected: storage technologies comparison. The 15 grid-connected scenarios cover four CGH₂ families (Types I–IV at 30/200/350/700 bar), UHS, and two MHs (MgH₂, LaNi₅) each with three heat-supply variants (100% WH, 100% EH, EH+PCM). Results are organised as storage characteristics (Figure 4.22), P2H component sizing (Figure 4.23), and economics (Figure 4.24).

(i) Storage characteristics: Required storage capacities for CGH₂ vessels cluster at 0.52–0.63 t H₂ because the grid connection suppresses seasonal cycling. Structural implications differ by pressure and type: within Type I, moving 30 $\rightarrow$ 200 bar reduces gas volume (253 $\rightarrow$ 43 m³), footprint (672 $\rightarrow$ 370 m²), and vessel mass (285 $\rightarrow$ 58 t) for essentially the same capacity—reflecting container-count penalties at very low pressure. In Types II–IV, raising pressure 350 $\rightarrow$ 700 bar increases footprint (162 $\rightarrow$ 295 m²) and compression duty, with only minor changes in capacity; mass trends are technology-driven (composites in Types III–IV). Optimal UHS capacity is much larger (11.5 t H₂) because of its low specific cost, making UHS the only technology that provides seasonal cycling in the optimum. For MHs, capacities again lie near 0.51–0.64 t H₂, footprint is very compact (25 m²), but total installed mass is high: MgH₂ weighs 68 t in 100% WH (rising to 128 t with PCM), LaNi₅ 55 t (rising to 97 t with PCM), consistent with Table 4.10.

(ii) Component sizing: All options converge to a narrow band for the primary assets: PV 8.0–8.4 MW and EL 4.3–4.9 MW. Differences stem from auxiliaries: CGH₂ tanks require compression that scales with pressure, whereas MHs avoid high-pressure compression but add desorption-heater load. In MgH₂–EH cases, the higher night-time electric duty increases WT capacity. UHS slightly reduces EL and PV while raising WT to 1.8 MW: with larger storage, the optimiser performs stronger temporal shifting under the annual GHG constraint.

(iii) Economics: UHS attains the lowest LCOH (7.60 €/kg) by selecting a larger storage while limiting grid purchases; despite a high storage CAPEX entry (400 k€), the system-wide balance remains favourable. Among CGH₂, low-pressure Type I leads: 7.63 €/kg at 200 bar

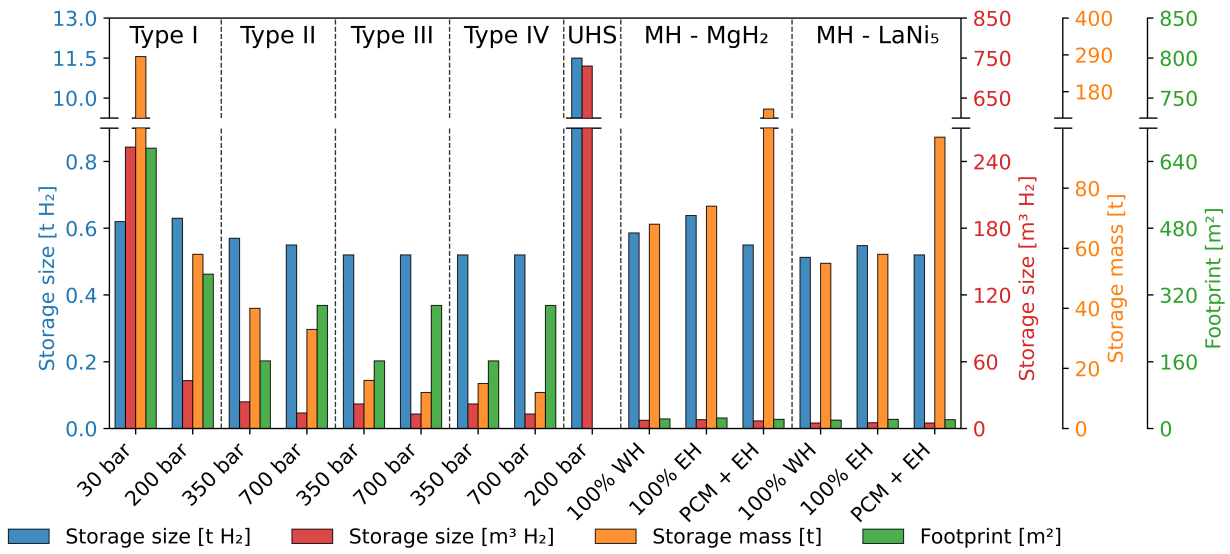


Figure 4.22: Hajira, grid-connected: storage characteristics across 15 options—storage size, gas volume, installed mass, and footprint.

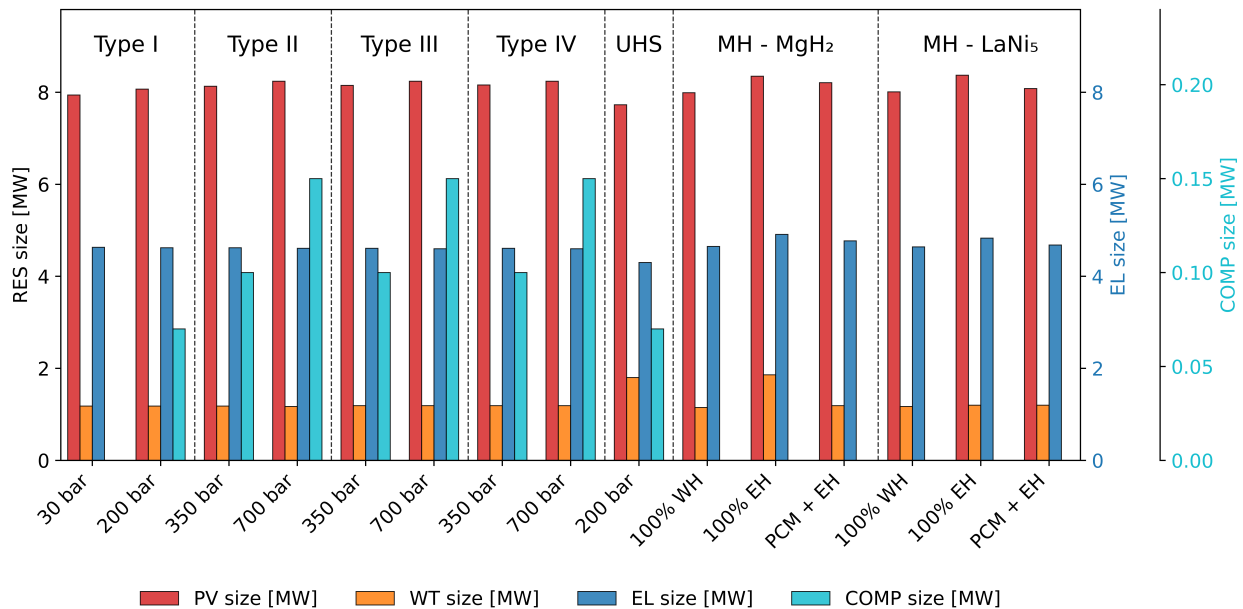


Figure 4.23: Hajira, grid-connected: optimal component sizes across 15 storage options.

(LCOS = 0.11 €/kg; storage CAPEX 125 k€). Increasing pressure within a family raises LCOH due to higher compression and higher storage specific cost; the within-family spread is 8% (0.6 €/kg). MHs split clearly: waste-heat variants are competitive (MgH₂ 7.65 €/kg; LaNi₅ 7.89 €/kg), whereas 100% EH penalises costs (MgH₂ 8.51 €/kg; LaNi₅ 8.17 €/kg). Adding PCM lowers LCOH despite higher investment (MgH₂ 7.91 €/kg; LaNi₅ 8.04 €/kg), at the expense of higher installed mass.

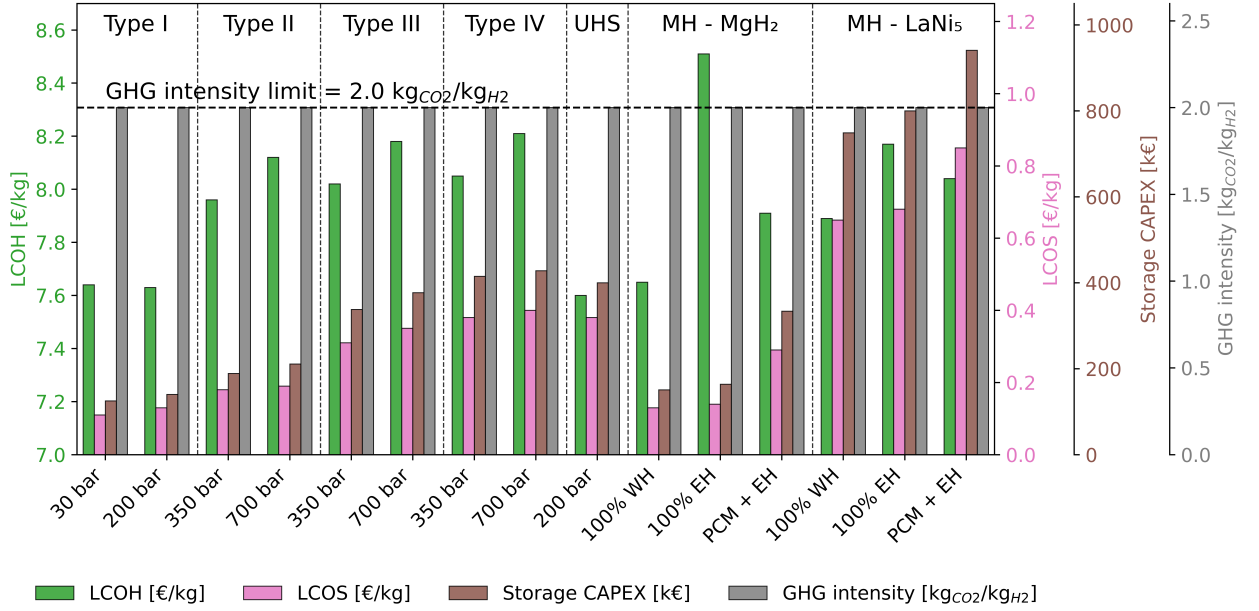


Figure 4.24: Hajira, grid-connected: economic KPIs — LCOH, LCOS, storage CAPEX, and achieved annual GHG intensity (cap at 2 kg_{CO2}/kg_{H2}).

All Hajira configurations operate exactly at the 2 kg_{CO2}/kg_{H2} limit. Absent this cap, a larger grid share would further reduce LCOH (price sensitivity not shown here), unlike Bari and Bremen, where the cap is not binding and additional purchases do not improve costs (see below).

The main outcomes can be summarised as follows:

- *Ranking.* UHS and low-pressure Type I tanks yield the lowest LCOH; MgH₂ with 100% WH follows. Higher-pressure tanks (Types II–IV at 350–700 bar) incur a 0.3–0.6 €/kg penalty; EH-heated MHs—especially LaNi₅—are least competitive.
- *Drivers.* With the grid cap binding, differences stem from compression duty, storage specific cost, and (for MHs) heat-supply strategy.
- *Siting.* If land is the binding constraint, containerised MH units provide the smallest site area (25 m²) due to low-pressure operation and high installed mass. Where a mass–area balance is preferred, Types III–IV at 350 bar offer compact footprints (162 m²) and low installed mass (12–16 t for ~ 0.52 t H₂), potentially justifying a higher LCOH. UHS performance presupposes suitable geology (and, if off-site, a transmission solution not costed here).

Hajira — Type I tanks at 200 bar: sensitivity analysis. UHS attains a slightly lower LCOH than Type I tanks in Hajira, but it presupposes suitable salt geology and dedicated site development. To keep findings broadly applicable, the sensitivity is performed on Type I tanks at 200 bar. The annual GHG-intensity cap is removed so that the optimiser can freely

choose the grid share and expose grid-price breakpoints. Figure 4.25 reports optimal designs as the grid purchase price varies from 0.05 to 0.50 €/kWh. Panel (a) shows the optimal $P_{\text{nom}}^{\text{PV}}$, $P_{\text{nom}}^{\text{WT}}$, $P_{\text{nom}}^{\text{EL}}$, $m_{\text{nom}}^{\text{HS}}$ and the resulting annual GHG intensity; Panel (b) shows LCOH, LCOS, and the tank contribution to LCOH ($\text{LCOH}_{\text{tank}}$). Three regimes emerge:

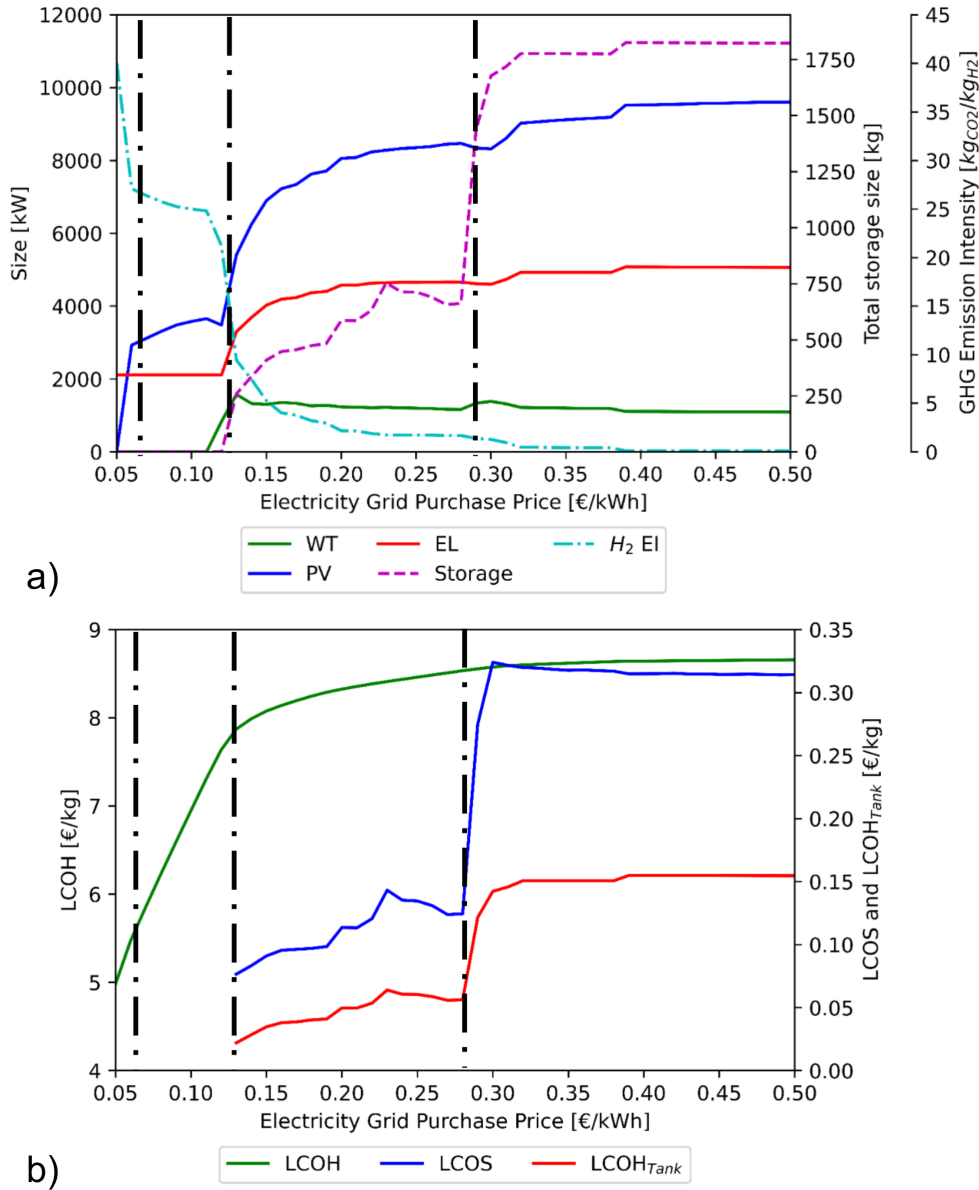


Figure 4.25: Hajira, grid-connected sensitivity (Type I tanks, 200 bar; GHG-intensity cap removed). (a) Optimal capacities ($P_{\text{nom}}^{\text{PV}}$, $P_{\text{nom}}^{\text{WT}}$, $P_{\text{nom}}^{\text{EL}}$, $m_{\text{nom}}^{\text{HS}}$) and achieved annual GHG intensity versus grid purchase price. (b) LCOH, LCOS, and $\text{LCOH}_{\text{tank}}$ versus price.

- Low price (≤ 0.06 €/kWh). The least-cost solution buys all electricity from the grid; PV, WT and HS are not installed. Emissions equal the EL's specific electricity use times the grid factor, yielding 41.6 kgCO₂/kgH₂. LCOH is low and dominated by purchased energy, while LCOS and $\text{LCOH}_{\text{tank}}$ are undefined (no HS).
- Mid price (0.12 €/kWh, Hajira average). Storage remains non-economic; WT is not adopted and a modest PV capacity appears (4 MW). LCOH rises nearly linearly with the tariff because capital outlays are limited. For prices above 0.12 €/kWh, WT

(1.5 MW) is added and storage grows roughly linearly with price; LCOS and $\text{LCOH}_{\text{tank}}$ therefore appear and increase accordingly.

- High price (≥ 0.28 €/kWh). A sharp increase in total HS capacity occurs—consistent with container modularity and NFPA spacing—together with slightly higher PV and EL sizing, as renewables-plus-shifting becomes cheaper than grid purchases. Emissions drop to $1 \text{ kg}_{\text{CO}_2}/\text{kg}_{\text{H}_2}$ as grid use collapses. LCOS and $\text{LCOH}_{\text{tank}}$ step up with the added HS, while overall LCOH becomes less sensitive to further price increases.

These results quantify the role of the certification cap discussed before: with the $2 \text{ kg}_{\text{CO}_2}/\text{kg}_{\text{H}_2}$ limit enforced, the permissible grid share is lower than $2/41.6 \approx 4.8\%$, which aligns with the optimal grid-connected design found previously for Hajira. Without the limit, the system is grid-dominant at low tariffs, transitions to renewables without storage near 0.06 €/kWh, adopts storage near 0.13 €/kWh, and becomes storage-led only beyond 0.28 €/kWh.

Location-dependent optima with Type I tanks at 200 bar. The analysis carried out for Hajira is extended to Bari (Italy), Bremen (Germany), and Houston (USA). Detailed time-series plots of balances, mass/footprint, and cross-technology rankings are omitted, since their qualitative behaviour mirrors the Hajira results discussed above. What varies—and ultimately sets the optimal design—is the combination of resource seasonality (Figure 4.20) and the electricity price / grid emission intensity / GHG limit triplet in Table 4.13. Together, these determine the PV/WT mix, HS size, and LCOH. Figure 4.26 summarises the site-by-site optima in the grid-connected configuration for Tank Type I at 200 bar.

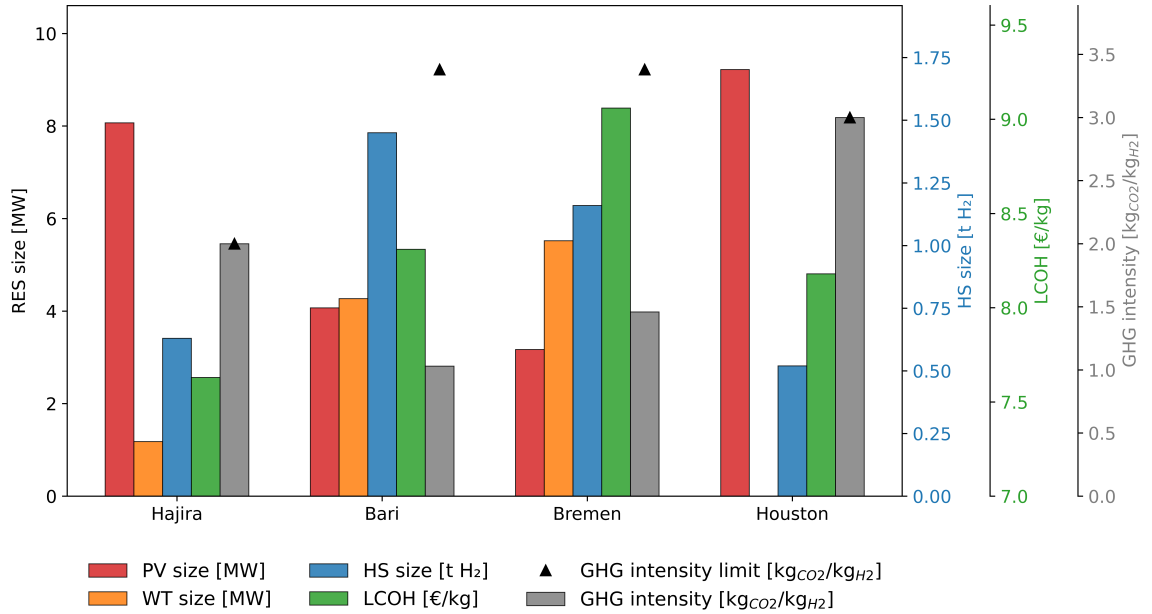


Figure 4.26: Grid-connected, Type I tanks at 200 bar: site-by-site optima for PV and WT ratings (left axis), storage size (blue), LCOH (green), and achieved annual emission factor (grey). Black triangles mark the site-specific limit.

- Bari (Italy). With complementary resources (PV summer-peaked, WT winter-peaked) and a higher average purchase price (0.20 €/kWh), the optimiser limits grid use and installs a balanced hybrid (PV and WT of comparable scale) and a larger storage ($1.45 \text{ t}_{\text{H}_2}$) than Hajira. The achieved annual GHG intensity lies well below the EU limit

($CI^{\text{H}_2} = 1.03 \text{ kg}_{\text{CO}_2}/\text{kg}_{\text{H}_2}$ vs. $CI^{\text{limit}} = 3.38 \text{ kg}_{\text{CO}_2}/\text{kg}_{\text{H}_2}$), but the extra CAPEX lifts the cost to $\text{LCOH} = 8.31 \text{ €/kg}$.

- Bremen (Germany). A wind-dominant resource (high WT capacity factor, low PV capacity factor) drives a wind-heavy mix and a modest storage ($1.16 \text{ t}_{\text{H}_2}$). As in Bari, the GHG-intensity cap does not bind ($CI^{\text{H}_2} = 1.46 \text{ kg}_{\text{CO}_2}/\text{kg}_{\text{H}_2}$) because grid electricity is relatively expensive (0.22 €/kWh). The larger wind build raises CAPEX and yields $\text{LCOH} = 9.06 \text{ €/kg}$.
- Houston (USA). Here the wind capacity factor is very low (12%), so the optimum is PV-only ($P_{\text{nom}}^{\text{WT}}=0$) with $P_{\text{nom}}^{\text{PV}} = 9.22 \text{ MW}$ and a small storage ($0.52 \text{ t}_{\text{H}_2}$), leaning on the grid up to the U.S. limit. The lower electricity price (0.13 €/kWh) keeps total cost below the EU sites: $\text{LCOH} = 8.18 \text{ €/kg}$.

For the same storage technology, price + seasonality + limit jointly set the PV/WT mix, HS size, and cost. In Bari and Bremen, higher electricity price makes the cap non-binding; grid use is minimal and larger PV/WT (and larger storage) are installed, lowering emissions but raising LCOH ($8.31\text{--}9.06 \text{ €/kg}$). In Houston, weak wind and lower electricity price make the limit binding; the solution leans on the grid, keeps storage small, and achieves a lower LCOH (8.18 €/kg). Among the four sites, Hajira retains the lowest cost for Type I at 200 bar ($\text{LCOH} = 7.63 \text{ €/kg}$), reflecting favourable PV resource and modest storage needs under the binding cap.

4.3.5 Main findings and methodological reflections

Findings. (i) With a binding cap (Hajira), small grid shares ($\sim 5\%$) suffice to markedly reduce oversizing of PV/EL/HS, lowering LCOH and footprint; (ii) without the cap, the LCOH-optimal pathway transitions from grid-only $\rightarrow$ PV-only $\rightarrow$ hybrid+storage as tariffs rise, with distinct price breakpoints ($\sim 0.06, 0.13, 0.28 \text{ €/kWh}$); (iii) across sites, UHS and low-pressure CGH₂ (Type I, 200 bar) lead on LCOH; MHs are competitive only with assured waste heat; electrically heated MHs are penalised by night-time loads.

Methodological reflections. Relative to the rule-based, GA-driven design workflow discussed earlier, the present section adopts a single perfect-foresight MILP that jointly sizes and schedules under explicit balances, exclusivities, and inventory dynamics. This strengthens optimality on operations (hourly routing is optimised, not imposed by rules) while preserving linear device physics and only the binaries that are physically necessary (HS direction, grid import/export). However, perfect foresight abstracts from uncertainty in prices, availability, and certification accounting signals; therefore, the obtained optima represent lower bounds under the assumed exogenous trajectories. Motivated by these limits, the next subsection introduces a two-stage stochastic optimisation shell to quantify the value of recourse and of hedging against uncertainty in VRE availability, while retaining the same device cards and feasibility guards as the deterministic MILP.

4.4 Two-stage stochastic MILP — Island decarbonisation

4.4.1 Motivation, scope and contributions

The perfect-foresight MILP of Section 3.2.3 provides a unified, physics-faithful baseline for joint sizing-scheduling, but it cannot capture the variability that governs stand-alone

design: multi-day wind lulls, cloudy spells, and seasonal swings that stress inventories and trigger costly recourse to diesel. This subsection therefore activates the risk-neutral two-stage shell of Section 3.2.4: a single here-and-now design s is chosen before uncertainty is realised, while hourly operations $\{v_{t,\omega}, \delta_{t,\omega}, x_{t,\omega}\}$ adapt scenario-wise under non-anticipativity on s . The plant is a fully islanded Hybrid Renewable Energy System (HRES); there is no grid interface and hydrogen is used as an internal carrier (EL→COMP→HS→FC) to buffer renewable variability and guarantee security of supply for the site electrical demand $p_t^{\text{el,dem}}$. The architecture is motivated by policy and system needs: net-zero trajectories and EU decarbonisation packages drive deep electrification and renewable penetration [24], while remote islands remain diesel-reliant with high energy costs and security-of-supply concerns [305–307]. In these settings, combining BESS (short-term) with hydrogen storage (long-duration) is recognised as reliability-enhancing and cost-curbing [308, 309]. The shell is applied to a real Mediterranean island with no feasible grid connection (Pantelleria), quantifying how variability reshapes capacities, dispatch, and the premium paid for reliability and emissions compliance relative to the deterministic baseline, as further documented in [234].

Contributions. Building on Section 3.2, this section: (i) formulates a risk-neutral two-stage stochastic MILP for joint sizing and dispatch of an off-grid HRES, enforcing non-anticipativity on s and scenario-adaptive recourse on hourly operations; security of supply is guaranteed in every scenario, and a DG ϵ^{CO_2} budget yields explicit cost–emissions trade-offs; (ii) embeds the full off-grid energy hub (PV, WT, EL+COMP+HS, FC, BESS, DG) in one optimisation, preserving linear plant physics and retaining only physically necessary binaries so that year-long horizons with $|\Omega|$ scenarios remain tractable while honouring balances, exclusivities, and inventory dynamics; (iii) constructs Ω via Monte Carlo with bootstrap daily recombination and k -means reduction, then forms a Cartesian PV×WT set (Section 3.2.4), preserving seasonality and low-renewables persistence that drive hydrogen-storage value; (iv) produces cost–emissions Pareto fronts under uncertainty by tightening ϵ^{CO_2} , and contrasts them with deterministic fronts to quantify the premium of reliability/compliance and the value of recourse (capacity shifts and dispatch flexibility that only emerge when operations adapt to scenarios); (v) reports decision-relevant metrics beyond TAC: coverage shares of $p_t^{\text{el,dem}}$ (direct VRE vs. BESS vs. FC vs. DG), curtailment patterns, and the dispersion of $\text{LOH}_{t,\omega}/\text{SOC}_{t,\omega}$ across ω .

4.4.2 Configuration

Figure 4.27 shows the Pantelleria off-grid HRES considered. The AC node couples: (i) variable RES (PV, WT), (ii) short-duration storage (BESS), (iii) the PtH chain composed of PEM EL, COMP and HS (Type I CGH₂ tank at high pressure), (iv) the HtP reconversion (PEM FC), (v) a last-resort DG, and (vi) the fixed site load $p_t^{\text{el,dem}}$. Two resource loops close at every (t, ω) : the electrical balance of Eq. 3.126 in its off-grid form, and the internal hydrogen balance of Eq. 3.127 (no external H₂ offtake). PV and WT are curtailable; BESS and HS provide temporal shifting (hour–day and day–season), and the DG ensures feasibility during extended calm-and-cloudy periods under an explicit annual emissions budget. The objective is the expected Total Annualised Cost TAC of Eq. 3.180, subject to capacity limits, cyclic inventories, and the ϵ -constraint on annual DG emissions (Eqs. 3.184–3.185). Uncertainty enters through full-year hourly PV/WT availability profiles $\xi_{t,\omega}$, generated via Monte Carlo with bootstrap daily recombination and reduced by k -means before forming the Cartesian PV×WT scenario set (Section 3.2.4); the demand profile $p_t^{\text{el,dem}}$ is fixed and common to all scenarios in the baseline. The complete two-stage formulation for the off-grid case is summarised in Eq. 3.186 where all plant physics, bounds, inventories, and exclusivities are

specified.

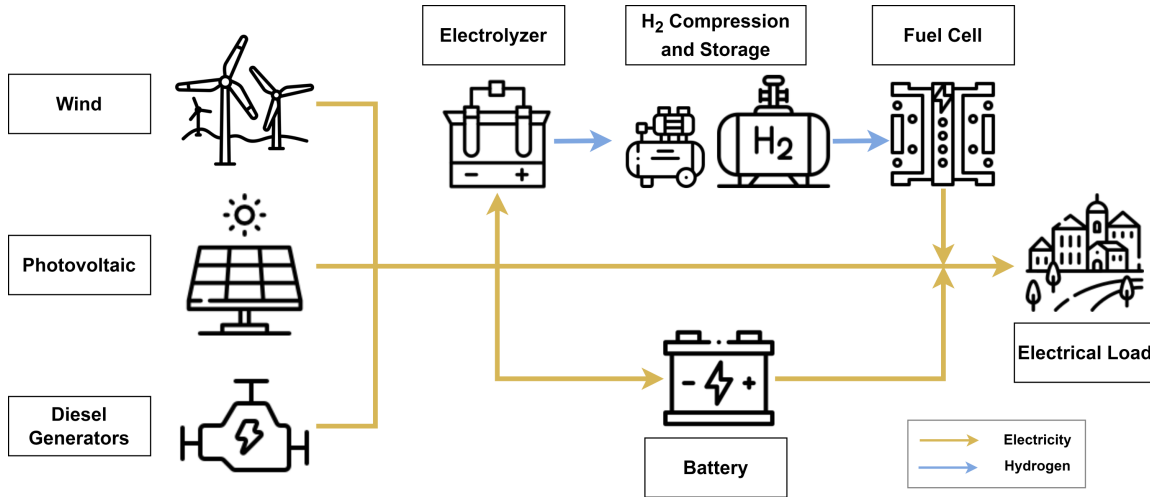


Figure 4.27: Configuration of the off-grid hybrid renewable energy source system on Pantelleria (Italy).

Site motivation. Pantelleria is geographically isolated and currently diesel-reliant; connection to the national grid is economically unfeasible [306]. Historical RES producibility (2005–2023) indicates mean annual PV yield $\approx 1619 \text{ kWh/kW}$ ($CF^{\text{PV}} \approx 18.5\%$) and wind yield $\approx 3495 \text{ kWh/kW}$ ($CF^{\text{WT}} \approx 39.9\%$), with marked interannual and seasonal variability as represented in Figure 4.28.

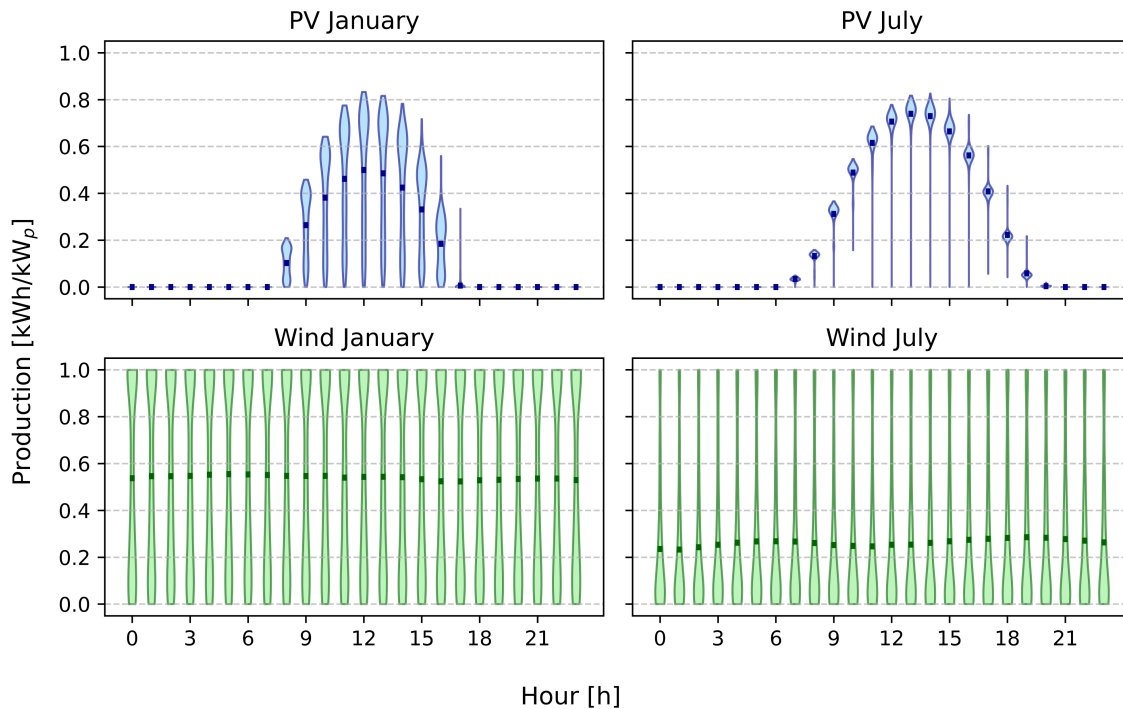


Figure 4.28: Historical PV and WT producibility: January and July violin plots. Dark points mark month–hour means.

The site electrical demand totals 31.1 GWh/yr , with a summer peak driven by tourism; monthly totals are from [306], and the hourly shape is derived with RSE’s TOTEM tool for the Province of Trapani [310]. For deterministic benchmarking, year 2005 is used as

a representative baseline (PV: 1633.7 kWh/kW; WT: 3534.7 kWh/kW), being closest to long-run means. Figure 4.29 summarises the hourly and monthly reference signals (load, PV, WT), showing summer-peaked demand and the PV–WT seasonal complementarity.

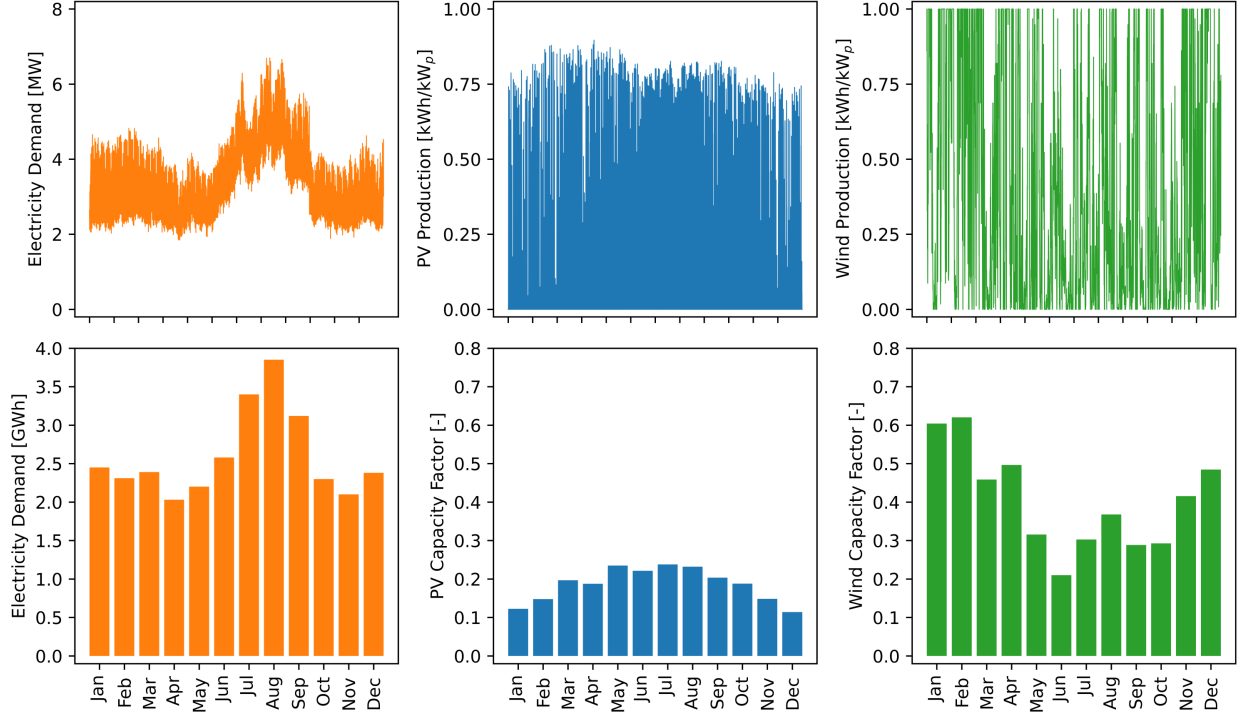


Figure 4.29: Reference inputs (deterministic baseline year): hourly (top) and monthly (bottom) profiles for electrical load, PV and WT specific power.

4.4.3 Technical and economic inputs

Table 4.17 compiles the technical parameters used in the case study, while Tables 4.18–4.19 report the economic datasets used to compute $\text{CAPEX}^{\text{ann}}(s)$ and OPEX in Eq. 3.180. Here, LT denotes the assumed component lifetime (in years) used for annualising CAPEX; for clarity, $\text{LT}^{\text{BESS}}=15$ years refers to the battery system, while the electrolyser lifetime in Table 4.17 is $\text{LT}^{\text{EL}}=10$ years (stack-level assumption), with replacements handled as year-specific $\text{CAPEX}_y^{\text{repr}}$ in the discounted economic KPIs.

4.4.4 Scenario construction

Uncertainty is placed on renewable availability only; the site demand $p_t^{\text{el,dem}}$ is fixed across ω (Section 3.2.4). Historical producibility (2005–2023) reveals two salient features: (i) PV is seasonally higher in summer with a clear diurnal structure; (ii) wind exhibits winter-leaning productivity and a distribution concentrated at extremes, so hourly means are not representative.

Methodological summary. Each scenario $\omega \in \Omega$ carries full-year hourly exogenous signals $\xi_{t,\omega} = (\bar{p}_{t,\omega}^{\text{PV,1kW}}, \bar{p}_{t,\omega}^{\text{WT}})$. Scenarios are generated by a Monte Carlo + Bootstrap daily recombination procedure that preserves intra-day correlation and seasonality: within each month m , whole daily profiles are drawn with replacement from historical sets $\mathcal{X}_m^r = \{\mathbf{x}_{m,d}^r \in \mathbb{R}^{24}\}$ and concatenated as in Eq. 3.187 to produce annual vectors $\mathbf{X}_s^{\text{PV}}, \mathbf{X}_s^{\text{WT}} \in \mathbb{R}^{N_T}$ [235–237]. In this study, we generate $S_{\text{MC}}^{\text{PV}} = S_{\text{MC}}^{\text{WT}} = 10\,000$ annual realisations per resource. For tractability,

Table 4.17: Technical parameters and operating conditions for the Pantelleria HRES.

Component	Parameter [unit]	Symbol	Value	Ref.
PV	Tilt angle [°]	-	32	[177]
	Azimuth angle [°]	-	7	[177]
	Total system losses [%]	-	14	[177]
	Specific production [kW h/kW]	$\bar{p}_t^{\text{PV},1\text{kW}}$	time series	[177]
	Lifetime [y]	LT^{PV}	20	–
WT	Hub height [m]	z_{hub}	80	–
	Reference height [m]	z_{ref}	10	–
	Power-law exponent [–]	α	0.17	[181]
	Cut-in speed [m/s]	w_{ci}	3	[180]
	Cut-out speed [m/s]	w_{co}	25	[180]
	Rated speed [m/s]	w_{rat}	13	[180]
	Lifetime [y]	LT^{WT}	20	–
BESS	Charging efficiency [–]	$\eta^{\text{BESS,ch}}$	0.95	[311]
	Discharging efficiency [–]	$\eta^{\text{BESS,dis}}$	0.95	[311]
	C-rate [h^{-1}]	$\mathcal{C}$	0.9	[222]
	Self-discharge rate [%/mon]	SDR	5	[312]
	Min. SOC [–]	SOC_{min}	0.20	[312]
	Max. SOC [–]	SOC_{max}	1.00	–
	Lifetime [y]	LT^{BESS}	15	–
EL	Operating pressure [bar]	$\mathcal{P}^{\text{EL}}$	30	–
	Spec. elect. cons. [kWh/kg _{H₂}]	SEC^{EL}	50.5	[248]
	Water use [m ³ /kg _{H₂}]	$sc_{\text{H}_2\text{O}}$	0.015	[191]
	Lifetime [y]	LT^{EL}	10	[222]
FC	Operating pressure [bar]	$\mathcal{P}^{\text{FC}}$	1	–
	Spec. fuel. cons. [kg _{H₂} /kWh]	SFC^{FC}	0.060	[222]
	Lifetime [y]	LT^{FC}	10	[313]
HS (CGH ₂)	Nominal pressure [bar]	$\mathcal{P}^{\text{HS}}$	200	[314]
	Charging efficiency [–]	$\eta^{\text{HS,ch}}$	0.995	–
	Discharging efficiency [–]	$\eta^{\text{HS,dis}}$	0.995	–
	Lifetime [y]	LT^{HS}	20	–
COMP	Specific consumption [kWh/kg _{H₂}]	$\text{SEC}_{30 \rightarrow 200}^{\text{COMP}}$	1.76	[197]
	Lifetime [y]	LT^{COMP}	20	–
DG	Nominal efficiency [–]	η^{DG}	0.37	[222]
	CO ₂ intensity [kg _{CO₂} /kWh]	CI^{DG}	0.805	[315]
	Lifetime [y]	LT^{DG}	20	–

Table 4.18: Per-asset economic inputs for the HRES.

Asset	Cost [€/kW;€/kWh;€/kg]	O&M [%/y]	Repl. [% CAPEX]	Ref.
PV	1060	2.0	–	[316, 317]
WT	1200	3.0	–	[318, 319]
BESS [€/kWh]	450	2.5	50	[320, 321]
EL	1196	5.0	50	[266, 322]
FC	1300	5.0	20	[222, 313]
HS [€/kg]	230	2.0	–	[253, 282]
COMP	4577	4.0	–	[248, 303]
DG	343	2.5	–	[222]

Table 4.19: Financial inputs.

Item	Value	Notes	Ref.
Diesel specific cost [€/m ³]	1800	Site-specific cost level	[306]
Water specific cost [€/m ³]	4	Deionised water for EL	[323]
Discount rate [%]	7	Entering Fisher equation	–
Engineering add-on [%]	15	Applied to bare CAPEX	–
Installation add-on [%]	15	Applied to bare CAPEX	–
Personnel [€/y]	200000	24 h supervision (3×8 h)	–
Project lifetime [y]	20	–	–

each Monte Carlo pool is reduced by k -means on $\mathbb{R}^{N_T}$ (Eq. 3.188) to $S_{CL}^{PV} = S_{CL}^{WT} = 10$ centroids $\{\mu_i^r\}$, with empirical probabilities π_i^r equal to cluster masses (Eq. 3.189). Figure 4.30 displays the cluster-wise histograms; red markers denote the selected centroids and their π_i^r . Assuming independence after reduction, the global set is the Cartesian product $\Omega = \Omega^{PV} \times \Omega^{WT}$ with $|\Omega| = 100$ and $\pi_{(i,j)} = \pi_i^{PV} \pi_j^{WT}$ (Eq. 3.190). These $\{\pi_\omega\}$ weight OPEX $_\omega$ and E^{DG} in Eqs. 3.180 and 3.184.

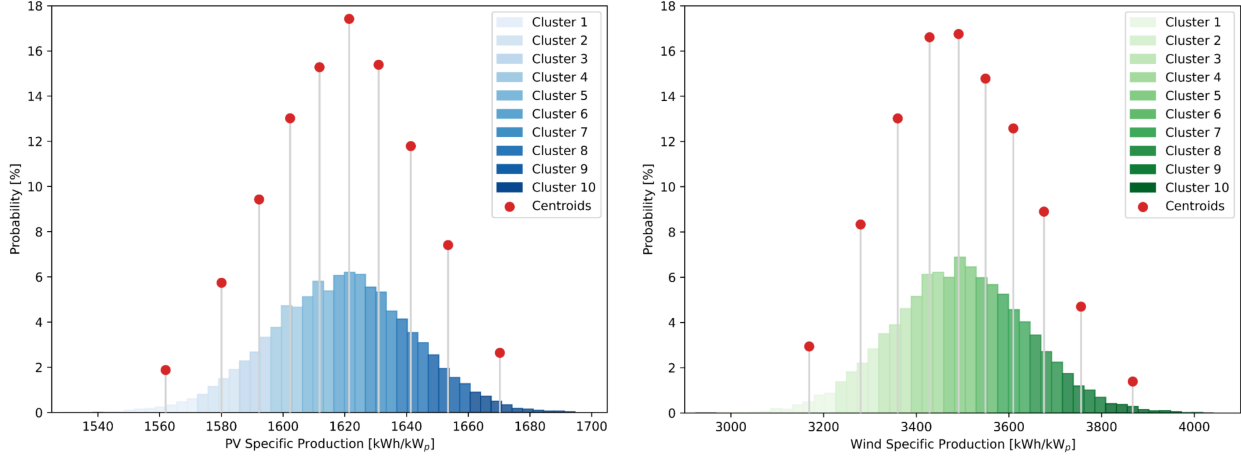


Figure 4.30: Scenario generation and reduction: histograms of annual PV and wind specific production from Monte Carlo pools (colours by cluster). Red circles: k -means centroids with empirical probabilities.

Table 4.20 reports the reduced centroids for PV and wind: the annual specific production (kWh/kW), the empirical probability (%), the weighted mean, and the distance from that mean. Consistent with Figure 4.28 and the literature [324], wind exhibits a larger spread than PV, indicating a higher incidence of both lull and very windy years.

These reduced scenario statistics quantify the persistence and depth of low-renewables periods that determine the value of hydrogen storage and the potential binding of the DG emissions cap.

4.4.5 Results and discussion

Deterministic baseline and Pareto frontier. The current configuration on Pantelleria (22 MW of DGs plus 1 MW of PV [306]) supplies the annual demand with 5.2% covered by PV and 94.8% by DGs, requiring 7900 m³ of diesel per year. The resulting TAC is 15.5 M€/yr and the associated emissions are 23.7 kt/yr, corresponding to 762 gCO₂/kWh, which exceeds by more than a factor of three the 2024 Italian grid intensity (274 gCO₂/kWh [325]). Figure 4.31 shows the cost–emissions Pareto front from the ϵ -constraint procedure (objective: TAC; constraint: annual CO₂ emission cap). The cap is tightened in 0.4 kt/yr steps, with two additional points at 0.25 and 0.10 kt/yr to resolve the approach to zero. The minimum-TAC configuration occurs at 3.2 kt/yr (i.e. 103 gCO₂/kWh) with TAC = 6.38 M€/yr. The zero-emissions configuration (100% RES-based) exhibits TAC = 8.10 M€/yr (+27% relative to the minimum-TAC point) while fully eliminating direct CO₂ emissions. In Figure 4.31, the pie charts explicitly show that, at minimum TAC, the electrical demand is covered 66.2% directly by RES, 15.1% by BESS, 6.2% by the hydrogen storage system (HSS) composed of EL+COMP+HS+FC and 12.5% by DGs; in the zero-emissions case the shares become 65.8% direct RES, 24.9% BESS and 9.3% HSS (no DG).

Table 4.20: Representative PV and wind scenarios after reduction: centroid annual specific production, probability, weighted mean and distance.

Scenario	Prod. [kW h/kW]	Prob. [%]	Weighted mean [kW h/kW]	Distance [%]
PV-1	1562.0	1.88	1618.7	-3.50
PV-2	1580.1	5.74	1618.7	-2.38
PV-3	1592.2	9.43	1618.7	-1.64
PV-4	1602.3	13.02	1618.7	-1.01
PV-5	1611.8	15.28	1618.7	-0.43
PV-6	1621.4	17.42	1618.7	0.17
PV-7	1631.0	15.39	1618.7	0.76
PV-8	1641.4	11.74	1618.7	1.40
PV-9	1653.4	7.41	1618.7	2.14
PV-10	1670.2	2.64	1618.7	3.18
WT-1	3169.0	2.94	3494.2	-9.31
WT-2	3279.8	8.33	3494.2	-6.14
WT-3	3359.9	13.02	3494.2	-3.84
WT-4	3428.7	16.61	3494.2	-1.87
WT-5	3491.3	16.75	3494.2	-0.08
WT-6	3549.5	14.78	3494.2	1.58
WT-7	3609.5	12.58	3494.2	3.30
WT-8	3675.7	8.90	3494.2	5.19
WT-9	3755.6	4.70	3494.2	7.48
WT-10	3867.2	1.39	3494.2	10.67

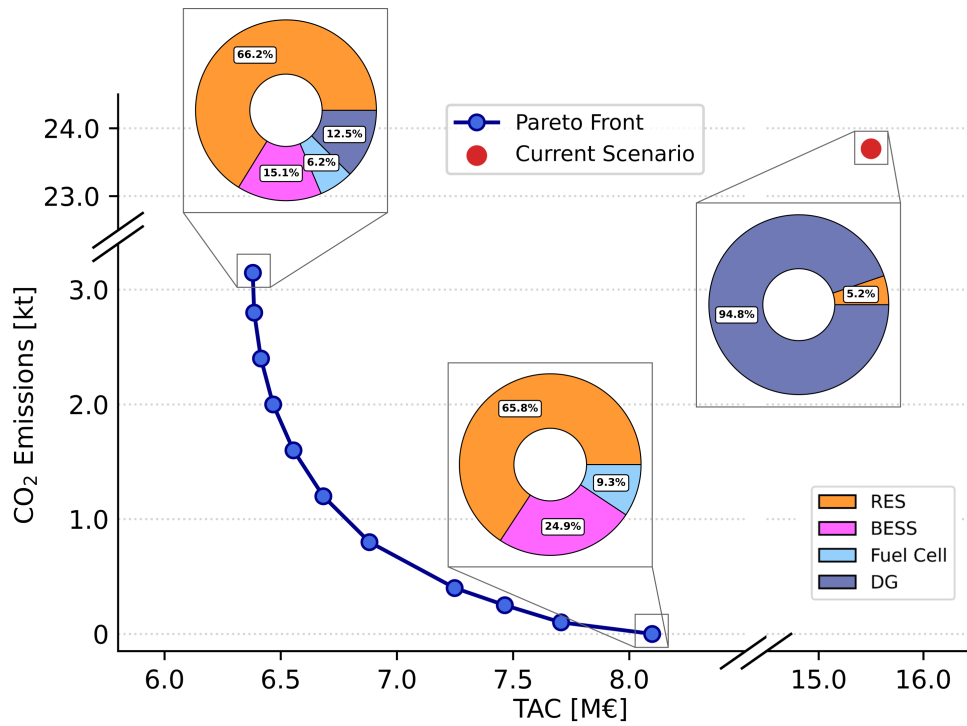


Figure 4.31: Cost–emissions Pareto front for the deterministic reference year against the current mix. The pie charts display the demand coverage shares (direct RES, BESS, HSS, DG) for the current, minimum-TAC, and zero-emissions points.

Capacity evolution along the Pareto front. Figure 4.32 shows how optimal component sizes evolve as the CO₂ cap is tightened. At the minimum-TAC point the selected capacities are: PV 9.7 MW, WT 8.8 MW, DG 3.3 MW, BESS 11.2 MWh, EL 1.6 MW, FC 1.0 MW, and HS 4.2 t (about 139 MWh, LHV basis). As the cap approaches zero, Figure 4.32 makes clear that DG capacity is eliminated and both RES and storage expand: PV reaches 15.8 MW (+62.9%), WT 10.8 MW (+22.7%), BESS 24.6 MWh (+119.6%), EL 3.4 MW (+116.6%), FC 3.5 MW (+253.5%), and HS 28.1 t (about 936 MWh, +564.3%). Figure 4.32 therefore indicates a pronounced scaling of long-duration elements at very low ϵ^{CO_2} , reflecting the need to bridge multi-day and seasonal deficits once DG flexibility is removed.

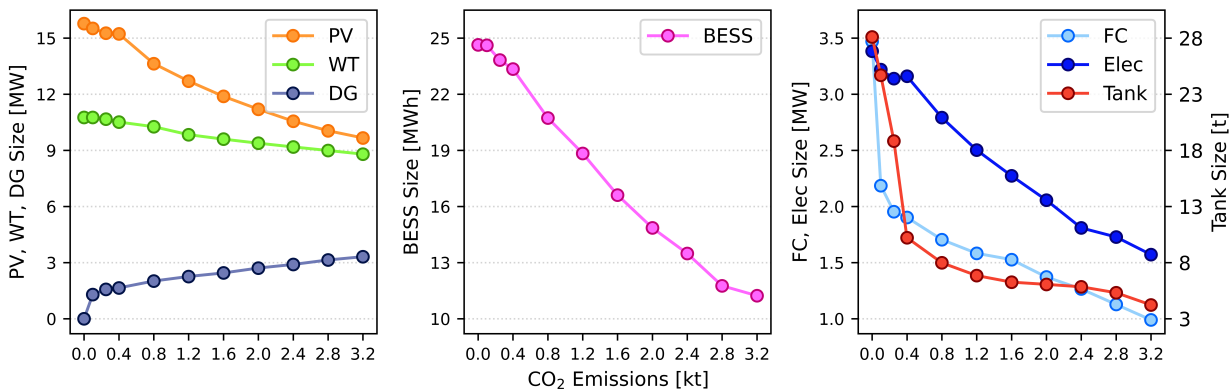


Figure 4.32: Optimal component sizes versus the annual CO₂ cap (deterministic).

Cost structure and component contributions. Figure 4.33 reports the TAC decomposition by component along the Pareto front. As the cap tightens, the DG contribution decreases to zero with falling diesel purchases, while the shares of PV, WT, BESS and HSS increase.

Specifically, Figure 4.33 shows DG-related costs declining from about 2.00 M€/yr at the minimum-TAC point to zero at the zero-emissions point; PV and WT contributions ranging from 1.00 to 1.64 M€/yr and from 1.14 to 1.39 M€/yr, respectively; and BESS and HSS increasing from 0.60 to 1.32 M€/yr and from 0.69 to 2.23 M€/yr. “Others” (engineering, installation, personnel) increase with plant scale from 0.93 to 1.52 M€/yr. Table 4.21 provides the numerical values at the two extremes (minimum TAC and zero emissions) and, consistently with Figure 4.33, disaggregates the HSS into EL, HS (including COMP), and FC contributions.

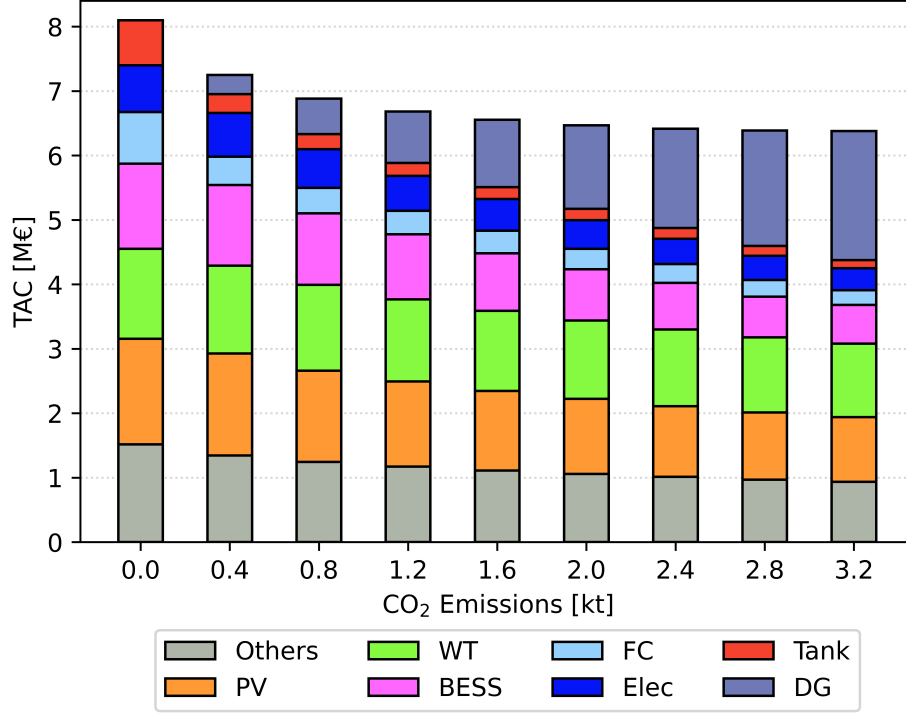


Figure 4.33: TAC breakdown versus the CO₂ cap (deterministic). Bars include CAPEX and OPEX.

Synthesis. Figure 4.31 indicates that all optimised points reduce TAC by roughly 48%–59% and emissions by 86.5% up to 100% relative to the current diesel-reliant mix. Figure 4.32 and Table 4.21 together show that BESS predominantly provides short-term balancing in both the minimum-TAC and zero-emissions configurations, while HSS (EL+COMP+HS+FC) scales to cover multi-day and seasonal deficits as DG use is phased out. Finally, Figure 4.33 makes explicit that the sharp TAC increase in the final decarbonisation steps is driven by the need to replace DG operational flexibility with long-duration storage and additional RES capacity.

Stochastic optimisation and effect on the Pareto frontier. Figure 4.34 compares the deterministic cost–emissions Pareto front with the stochastic counterpart obtained by enforcing feasibility (including the CO₂ cap ϵ^{CO_2}) across all scenarios. Figure 4.34 (left) shows a fan-shaped stochastic front: for a given emissions cap, the envelope (min–max band) across scenarios widens as the cap is tightened. The mean stochastic curve exhibits lower average emissions than the deterministic front at the same ϵ^{CO_2} , as sizing must guarantee security of supply in all ω . At relaxed caps (high allowable emissions), DGs buffer variability and the mean TAC remains close to the deterministic value, but with larger dispersion (primarily due to the variability of diesel use; water use variability has negligible cost impact). At stringent caps, the loss of DG flexibility requires larger capacities to cover worst-case low-VRE

Table 4.21: Component contributions to TAC at the Pareto extremes (deterministic). The COMP is included in HS costs.

Component	Zero emissions		Minimum TAC	
	Cost [M€]	Impact [%]	Cost [M€]	Impact [%]
PV	1.64	20.24	1.00	15.67
WT	1.39	17.16	1.14	17.87
BESS	1.32	16.30	0.60	9.40
FC	0.80	9.88	0.23	3.61
EL	0.73	9.01	0.34	5.33
HS	0.70	8.64	0.13	2.04
DG	–	–	2.01	31.50
Others	1.52	18.77	0.93	14.58
Total	8.10	100	6.38	100

realisations, and costs rise accordingly. In particular, Figure 4.34 (right) shows that at zero emissions the stochastic TAC increases by 15.7%, from 8.10 to 9.37 M€/yr. Table 4.22 quantifies these effects over the full cap range: the mean TAC increment grows monotonically from 0.3% (at 3.2 kt/yr) to 15.7% (at 0.0 kt/yr).

Table 4.22: Impact of stochastic optimisation on TAC at different CO₂ caps ϵ^{CO_2} . Mean/min/max refer to the distribution across $\omega \in \Omega$.

CO ₂ emissions [kt/yr]	Deterministic TAC [M€/yr]	Mean TAC [M€/yr]	Min TAC [M€/yr]	Max TAC [M€/yr]	Mean Δ TAC [%]
3.2	6.38	6.40	5.38	6.89	0.3
2.8	6.39	6.45	5.93	6.92	0.9
2.4	6.41	6.54	6.09	6.97	2.0
2.0	6.47	6.67	6.30	7.07	3.1
1.6	6.55	6.86	6.57	7.23	4.7
1.2	6.68	7.12	6.90	7.43	6.6
0.8	6.88	7.47	7.31	7.72	8.6
0.4	7.25	8.06	8.00	8.21	11.2
0.0	8.10	9.37	9.37	9.37	15.7

Zero-emissions design under uncertainty. Figure 4.35 shows the optimal component sizes for the zero-emissions configuration in deterministic and stochastic settings, together with the corresponding TAC impact. The figure indicates that, under uncertainty, PV increases from 15.8 to 18.6 MW and BESS from 24.6 to 38.8 MWh (+59.0%), while HS rises from 28.1 to 34.6 t (+23.1%). WT exhibits a modest decrease from 10.8 to 10.3 MW. On the right panel, Figure 4.35 makes explicit the TAC increase (+15.7%) driven by conservative sizing of storage and PV needed to ensure feasibility across all ω .

Operational variability across scenarios. Figure 4.36 presents the annual trajectories of the hydrogen level $\text{LOH}_{t,\omega}$ for the zero-emissions design (stochastic solution). The shaded band (interquartile range) and thin bounds (min–max) quantify the dispersion across ω ,

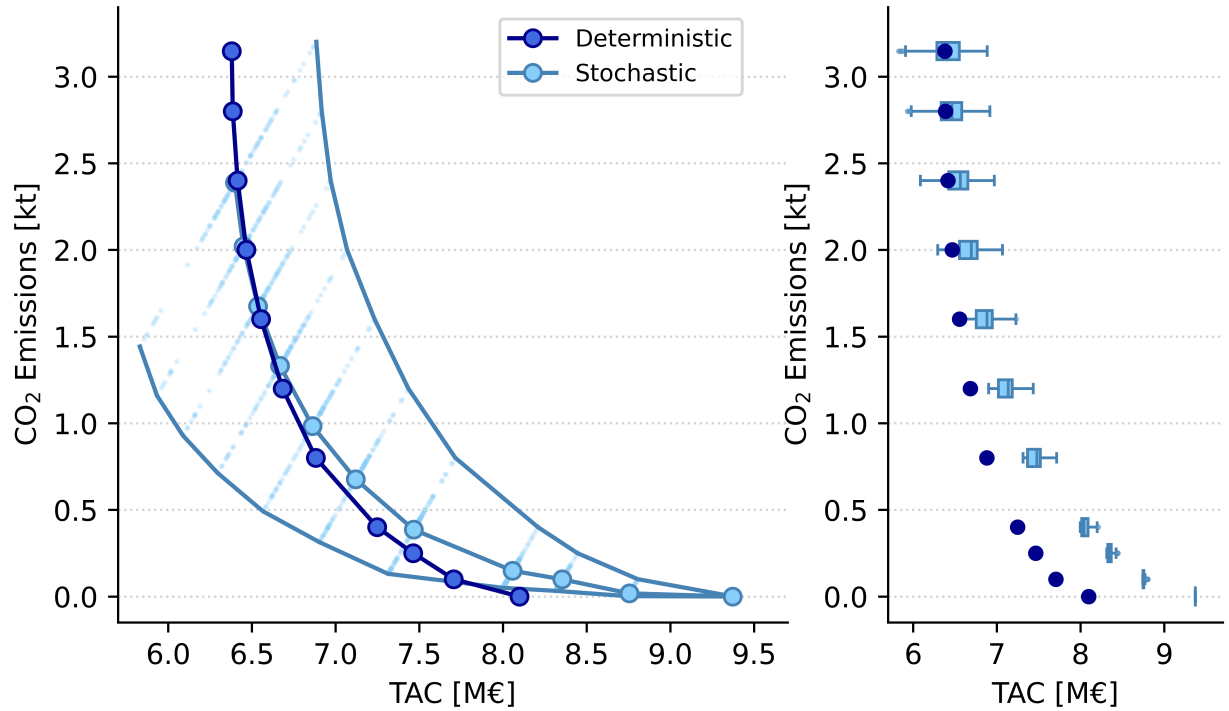


Figure 4.34: Cost-emissions Pareto fronts: deterministic vs. stochastic. Left: fan-shaped stochastic front with min-max envelope across scenarios. Right: boxplots of stochastic TAC at selected emission levels compared with deterministic values at the same CO₂ cap.

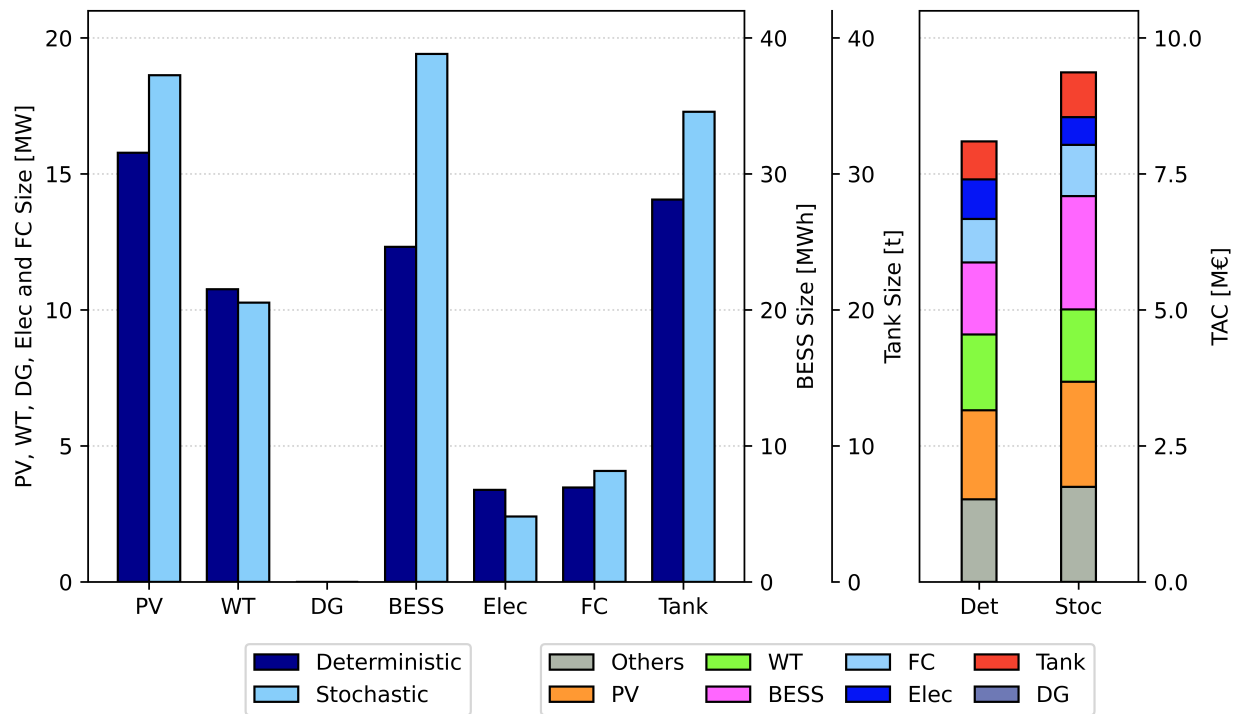


Figure 4.35: Zero-emissions configuration: deterministic vs. stochastic optimal sizes (left) and TAC impact (right).

while the solid line reports the deterministic trajectory for reference. Figure 4.36 shows that high-VRE scenarios (illustrative dashed green) operate with a smaller seasonal swing of LOH (implying that a smaller HS would have sufficed), whereas low-VRE scenarios (illustrative dashed red) require deeper drawdowns and more frequent FC utilisation, thereby justifying the larger HS selected by the stochastic design. This dispersion across ω mirrors the spread discussed in Figure 4.34 and in Table 4.22, and reflects the multi-day/seasonal coverage role of HS once DG is excluded.

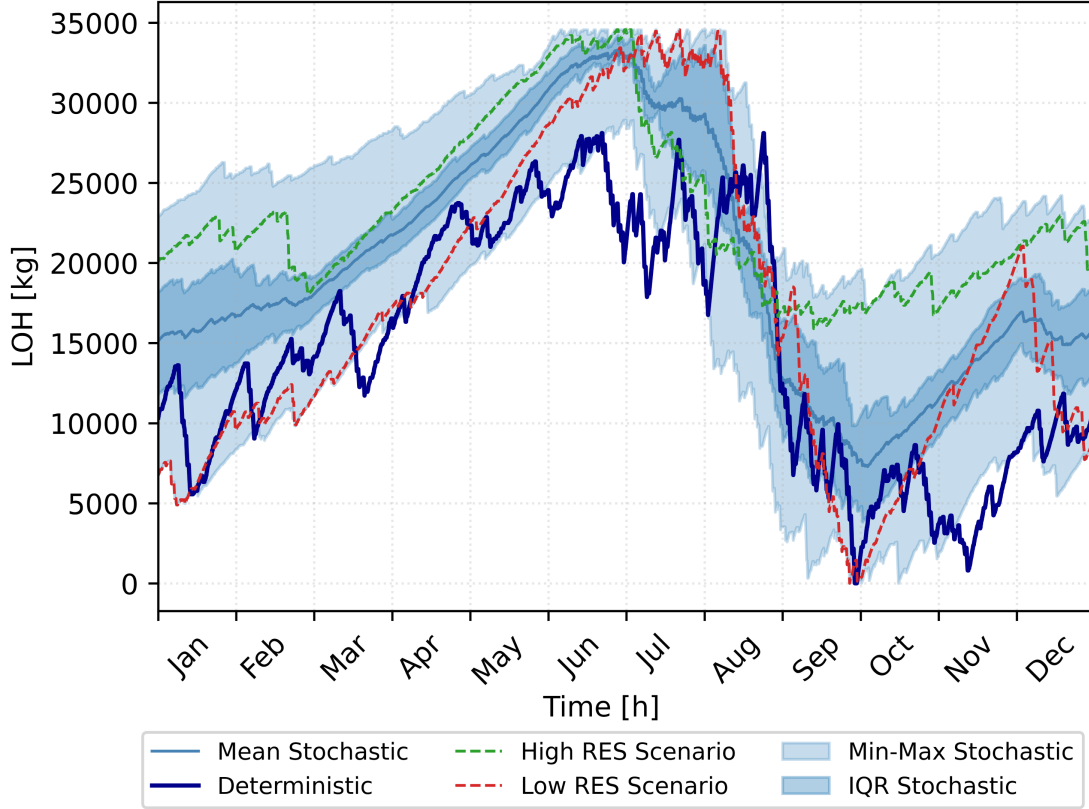


Figure 4.36: Hydrogen inventory trajectories $\text{LOH}_{t,\omega}$ for the zero-emissions configuration (stochastic solution). Shading: interquartile range; thin lines: min-max; solid: deterministic.

Summary. Figure 4.34 and Table 4.22 indicate that accounting for renewable-generation uncertainty shifts the Pareto front upward at tight caps and introduces dispersion due to scenario-dependent diesel usage at relaxed caps. Figures 4.35 and 4.36 together show that robust zero-emissions designs require materially larger BESS and HS (and somewhat larger PV) to bridge persistence of low-renewables periods across ω , which explains the observed TAC premium under uncertainty.

4.4.6 Main findings and methodological reflections

Findings. (i) Accounting for renewable-generation uncertainty reshapes the cost-emissions trade-off: Figure 4.34 shows a fan-shaped stochastic Pareto front, with the mean stochastic curve achieving lower average emissions than the deterministic curve at the same ϵ^{CO_2} due to non-anticipative sizing across ω (i.e., design variables common to all scenarios). The associated TAC dispersion widens as the emissions cap tightens. Quantitatively, Table 4.22 reports mean TAC increases from 0.3% at 3.2 kt/yr to 15.7% at zero emissions. (ii) The zero-emissions design is materially more storage- and PV-intensive under uncertainty: Figure 4.35 indicates

$P_{\text{nom}}^{\text{PV}}$ rises from 15.8 to 18.6 MW, BESS energy from 24.6 to 38.8 MWh (+59.0%), and HS from 28.1 to 34.6 t (+23.1%), while $P_{\text{nom}}^{\text{WT}}$ slightly decreases (from 10.8 to 10.3 MW). This capacity shift explains the TAC premium at zero emissions in Figure 4.34 (right). (iii) Operations display marked scenario-to-scenario variability even with a fixed design: Figure 4.36 shows wide interquartile and min–max bands for $\text{LOH}_{t,\omega}$ over the year. High-VRE realisations (illustrative dashed green) operate with tighter LOH swings, whereas low-VRE realisations (illustrative dashed red) require deeper seasonal drawdowns and more frequent FC utilisation, justifying the larger HS selected by the stochastic sizing.

Methodological reflections. The two-stage, risk-neutral shell proves appropriate for joint sizing–scheduling under uncertainty when non-anticipativity is imposed on the design s and recourse is allowed on hourly operations $\{v_{t,\omega}, \delta_{t,\omega}, x_{t,\omega}\}$. The scenario pipeline (Monte Carlo + Bootstrap daily recombination, followed by k -means reduction and Cartesian PV×WT combination) preserves diurnal structure and seasonality, enabling tractable year-long studies while retaining physics-faithful balances (cf. Figs. 4.34–4.36 and Table 4.22). At the same time, the separation between here-and-now s and recourse operations entails that sequential, information-adaptive scheduling decisions within the year are not optimised beyond a single stage of recourse. Moreover, the analysis is risk-neutral and places uncertainty only on VRE availability (PV, WT), with independence assumed after reduction.

Transition to multi-stage scheduling. Motivated by these limits, the next (and last) subsection focuses on multi-stage stochastic optimisation of operations when considering that the plant has already been built. The design s is fixed (e.g., to a representative two-stage solution on the Pareto front), and the hourly schedules $\{v_t, \delta_t, x_t\}$ are optimised over a scenario tree consistent with the information filtration, enforcing non-anticipativity at every stage. This setting captures the value of sequential recourse under unfolding uncertainty (e.g., persistent low-VRE spells) without incurring the prohibitive complexity of simultaneous size–schedule multi-stage optimisation.

4.5 Multi-stage stochastic MILP — Market-coupled scheduling

4.5.1 Motivation, scope and contributions

The two-stage results in Section 4.4 established how variability in renewable availability reshapes design and operations when the system is islanded and jointly sized–scheduled. Once capacities are commissioned, however, economic value is created (or eroded) hour by hour through scheduling and market participation. In the operating phase, the PtH plant, which in this case is represented by a hydrogen refuelling station (HRS), behaves as a hydrogen-enabled virtual power plant (VPP): it must meet its hydrogen offtake while arbitraging across sequential electricity markets—day-ahead, secondary reserve, multiple intraday auctions, and ex-post imbalance settlement—under uncertainty that is revealed progressively through the day (Section 3.2.5). In this context, effective market-coupled scheduling is central to lowering the LCOH: disciplined participation in DA/RM/IM and prudent imbalance management can monetise flexibility, mitigate penalties, and internalise degradation, thereby reducing operating expenditures per kilogram of H_2 .

Compared with the stand-alone sizing problem, several features become pivotal: (i) bids must be implementable ex post, so that DA commitments remain deliverable under later realisations of PV and prices; (ii) reserve capacity offers must honour instantaneous headroom/footroom and energy margins over the activation window; (iii) intraday redis-

patch should absorb forecast updates without speculative reshaping; and (iv) imbalance settlement must be represented financially consistently (Section 3.2.5). Casting this as a multi-stage stochastic MILP aligned with the pre-June 2024 Iberian market sequence (DA→RM→IM1–IM6→IM7→IB) enables gate-wise non-anticipative decisions that adapt as information arrives (scenario tree generation and reduction as described in Section 3.2.5), while keeping the daily horizon tractable. The present subsection therefore fixes the design s and focuses on the market-coupled scheduling problem under sequential uncertainty, as further documented in [238].

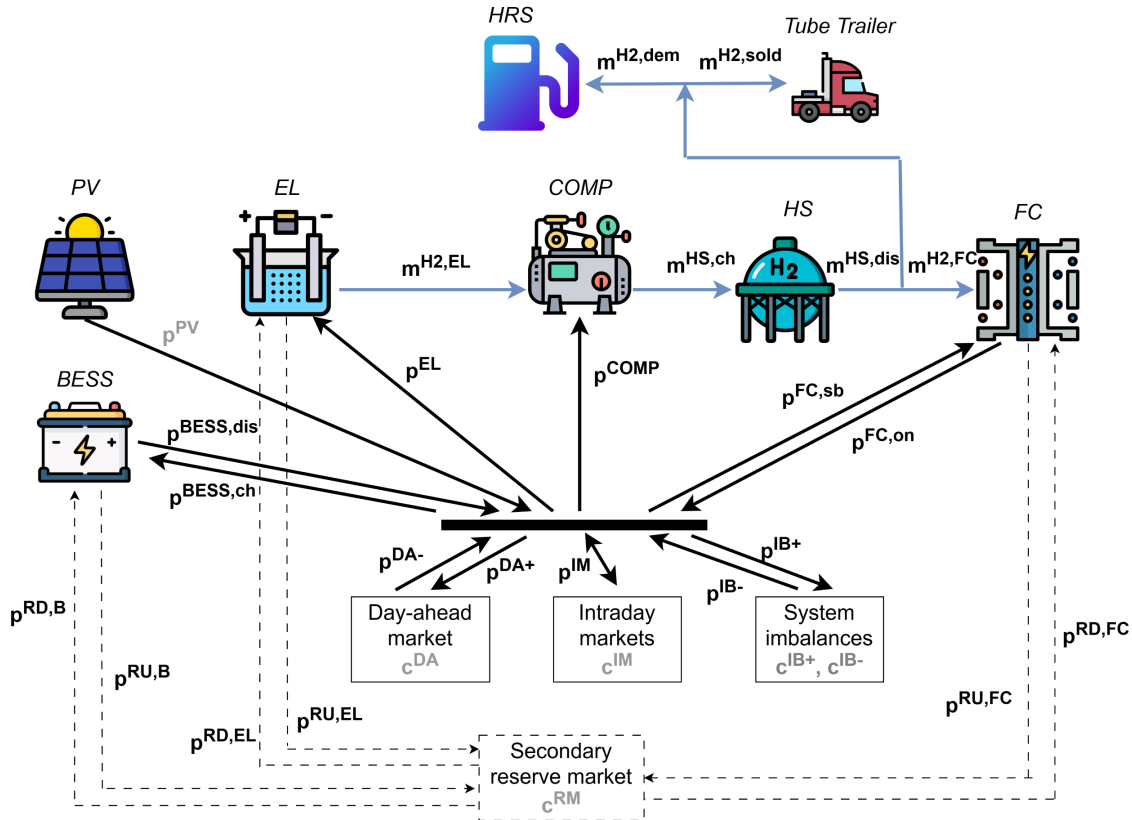


Figure 4.37: Overview of the hydrogen-enabled VPP. Random parameters (grey) and decision variables (black).

Contributions. Building on Section 3.2.5, this section: (i) formulates a risk-neutral multi-stage stochastic MILP that co-optimises DA bidding, secondary-reserve capacity, all intraday redispatches, delivery-stage set-points, and IB settlement, enforcing gate-wise non-anticipativity and the DA bidding-curve structure with explicit monotonicity and minimum-block rules; (ii) embeds state-dependent operating dynamics for electrolyser and fuel cell—minimum load, standby draw, warm/cold starts, and time-at-load degradation—together with a throughput-based BESS ageing proxy, so that reserve headroom/footroom and activation-energy feasibility are honoured without sacrificing tractability; (iii) represents all market layers coherently—DA, six IM sessions plus IM7, secondary reserve, and IB—so that early commitments are deliverable and later recourse mirrors actual operational degrees of freedom (price-accepting quantities at RM/IM decision times; ex-post IB with positive/negative parts), capturing full uncertainty in PV availability and prices at each market layer via a scenario tree; (iv) yields implementable artefacts for operations and trading: hourly DA supply/demand curves, price-accepting RM/IM volumes consistent with technical limits, and delivery-stage schedules that co-evolve with SOC and LOH, enabling an OPEX-phase assessment of LCOH drivers under market uncertainty.

4.5.2 Model outputs

The scheduling problem has been modelled exactly as in Section 3.2.5. The HRS under study is represented in Figure 4.37 as a VPP comprising PV, BESS, EL, COMP, HS, and (optionally) FC, with linear device physics and inter-hour recursions taken from Secs. 3.2.1–3.2.2. Market participation follows the pre-June 2024 DA→RM→IM1–IM6→IM7→IB sequence; uncertainty affects PV availability and prices at all gates. The complete compact formulation for the daily problem is summarised in Eq. 3.225.

Output (i): Optimal DA bidding curves. For each hour t , the model returns monotone step-wise supply/demand curves obtained a posteriori by sorting scenarios by $c_{t,\omega}^{\text{DA}}$ and pairing the price rank with the matched $p_{t,\omega}^{\text{DA}+}$ (sell) or $p_{t,\omega}^{\text{DA}-}$ (buy) as represented in Figure 4.38. Buying-only bids (negative quantities) express willingness to purchase that decreases with price; selling-only bids (positive quantities) increase with price; mixed bids cross the quantity axis near an indifference price. These curves are implementable by construction and consistent with market rules.

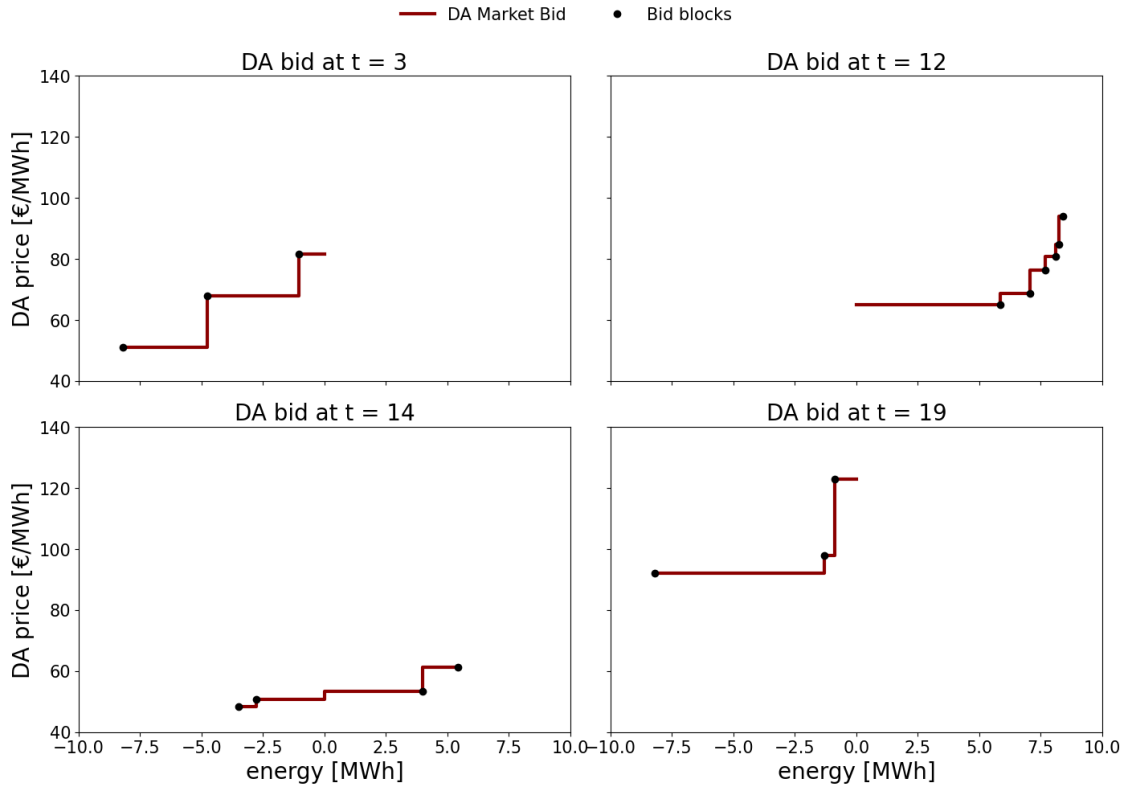


Figure 4.38: Representative DA bids for four hours: buying-only (negative), selling-only (positive), and mixed (axis-crossing) cases. Markers show block pairs (quantity–price); lines connect blocks to illustrate the monotone step-wise curve.

Output (ii): Price-accepting RM/IM quantities. Upward/downward secondary-reserve capacities $\{p_{t,\omega}^{\text{RU}}, p_{t,\omega}^{\text{RD}}\}$ (with technology splits from BESS, EL, FC) are committed at RM clearing. Similarly, intraday positions $\{p_{t,\omega}^{\text{IM}_i}\}$ are price-accepting at each session i . This yields implementable redispatch consistent with technical limits and with the sequential information structure.

Output (iii): Delivery-stage schedules, commitments, and inventories. To honour submitted bids in every scenario, the model produces hourly set-points for grid exchanges and plant operation (BESS charge/discharge; EL ON/STANDBY loads; COMP consumption; HS

charge/discharge; FC *ON*/*STANDBY* output) together with $\text{SOC}_{t,\omega}$, $\text{LOH}_{t,\omega}$, and imbalance volumes $p_{t,\omega}^{\text{IB}\pm}$. Figure 4.39 reports a one-day mean across scenarios: The DA position is decomposed into DA sell (solid dark red) and DA buy (dark red, cross-hatched). Subsequent intraday adjustments appear as IM sell (solid dark yellow) and IM buy (dark yellow, cross-hatched), while any residual deviations are captured as positive imbalances (solid grey) and negative imbalances (grey, cross-hatched). On the physical side, PV generation (light green) is allocated between export and internal use, primarily the EL (dark blue) and the COMP (turquoise). The FC dispatch is shown in purple, cross-hatched, with FC standby consumption indicated in purple. The bottom timelines highlight unit-commitment states for the EL and the FC: *ON* (orange), *STANDBY* (grey), and *OFF* (white). The LOH in the HS co-evolves with these flows, increasing when electrolysis dominates and decreasing when meeting hydrogen demand or generating via the FC.

Output (iv): Variability bands and endogenous responses. Finally, Figure 4.40 illustrates scenario dispersion for key drivers and one endogenous response. Exogenous inputs from the scenario tree (PV generation; DA and RM prices) are shown as hourly percentiles (10–90 and 25–75 bands, median line). The electrolyser load is endogenous: its percentile bands reflect the scheduler’s response to price/PV realisations, reserve commitments, start-up costs, and ageing penalties.

4.5.3 Configurations

Four operational configurations are assessed; all enforce exact daily hydrogen delivery and differ only in market participation options and flexibility carriers:

- *Base.* PV–EL–COMP–HS–FC with secondary-reserve participation; hydrogen spot sales disabled ($\phi = 0$). The scheduler maximises expected profit from electricity markets while satisfying the contracted hydrogen demand and internal constraints; this serves as the operational benchmark.
- *No-reserve.* Same asset portfolio as Base, with reserve offers disallowed, to isolate the contribution of reserve remuneration and its scheduling effects.
- *BESS instead of FC.* The FC is replaced by a BESS sized to provide comparable reserve capacity (Table 4.24), allowing a like-for-like comparison between PtHtP reversion and electrochemical storage.
- *H₂ sales enabled.* Base portfolio with optional surplus hydrogen sales ($\phi = 1$), to test the optimal split between electricity-market arbitrage and hydrogen export when sales are permitted.

The HRS is located in Barcelona (postal code 08028), where a baseline daily hydrogen demand of 1440 kg_{H₂}/day at 700 bar is imposed via the refuelling load. In fleet equivalence, 1440 kg_{H₂}/day would correspond roughly to 50–60 heavy-duty trucks (about 27 kg/day each over 300 km/day), or 150 transit buses (10 kg/day each), or 2500 passenger FCEVs (0.5 kg/day each for 50 km/day). A plausible mixed-fleet combination is therefore on the order of 20 trucks, 40 buses and 1000 cars, which sums to the imposed baseline demand. The hydrogen sale-price parameter is set to $c^{\text{H}_2} = 3\text{€}/\text{kg}$, aligned with recent estimates of the prevailing cost of grey hydrogen in Southern Europe [267].

The hourly H₂ demand profile used in the daily optimisations represented in Figure 4.41 is constructed by averaging demand curves for mixed-fleet refuelling reported in the literature [326–329]. The resulting 24-hour profile, normalised so that its daily integral equals

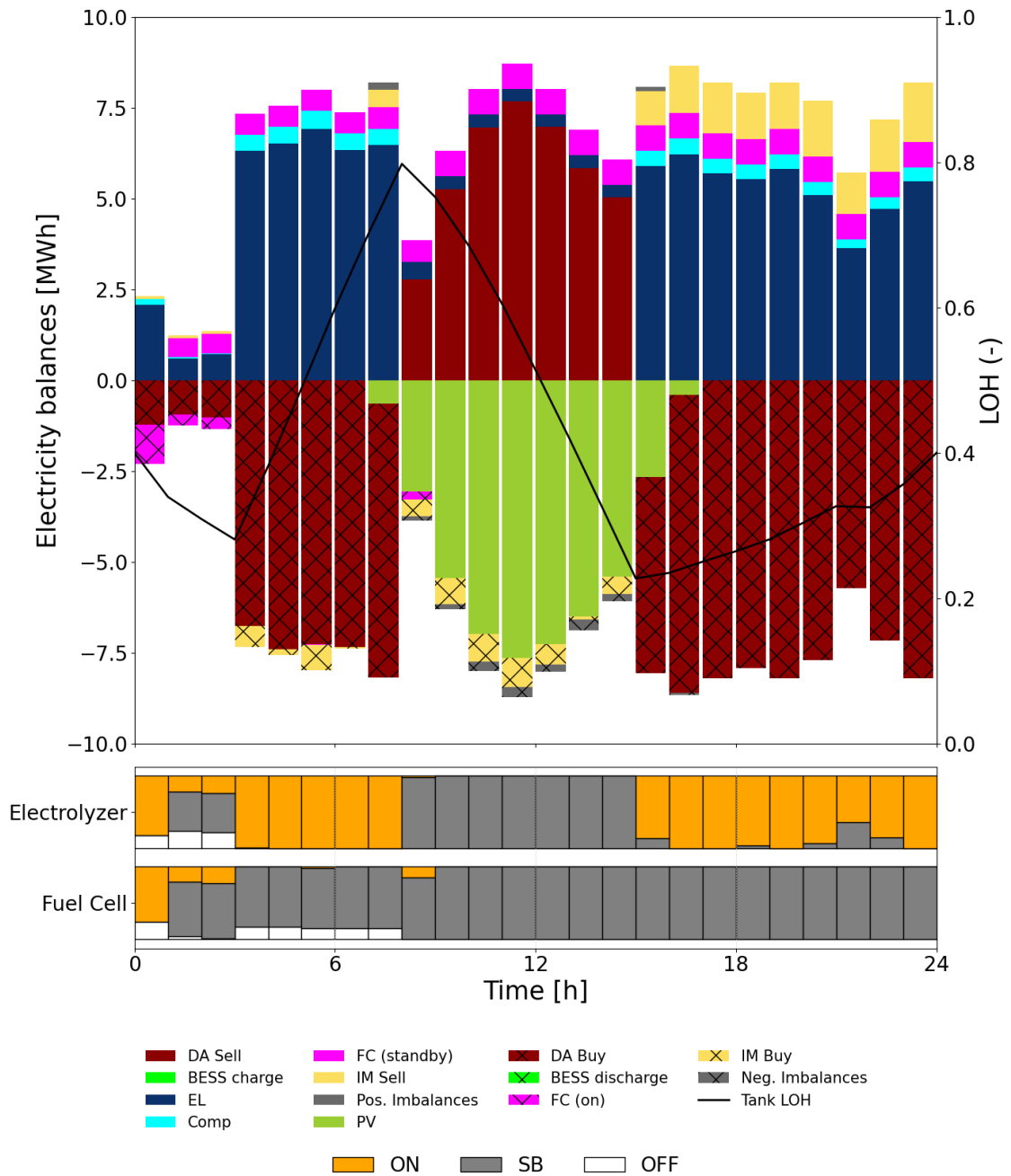


Figure 4.39: Behaviour summary over one day (means across scenarios): DA sell/buy, IM sell/buy, positive/negative imbalances; PV production; EL and COMP consumption; FC dispatch and standby draw; EL/FC ON/*STANDBY*/*OFF* timelines; co-evolution of the hydrogen inventory LOH.

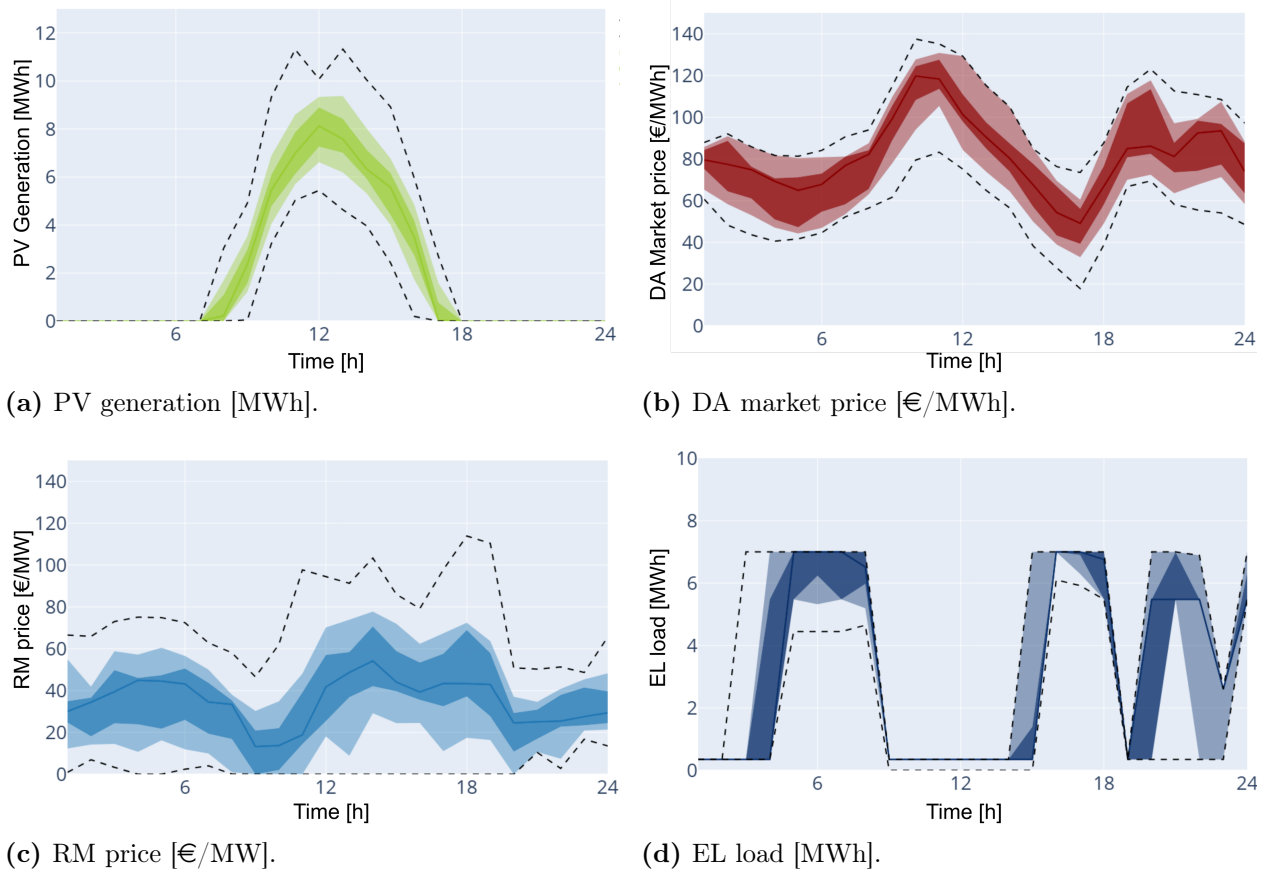


Figure 4.40: Percentiles of PV generation [MWh] (top left), DA market price [€/MWh] (top right), RM price [€/MW] (bottom left), and EL load [MWh] (bottom right) over a day. In every plot, there are: maximum and minimum (dashed black line), 10–90 percentile (light), 25–75 percentile (dark), and median (solid line).

1440 kg_{H₂}/day, exhibits a pronounced midday peak between 12:00 and 15:00, with low demand during the night and moderate morning and evening shoulders. Empirical studies of comparable fleets suggest that weekly and seasonal deviations around this mean shape remain typically within ± 10 – $\pm 15\%$ of the baseline level [330], which supports reusing the same normalised profile on consecutive days and scaling it only by the daily total.

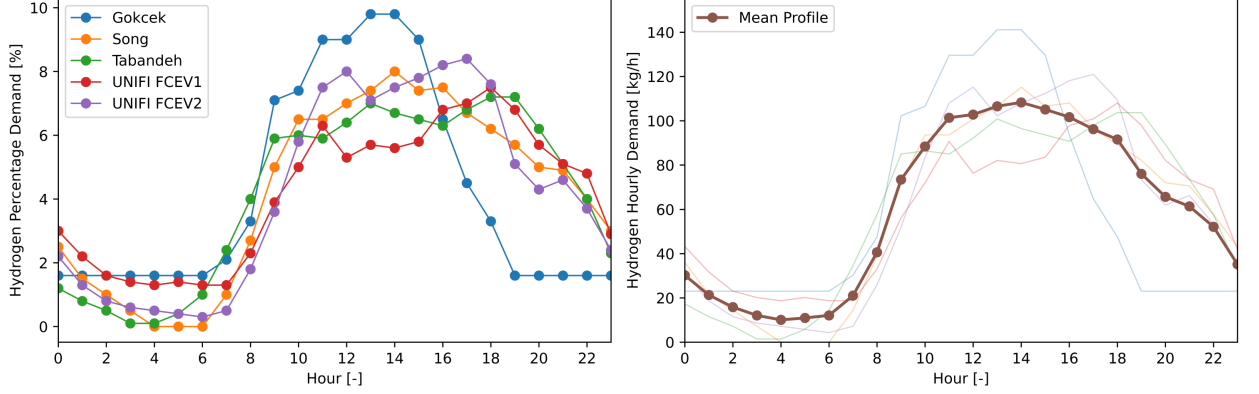


Figure 4.41: Mean hourly hydrogen demand profile normalised to 1440 kg_{H₂}/day; pronounced midday peak and moderate dispersion support a fixed daily profile [326–330].

4.5.4 Technical and economic inputs

The PV, EL, COMP and HS capacities used here were not tuned directly in the market-optimisation layer. Instead, they were sized in prior design work using a Genetic Algorithm (GA) embedded in the MESS platform (Section 3.1), a multi-energy simulation tool capable of long-horizon techno-economic assessment with component ageing. Following [249], the GA minimised the LCOH over a 25-year horizon subject to: (i) exact satisfaction of the baseline daily demand profile at the HRS, (ii) compliance with the RED III RFNBO carbon-intensity limit, and (iii) hourly operational feasibility of all devices, including storage and compression. The optimal configuration adopted as input to the market study comprises a 12 MW PV array, a 7 MW EL capable of producing approximately 140 kg_{H₂}/h at full load, and a 500 kW COMP sized to lift the EL outlet from 30 bar to the 700 bar storage/refuelling level. The HS capacity is set to 1120 kg_{H₂}, corresponding to roughly eight hours of continuous EL operation at nameplate, in line with literature indicating that beyond-diurnal HS is generally not cost-effective under current European energy and ancillary-service markets [331]. For reconversion, the SOFC block is sized at 7 MW, matching the EL nameplate to simplify comparison between production and HtP use. Component-level technical parameters and economic parameters are summarised in Tables 4.23 and 4.24; in this case study the electrolyser (EL) is parameterised as a PEM electrolyser (PEMEL).

Market and stochastic inputs The HRS participates in the Iberian electricity market through its EL, BESS (where applicable), and FC. The IM-to-DA cap is set at $R^{\text{IM/DA}} = 0.20$ in Eqs. 3.212–3.213, which means that in each intraday (IM) session the absolute volume that can be reshaped (bought or sold) is limited to at most 20% of the corresponding day-ahead (DA) position for that hour. This reflects a practical limit on active position management rather than a hard market rule, and avoids unrealistic full re-optimisation of DA commitments at each IM gate.

For reserve provision, we adopt a secondary-reserve (automatic Frequency Restoration Reserve, aFRR) product with activation window $T^{\text{RM}} = 0.25$ h (15 min), consistent with the

Table 4.23: Component characteristics and case-study inputs (PV–EL–COMP–HS–FC).

Component	Parameter [unit]	Symbol	Value	Ref.
PV	Nominal power [MW]	$P_{\text{nom}}^{\text{PV}}$	12	–
	Tilt angle [°]	–	optimal	[177]
	Azimuth angle [°]	–	0 (south)	[177]
	Reference year [–]	–	2023	–
EL	Nominal power [MW]	$P_{\text{nom}}^{\text{EL}}$	7	–
	Spec. elect. cons. [kWh/kg _{H₂}]	SEC^{EL}	50	–
	Minimum load fraction [–]	$u_{\text{min}}^{\text{EL}}$	0.20	[78]
	Standby fraction [–]	$u_{\text{sb}}^{\text{EL}}$	0.05	[78, 79]
	Operating pressure [bar]	$\mathcal{P}^{\text{EL}}$	30	–
	Water use [m ³ /kg _{H₂}]	$s_{\text{CH}_2\text{O}}$	0.015	–
	Water price [€/L]	$c_{\text{H}_2\text{O}}$	0.004	–
	Lifetime [h]	LT^{EL}	80000	[332]
	Replacement cost [M€/MW]	SRC^{EL}	1.2	–
	Warm start cost [€/(MW event)]	$c^{\text{EL,warm}}$	0.8	[333, 334]
	Cold start cost [€/(MW event)]	$c^{\text{EL,cold}}$	8.2	[333, 334]
	Initial state (day one) [–]	$\delta_{\text{ini}}^{\text{EL,on}}, \delta_{\text{ini}}^{\text{EL,sb}}, \delta_{\text{ini}}^{\text{EL,off}}$	0, 0, 1	–
COMP	Nominal power [MW]	$P_{\text{nom}}^{\text{COMP}}$	0.5	–
	Specific consumption [kWh/kg _{H₂}]	$\text{SEC}_{30 \rightarrow 700}^{\text{COMP}}$	3.5	[197]
	Inlet→outlet pressure [bar]	$\mathcal{P}^{\text{in}} \rightarrow \mathcal{P}^{\text{out}}$	30 → 700	–
HS	Nominal capacity [kg]	$m_{\text{nom}}^{\text{HS}}$	1120	–
	Operating pressure [bar]	$\mathcal{P}^{\text{HS}}$	700	–
	Max (dis)charge rate [kg/h]	$\dot{m}^{\text{HS,max}}$	600	–
	Charging efficiency [–]	$\eta^{\text{HS,ch}}$	0.995	–
	Discharging efficiency [–]	$\eta^{\text{HS,dis}}$	0.995	–
	LOH _{max} , LOH _{min} [–]	LOH _{max} , LOH _{min}	0.99, 0.10	–
	Initial/final LOH [–]	LOH ₀ , LOH _T	0.40, 0.40	–
FC	Nominal power [MW]	$P_{\text{nom}}^{\text{FC}}$	7	–
	Spec. fuel cons. [kg _{H₂} /kWh]	SFC^{FC}	0.06	–
	Minimum load fraction [–]	$u_{\text{min}}^{\text{FC}}$	0.20	[335]
	Standby fraction [–]	$u_{\text{sb}}^{\text{FC}}$	0.10	[335]
	Operating pressure [bar]	$\mathcal{P}^{\text{FC}}$	1.05	–
	Lifetime [h]	LT^{FC}	60000	[336]
	Replacement cost [M€/MW]	SRC^{FC}	1.5	–
	Warm start cost [€/(MW event)]	$c^{\text{FC,warm}}$	0.8	[333, 334]
	Cold start cost [€/(MW event)]	$c^{\text{FC,cold}}$	8.2	[333, 334]
	Initial state (day one) [–]	$\delta_{\text{ini}}^{\text{FC,on}}, \delta_{\text{ini}}^{\text{FC,sb}}, \delta_{\text{ini}}^{\text{FC,off}}$	0, 0, 1	–

Table 4.24: BESS characteristics for the “BESS instead of FC” configuration.

Parameter [unit]	Symbol	Value	Ref.
Energy capacity [MW h]	$E_{\text{nom}}^{\text{BESS}}$	10	–
C-rate [h^{-1}]	$\mathcal{C}$	0.35	[222]
Charging efficiency [–]	$\eta^{\text{BESS,ch}}$	0.9	–
Discharging efficiency [–]	$\eta^{\text{BESS,dis}}$	0.9	–
Max/Min SOC [–]	$\text{SOC}_{\text{max}}, \text{SOC}_{\text{min}}$	0.90, 0.10	–
Initial/final SOC [–]	$\text{SOC}_0, \text{SOC}_T$	0.40, 0.40	–
Replacement cost [M€ h/MW]	SRC^{BESS}	0.35	–
Life cycles [–]	cyc_{max}	10000	[337]

Spanish implementation of aFRR on the PICASSO platform and the current technical rules of the transmission system operator [241, 242]. Reserve bids $p_{t,\omega}^{\text{RU}}$ and $p_{t,\omega}^{\text{RD}}$ therefore represent up/down capacities that must be deliverable within this time frame.

Stochastic inputs for prices and PV are generated as in Section 3.2.5. For each target delivery day, hourly DA, RM, IM and imbalance (IB) prices, together with site-specific PV generation time series, are collected from historical data for 2022–2023 up to the day before the optimisation (sources: OMIE for prices [338] and PVGIS for PV production [177]). These historical trajectories are then processed through a TSFA→VAR pipeline to capture temporal correlations, and bootstrap fans are drawn to generate an ensemble of plausible future realisations around the latest observations. Finally, a forward-selection algorithm reduces the ensemble to a 100-scenario tree aligned with the DA, IM and reserve gate structure, striking a balance between capturing uncertainty and keeping the MILP tractable.

Solver settings. Each day is modelled as a 24-hour multistage MILP on the above 100-scenario tree and solved with Gurobi, using a relative MIP optimality gap of 1%. All runs are executed on a shared HPC node equipped with two 48-core AMD CPUs (96 physical cores in total). Under these settings, the median wall-clock time per daily instance is approximately three minutes (December 2023 runs), which is compatible with a day-ahead decision-support workflow.

4.5.5 Results and discussion

Results are reported for the four configurations of Section 4.5 over December 2023 (Barcelona).

Common exogenous drivers. Across all configurations, the same representative December day with pronounced PV uncertainty is examined to enable like-for-like comparisons. The exogenous inputs for that day are those already shown in Figure 4.40: percentiles of PV generation, the day-ahead price $c_{t,\omega}^{\text{DA}}$, and the reserve-market price $c_{t,\omega}^{\text{R}}$. These inputs are identical for the Base, No-reserve, and BESS-instead-of-FC cases; only market-participation choices and flexibility portfolios differ, while the stochastic drivers remain the same.

Base configuration. Figure 4.42 collects, for the same representative day, the main outputs of the optimisation under the *Base* configuration: Panel (a) reports the net DA position percentiles $p_t^{\text{DA}+} - p_t^{\text{DA}-}$ (dark-red ribbons), the mean total intraday correction $p_t^{\text{IM,tot}}$ (yellow line), and the mean scheduled upward/downward reserve $p_t^{\text{RU}}, p_t^{\text{RD}}$ (blue lines). Panel (b) shows the percentiles of the hydrogen inventory $\text{LOH}_{t,\omega}$ in the HS. Panel (c) presents the expected hourly energy balance as stacked bars, separating positive contributions (DA sell,

EL and COMP consumption, FC standby, IM sell, positive imbalances $p_{t,\omega}^{\text{IB}+}$) and negative contributions (DA buy, FC ON, IM buy, PV production). Bottom timelines display, for each hour, the scenario shares of EL and FC operating states (*ON/STANDBY/OFF*).

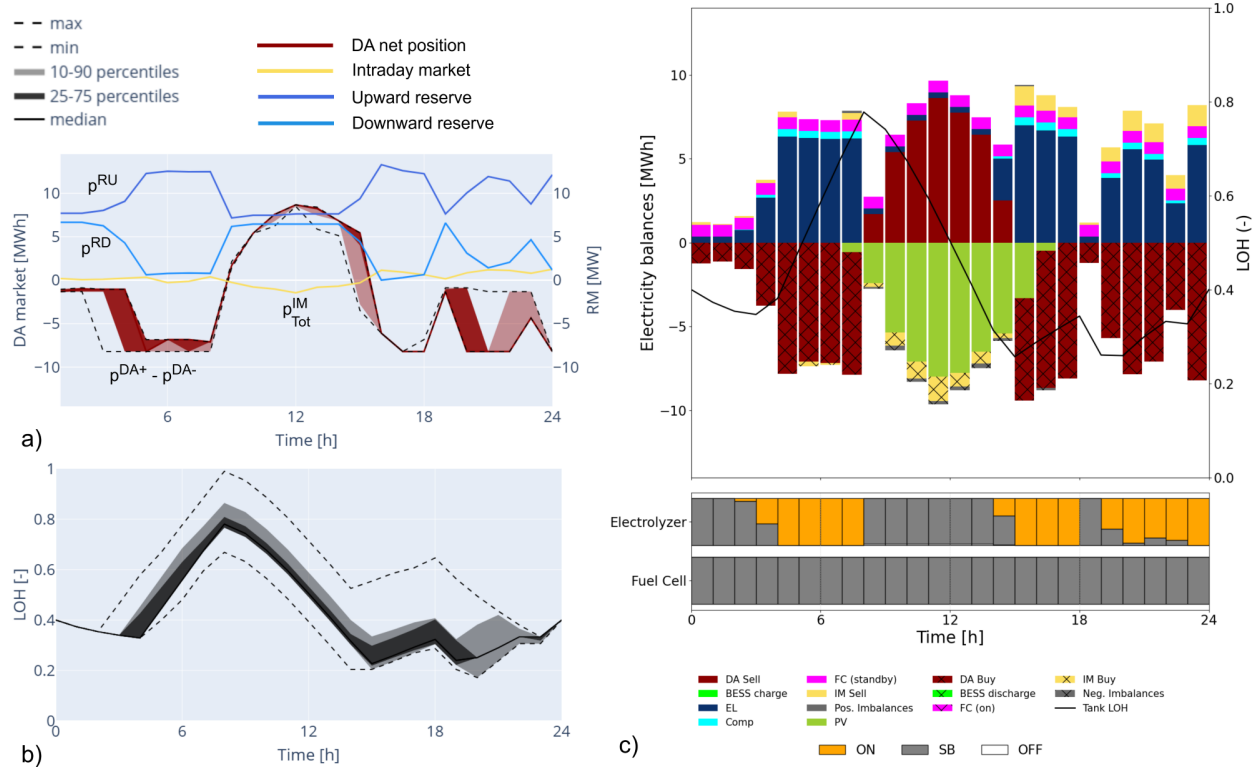


Figure 4.42: Representative day (December 2023, Barcelona) — *Base* configuration with reserve. (a) Net DA position percentiles $p_t^{\text{DA}+} - p_t^{\text{DA}-}$ (dark-red ribbons); mean total intraday correction $p_t^{\text{IM,tot}}$ (yellow line); mean scheduled reserve p_t^{RU} , p_t^{RD} (blue). (b) LOH_{t,ω} percentiles in the HS. (c) Expected hourly energy balance (stacked). Bottom: EL/FC operating-state shares by hour.

Given the drivers in Figure 4.40, the model builds, for each hour t , the DA bidding curve as an ordered set of blocks $\{(p_{t,\omega}^{\text{DA}}, c_{t,\omega}^{\text{DA}})\}_{\omega \in \Omega}$. Figure 4.38 represents the results obtained in this case showing that off-peak hours (low $c_{t,\omega}^{\text{DA}}$) produce buying-only bids, solar-noon hours with stronger $c_{t,\omega}^{\text{DA}}$ and PV yield selling-only bids, and transition hours often cross the quantity axis near an indifference price. Aggregating blocks yields $p_t^{\text{DA}+}$ and $p_t^{\text{DA}-}$, whose percentiles in Figure 4.42a show a net buying stance in off-peak hours and net selling around midday.

Intraday reshaping $p_t^{\text{IM,tot}}$ remains modest on average, indicating that most price/volume risk is hedged at the DA gate. Scheduled upward reserve p_t^{RU} exceeds downward reserve p_t^{RD} , because the FC is kept hot in *STANDBY* (able to contribute only to up capacity), whereas the EL contributes up/down when operated. Panel (c) confirms that the FC never turns *ON* to generate energy: the poor PtHtP round-trip efficiency and explicit degradation/usage costs make capacity remuneration preferable to energy production. The EL meets the exact daily delivery with concentrated *ON* blocks (average load factor 42%), limiting starts and time-at-load costs and using *STANDBY* strategically to keep response available without incurring additional cold starts. The LOH bands in Figure 4.42b stay comfortably within bounds, preserving headroom/footroom for reserve. Imbalances $p_{t,\omega}^{\text{IB}\pm}$ are small on average and peak in hours where PV uncertainty is widest (Figure 4.40a), consistent with the financially coherent imbalance settlement in Section 3.2.5.

No-reserve configuration. Relative to the previous configuration, the *No-reserve* case removes scheduled capacity $p_t^{\text{RU}} \equiv 0$, $p_t^{\text{RD}} \equiv 0$ and, with it, the economic role of *STANDBY*,

as shown in Figure 4.43. The optimiser therefore suppresses idle consumption and keeps the FC *OFF* at all hours. The EL exhibits a more pronounced bang–bang pattern: hydrogen production is concentrated in fewer, larger *ON* blocks to (i) meet the exact daily delivery and (ii) minimise the number of start events and time-at-load costs. As a result, $\text{LOH}_{t,\omega}$ shows larger step changes between fill and drawdown episodes, with wider interquartile bands when the production blocks straddle hours of PV/price uncertainty.

Without reserve remuneration, value shifts toward DA positioning and intraday arbitrage. The mean intraday correction $p_t^{\text{IM,tot}}$ is typically higher than in the *Base* case around the EL *ON* windows, reflecting more frequent reshaping to track updated price and PV information. Net DA positions remain negative (buying) off-peak and positive (selling) near solar noon, but the ribbons are somewhat wider because DA bids can no longer “lean” on up/down headroom monetised in RM. Imbalances $p_{t,\omega}^{\text{IB}\pm}$ modestly increase in hours with the largest PV dispersion, since there is no reserve-enabled buffer to absorb residual forecast errors.

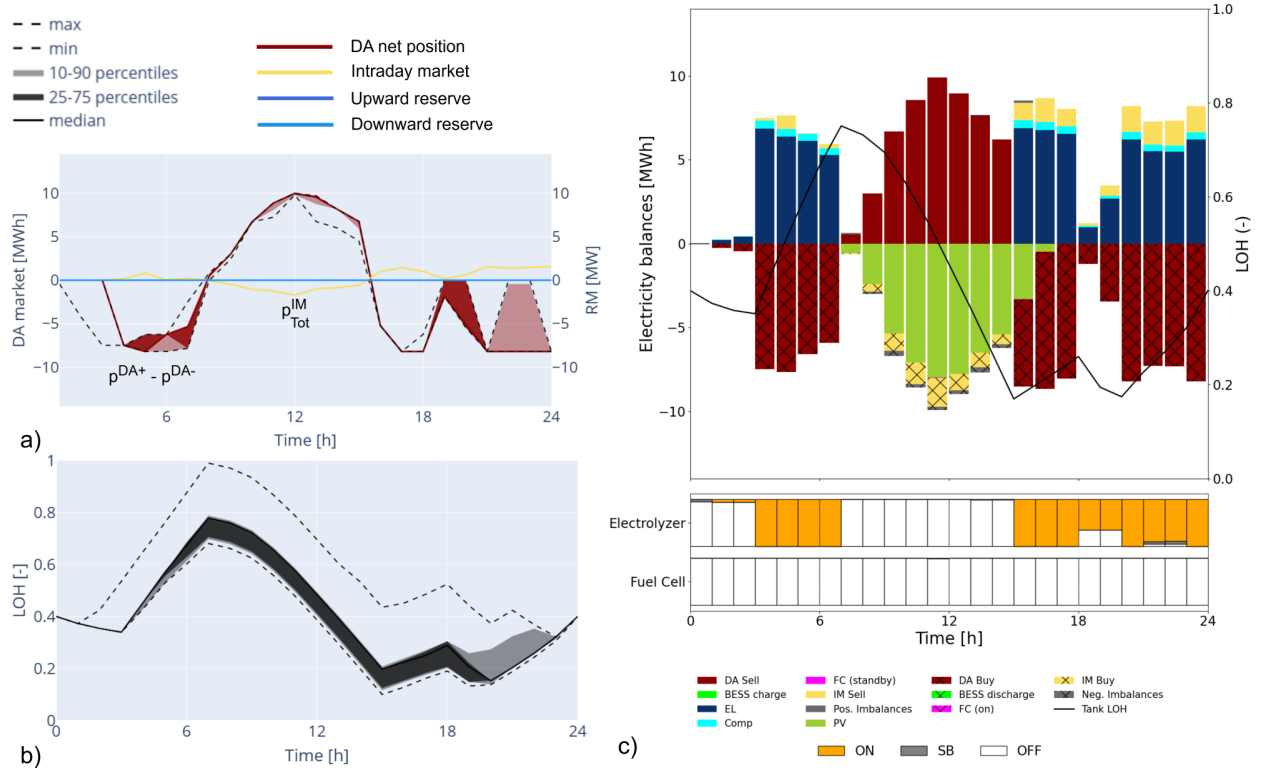


Figure 4.43: Representative day (December 2023, Barcelona) — *No-reserve* configuration.

BESS-instead-of-FC configuration. Replacing the FC with a BESS (Figure 4.44) restores fast flexibility without PtHtP losses. Scheduled reserves become more bidirectional and symmetric: p_t^{RU} and p_t^{RD} are of comparable magnitude across most hours, in contrast with the *Base* case where $p_t^{\text{RU}} > p_t^{\text{RD}}$ due to FC *STANDBY*-only up capability. The net DA stance tightens around high-price hours: additional discharge capability allows shifting some margin from IM/IB to DA when spreads justify it. Consistently, the mean intraday correction $p_t^{\text{IM,tot}}$ often increases relative to the *Base* case, signalling that the BESS enlarges the feasible (and profitable) redispatch space across sessions.

Operationally, $\text{SOC}_{t,\omega}$ executes two–three bounded cycles per day (aligned with PV and price peaks), while the HS $\text{LOH}_{t,\omega}$ trajectory is smoother than in the *Base* case because sub-hour/fast balancing is delegated to the BESS. This reduces expected imbalances $p_{t,\omega}^{\text{IB}\pm}$ and eliminates FC *STANDBY* draw. The throughput-based ageing term in the objective discourages gratuitous cycling, so extra charge–discharge swings only appear where expected

spreads (net of round-trip losses) compensate the implicit degradation cost; this curbs SOC churning during flat-price hours and pushes flexibility toward the most valuable gates.

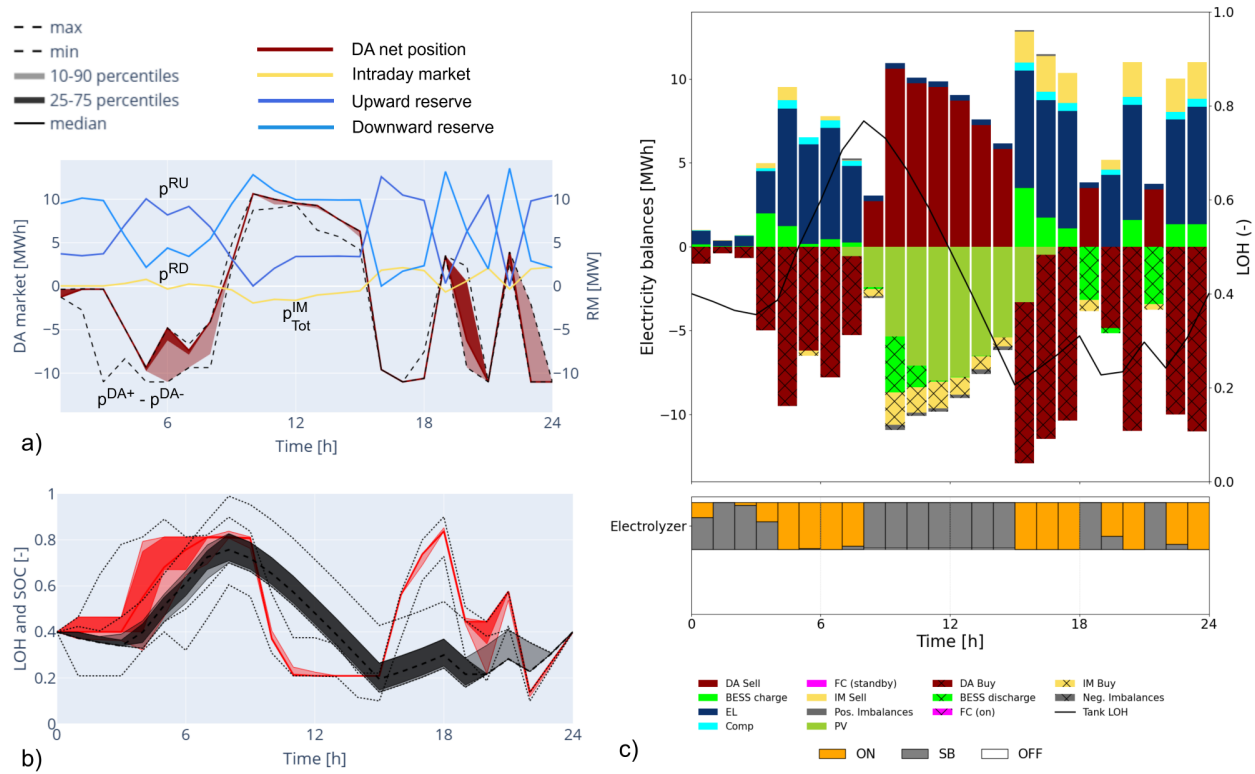


Figure 4.44: Representative day (December 2023, Barcelona) — *BESS instead of FC* with reserve.

Monthly results. Figure 4.45 aggregates December 2023 outcomes (31 daily optimisations) for the four configurations analysed here, including the *H₂ sales enabled* case. Each panel reports, via box plots, statistics across daily runs for total profit and for all objective-function terms defined in Section 3.2.5: DA/IM energy, reserve capacity, imbalance settlement, water consumption, start-up costs (warm and cold combined), ageing penalties, the fixed revenue associated with the contracted H₂ delivery, and—where permitted—hydrogen-sales revenue.

In panel (a) (*Base*), profits are primarily sustained by reserve-capacity payments and by the fixed hydrogen-delivery revenue remunerated at $c^{H_2} = 3 \text{ €/kg}$; DA/IM energy and imbalance terms remain comparatively small. The FC operates almost exclusively in *STANDBY* (average load factor $\sim 2\%$), monetising reserve capacity while avoiding inefficient PtHtP energy production and associated degradation.

Panel (b) (*No-reserve*) exhibits a marked drop in median profit and a narrower dispersion: the disappearance of capacity revenues is not compensated by DA/IM arbitrage. Exposure to price and PV variability increases, consistent with the day-level patterns discussed previously.

Panel (c) (*BESS instead of FC*) raises the median profit and tightens the spread. The BESS delivers symmetric, bidirectional reserve and short-horizon time shifting that jointly (i) reduce expected imbalance payments and (ii) improve DA/IM contributions despite round-trip losses; ageing costs are present but are more controllable (cycle-cost proxy) and lower than FC running/degradation costs.

Panel (d) (*H₂ sales enabled*) introduces a positive hydrogen-sales component that slightly relaxes dependence on electricity arbitrage. Gains materialise episodically—e.g., when DA prices fall below $\sim 40\text{--}50 \text{ €/MWh}$, conditional on the EL state inherited from the previous hour—yet, at the monthly scale, lift the profit distribution relative to (a) while leaving reserve revenues essentially unchanged.

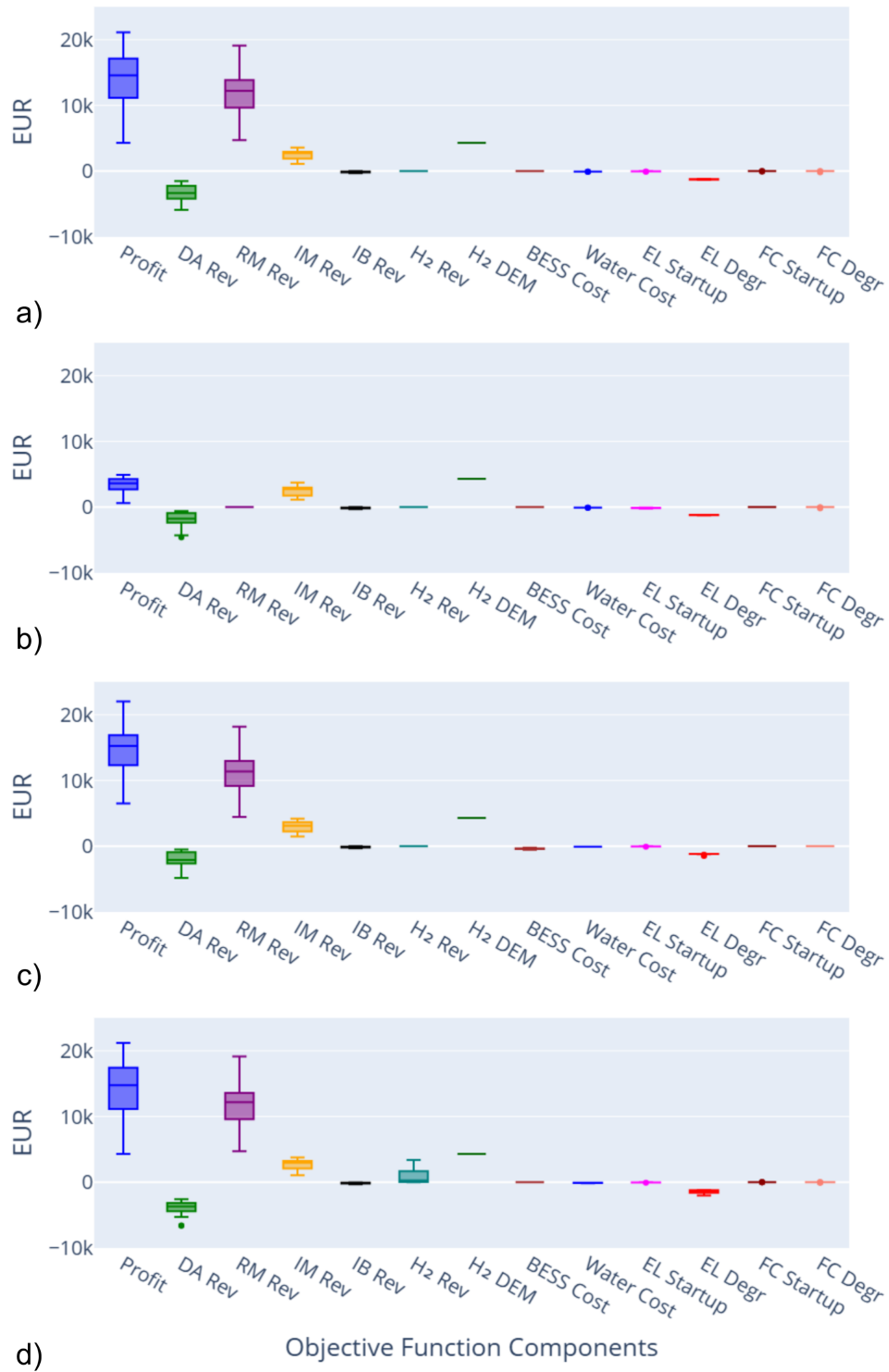


Figure 4.45: Monthly objective breakdown (December 2023; 31 daily optimisations). Box plots show median (line), interquartile range (box), and Tukey whiskers with outliers (1.5 IQR). (a) *Base:* FC with reserve, no H₂ sales; (b) *No-reserve:* same portfolio without reserve; (c) *BESS instead of FC* with reserve; (d) *H₂ sales enabled:* FC with reserve and H₂ sales enabled.

Summary. Across daily and monthly views, reserve reshapes operating states and improves profitability without entering the physical energy balance. Disabling reserve reduces expected profit and heightens exposure to DA/IM variability. Substituting the FC with a BESS preserves reserve revenues, increases controllable DA/IM contributions, reduces expected imbalances, and yields a more symmetric flexibility mix. Allowing H_2 sales adds a price-contingent uplift; however, the BESS substitution remains the more robust lever for stabilising and raising monthly profits.

4.5.6 Main findings and methodological reflections

Main findings. A multi-stage stochastic MILP has been developed and tested for a hydrogen-enabled VPP represented by an HRS with PV, EL, COMP, HS, and an optional FC or BESS. The model co-optimises participation in DA, secondary reserve (aFRR), six intraday auctions, and imbalance settlement while enforcing exact hydrogen off-taker fulfilment. Device behaviour is represented with tri-state operation (*ON/STANDBY/OFF*), warm/cold starts, and degradation for EL/FC; BESS ageing is captured via a cycle-cost term, yielding operationally realistic schedules. Uncertainty in PV and market prices is represented with scenario trees aligned to the information filtration ($DA \rightarrow RM \rightarrow IM_1-IM_6 \rightarrow IM_7 \rightarrow IB$), following the OMIE timing pre-June 2024.

Four case studies were examined: (i) *Base* with FC and reserve; (ii) *No-reserve*, which has the same portfolio without reserve; (iii) *BESS instead of FC* sized to provide comparable reserve; and (iv) *H_2 sales enabled*. The main behavioural and economic takeaways are:

- (i) *Base with reserve.* Reserve remuneration reshapes operating states and economics without entering the energy balance: near-flat DA posture off-peak and net selling around solar noon; modest intraday corrections; $p_t^{RU} > p_t^{RD}$ due to hot-standby FC; EL delivers $1440 \text{ kg}_{H_2}/\text{d}$ at $\sim 42\%$ average load factor via concentrated *ON* blocks; LOH stays within bounds; imbalances remain small on average. (ii) *No-reserve.* Without capacity revenues, *STANDBY* becomes a pure cost; EL behaves bang-bang (with occasional standby to avoid cold starts), FC remains *OFF*, exposure to DA/IM variability increases, LOH shows larger steps, and monthly profits decrease.
- (iii) *BESS instead of FC.* Reserve becomes more bidirectional and symmetric; DA net-position bands tighten around solar hours; DA/IM adjustments increase in a controllable way; expected imbalances fall; median monthly profit increases.
- (iv) *H_2 sales enabled.* Surplus H_2 sales provide episodic uplift when DA market price is low, improving overall profit while leaving reserve income essentially unchanged; nevertheless, the BESS substitution in the third configuration yields the larger and more robust monthly gain.

Methodological reflections. Three elements are pivotal for implementable bids and feasible schedules: (i) tri-state EL/FC modelling with warm/cold starts and running/degradation costs; (ii) multi-stage, non-anticipative coordination across DA, RM, IM, and IB decisions with a posteriori recovery of monotone DA bid curves consistent with market rules; and (iii) ageing-aware costs (BESS cycles and EL/FC usage) to prevent chattering, ensure reserve deliverability, and respect storage bounds.

Limitations and future work. Rolling-horizon re-optimisation with forecast updates and explicit modelling of reserve activation energy merit further development. In practice, once DA clears, the problem can be re-solved with updated information for RM; the process then iterates at each IM session through to IB, regenerating scenario trees aligned with the evolving information set and data sources.

5. ORIGINAL CONTRIBUTION

5.1 List of publications

- P1. A. Ademollo, A. S. Vilalta, C. Carcasci, F. J. Heredia, “Multi-stage stochastic optimization of hydrogen-enabled virtual power plants for co-optimized electricity market bidding and off-taker fulfilment”, working paper, planned submission to *Applied Energy*, 2025.
- P2. A. Ademollo, N. Ulivi, L. Ferretti, F. Serafini, C. Carcasci, C. Pacini, “Policy-constrained agrivoltaics in Italy: A potato case study linking shading, crop and economics”, *Applied Energy*, vol. 405, 127225, 2026 (open access). DOI: 10.1016/j.apenergy.2025.127225
- P3. A. Ademollo, M. Calabrese, C. Carcasci, I. Joshi, M. Vaccaro, “Comparative techno-economic assessment of stationary hydrogen storage technologies”, *International Journal of Hydrogen Energy*, vol. 199, 152849, 2026 (open access). DOI: 10.1016/j.ijhydene.2025.152849
- P4. M. Calabrese, A. Ademollo, C. Carcasci, “Designing off-grid hybrid renewable energy systems under uncertainty: A two-stage stochastic programming approach”, *Renewable Energy*, vol. 256, 124193, 2025. DOI: 10.1016/j.renene.2025.124193
- P5. A. Franco, C. Carcasci, A. Ademollo, M. Calabrese, C. Giovannini, “Integrated plant design for green hydrogen production and power generation in photovoltaic systems: Balancing electrolyzer sizing and storage”, *Hydrogen*, 6(1):7, 2025. DOI: 10.3390/hydrogen6010007
- P6. A. Ademollo, M. Calabrese, C. Carcasci, “An up-to-date perspective of levelized cost of hydrogen for PV-based grid-connected power-to-hydrogen plants across all Italy”, *Applied Energy*, vol. 379, 124958, 2025. DOI: 10.1016/j.apenergy.2024.124958
- P7. A. Ademollo, A. Mati, M. Pagliai, C. Carcasci, “Exploring the role of hydrogen in decarbonizing energy-intensive industries: A techno-economic analysis of a solid oxide fuel cell cogeneration system”, *Journal of Cleaner Production*, 469:143254, 2024. DOI: 10.1016/j.jclepro.2024.143254

- P8. M. Calabrese, A. Ademollo, L. Busi, M. Meazzini, C. Carcaschi, “Techno-economic assessment of green hydrogen production for blending in the natural gas network”, *Journal of Physics: Conference Series*, vol. 2893, 012066, 2024. DOI: 10.1088/1742-6596/2893/1/012066
- P9. A. Ademollo, C. Carcaschi, A. Ilo, “Behavior of the electricity and gas grids when injecting synthetic natural gas produced with electricity surplus of rooftop PVs”, *Sustainability*, 16(22):9747, 2024. DOI: 10.3390/su16229747
- P10. A. Mati, A. Ademollo, C. Carcaschi, “Assessment of paper industry decarbonization potential via hydrogen in a multi-energy system scenario: A case study”, *Smart Energy*, 11:100114, 2023. DOI: 10.1016/j.segy.2023.100114
- P11. A. Ademollo, A. Ilo, C. Carcaschi, “End-use sector coupling to turn customer plants into prosumers of electricity and gas”, *IET Conference Proceedings* (CIRED 2023), pp. 357–361, 2023. DOI: 10.1049/icp.2023.0308

5.2 Mapping between thesis chapters and peer-reviewed outputs

Table 5.1 summarises how the main thesis chapters and case studies correspond to the core peer-reviewed publications produced during the PhD. This complements the narrative discussion below and provides a concise navigation aid for readers.

Table 5.1: Mapping between thesis chapters and the primary peer-reviewed publications.

Thesis location	Model family	Related publication	Journal and status
Section 4.1	Rule-based simulation: paper-mill cogeneration (solid oxide fuel cell combined heat and power)	[P7]; [P10]	<i>Journal of Cleaner Production</i> (published); <i>Smart Energy</i> (published)
Section 4.2	Rule-based simulation + GA optimisation: Italy-wide PV-based PtH screening	[P6]	<i>Applied Energy</i> (published)
Section 4.3	Deterministic optimisation: stationary hydrogen storage technology comparison	[P3]	<i>International Journal of Hydrogen Energy</i> (published)
Section 4.4	Two-stage stochastic optimisation: island system design under renewable uncertainty	[P4]	<i>Renewable Energy</i> (published)
Section 4.5	Multi-stage stochastic optimisation: market-coupled scheduling for hydrogen refuelling station	[P1]	Planned submission: <i>European Journal on Operations Research</i>
Appendix 7	Agrivoltaics extension under land constraints	[P2]	<i>Applied Energy</i> (published)

5.3 Discussion

The thesis is primarily based on the publications that directly underpin the modelling developments and case studies presented in the chapters, namely [P10], [P7], [P6], [P3], [P4], [P1] and [P2]. The other works [P11], [P9], [P8] and [P5] are related outputs that extend the same research line to additional applications (sector coupling, blending, PV–hydrogen integration) but are not central to the structure of the thesis. In this section, the focus is therefore on the papers that were effectively used to write the thesis.

Rule-based multi-energy system modelling and industrial applications

The first step of the thesis is grounded in rule-based simulation of hydrogen-enabled industrial energy systems. In [P7], a hydrogen-based solid oxide fuel cell (SOFC) cogeneration system is assessed for an energy-intensive paper mill, comparing three options: a conventional natural gas-fuelled gas turbine, a SOFC fed with grey hydrogen produced via steam methane reforming, and a SOFC supplied with green hydrogen produced on-site. This work provides the detailed thermo-economic treatment of cogeneration options, explicit modelling of SOFC behaviour and steam supply, and a consistent link between component-level performance and plant-level indicators such as LCOH and net present cost.

In [P10], the focus shifts to retrofitting an existing cogeneration plant. Starting from the real energy consumption of a paper mill, the paper analyses the conversion of a conventional natural gas turbine-based cogeneration system to a hydrogen-fuelled gas turbine supplied by locally produced green hydrogen. The hydrogen-fuelled gas turbine is modelled in detail, and a multi-energy system model is built for the upstream hydrogen production chain, including PV-powered PEM electrolyzers, hydrogen storage and gas-turbine utilisation. The main contribution is a thorough techno-economic assessment of this retrofit pathway, quantifying the cost of green hydrogen and highlighting the sensitivity of project profitability to natural gas prices and investment costs.

The nation-wide analysis in [P6] then combines the rule-based MESS framework with a genetic algorithm to design PV-based, grid-connected power-to-hydrogen plants supplying constant hydrogen demand across all Italian bidding zones under evolving European regulations for green-hydrogen certification. This work contributes to the thesis by: (i) establishing the methodology used to link plant design, degradation and temporal-correlation rules to LCOH and grid dependence; and (ii) clarifying which design levers (PV-to-electrolyser ratio, hydrogen storage, battery storage, correlation rules) most strongly affect plant economics and certified green hydrogen shares.

Together, [P10], [P7] and [P6] provide the industrial case studies, data and rule-based modelling insights used in the early chapters of the thesis. They also reveal the limitations of rule-based approaches: the absence of guaranteed optimality, the difficulty of systematically valuing flexibility, and the lack of a formal treatment of uncertainty. These limitations motivate the transition to optimisation-based models.

Deterministic optimisation for hydrogen storage technology choice

The deterministic mixed-integer linear programming (MILP) formulation developed in the thesis for comparing stationary hydrogen storage technologies is captured in the manuscript [P3]. Building on the techno-economic and regulatory insights from [P6], this work embeds different storage technologies into a single optimisation framework where plant capacities and hourly operation are co-optimised over a representative year.

The original contribution relevant to the thesis lies in showing that once plant-level design and operation are jointly optimised, storage technologies that look quite different at component level can yield similar LCOH, and that non-economic aspects such as geology, footprint and required buffering duration can be decisive. This deterministic layer marks the transition from rule-based scenario exploration to rigorous cost-optimal design under a single, representative future, and highlights why a more explicit treatment of uncertainty is needed for robust capacity decisions.

Two-stage stochastic optimisation for design under uncertainty

The two-stage stochastic MILP framework used in the thesis for off-grid hybrid renewable-hydrogen systems is presented in [P4]. In this framework, first-stage variables represent investments (PV, wind, batteries, hydrogen storage, diesel backup), while second-stage variables represent hourly operation across multiple renewable scenarios. The Pantelleria case study directly corresponds to one of the main thesis case studies.

For the purposes of the thesis, the key contributions of [P4] are: (i) the explicit separation between design decisions and operational recourse under uncertainty; (ii) the quantification of the cost of robustness by comparing two-stage solutions against deterministic, perfect-foresight ones; and (iii) the demonstration that deterministic designs can misrepresent both cost and emissions when variability in renewable generation is neglected. This paper provides the methodological and numerical backbone for the thesis chapters dealing with design under uncertainty.

Multi-stage stochastic optimisation for market-coupled operation

Once the plant is built, capacity decisions are fixed and the main lever left to reduce effective hydrogen cost is operation, particularly through interaction with electricity markets. The multi-stage stochastic optimisation model developed in the thesis and summarised in [P1] addresses this operational problem for a grid-connected power-to-hydrogen plant serving a hydrogen refuelling station.

[P1] encapsulates the main methodological advances of the final part of the thesis: scenario-tree-based representation of prices and renewable output across day-ahead, intraday and reserve markets; non-anticipativity constraints that enforce a realistic information structure; and detailed modelling of state variables for batteries, fuel cells and hydrogen storage. This work supplies the multi-stage framework and case-study results used in the thesis to show how co-optimised bidding and recourse operation can increase expected profit and reduce downside risk compared with deterministic or rule-based strategies.

Agrivoltaics and land-constrained extensions

The agrivoltaic modelling framework described in [P2] is used in the thesis as an extension to discuss land-constrained PV deployment and its implications for hydrogen systems. Although the paper focuses on a potato case study in Italy, it contributes a way to link shading, crop yield and farm economics under policy constraints. In the thesis, this work provides the conceptual and modelling basis for incorporating alternative PV layouts and land-use constraints into the plant design problem without changing the core optimisation structure.

Additional related publications

The remaining publications [P11], [P9], [P8] and [P5] form part of the broader research activity carried out during the PhD, but they are only indirectly used in the thesis. [P11] addresses end-use sector coupling and prosumer-level flexibility from a power and gas perspective. [P9] extends the sector-coupling view to synthetic natural gas produced from rooftop PV surplus, and [P8] analyses green hydrogen production for blending in the natural gas grid. [P5] studies integrated PV–hydrogen plants with a stronger focus on combined power and hydrogen services. These works support the general background and motivation of the thesis and illustrate the wider applicability of the modelling expertise developed, but they are not central to the thesis structure and are therefore only briefly referenced here.

Overall, the core publications [P10], [P7], [P6], [P3], [P4], [P1] and [P2] underpin the main chapters of the thesis and reflect its methodological trajectory: from detailed rule-based simulation, through deterministic and two-stage stochastic optimisation for design, to multi-stage stochastic optimisation for market-coupled operation of hydrogen-enabled multi-energy systems.

6. CONCLUSIONS

This thesis set out to develop a coherent modelling path for green-hydrogen-based power-to-hydrogen (PtH) plants embedded in multi-energy systems. The path is deliberately incremental: it starts from rule-based simulation with detailed component models, then moves to deterministic mixed-integer linear programming (MILP) for joint design and operation, and finally to two-stage and multi-stage stochastic MILP formulations for sizing and scheduling under uncertainty and electricity-market exposure. Along this path, the focus gradually shifts from *design decisions* that shape the levelised cost of hydrogen (LCOH) at planning stage to *operational decisions* that exploit market opportunities once a plant is already built. This chapter summarises the main methodological contributions of each step, highlights cross-cutting insights on plant design and operation, and outlines limitations and directions for future work.

Summary of the methodological path

The first part of the work focuses on rule-based simulation via the Multi Energy System Simulator (MESS). Within this framework, different configurations of hydrogen technologies, renewable generation and conventional equipment are tested under realistic operating constraints, using priority rules to emulate industrial control philosophies. Two case studies are considered: a solid oxide fuel cell (SOFC) cogeneration system for a paper mill, and grid-connected PV-based PtH plants supplying a constant hydrogen demand across Italian bidding zones. These studies show how fuel substitution, PV-to-electrolyser ratios, component degradation and green-hydrogen certification rules affect energy flows, emissions and approximate levelised costs. At the same time, they expose the inability of rule-based approaches to guarantee optimality or to systematically value flexibility options, motivating the transition to optimisation-based methods.

The second step introduces a deterministic MILP formulation for the joint design and operation of PtH plants, with particular emphasis on hydrogen storage technology selection. By embedding different storage options (pressurised tanks, underground storage and metal hydrides) into a common plant model, the MILP provides cost-optimal designs under perfect foresight and clarifies which techno-economic factors actually drive LCOH differences. This reveals that, under consistent boundary conditions, several storage technologies can produce similar LCOH, and that geology, footprint and required buffering duration may matter more than marginal efficiency differences. However, the deterministic formulation assumes a single

representative future, making it ill-suited for robust investment decisions in the presence of strong variability in renewable generation.

To address this limitation at the design stage, the third step develops a two-stage stochastic MILP framework in which capacity decisions are taken before uncertainty is revealed, while hourly operation is optimised afterwards for multiple scenarios. The application to an off-grid hybrid renewable energy system for the island of Pantelleria illustrates how stochastic design can hedge against variability in resource availability. Comparing two-stage solutions with deterministic designs quantifies the cost of robustness and shows that ignoring uncertainty can lead to mis-sized assets and systemic underestimation of both total cost and emissions when tight emission budgets are imposed. At this point, the modelling focus remains primarily on investment: uncertainty is introduced to improve sizing decisions and obtain more realistic LCOH estimates, but operational behaviour is still aggregated into a single recourse block and not explicitly linked to detailed market mechanisms.

In practice, once a PtH plant has been built, LCOH and economic performance can only be improved through operational choices, in particular by optimising how the plant interacts with electricity markets on a daily basis. The methodological path therefore culminates in a multi-stage stochastic MILP for the market-coupled scheduling of a grid-connected PtH plant, already in place, serving a hydrogen refuelling station. Scenario trees for electricity prices and renewable generation represent day-ahead, intraday and reserve markets, with non-anticipativity constraints and detailed device dynamics. This formulation captures how information is gradually revealed and how bids, setpoints and storage states co-evolve over time. The case studies show that co-optimised bidding and recourse scheduling can increase expected operating profit and substantially reduce downside risk relative to strategies that treat prices as deterministic or ignore reserve-market participation, thereby providing a consistent way to value flexibility from batteries, fuel cells and hydrogen storage once the plant configuration is fixed.

Comparative synthesis across modelling layers

Table 6.1 provides a compact comparison of the four modelling layers developed in this thesis. The intent is to make explicit what is gained and what is traded off when moving from rule-based simulation to deterministic optimisation and then to stochastic formulations, in terms of physical realism, computational burden and decision relevance.

Table 6.1: Comparison of modelling layers: decision relevance, realism and computational burden.

Layer	Decision relevance	Realism and uncertainty treatment	Computational burden / main limitations
Rule-based simulation (MESS)	Rapid screening of configurations and control heuristics; transparent “engineering” benchmarking	High physical detail and interpretable logic; uncertainty explored via parametric/sensitivity studies rather than embedded decisions	Very low; results depend on heuristic rules and do not guarantee optimality
Deterministic MILP	Cost-optimal sizing/dispatch under perfect-foresight assumptions; consistent KPI calculation (LCOH, emissions)	Optimisation provides a globally optimal solution for the linearised model; uncertainty not represented explicitly	Medium; requires simplifications/linearisation; may mis-size assets when variability is strong
Two-stage stochastic MILP	Robust “here-and-now” design with recourse operation; quantifies the cost/value of robustness	Uncertainty represented through scenarios with non-anticipativity on investment; chronology within the recourse block is limited	High; scenario generation/reduction is needed; computational cost grows with scenarios
Multi-stage stochastic MILP	Market-aware scheduling and bidding with sequential information revelation; values flexibility and downside risk	Captures market timeline and non-anticipativity across stages; directly links uncertainty to decisions and cashflows	Very high; tree size grows rapidly and requires aggressive reduction and careful implementation

Practical takeaway. Rule-based models prioritise physical fidelity and transparency; deterministic MILP prioritises optimality and scalability; stochastic MILP prioritises robustness and market relevance at the cost of computational complexity. The appropriate layer therefore depends on the decision at hand (concept screening, investment sizing, or operational scheduling).

Methodological contributions by modelling layer

Rule-based simulation with MESS

MESS provides a modular, component-resolved simulation environment in which electrolyzers, fuel cells, compression systems, storage, batteries and conventional units are linked through multi-carrier energy and mass balances. Rule-based dispatch is useful for several reasons. First, it is transparent: the mapping from control rules to operating patterns is easy to inspect and explain to industrial stakeholders. Second, it is flexible: new technologies or operating modes can be added without reformulating a global optimisation problem. Third, it is computationally light, which enables extensive parametric studies over plant sizes, control heuristics and policy constraints.

The SOFC cogeneration study demonstrates that, under suitable operating conditions, hydrogen-fed SOFCs can significantly reduce natural-gas consumption and emissions while supporting high electrical self-sufficiency. The Italian PV-based grid-connected PtH study

shows that, within realistic ranges of PV and electrolyser costs, optimal-looking designs tend to concentrate around a narrow PV-to-electrolyser capacity band, and that component degradation and certification rules materially affect the required grid backup and the share of hydrogen that can be labelled as green. These insights are valuable, but they are obtained under manually tuned control rules, without guarantees that the resulting designs are cost-optimal or that the chosen flexibility options are efficiently used.

Methodologically, this highlights the main weaknesses of a pure rule-based approach. It does not provide a principled way to choose capacities or to quantify the marginal value of adding storage or flexibility and, while it can replay historical time series, it offers no natural mechanism to explore the impact of alternative futures beyond additional trial-and-error runs. These limitations motivate the move to optimisation-based formulations for both design and operation.

Deterministic optimisation for joint design and operation

The deterministic MILP formulation introduced in this thesis replaces rule-based control with optimisation over a full year of representative data. By defining decision variables for capacities, hourly operating points and storage trajectories, subject to techno-economic constraints, the model yields plant configurations that minimise total cost under perfect foresight. This enables a consistent comparison of hydrogen storage technologies within a single PtH plant architecture, rather than at the level of isolated components.

The storage comparison shows that, when all technologies are sized and operated optimally with respect to a single assumed future, the spread in LCOH can be relatively small across compressed-gas tanks and underground storage for sites with suitable geology. Metal-hydride storage tends to be more expensive but may become competitive when low-grade waste heat is available or when footprint constraints dominate. Importantly, the MILP reveals that intuitive preferences based solely on round-trip efficiency can be misleading once capital costs, operating profiles and coupled constraints are considered.

From a methodological standpoint, the deterministic MILP represents a clear step forward over rule-based simulation: it guarantees optimality with respect to the assumed data. At the same time, its main weakness is structural: by assuming a single, known realisation of loads and renewable generation, it effectively captures only one possible future. In contexts where PtH assets are exposed to substantial variability and long lifetimes, this can lead to undersized designs that perform poorly under different conditions, and to LCOH estimates that are overly optimistic. This limitation motivates the adoption of stochastic formulations for design under uncertainty.

Two-stage stochastic optimisation for design under uncertainty

The two-stage stochastic MILP framework addresses design under uncertainty by distinguishing between first-stage capacity decisions and second-stage operational recourse decisions across multiple scenarios. In the island of Pantelleria application, scenarios represent different realisations of wind and solar availability and, indirectly, different emission outcomes under alternative resource mixes and diesel usage.

The two-stage model preserves much of the structure of the deterministic MILP but embeds it into a scenario set with probability weights. This allows the trade-off between investment in flexibility (e.g. batteries, hydrogen storage, backup generators) and expected operating cost to be quantified explicitly. Solutions are no longer “perfectly adapted” to one historical year; instead, they represent compromises that perform reasonably well across all considered scenarios. Comparing two-stage solutions with deterministic designs shows that

the latter can underestimate total cost and emissions when variability is high, especially when stringent emission caps are enforced. In this sense, the two-stage framework is primarily a *design tool*: it improves sizing decisions and produces more robust LCOH estimates by internalising the cost of unfavourable operating conditions.

Methodologically, the two-stage framework provides a natural way to introduce uncertainty without sacrificing linear structure. It clarifies the separation between decisions that must be fixed before uncertainty is realised and those that can adapt in operation. Its main weaknesses stem from the scenario representation: the choice of scenario set and reduction method strongly influences both results and computational burden, and the two-stage structure still aggregates all operational decisions into a single block. It cannot represent sequential markets, dynamic bidding strategies or the stepwise revelation of information, which are essential to fully exploit the operational value of a PtH plant once it is built. This motivates the final extension towards a multi-stage perspective focused on daily operation and market interaction.

Multi-stage stochastic optimisation for market-coupled operation

The multi-stage stochastic MILP developed in this thesis targets the operational problem of a PtH plant participating in day-ahead, intraday and reserve electricity markets while supplying a hydrogen refuelling station. In contrast to the two-stage design model, the plant configuration is assumed to be fixed; the remaining degrees of freedom are the operating schedules and market bids. Scenario trees are used to represent the evolution of prices and renewable generation over time, with non-anticipativity constraints ensuring that decisions at each stage depend only on information that is actually available. State variables track the dynamics of batteries, hydrogen storage, electrolyser loading and, where relevant, fuel cells.

This formulation strengthens the link between PtH modelling and actual market design. It captures price spreads and reserve remuneration, and it highlights how different flexibility options (electrolyser modulation, fuel cells, batteries, hydrogen storage) contribute to both expected profit and risk reduction. By focusing on operational recourse, it shows that once a plant is in place, a significant fraction of the achievable reduction in effective hydrogen cost comes from using its assets in a market-aware way, rather than from further changes in hardware. The case studies show that reserve participation reshapes operating states, shifting the balance between energy arbitrage and capacity revenues, and that enabling additional revenue streams (for example through hydrogen sales) can significantly improve and stabilise monthly profits.

Methodologically, the multi-stage approach demonstrates how sequential markets and recourse can be integrated into PtH scheduling without abandoning MILP structure. It provides a consistent framework to evaluate operating policies that would be difficult to benchmark with rule-based or deterministic models. Its weaknesses are the increased computational burden, the need for carefully constructed scenario trees, and the reliance on stylised representations of forecast errors and bidding rules. As a result, it is best seen as a detailed operational tool complementing the design-oriented deterministic and two-stage models, rather than as a universal replacement for simpler approaches.

Cross-cutting insights for PtH in multi-energy systems

Across the different modelling layers and case studies, several cross-cutting insights emerge for the design and operation of green-hydrogen-enabled multi-energy systems:

- **Complementarity of modelling layers and decision focus.** Rule-based simulation is well suited to early exploratory work and stakeholder communication. Deterministic

and two-stage MILP formulations are primarily *design tools*, aimed at choosing plant capacities and estimating LCOH under different assumptions about uncertainty. The multi-stage MILP is an *operational tool*, aimed at extracting value from electricity markets for an existing plant. No single model is sufficient: robust PtH planning and operation require moving across layers as the decision focus shifts from concept, to sizing, to daily market participation.

- **Role of storage and flexibility.** Hydrogen storage technologies that look quite different at the component level can be nearly interchangeable at plant level once optimally sized and operated in deterministic or two-stage models; non-economic factors such as geology, footprint and regulatory context often dominate. Electrical storage and flexible converters (fuel cells, modulating electrolyzers) become particularly valuable in the multi-stage formulation, where they enable profitable and less risky participation in multiple electricity markets.
- **Impact of uncertainty on design.** Designs obtained under deterministic assumptions can perform acceptably in mild conditions but risk mis-sizing storage and backup capacity when variability is higher than anticipated or when very low emission targets are imposed. Two-stage stochastic design quantifies the cost of robustness and helps avoid over-optimistic LCOH estimates by internalising the cost of adverse scenarios.
- **Value of market coupling for operation.** Incorporating day-ahead, intraday and reserve markets reveals additional operational value streams and allows the risk profile of PtH plants to be shaped through flexibility investments and bidding strategies. Simplified models that ignore reserve or treat prices as deterministic can misrepresent both the average profitability and the downside risk of market-exposed plants, and therefore underestimate the operational levers available once the plant is built.
- **Extensions to siting and land use.** The agrivoltaic extension outlined in this thesis shows that land-use constraints and alternative PV layouts can be incorporated with relatively minor changes to the optimisation structure, suggesting a route to integrate PtH modelling with land-use planning in future work.

Overall, the combination of rule-based and optimisation-based approaches provides a richer picture than any single model could offer alone. It highlights both how to *design* PtH plants so as to achieve robust LCOH under uncertainty and how to *operate* them in electricity markets to fully exploit their flexibility once they are in place.

Limitations and future work

The work presented in this thesis has several limitations that offer opportunities for further research. A first limitation concerns the level of physical detail that can be retained in optimisation-based models. Rule-based simulations in MESS include detailed component models and non-linear performance maps, which are difficult to reproduce exactly within a MILP framework. For the deterministic and stochastic formulations, efficiencies and losses are therefore represented in a simplified way, and ageing is treated as a virtual cost. This is a conscious trade-off between model fidelity and computational tractability. Future work could explore more systematic use of piecewise-linear approximations for efficiency curves, temperature-dependent performance and part-load behaviour, as well as richer degradation models for electrolyzers, fuel cells and batteries, accepting higher computational cost where

needed. Hybrid approaches that couple high-fidelity simulation or surrogate models with optimisation, for example via decomposition or iterative schemes, also appear promising.

A second limitation is related to how uncertainty is represented. The scenario sets and scenario trees used in the two-stage and multi-stage models are constructed from historical time series and simple clustering or reduction techniques. While this ensures consistency with past data, it does not fully exploit advanced forecasting capabilities, nor does it guarantee that rare but impactful patterns are adequately represented. Future work could combine the current frameworks with data-driven or machine learning-based forecasting tools, using them to generate ensembles of trajectories that preserve temporal correlations and capture different regimes. These forecasts could then be fed into more sophisticated scenario-generation and reduction procedures, or into distributionally robust optimisation formulations, to better reflect forecast uncertainty and improve the robustness of both design and operational decisions.

Third, network constraints and spatial aspects are represented in a simplified way. The models focus on site-scale balances and treat the point of connection to the grid as a single node without explicit network limits. As a result, congestion and the interaction with distribution networks are not captured. Extending the framework to include reduced grid models, or coupling it with power-system tools that provide locational marginal prices and curtailment risk, would allow the assessment of siting decisions and the locational value of PtH plants.

Finally, the market models considered focus on a specific set of products and tariff structures. Day-ahead, intraday and a simplified reserve product are represented, but real-world PtH projects may face more complex arrangements, including distribution network charges, multiple reserve and ancillary services, capacity mechanisms and long-term bilateral contracts for hydrogen and electricity. Extending the multi-stage formulation to a broader set of markets, possibly within a rolling-horizon framework with forecast updates, and considering risk-averse objective functions or chance constraints, would bring the analysis closer to real decision problems and further clarify how operational strategies can reduce effective LCOH for an existing plant.

In summary, future work could proceed along several lines: (i) enriching the physical fidelity of optimisation models through piecewise-linear or surrogate representations and more detailed ageing; (ii) combining the current stochastic formulations with advanced forecasting and data-driven scenario generation; (iii) integrating site-scale PtH optimisation with simplified grid and spatial models; (iv) expanding the market representation to include additional products, tariff structures and risk metrics; and (v) extending the paper-mill case study by evaluating the valorisation of electrolyser co-product oxygen (e.g., for bleaching-related processes) and its impact on both profitability and environmental performance. Together, these extensions would strengthen the ability of the proposed methodological toolbox to support decision-making for green-hydrogen projects, from early concept development and robust sizing to market-aware operation of plants that are already in place.

7. APPENDIX — AGRIVOLTAICS

This appendix documents an additional siting option for the PV supply of PtH plants when land availability, policy or social acceptance constrain conventional ground-mounted PV (GMPV). It does not alter the per-kWp PV production model used for scheduling: PV power is still modelled as in Section 3.1.1 (PVGIS or Hay–Davies → Durisch). Instead, it informs capacity planning and economics by changing feasible layout, installable MW per hectare, and CAPEX/O&M structure under agronomic constraints.

7.1 Introduction

Solar deployment at utility scale intensifies competition for agricultural land and tightens the water–food–energy nexus [339, 340]. Agrivoltaics (AV)—co-locating elevated PV arrays with crops—aims to relieve that land-use conflict by producing electricity and food on the same area [341, 342]. Early experiments showed that several crops tolerate or even benefit from partial shade depending on climate and season [343, 344], while reviews now frame AV as a promising tool to enhance resilience during heat and drought [345]. Against this backdrop, policy support has emerged internationally, although criteria differ: Japan links support to minimum yield retention [346], France requires yields comparable to regional references [347], Germany caps land loss [348], and Italy defines “advanced AV” mainly via structural prescriptions [349]. In practice, these heterogeneous rules shift project feasibility and the PV-to-PtH capacity split from a purely technical to a techno-agronomic decision.

State of the art

Shading and irradiance at canopy. AV performance depends on a small set of layout variables with non-linear interactions: row spacing, clearance, tilt, azimuth, and tracking strategy [350]. Two modelling families are used to map ground-level irradiance and Photosynthetically Active Radiation (PAR): (i) analytic geometric/view-factor approaches that project module outlines at fine temporal resolution with modest cost, and (ii) 3D ray-tracing that resolves direct, diffuse and reflected components at higher fidelity but higher cost [345]. Choice of method is typically dictated by the need to scan many layouts and years versus capturing rear-side or complex structures.

Crop-growth modelling. After PAR and microclimate are estimated, biomass and yield are simulated either with (i) radiation-/light-use efficiency models—fast and parsimonious but with stress responses implicit [351]—or (ii) process-based simulators that represent water, nutrients and phenology (e.g., AquaCrop [352], EPIC [353], CROPSIM-WHEAT [354], DSSAT [355]). AV-specific complications arise from repeated shade–sun transitions, altered vapour pressure deficit, humidity and temperature cycles [356], which motivate sub-hourly forcing and careful treatment of heat and water stress. Applications with STICS and GECROS have shown promising accuracy under partial shading when appropriately validated [342].

Metrics and economics. Joint evaluation relies on agronomic and energetic indicators: the Land Equivalent Ratio (LER) synthesises land productivity from crops and electricity [341], with complementary ratios to compare yields and PAR under shade [357]. Elevated structures and reduced module density make AV CAPEX and LCOE typically higher than ground-mounted PV [358]; however, AV can partly preserve crop revenue, improve water-use efficiency and facilitate on-farm self-consumption, with the balance shaped by policy incentives [346]. These trade-offs imply that the site choice (GMPV vs. AV) can be decisive even when the operational scheduling of the PtH plant per installed kW remains the same.

7.2 Scope and novelty

Scope. This appendix develops an AV siting option compliant with current Italian “advanced AV” constraints [349], coupling the PV power model already used in Section 3.1.1 with high-resolution shading-to-PAR mapping, a process-based crop model that captures temperature and water stress, and a techno-economic layer with the same KPIs as the main thesis (LCOE, NPV, IRR, PBT). The case is framed for central-Italian conditions representative of Mediterranean mixed farming where summer heat and water scarcity are material [359].

Novelty. Relative to prior AV workflows, the contribution is twofold: (i) a tractable, high-temporal-resolution pipeline that links layout-driven shading to process-based crop response at field scale and (ii) a consistent techno-economic comparison of AV versus GMPV that explicitly embeds policy constraints.

7.3 Materials and methods

The framework integrates four modules: (i) PV power production (as in Section 3.1.1), (ii) geometric shadow-casting to map under-array irradiance, (iii) a crop-growth simulator driven by PAR and stress factors, and (iv) a techno-economic layer consistent with the thesis KPIs (LCOE, NPV, IRR, PBT). Figure 7.1 sketches dataflow and dependencies.

7.3.1 Photovoltaic power production

PV production is modelled identically to Section 3.1.1. When PVGIS is selected, specific AC power per kWp $\bar{p}_t^{\text{PV},1\text{kW}}$ is retrieved and Eq. 3.2 is used [177]. Otherwise, the plane-on-array irradiance GTI_t is obtained via Hay–Davies [178] (Eq. 3.4 with geometry in 3.5), and electric power follows the Durisch efficiency model (Eq. 3.3) [179].

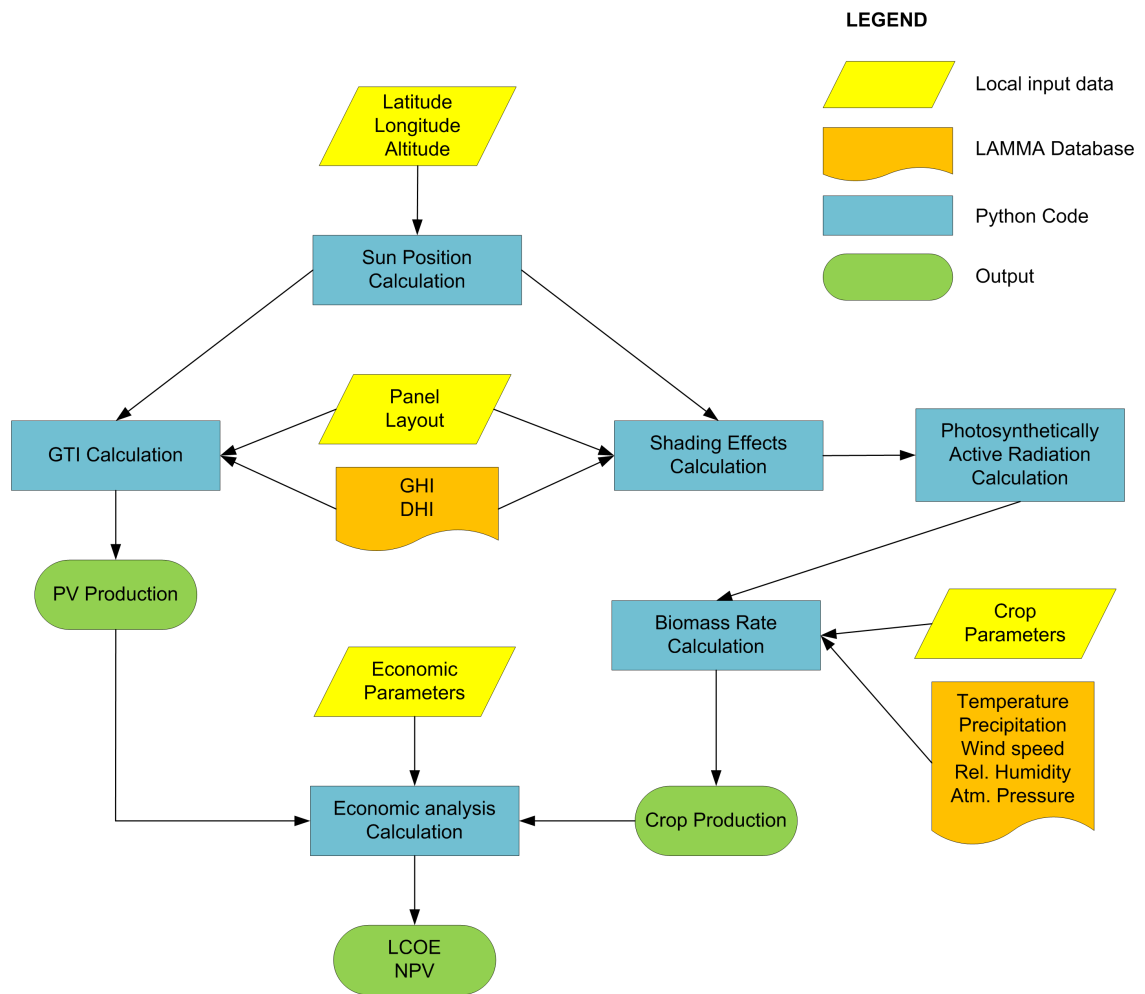


Figure 7.1: Integrated modelling workflow for agrivoltaics: solar geometry and irradiance feed both PV power and the shadow-casting routine; pixel-level PAR forces the crop model; energy and yield feed the techno-economic module.

7.3.2 Geometric shadow-casting

Shading beneath elevated, fixed-tilt rows is resolved with a parallel-ray geometric construction [360]. A rectangular module is defined by length L_{mod} , width W_{mod} , centre height z_{mod} , and tilt β ; the module is centred at $(0, 0, z_{\text{mod}})$ in a local (x, y, z) frame with z vertical. The four corners are denoted by indices $j \in \{A, B, C, D\}$ with coordinates $(X_j^{\text{mod}}, Y_j^{\text{mod}}, Z_j^{\text{mod}})$, where the upper edge is elevated by $\Delta Z_{\text{edge}} = W_{\text{mod}} \sin \beta$ relative to the lower edge (Figure 7.2).

At daylight time t (sun above the horizon, $\alpha_{z,t} < \pi/2$), the horizontal shadow displacement induced by the solar zenith $\alpha_{z,t}$ and solar azimuth $\alpha_{s,t}$ (symbols as in Section 3.1.1) is computed as in Eq. 7.1:

$$d_{j,t}^{\text{ray}} = \frac{Z_j^{\text{mod}}}{\tan(\frac{\pi}{2} - \alpha_{z,t})}, \quad \Delta X_{j,t}^{\text{ray}} = d_{j,t}^{\text{ray}} \sin \alpha_{s,t}, \quad \Delta Y_{j,t}^{\text{ray}} = d_{j,t}^{\text{ray}} \cos \alpha_{s,t}. \quad 7.1$$

The projected corner points on the ground plane are then obtained as represented in Eq. 7.2:

$$(X'_{j,t}, Y'_{j,t}) = (X_j^{\text{mod}} + \Delta X_{j,t}^{\text{ray}}, Y_j^{\text{mod}} + \Delta Y_{j,t}^{\text{ray}}). \quad 7.2$$

The quadrilateral $\{(X'_{j,t}, Y'_{j,t})\}$ defines the beam-shadow footprint at time t . The cultivated surface is discretised into square pixels indexed by p . A point-in-polygon test classifies each pixel by a Boolean sunlit indicator $\delta_{p,t}^{\text{SUN}} \in \{0, 1\}$ (sunlit = 1, shaded = 0). Pixel-level ground irradiance is then assigned as in Eq. 7.3. This methodology follows standard practice in AV PAR decomposition [361]:

$$\mathcal{G}_{p,t}^{\text{gnd}} = \text{GHI}_t \delta_{p,t}^{\text{SUN}} + \text{DHI}_t (1 - \delta_{p,t}^{\text{SUN}}). \quad 7.3$$

Iterating Eqs. 7.1–7.3 at the simulator timestep (e.g., 5 min) produces high-resolution spatio-temporal shade maps. Reflections, support-structure occlusions and rear-side effects are neglected; for monofacial, fixed-tilt arrays this yields slightly conservative under-canopy radiation.

Photosynthetically Active Radiation (PAR)

Crop-growth routines require PAR rather than broadband irradiance. In the absence of local PAR sensors, a constant conversion factor κ_{PAR} is applied to each pixel's ground irradiance, as shown in Eq. 7.4, consistent with mid-latitude measurements and AV practice [343, 362]:

$$\text{PAR}_{p,t} = \kappa_{\text{PAR}} \mathcal{G}_{p,t}^{\text{gnd}}, \quad \kappa_{\text{PAR}} = 0.48. \quad 7.4$$

Daily forcing for the crop model is obtained by time integration over the set of timestep indices $\mathcal{T}(d)$ for day d , as represented in Eqs. 7.5–7.6:

$$\text{PAR}_{p,d}^{\text{day}} = \sum_{t \in \mathcal{T}(d)} \text{PAR}_{p,t} \Delta t, \quad 7.5$$

$$\overline{\text{PAR}}_d^{\text{day}} = \frac{1}{N_{\text{pix}}} \sum_{p \in \mathcal{S}} \text{PAR}_{p,d}^{\text{day}}, \quad 7.6$$

where $\mathcal{S}$ is the set of ground pixels discretising the cultivated area, $N_{\text{pix}} = |\mathcal{S}|$ is the number of pixels, and Δt is the simulator timestep.

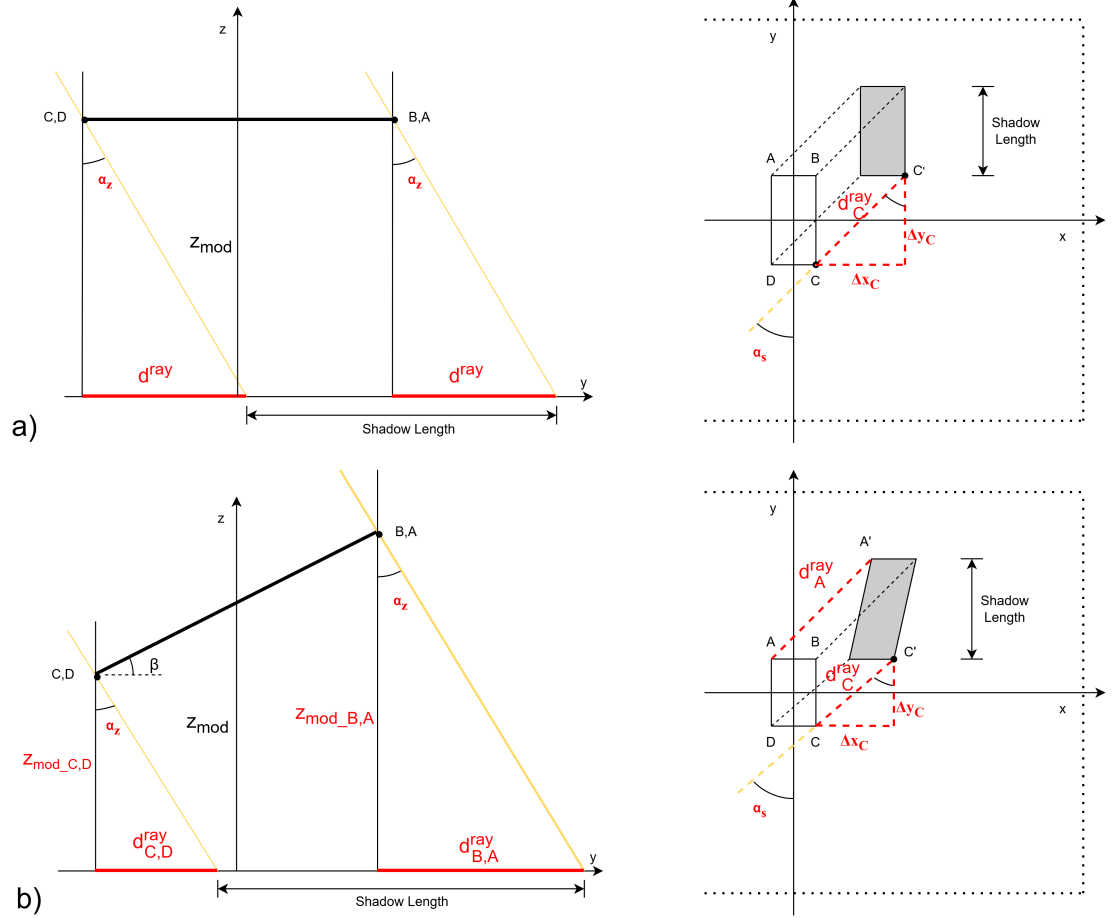


Figure 7.2: Geometric shadow-casting under the parallel-ray assumption. (a) $\beta = 0^\circ$ (shadow congruent with the module, displaced by $\alpha_{s,t}$). (b) $\beta = 30^\circ$ (upper edge produces longer rays, enlarging the footprint).

7.3.3 Potato growth modelling

Potato development is simulated with the SIMPLE crop model [363], which reproduces daily biomass accumulation with a compact parameter set while retaining sensitivity to the irradiance heterogeneity generated by the PV layout. Biomass increment on day d (g day^{-1}) is computed as shown in Eq. 7.7:

$$\dot{Y}_d = \text{PAR}_d^{\text{day}} \cdot f_{\text{Solar},d} \cdot \text{RUE} \cdot f_{\text{CO}_2,d} \cdot f_{\text{Temp},d} \cdot \min\{f_{\text{Heat},d}, f_{\text{Water},d}\}, \quad 7.7$$

where $\text{PAR}_d^{\text{day}}$ is the daily photosynthetically active radiation driver (linked to Eq. 7.6), RUE (g MJ^{-1}) is the radiation-use efficiency, and the multiplicative factors are dimensionless (0–1, except $f_{\text{CO}_2,d} > 1$), scaling growth under CO_2 , temperature, heat and water stresses. Phenology is driven by thermal time, keeping parameterisation compact. Full governing equations and parameter values are provided in the companion article [364].

Canopy light interception. The fraction of incident PAR intercepted by the canopy, $f_{\text{Solar},d}$, is modelled as a function of cumulative thermal time TT_d ($^\circ\text{C day}$) and the cultivar’s thermal requirement to maturity TT_{sum} . Its evolution follows the lower envelope of two sigmoids (leaf growth and senescence), as represented in Eq. 7.8:

$$f_{\text{Solar},d} = \min\left(\frac{f_{\text{Solar}}^{\max}}{1 + \exp[-0.01 (\text{TT}_d - \text{TT}_{50A})]}, \frac{f_{\text{Solar}}^{\max}}{1 + \exp[0.01 (\text{TT}_d - (\text{TT}_{\text{sum}} - \text{TT}_{50B,d}))]}\right), \quad 7.8$$

where TT_{50A} is the thermal time at which 50 % interception is reached during leaf growth, and $\text{TT}_{50B,d}$ is the (backward-counted) thermal time to 50 % interception along senescence. Under heat and water stress, $\text{TT}_{50B,d}$ increases, advancing senescence and reducing $f_{\text{Solar},d}$. The plateau interception is denoted $f_{\text{Solar}}^{\max}$.

Water stress. Water limitation is represented using the Agricultural Reference Index for Drought (ARID) [365]. The stress factor $f_{\text{Water},d}$ and ARID are computed as shown in Eq. 7.9:

$$f_{\text{Water},d} = 1 - SC_{\text{water}} \cdot \text{ARID}_d, \quad \text{ARID}_d = 1 - \frac{\text{Tr}_d}{\text{ET}_{0,d}}, \quad 7.9$$

where SC_{water} is a crop-specific sensitivity coefficient (–), Tr_d is the actual daily transpiration supplied by the root-zone water balance, and $\text{ET}_{0,d}$ is the reference evapotranspiration. In practice, $\text{ARID}_d = 0$ when $\text{Tr}_d = \text{ET}_{0,d}$ (no water stress, $f_{\text{Water},d} = 1$); as $\text{Tr}_d < \text{ET}_{0,d}$, ARID_d increases and $f_{\text{Water},d}$ decreases linearly. The full computation of Tr_d and $\text{ET}_{0,d}$ follows the companion article [364].

Spatial application and aggregation. To preserve heterogeneity, Eqs. 7.7–7.9 are applied at pixel level using $\text{PAR}_{p,d}^{\text{day}}$ from Eq. 7.6. Pixel biomass $\dot{Y}_{p,d}$ is accumulated over d to obtain per-pixel yields and then aggregated area-weightedly to field-scale indicators. This preserves the non-linear response to moving shade while remaining compatible with the thesis’ techno-economic layer.

7.3.4 Economic analysis

Three alternatives are evaluated on a per-hectare basis: Full-light Cropping System (FCS), Ground-Mounted Photovoltaics (GMPV), and Agrivoltaics (AV). Two land-use contexts are considered: Abandoned Farmland (AF) and Conventional Farming (CF). Investment and operating performance are computed with the KPIs defined in Section 3.1.2 (revenues,

operating expenditures, cash flows, and investment metrics), using the same yearly aggregators and price symbols.

Electricity valuation and self-consumption share. Electricity exported to the grid is valued via Eq. 3.94 using the export tariff $c_t^{\text{el,exp}}$. Self-consumed PV offsets imports and appears in $\text{OPEX}_y^{\text{el}}$ through Eq. 3.99, avoiding double counting. For tariff scenarios, a constant self-consumption share $\lambda^{\text{sc}} \in [0, 1]$ is imposed at the *annual* level. The split of yearly PV energy is then defined, as shown in Eq. 7.10 and Eq. 7.11:

$$E_y^{\text{PV,sc}} = \lambda^{\text{sc}} E_y^{\text{PV}}, \quad 7.10$$

$$E_y^{\text{PV,exp}} = (1 - \lambda^{\text{sc}}) E_y^{\text{PV}}. \quad 7.11$$

In the case studies, constant tariffs are adopted for clarity: $c_t^{\text{el,exp}} \equiv 0.09 \text{ €/kWh}$ [366] and $c_t^{\text{el,imp}} \equiv 0.17 \text{ €/kWh}$ [367].

Crop, irrigation water, and insurance terms. Crop revenue and irrigation cost are introduced additively to the KPI cash-flows. The yearly crop revenue and irrigation OPEX are defined, as shown in Eq. 7.12 and Eq. 7.13:

$$\text{REV}_y^{\text{crop}} = c_y^{\text{crop}} Y_y^{\text{crop}}, \quad 7.12$$

$$\text{OPEX}_y^{\text{irr}} = c_y^{\text{irr}} Q_y^{\text{irr}}, \quad 7.13$$

where c_y^{crop} [€/t] is the crop price, Y_y^{crop} [t/ha] is the tuber yield, c_y^{irr} [€/m³] is the irrigation-water price, and Q_y^{irr} [m³/ha] is the annual irrigation volume. PV insurance is modelled as a fixed annual charge per installed kilowatt, as shown in Eq. 7.14:

$$\text{OPEX}_y^{\text{ins}} = c^{\text{ins}} P_{\text{nom}}^{\text{PV}}, \quad 7.14$$

where c^{ins} [€/(kW yr)] is the specific insurance cost and $P_{\text{nom}}^{\text{PV}}$ [kW/ha] is the installed PV capacity per hectare. Annual PV O&M is parameterised in €/(kW yr).

Electricity value: export revenue and self-consumption benefit. The monetary value of PV electricity combines (i) grid-export revenue and (ii) the benefit of self-consumption (avoided purchase). The yearly export revenue is determined by the exported energy and the export tariff, and the yearly self-consumption benefit is determined by the self-consumed energy and the import tariff. The two components are defined as shown in Eq. 7.15 and Eq. 7.16:

$$\text{REV}_y^{\text{el,exp}} = c_y^{\text{el,exp}} E_y^{\text{PV,exp}}, \quad 7.15$$

$$\text{SAV}_y^{\text{el,sc}} = c_y^{\text{el,imp}} E_y^{\text{PV,sc}}, \quad 7.16$$

where $c_y^{\text{el,exp}}$ and $c_y^{\text{el,imp}}$ are the yearly export and import tariffs [€/kWh], and $E_y^{\text{PV,exp}}$, $E_y^{\text{PV,sc}}$ are yearly exported and self-consumed PV energy [kWh].

Upfront investment C_0 . The upfront investment is the capacity-weighted sum of the per-kW cost items in Table 7.1, multiplied by the installed PV nominal capacity. For each alternative, C_0 is expressed as shown in Eq. 7.17–7.19:

$$C_0^{\text{GMPV}} = P_{\text{nom}}^{\text{PV}} (c^{\text{mod}} + c^{\text{str,G}} + c^{\text{bop,G}} + c^{\text{inv}}), \quad 7.17$$

$$C_0^{\text{AV}} = P_{\text{nom}}^{\text{PV}} (c^{\text{mod}} + c^{\text{str,A}} + c^{\text{bop,A}} + c^{\text{inv}}), \quad 7.18$$

$$C_0^{\text{FCS}} = 0, \quad 7.19$$

where c^{mod} is the module cost [€/kW], $c^{\text{str},\cdot}$ and $c^{\text{bop},\cdot}$ are support-structure and installation/BOP costs for ground ($\cdot = G$) or agrivoltaic ($\cdot = A$) layouts, and c^{inv} is the inverter/miscellaneous cost [€/kW].

AF (abandoned farmland): cash-flow definitions by alternative. For abandoned farmland, cash flows are absolute (not incremental). The yearly revenue, operating expenditure, and operating cash flow for each alternative are defined as follows.

FCS (full-light cropping). The yearly revenue and OPEX are defined as shown in Eq. 7.20 and Eq. 7.21:

$$\text{REV}_y^{\text{FCS|AF}} = c_y^{\text{crop}} Y_y^{\text{FL}}, \quad 7.20$$

$$\text{OPEX}_y^{\text{FCS|AF}} = \text{O\&M}_y^{\text{crop}} + c_y^{\text{irr}} Q_y^{\text{FL}}, \quad 7.21$$

where Y_y^{FL} [t/ha] and Q_y^{FL} [m³/ha] are full-light yield and irrigation. The operating cash flow is defined as shown in Eq. 7.22:

$$CF_y^{\text{FCS|AF}} = \text{REV}_y^{\text{FCS|AF}} - \text{OPEX}_y^{\text{FCS|AF}}. \quad 7.22$$

GMPV (ground-mounted PV). The yearly revenue includes export revenue and self-consumption benefit; OPEX includes PV O&M and insurance, as shown in Eq. 7.23–7.25:

$$\text{REV}_y^{\text{GMPV|AF}} = \text{REV}_y^{\text{el,exp}} + \text{SAV}_y^{\text{el,sc}}, \quad 7.23$$

$$\text{OPEX}_y^{\text{GMPV|AF}} = \text{O\&M}_y^{\text{PV}} + \text{OPEX}_y^{\text{ins}}, \quad 7.24$$

$$CF_y^{\text{GMPV|AF}} = \text{REV}_y^{\text{GMPV|AF}} - \text{OPEX}_y^{\text{GMPV|AF}}. \quad 7.25$$

AV (agrivoltaics). The yearly revenue adds crop sales to the electricity value; OPEX adds cropping O&M and irrigation, as shown in Eq. 7.26–7.28:

$$\text{REV}_y^{\text{AV|AF}} = \text{REV}_y^{\text{el,exp}} + \text{SAV}_y^{\text{el,sc}} + c_y^{\text{crop}} Y_y^{\text{AV}}, \quad 7.26$$

$$\text{OPEX}_y^{\text{AV|AF}} = \text{O\&M}_y^{\text{PV}} + \text{OPEX}_y^{\text{ins}} + \text{O\&M}_y^{\text{crop}} + c_y^{\text{irr}} Q_y^{\text{AV}}, \quad 7.27$$

$$CF_y^{\text{AV|AF}} = \text{REV}_y^{\text{AV|AF}} - \text{OPEX}_y^{\text{AV|AF}}. \quad 7.28$$

Here Y_y^{AV} [t/ha] and Q_y^{AV} [m³/ha] are agrivoltaic yield and irrigation.

CF (conventional farming): incremental cash-flow definitions by alternative. For conventional farming, cash flows are computed as increments with respect to continued full-light cropping on the same hectare.

FCS baseline. The incremental terms are zero, as shown in Eq. 7.29:

$$\Delta \text{REV}_y^{\text{FCS|CF}} = 0, \quad \Delta \text{OPEX}_y^{\text{FCS|CF}} = 0, \quad \Delta CF_y^{\text{FCS|CF}} = 0. \quad 7.29$$

GMPV. The incremental revenue subtracts lost crop sales; the incremental OPEX removes baseline cropping costs, as shown in Eq. 7.30–7.32:

$$\Delta \text{REV}_y^{\text{GMPV|CF}} = \text{REV}_y^{\text{el,exp}} + \text{SAV}_y^{\text{el,sc}} - c_y^{\text{crop}} Y_y^{\text{FL}}, \quad 7.30$$

$$\Delta \text{OPEX}_y^{\text{GMPV|CF}} = \text{O\&M}_y^{\text{PV}} + \text{OPEX}_y^{\text{ins}} - \text{O\&M}_y^{\text{crop}} - c_y^{\text{irr}} Q_y^{\text{FL}}, \quad 7.31$$

$$\Delta CF_y^{\text{GMPV|CF}} = \Delta \text{REV}_y^{\text{GMPV|CF}} - \Delta \text{OPEX}_y^{\text{GMPV|CF}}. \quad 7.32$$

AV. The incremental revenue credits the crop delta under shade; incremental OPEX reflects the irrigation delta only (cropping O&M cancels), as shown in Eq. 7.33–7.35:

$$\Delta \text{REV}_y^{\text{AV|CF}} = \text{REV}_y^{\text{el,exp}} + \text{SAV}_y^{\text{el,sc}} + c_y^{\text{crop}} (Y_y^{\text{AV}} - Y_y^{\text{FL}}), \quad 7.33$$

$$\Delta \text{OPEX}_y^{\text{AV|CF}} = \text{O\&M}_y^{\text{PV}} + \text{OPEX}_y^{\text{ins}} + c_y^{\text{irr}} (Q_y^{\text{AV}} - Q_y^{\text{FL}}), \quad 7.34$$

$$\Delta CF_y^{\text{AV|CF}} = \Delta \text{REV}_y^{\text{AV|CF}} - \Delta \text{OPEX}_y^{\text{AV|CF}}. \quad 7.35$$

Investment metrics. For abandoned farmland (AF), investment appraisal uses the absolute yearly operating cash flows $CF_y^{\cdot|\text{AF}}$ defined above together with the upfront investment C_0 . For conventional farming (CF), appraisal uses the incremental cash flows $\Delta CF_y^{\cdot|\text{CF}}$ together with the same C_0 .

Net present value (NPV), AF. The NPV for alternative $\cdot \in \{\text{FCS}, \text{GMPV}, \text{AV}\}$ under AF is computed as shown in Eq. 7.36:

$$\text{NPV}^{\cdot|\text{AF}} = \sum_{y=1}^N \frac{CF_y^{\cdot|\text{AF}}}{(1 + \text{DR})^y} - C_0. \quad 7.36$$

Net present value (NPV), CF (incremental). The incremental NPV for alternative $\cdot \in \{\text{FCS}, \text{GMPV}, \text{AV}\}$ is computed as represented in Eq. 7.37:

$$\text{NPV}^{\cdot|\text{CF}} = \sum_{y=1}^N \frac{\Delta CF_y^{\cdot|\text{CF}}}{(1 + \text{DR})^y} - C_0. \quad 7.37$$

Levelised cost of electricity (LCOE), PV boundary. For PV-bearing alternatives $\cdot \in \{\text{GMPV}, \text{AV}\}$, the LCOE is evaluated on the PV boundary (numerator: PV capital and PV-related operating costs; denominator: discounted PV energy), as shown in Eq. 7.38:

$$\text{LCOE}^{\cdot|\text{PV}} = \frac{C_0 + \sum_{y=1}^N \frac{\text{OPEX}_y^{\text{PV},\cdot}}{(1 + \text{DR})^y}}{\sum_{y=1}^N \frac{E_y^{\text{PV},\cdot}}{(1 + \text{DR})^y}} \quad [\text{€/kWh}], \quad 7.38$$

where $\text{OPEX}_y^{\text{PV},\cdot} \equiv \text{O\&M}_y^{\text{PV}} + \text{OPEX}_y^{\text{ins}}$. For FCS, $\text{LCOE}^{\text{FCS}|\text{PV}}$ is not defined (no PV asset).

7.4 Configuration

The site is Sesto Fiorentino, Tuscany, Italy (43.819°N, 11.202°E; elevation 42 m). Meteorological forcing—air temperature (°C), relative humidity (%), GHI, DHI (W/m^2), surface pressure (kPa), wind speed at 2 m (m/s), and precipitation (mm)—was retrieved from the Consorzio LaMMA regional archive and pre-processed (screening, gap-handling) before use [372]. To evaluate PV production GHI/DHI are transposed to GTI_t with Hay–Davies (Eqs. 3.4–3.5) [178] and converted to power with the Durisch efficiency relation in Eq. 3.3 [179].

Policy background and constraints. Farmland abandonment reaches 10 % to 14 % in Italy [359]. To align agrivoltaic deployment with both energy and rural-development targets, national “advanced AV” guidelines impose three quantitative checks [349]. First, the *Land Area Occupation Ratio* (LAOR) limits the panelised footprint:

$$\text{LAOR} = \frac{A^{\text{PV}}}{A^{\text{tot}}} \times 100 \leq 40, \quad 7.39$$

Table 7.1: Data summary for the analysed alternatives and contexts. Note: GMPV installed density 1.0 MW/ha; AV installed density 0.8 MW/ha.

Item	FCS	GMPV	AV	Ref.
<i>Capital costs</i>				
PV modules [€/kW]	–	300	300	[349]
Supporting structure [€/kW]	–	65	350	[349]
Installation & BOP [€/kW]	–	250	414	[349]
Inverter & misc. [€/kW]	–	130	130	[349]
Total C_0 per kW [€/kW]	–	748	1194	[349]
<i>Operational costs (yearly)</i>				
PV O&M [€/(kW yr)]	–	18.7	16.3	[349]
Insurance [€/(kW yr)]	–	5	5	–
Crop O&M [€/(ha yr)]	10000	–	10000	[368]
<i>Utilities and prices</i>				
Export tariff $\bar{c}_y^{\text{el,exp}}$ [€/kWh]	–	0.09	0.09	[366]
Import tariff $\bar{c}_y^{\text{el,imp}}$ [€/kWh]	–	0.17	0.17	[367]
Irrigation water c_y^{irr} [€/m ³]	0.17	–	0.17	[369]
Crop price c_y^{crop} [€/t]	500	–	500	[370]
<i>Project parameters</i>				
Installed density [MW/ha]	–	1.0	0.8	[371]
Lifetime N [yr]	25	25	25	–
Discount rate DR [%]	5	5	5	–

where A^{PV} is the PV-module footprint and A^{tot} the total plot area. Second, the *Utilised Agricultural Surface* must remain mostly cultivable:

$$A^{\text{SAU}} \geq 0.7 A^{\text{tot}}. \quad 7.40$$

Third, the agrivoltaic specific installed capacity (MW/ha) must not fall below 60 % of a ground-mounted benchmark:

$$P_{\text{nom}}^{\text{PV,AV}} \geq 0.6 P_{\text{nom}}^{\text{PV,GMPV}}, \quad 7.41$$

where $P_{\text{nom}}^{\text{PV,AV}}$ and $P_{\text{nom}}^{\text{PV,GMPV}}$ denote the agrivoltaic and ground-mounted PV installed capacities per hectare, respectively. These constraints influence feasible $P_{\text{nom}}^{\text{PV,AV}}$ and row geometry, linking siting to both agronomy and energy yield.

Layout and PV parameters. A one-hectare strip of size 20 m $\times$ 500 m is configured to satisfy Eqs. 7.39–7.41 while preserving mechanised access (Figure 7.3). PV performance parameters follow Section 3.1.1: module efficiency $\eta_{\text{mod}}^{\text{PV}} = 0.19$, performance ratio $\text{PR} = 0.8$, array tilt $\beta = 30^\circ$, and array azimuth $\alpha_{\text{az}} = 0^\circ$ (south-facing). Row geometry for shading uses the symbols of Section 7.3.2: module length $L_{\text{mod}} = 2$ m, module width $W_{\text{mod}} = 1$ m, ground clearance (row midline) 3 m, inter-row spacing 5 m. The agrivoltaic installed density is set to $P_{\text{nom}}^{\text{PV,AV}} = 0.8$ MW/ha; the ground-mounted benchmark adopts $P_{\text{nom}}^{\text{PV,GMPV}} = 1.0$ MW/ha. With these choices, $\text{LAOR} \approx 40\%$ and $A^{\text{SAU}} \gtrsim 70\%$, satisfying the first two conditions [349]; the third condition holds with $P_{\text{nom}}^{\text{PV,AV}}/P_{\text{nom}}^{\text{PV,GMPV}} = 80\% > 60\%$. The selection $\beta = 30^\circ$, $\alpha_{\text{az}} = 0^\circ$ is consistent with annual-energy optimisation at this latitude [177]; minor intra-row gaps are neglected in the shading routine (conservative for under-canopy radiation).

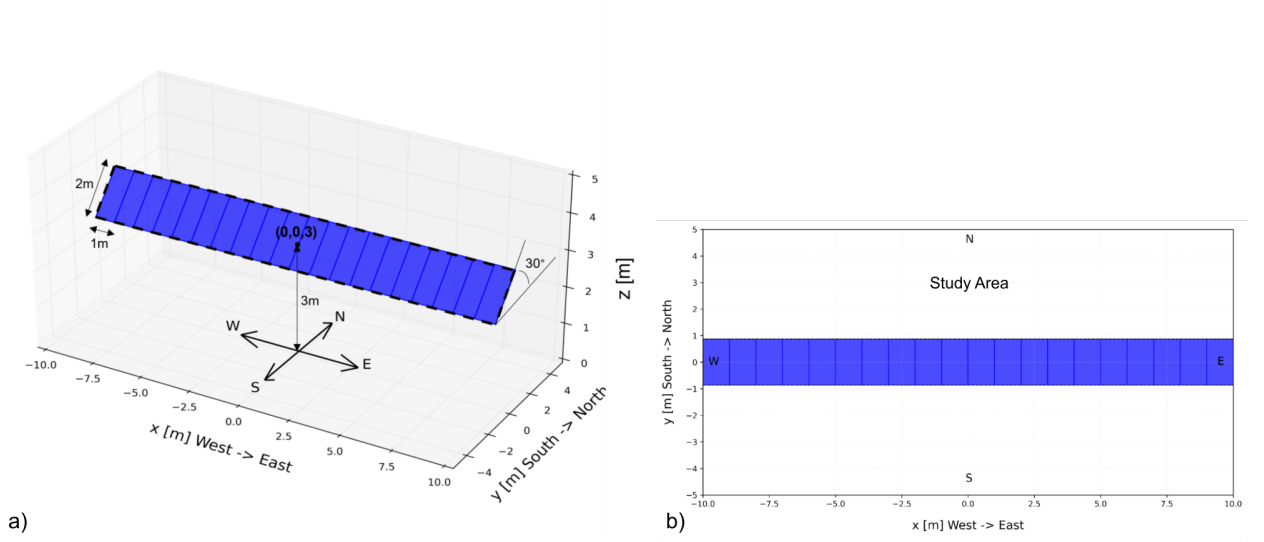


Figure 7.3: Case-study layout in Sesto Fiorentino: (a) 3D view; (b) top view. Elevated rows (3 m clearance) and 5 m inter-row spacing preserve A^{SAU} while panels are set at $\beta = 30^\circ$, $\alpha_{\text{az}} = 0^\circ$.

Comparative policy context. An EU-wide harmonised AV definition is not yet in force [371]. France (decree of Apr 8, 2024) adopts ground-coverage caps near 40 % together with yield-maintenance criteria [347]; Japan’s “solar-sharing” requires maintaining $\geq 80\%$ of average crop yield to retain farmland status [346]. Such rules map directly to $A^{\text{PV}}/A^{\text{tot}}$, yield ratios, and the choice of $P_{\text{nom}}^{\text{PV}}$ in this workflow.

Spatial–temporal resolution and agronomy settings. To resolve moving shade, the cultivated surface is discretised at 0.13 m along rows and 0.065 m across rows, and Eqs. 7.1–7.3 are iterated at $\Delta t = 5$ min. Meteorological fields not directly altered by the structure (air temperature, precipitation, relative humidity) are treated as spatially uniform; PAR, evapotranspiration and soil-water balance are computed per pixel where partial shading occurs (Sections 7.3.2 and 7.3.3). Planting is set to March 1 (regional practice). In the base run no irrigation is applied, so soil moisture evolves only with precipitation, consistent with field practice for potatoes in Tuscan Apennine settings [373]; under this assumption $Q_y^{\text{FL}} = Q_y^{\text{AV}} = 0$.

Performance indicators. The Land Equivalent Ratio (LER) combines crop and electricity outputs per hectare [341]. Including an explicit non-cultivable fraction L^{loss} (e.g., posts, service paths), LER is defined as represented in Eq. 7.42:

$$\text{LER} = \frac{Y^{\text{AV}}(1 - L^{\text{loss}})}{Y^{\text{FL}}} + \frac{E^{\text{PV,AV}}}{E^{\text{PV,GMPV}}}, \quad 7.42$$

where Y^{AV} is the AV tuber yield and Y^{FL} the full-light reference; $E^{\text{PV,AV}}$ and $E^{\text{PV,GMPV}}$ are the electrical energies (per hectare) from AV and ground-mounted layouts, respectively. Following field deployments with elevated rows, $L^{\text{loss}} = 0.083$ is adopted [344]. Because maximising LER alone can bias towards large $P_{\text{nom}}^{\text{PV}}$, recent studies recommend also reporting crop-yield and PAR ratios to keep the agronomic perspective explicit [357].

7.5 Results and discussion

The workflow in Section 7.3 is applied to the one-hectare site in Sesto Fiorentino (Tuscany, Italy), dimensioned to satisfy the Italian PNRR “advanced agrivoltaic” criteria (Eqs. 7.39–7.41) and driven by 2023 meteorological observations from Consorzio LaMMA [372]. Results

are organised as follows: Section 7.5.1 reports PV performance, Section 7.5.2 examines spatio-temporal shading, Section 7.5.3 presents simulated potato biomass and stresses, and Section 7.5.4 evaluates the economic metrics.

7.5.1 PV production

Figure 7.4 contrasts global horizontal irradiance (GHI) with global tilted irradiance (GTI) at the Sesto Fiorentino site for representative clear-sky days and for monthly aggregates. The array is fixed at $\beta = 30^\circ$ and south-facing azimuth, consistent with the design in Section 7.3.

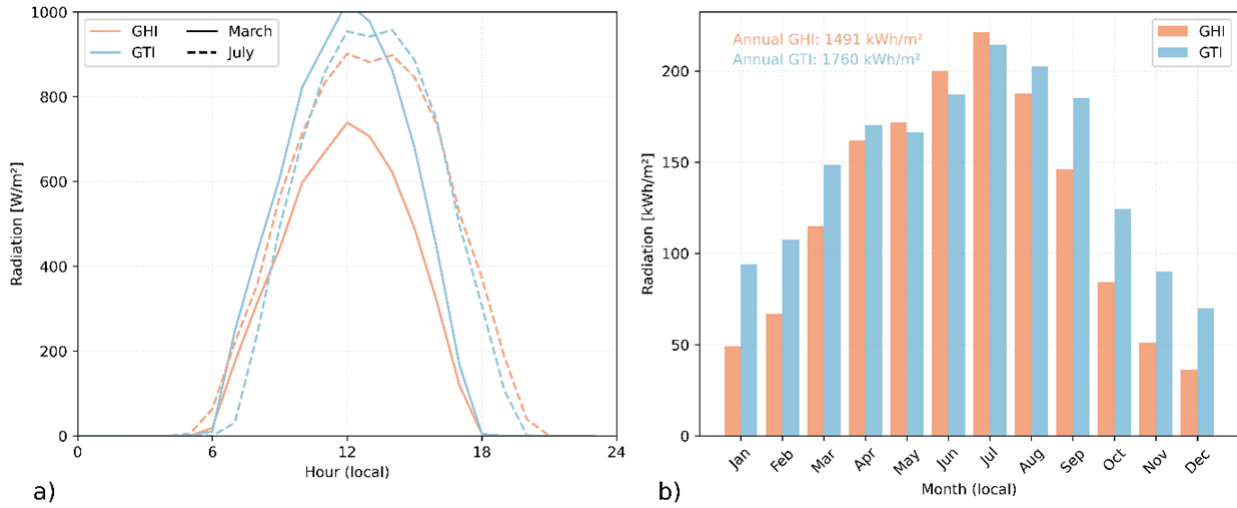


Figure 7.4: Irradiance at Sesto Fiorentino: (a) representative clear-sky days in March and July, GHI vs. GTI; (b) monthly aggregates.

On representative clear-sky days (panel a), GTI exceeds GHI in March (midday solar zenith $\approx 55^\circ$ to 60°) because the beam component is closer to normal incidence on the tilted plane; in July (zenith $\approx 25^\circ$ to 30°) GTI and GHI converge with the higher sun path. Aggregated by month (panel b), the seasonal cycle yields $\text{GTI/GHI} > 1$ in winter and approaching unity in summer. On an annual basis, the site receives about 1500 kWh/m^2 of GHI and 1760 kWh/m^2 of GTI. Applying the fixed-efficiency relation (as shown in Eq. 3.3) with $\eta_{\text{mod}}^{\text{PV}} = 0.19$ and $\text{PR} = 0.8$ yields a specific production near 1300 kWh/kW , consistent with fixed-tilt benchmarks for Tuscany [177].

For context, the resulting capacity factor is approximately $1300/8760 \simeq 14.8\%$. Using the installed densities in Table 7.1, the annual electricity per hectare is 1300 MWh/ha for GMPV (1.0 MW/ha) and 1040 MWh/ha for AV (0.8 MW/ha). These values align with the policy constraint that AV specific power and energy densities approach a substantial fraction of a conventional GMPV benchmark while respecting ground-coverage limits [349, 371].

7.5.2 Shading patterns

The geometric routine in Section 7.3.2 is executed every $\Delta t = 5 \text{ min}$ over a spatial grid of $0.13 \text{ m} \times 0.065 \text{ m}$, producing pixel-level ground irradiance $\mathcal{G}_{p,t}^{\text{gnd}}$ as shown in Eq. 7.3. Figure 7.5 reports hourly maps across a $20 \text{ m} \times 10 \text{ m}$ subsection on two clear-sky days (March and July) to illustrate the diurnal movement of the beam-shadow quadrilateral (as in Eqs. 7.1–7.2) around a single module of $1 \text{ m} \times 2 \text{ m}$.¹

¹Each row contains 20 modules; a single-module window isolates local dynamics before row repetition.

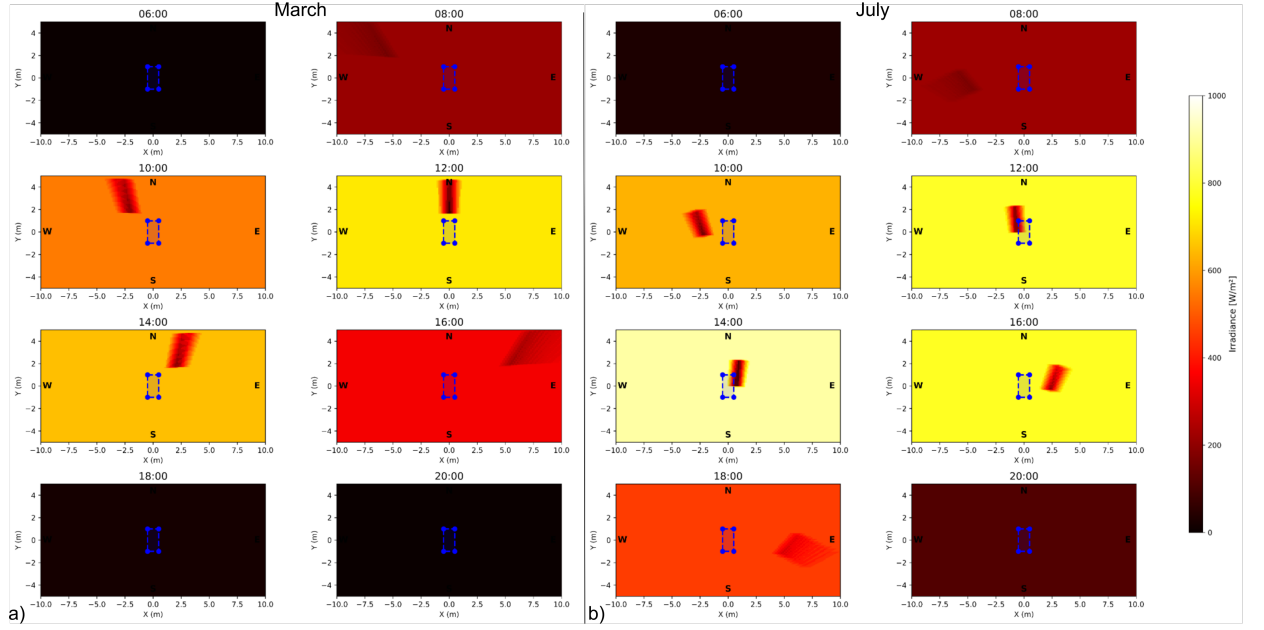


Figure 7.5: Hourly ground-level irradiance [W/m^2] on a clear-sky day over a $20\text{ m} \times 10\text{ m}$ window around one module; (a) March; (b) July.

During morning hours, the shadow lies up-sun of the module line (northwest in March; southwest in July), then contracts and shifts at midday with solar zenith $\alpha_{z,t}$, and elongates again in late afternoon toward the opposite quadrant. At midday in March, lower solar altitude extends the footprint up to $\sim 3\text{ m}$ north of the lower edge; in July, higher altitude reduces the offset to $\sim 0.9\text{ m}$ south of the lower edge. Peak $\mathcal{G}_{p,t}^{\text{gnd}}$ near 13 h is about $700\text{ W}/\text{m}^2$ in March and $930\text{ W}/\text{m}^2$ in July for the illustrative days.

Monthly ground-level radiation totals from March (sowing) to August (maturity) are mapped in Figure 7.6. Persistent low- $\mathcal{G}$ bands appear just north of the module line where the direct beam is frequently intercepted; in those bands, diffuse irradiance (DHI) underpins the residual PAR forcing (Section 7.3.2). Monthly maxima range from $\sim 106\text{ kWh}/\text{m}^2$ (March) to $\sim 225\text{ kWh}/\text{m}^2$ (July), with spatial variance increasing in months with more frequent clear-sky periods.

Row repetition composes single-module footprints into the full agrivoltaic swath. Figure 7.7 accumulates ground-level radiation over March–August for an entire 20-module row. The lower half (negative y) shows the full-light field margin for contrast; the upper half (positive y) shows the repeating AV band. When aggregated over the cropping period, pixel-level PAR reductions reach up to 55 % relative to the full-light margin at the most affected stripes, while moderately shaded corridors experience smaller PAR reductions that, as discussed later (Section 7.5.3), may partially mitigate heat and water stress.

7.5.3 Potato growth

Pixel-level photosynthetically active radiation (PAR) is computed from ground irradiance via Eq. 7.4 and time-integrated to daily drivers with Eqs. 7.5–7.6. Daily biomass accumulation then follows Eq. 7.7, with canopy interception f_{Solar} and water-stress factor f_{Water} evolving as in Eqs. 7.8–7.9.

Figure 7.8 summarises spatial outcomes for the 2023 season. Panel (a) maps the final potato yield ratio (AV yield normalised to the full-light, FL, reference) over three consecutive PV rows. Panel (b) reports, along the central south–north transect of the first row ($x = 0$),

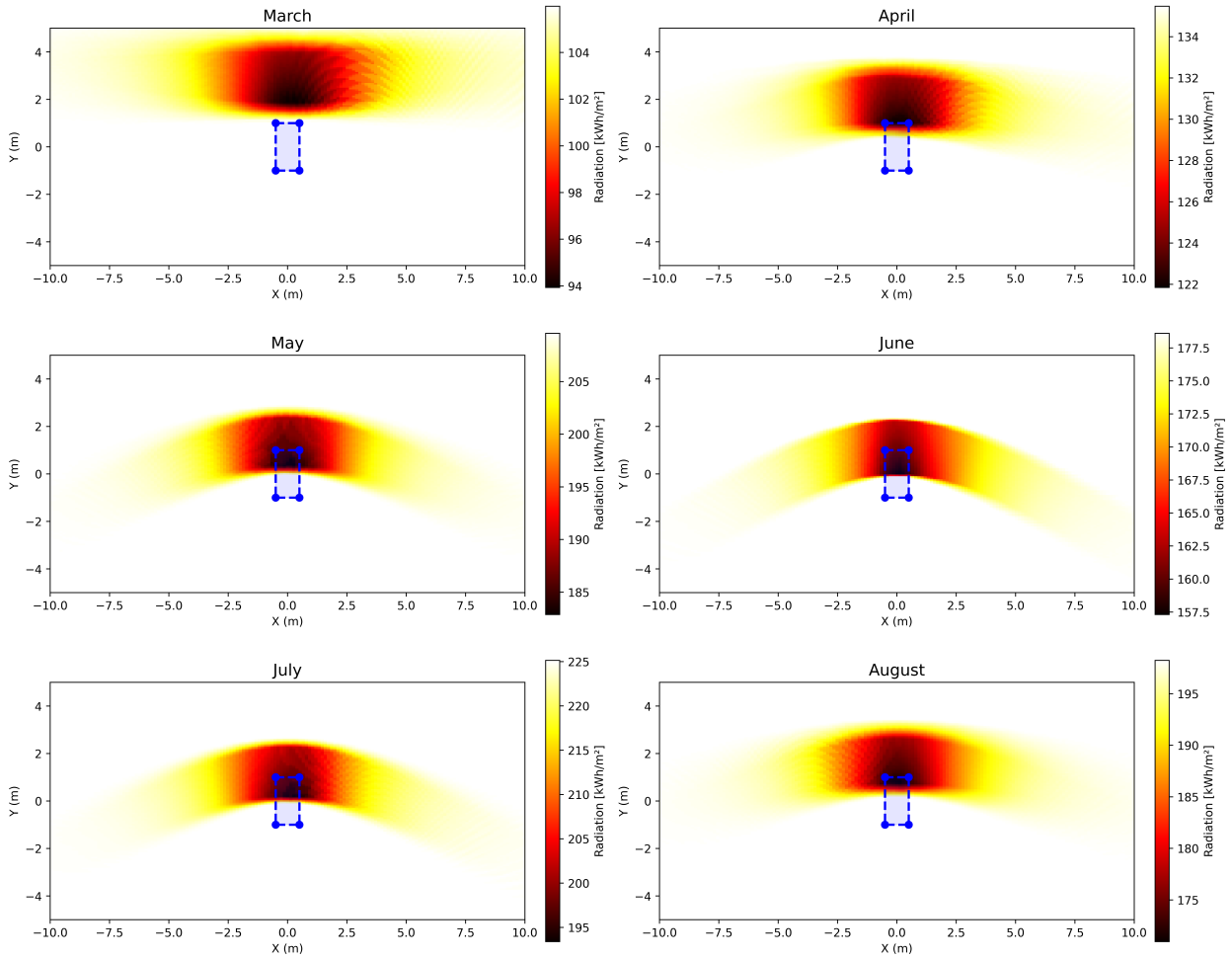


Figure 7.6: Monthly ground-level radiation [kWh/m²] across the 20 m × 10 m window (March–August).

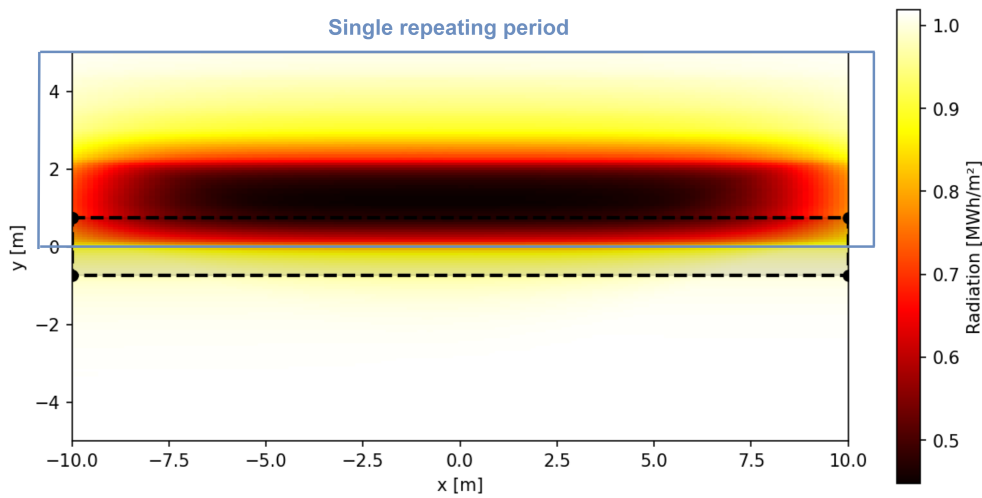


Figure 7.7: Cumulative ground-level radiation (March–August) over a full 20-module row. The lower half ($y \in [-5, 0]$ m) is the full-light margin; the upper half ($y \in [0, 5]$ m) is the AV band that tiles across the site.

the yield ratio and the PAR ratio, each value normalised to the FL zone (100%) so that direct comparisons are scale-free.

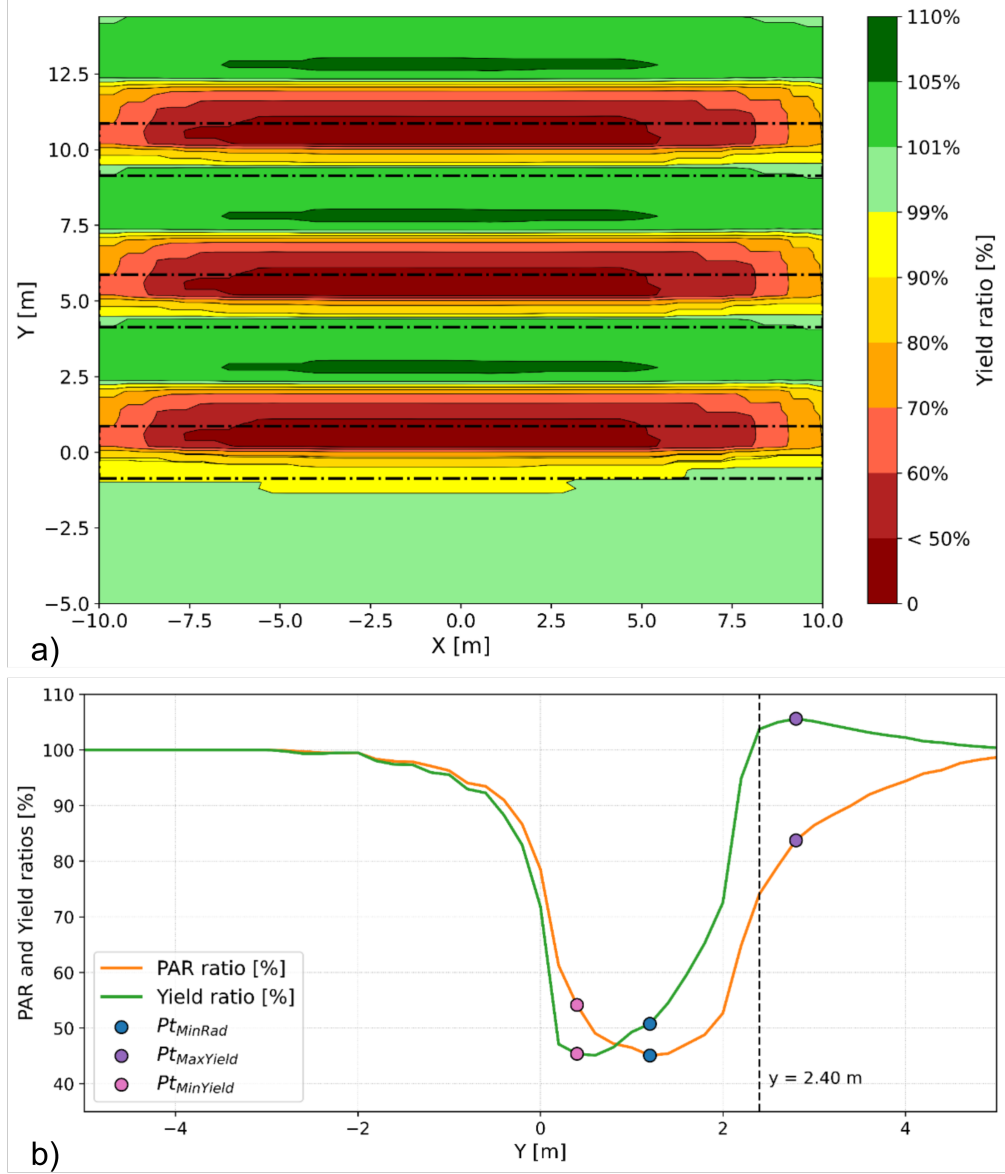


Figure 7.8: Potato yields under AV shading. (a) Final yield ratio (normalised to FL) across three PV rows. (b) Yield ratio and PAR ratio along the central south–north transect of the first row ($x = 0$); ordinates normalised to FL = 100%.

Yield and PAR begin to decline for $y > -2$ m as repeated shadows from the PV rows reach the crop. The two curves diverge in sensitivity: along the transect, the minimum yield ratio is 46% at $y = 0.2$ m whereas the PAR ratio there is 60%; their intersection occurs near $y = 0.8$ m, delineating a zone where effects are predominantly negative (yield ratio < PAR ratio for $y < 0.8$ m) and a zone where moderate shade is beneficial (yield ratio > PAR ratio for $y > 0.8$ m). At the minimum-PAR location ($y = 1.2$ m; PAR ratio $\approx 45\%$), the yield ratio remains higher ($\approx 52\%$), indicating partial mitigation of water stress under extended shading. Beyond $y \approx 2.4$ m, the yield ratio exceeds 100% and peaks at 106% even though the PAR ratio is 85%, suggesting an agronomic advantage associated with mild early-season shade.

To explain these patterns, Figure 7.9 compares time series of (i) cumulative biomass (green), (ii) canopy interception f_{Solar} (red), (iii) weekly PAR (orange bars), and (iv) water-stress factor f_{Water} (blue) at two representative transect points, each overlaid against the FL

reference (dashed). Panel (a) shows the maximum-yield point ($y = 2.4$ m); panel (b) shows the minimum-yield point ($y = 0.2$ m).

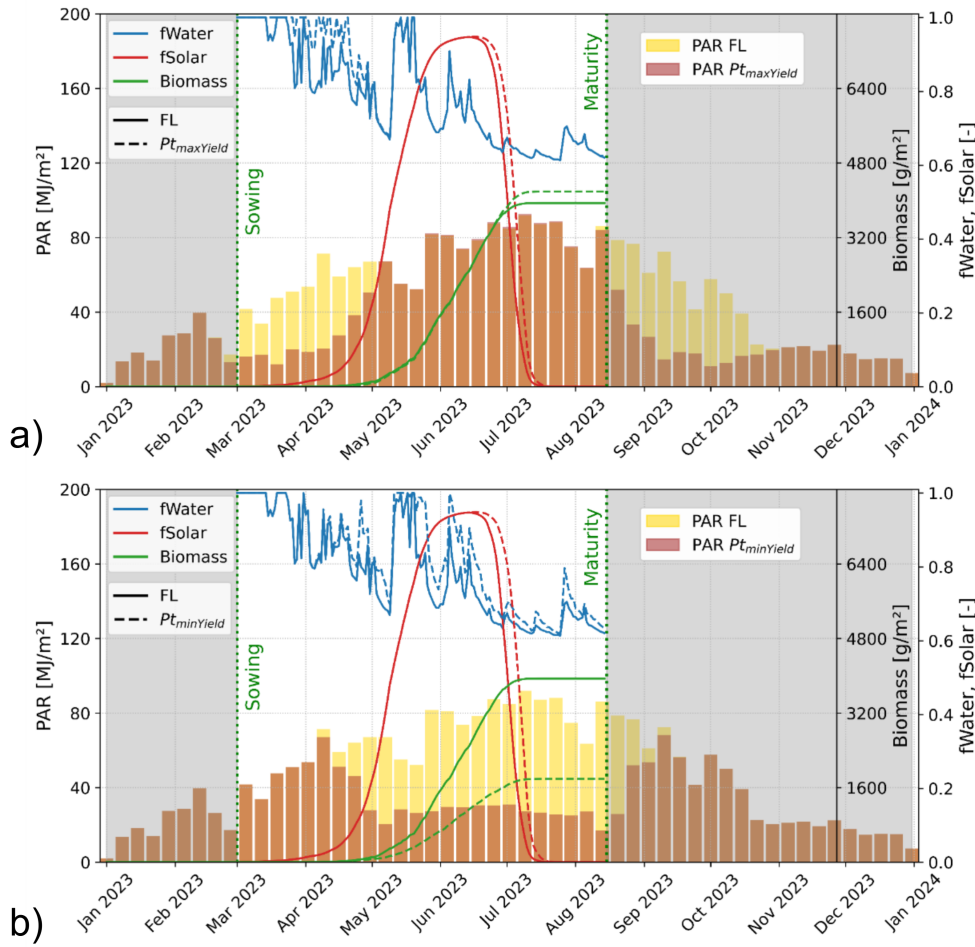


Figure 7.9: Time-series comparison with FL reference (dashed) at two transect locations: (a) maximum-yield point $y = 2.4$ m; (b) minimum-yield point $y = 0.2$ m. Variables: cumulative biomass (green), f_{Solar} (red), weekly PAR (orange bars), f_{Water} (blue).

In the FL reference, biomass follows the expected S-shape: a lag during emergence, rapid growth as tubers enlarge, and a plateau at senescence; physiological maturity is reached around 15 August. The f_{Solar} trajectory peaks during the rapid growth phase as the canopy saturates interception, and f_{Water} stays near unity until soil-water depletion triggers stress; rainfall events partly restore f_{Water} before summer drought lowers it again.

At the minimum-yield point, mid-season shade cuts PAR by 40%, which lowers evaporative demand and delays water stress (i.e., f_{Water} remains closer to 1 for longer). Nevertheless, lower PAR outweighs the benefit of delayed stress, so the yield ratio (46%) undershoots the PAR ratio (60%). At the minimum-PAR point (not plotted), shade is more prolonged early, producing a PAR ratio of 45% but a higher yield ratio (52%) because extended stress relief preserves growth duration. Conversely, Figure 7.9a shows the maximum-yield point achieves the most favourable balance: mild shading from sowing to early May reduces early PAR by 15% yet slows soil drying, keeps f_{Water} elevated, and extends the period with $f_{\text{Solar}} \approx 0.95$ by 6 days, resulting in 106% yield despite reduced PAR. This agrees with reports that potato is more penalised by early water deficit than by late deficit [374].

Aggregating pixel-level tuber yield over the site area A_{site} yields $Y^{\text{AV}} = 26.8$ t/ha under AV against $Y^{\text{FL}} = 31.5$ t/ha under FL (−15%). The simulated AV penalty is consistent with temperate-Europe AV trials on potato (Heggelbach, Germany) reporting −11% to −18% at

35 % shading [375]; the FL yield is aligned with national benchmarks of 30 t/ha to 35 t/ha [376, 377].

The land-equivalent ratio (LER), defined earlier (as shown in Eq. 7.42), evaluates to $LER = 1.58$ for the baseline design. As indicated by Eq. 7.42, LER decreases linearly with land loss L^{loss} with slope equal to the AV/FL yield ratio. Using the simulated yield ratio 0.851, an increase $\Delta L^{\text{loss}} = 0.01$ lowers LER by ≈ 0.0085 in absolute terms. Illustratively, $L^{\text{loss}} = 5\% \Rightarrow LER \approx 1.61$, $L^{\text{loss}} = 12\% \Rightarrow LER \approx 1.55$; with the baseline $L^{\text{loss}} = 0.083$, $LER = 1.58$, holding other terms fixed. Alternative AV designs (e.g., single/dual-axis tracking, bifacial modules) increase the energy contribution in LER; they may also alter L^{loss} via clearances/structures and reshape shade patterns that affect the yield ratio. The net effect on LER is the balance of these changes and is therefore layout- and site-specific [371].

Overall, the yield response is non-linear and site-dependent: heavy shading reduces production, whereas light-to-moderate shading around critical stages can improve water status and prolong effective growth, delivering yields comparable to or higher than FL despite reduced PAR [374].

7.5.4 Economic analysis

The economic assessment compares Full-light Cropping System (FCS), Ground-Mounted PV (GMPV), and Agrivoltaics (AV) under Abandoned Farmland (AF) and Conventional Farming (CF), using the cash-flow constructs of Section 7.3.4 (absolute CF_y^{AF} and incremental ΔCF_y^{CF}) and investment metrics on a 25 yr horizon at $DR = 5\%$. Two annual self-consumption shares are analysed: $\lambda^{\text{sc}} = 0.70$ and $\lambda^{\text{sc}} = 0.30$, with $c_y^{\text{el,exp}} = 0.09 \text{ €/kWh}$ and $c_y^{\text{el,imp}} = 0.17 \text{ €/kWh}$. Capital items per kW are those in Table 7.1; installed densities are 1.0 MW/ha (GMPV) and 0.8 MW/ha (AV).

LCOE (PV boundary). Using Eq. 7.38, the GMPV configuration ($C_0 = 748 \text{ €/kW}$) yields $LCOE^{\text{GMPV|PV}} = 0.061 \text{ €/kWh}$. The AV configuration ($C_0 = 1194 \text{ €/kW}$) yields $LCOE^{\text{AV|PV}} = 0.084 \text{ €/kWh}$. The higher AV value reflects elevated supporting-structure and BOP costs at comparable specific generation.

Per-hectare cash-flow and investment outcomes. Figure 7.10 reports cumulative NPV per hectare (panel a) and per installed MW (panel b) under AF and CF for $\lambda^{\text{sc}} = 0.70$ and 0.30. Per-hectare, GMPV naturally accrues larger electricity value than AV because of its higher installed capacity. Under AF with $\lambda^{\text{sc}} = 0.70$, GMPV repays sooner (discounted PBT 6 years) and attains a higher IRR (21%); AV repays in 10 years at IRR 13%. Under CF, displacement of the baseline crop matters: GMPV forfeits 31.5 t/ha potato revenue (Section 7.5.3), reducing annual net cash by 5.5 k€/ha and lowering IRR to 19%; AV forfeits only the shaded delta (from 31.5 t/ha to 26.8 t/ha), i.e., 0.8 k€/ha, so IRR decreases by 1 pp (12%).

Normalising by installed capacity (panel b of Figure 7.10), AV's NPV trajectory steepens and narrows the gap to GMPV by year 25 despite higher C_0 . This convergence occurs because the capacity differential (0.8 vs. 1.0 MW/ha) is removed while the dual revenue stream (electricity + crop) accumulates.

Summary table (per hectare). Table 7.2 collects annualised operating figures and investment outcomes for the two λ^{sc} values. Here “Crop revenue” corresponds to REV_y^{crop} under AF or to its increment under CF; “Electricity value” corresponds to the yearly electricity value $REV_y^{\text{el,exp}} + SAV_y^{\text{el,sc}}$. “Cash flow” is the representative steady-year operating cash flow (AF: CF_y^{AF} ; CF: ΔCF_y^{CF}). NPV, IRR, and discounted PBT are also reported.

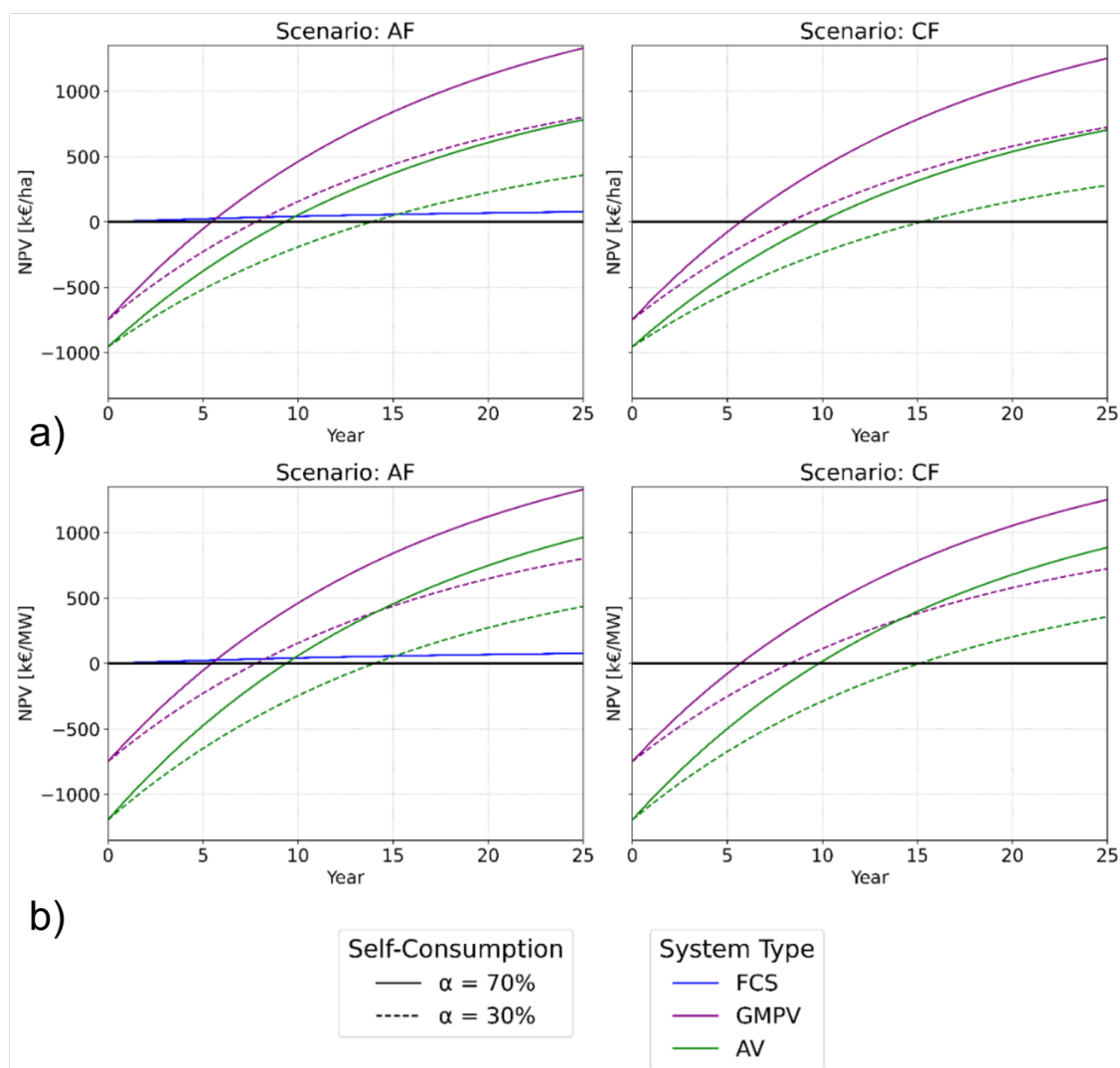


Figure 7.10: Cumulative NPV trajectories for FCS, GMPV and AV under AF and CF at $\lambda^{sc} = 0.70$ and $\lambda^{sc} = 0.30$: (a) per hectare of land; (b) per installed megawatt.

Table 7.2: Economic performance of FCS, GMPV and AV under AF and CF, for $\lambda^{\text{sc}} = 0.70$ and $\lambda^{\text{sc}} = 0.30$. All values per hectare.

Scenario		$\lambda^{\text{sc}} = 0.70$					
		Crop rev. [k€/yr]	Electricity rev. [k€/yr]	Cash flow [k€/yr]	NPV [k€]	IRR [%]	PBT [yr]
FCS	AF	15.7	–	5.5	78	–	15
FCS	CF	–	–	–	–	–	–
GMPV	AF	–	188	164	1330	21	6
GMPV	CF	–15.7	188	158	1252	19	6
AV	AF	13.5	150	136	781	13	10
AV	CF	–2.2	150	131	703	12	10

Scenario		$\lambda^{\text{sc}} = 0.30$					
		Crop rev. [k€/yr]	Electricity rev. [k€/yr]	Cash flow [k€/yr]	NPV [k€]	IRR [%]	PBT [yr]
FCS	AF	15.7	–	5.5	78	–	15
FCS	CF	–	–	–	–	–	–
GMPV	AF	–	147	123	800	15	8
GMPV	CF	–15.7	147	117	720	13.5	9
AV	AF	13.5	117	109	358	9	14
AV	CF	–2.2	117	98	280	8	15

Table 7.2 shows that lowering λ^{sc} from 0.70 to 0.30 extends discounted payback by 2–3 yr and reduces IRR by 4–6 pp for both PV-bearing options, without altering their ranking. Crop-only FCS is insensitive to λ^{sc} . A $\pm 10\%$ change in C_0 (other items fixed) shifts IRR by roughly ± 1 pp– ± 2 pp and PBT by ± 1 yr; AV is somewhat more sensitive (larger structural share), while GMPV is slightly more tariff-sensitive. Differences in irrigation outlays between AV and FCS (no irrigation in the baseline simulations) correspond to 50 €/yr and are negligible at the project scale.

AV’s elevated C_0 drives a higher LCOE^{PV} and longer PBT than GMPV; however, on an equal-capacity basis (Figure 7.10b), the combined electricity and crop revenue streams narrow the long-run NPV gap. As larger PV penetrations depress wholesale prices, the relative stabilising contribution of agricultural income grows, improving AV’s resilience as a dual-use land strategy [371].

7.6 Main findings

A Python workflow was developed that integrates: (i) PV power modelling, (ii) high-resolution shadow-casting at five-minute cadence, (iii) process-based potato growth simulation, and (iv) techno-economic analysis. The framework was applied to a one-hectare agrivoltaic (AV) layout in Sesto Fiorentino (Tuscany, Italy) designed to satisfy the Italian PNRR “advanced AV” criteria: 2 m $\times$ 1 m modules (400 W), fixed tilt 30°, clearance 3 m, inter-row spacing 5 m, ground coverage $\leq 40\%$, cultivated surface $\geq 70\%$, and installed density 0.8 MW/ha.

- **PV performance.** Annual GTI and GHI at the site are about 1760 kW h/m² and 1500 kW h/m², respectively. Using the fixed-efficiency relation (Durisch) with $\eta_{\text{mod}}^{\text{PV}} =$

0.19 and $PR = 0.8$ yields a specific production near 1300 kWh/kW, consistent with regional fixed-tilt benchmarks.

- **Shading and under-canopy light.** Five-minute, $0.13\text{ m} \times 0.065\text{ m}$ maps show local growing-season reductions of ground-level irradiance up to 55 % directly beneath arrays, with persistent low- $\mathcal{G}$ bands north of module centres where beam shielding dominates.
- **Crop response and LER.** Simulated field-average potato yield under AV is 26.8 t/ha, 15 % below the full-light (FL) reference of 31.5 t/ha. The Land-Equivalent Ratio is $LER = 1.58$, indicating superior land productivity versus separate siting. Intra-field variability is marked: minima reach 46 % of FL beneath modules, while a band 2.4 m north of module centres attains 106 % of FL with 85 % of FL PAR, evidencing that moderate early-season shading delays soil-moisture depletion and senescence, improving water-use efficiency.
- **Economics.** Ground-mounted PV (GMPV, 1.0 MW/ha) requires $C_0 = 748\text{ €/kW}$; AV (0.8 MW/ha) requires $C_0 = 1194\text{ €/kW}$. The resulting PV-boundary levelised costs are $LCOE = 0.061\text{ €/kWh}$ (GMPV) and $LCOE = 0.084\text{ €/kWh}$ (AV). On abandoned farmland, with annual self-consumption share $\lambda^{sc} = 0.70$, GMPV exhibits shorter discounted payback (6 years) and higher IRR (21 %) than AV (10 years; 13 %). On conventional farmland, the baseline-crop displacement penalises GMPV more strongly (loss of 31.5 t/ha) than AV (loss of 4.7 t/ha), reducing the IRR gap (GMPV 19 %, AV 12 %). When normalised per installed megawatt, the AV NPV trajectory closes part of the gap over 25 yr as dual revenue streams (electricity + crop) accumulate.

Implications for PtH siting and planning. The AV option leaves the per-kW PV production model used for the rule-based scheduling of the PtH plant unchanged (Section 3.1.1); it acts upstream, by altering feasible layouts, MW/ha, and the CAPEX/O&M structure under agronomic constraints. Where GMPV is constrained by land availability, permitting, or social acceptance, AV can supply on-site PV to PtH while preserving agricultural function. Capacity planning should therefore consider AV as a siting class with: (i) higher LCOE per kW, (ii) lower installable MW/ha, and (iii) additional crop-linked cash flows. At system level, these differences propagate into the economic KPIs (NPV, IRR, discounted payback) without modifying the operational scheduling logic per installed kW; portfolio mixes of GMPV and AV can be optimised against land constraints and the hydrogen cost target.

Limitations and next steps. The present implementation assumes uniform micrometeorology (air temperature, humidity, wind) beneath arrays and in open field; soil and canopy microclimate are not yet coupled to shading. Including an under-panel micrometeorology submodule (radiative, thermal and aerodynamic effects) is expected to increase the estimated heat-stress relief and refine long-term resilience signals. Extensions to tracking and bifacial systems, and jurisdiction-specific policy constraints, can be incorporated by updating the geometric/PAR layer and the techno-economic parameters while retaining the same KPI machinery.

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