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Towards the Resilient Design of Power-to-Ammonia Systems via Linear Optimization Tools

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ABSTRACT

The design of Power-to-Ammonia systems (P2A) is a challenging task. While the technology for all its components, including renewable energy harnessing, electrolysis, Haber-Bosch synthesis, and auxiliary buffers, is mature, assembling such a system to meet the challenges of varying power profiles is not trivial. To ensure resilient, cost-effective designs, careful selection of unit capacities and coordination of all system operations are required. Specifically, this requires modeling system behaviour and enforcing operational constraints to capture system flexibility over a representative time frame. The first steps towards a novel P2A design framework are presented, with a focus on enhanced process operations and exploring new options for process flexibility. A general methodology is proposed, where the full system can be customized, namely by enabling or disabling: (i) multiple renewable energy harnessing sources, (ii) grid operations, and (iii) buffers, including battery and/or an H_2 tank. The model is defined as a linear function of a set of design and operation variables, expressed through a set of matrices and vectors, which are then used to formulate and solve a Linear Programming problem. The design methodology is presented and illustrated via 3 distinct P2A configurations, with key results and analyses of system flexibility and performance. A discussion of future steps towards developing this design framework is also presented.

Keywords: Power-to-Ammonia, Process Design, Optimization, Sustainability, Resilience

INTRODUCTION

Ammonia (NH_3) is a key building block in the modern economy, with a global production of 183 million metric tons in 2020. Its relevance stems from its role as a precursor in fertilizer production, supporting an estimated 50% of food chains [1]. Given its potential as an energy vector, demand is forecast to increase and to capture new markets, such as maritime transportation [1].

The Haber-Bosch (HB) process is the industry's standard for ammonia production, accounting for more than 90% of the total output [2]. It reports roughly 63% energy efficiency and 1.5-1.6 ton CO_2 / ton NH_3 for the Best Available Technology, via the Steam Methane Reforming (SMR) process [3]. While the HB process has long achieved full technological maturity, the industry accounts for an estimated 1-2% of CO_2 emissions, making it a primary target for decarbonization and achieving the UN's Sustainable Development Goals [4].

The primary source of carbon dioxide (CO_2) emissions in this process is related to the operation of the SMR section, where a 3:1 molar syngas mixture of hydrogen (H_2) and nitrogen (N_2) is produced. Natural gas (primarily composed of methane – CH_4) is used in this section as a feedstock to manufacture H_2, and as a fuel to achieve high temperatures in the reforming units [5].

The last section of the process is the HB synthesis, where the syngas from the SMR section is catalytically converted to NH_3 in a reaction loop. Direct CO_2 emissions are much lower and are mainly due to CH_4 purge from the loop, where it remains chemically inert. The synthesis reaction is autothermal, avoiding fuel consumption except during process start-up, but it requires a power supply to achieve the high pressures in the synthesis loop [2].

Water electrolysis is a more sustainable route to hydrogen production, as it avoids the use of fossil fuels.

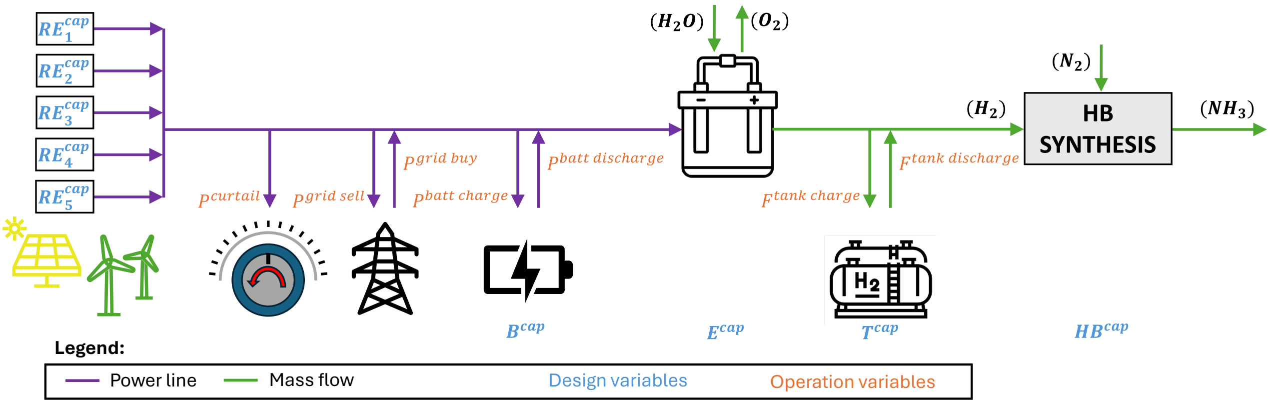

Figure 1. P2A system superstructure (adapted from [4]). Multiple renewable sources (e.g., solar and wind) may be enabled to power the system. Their installed capacities are represented as RE_i^{cap} ($i = 1, \ldots, 5$). Power curtailment ($P^{curtail}$) may be activated at periods when a large excess of energy is available from the renewable sources to protect the system from excessive power. Buying ($P^{grid\ buy}$) and selling ($P^{grid\ sell}$) energy to the grid may also be enabled, subject to the local power grid's restrictions. A battery (B^{cap}) may be used as a buffer to store energy ($P^{batt\ charge}$) during peak energy availability and supply ($P^{batt\ discharge}$) the system when the harnessed power is low. These 3 auxiliary services may be enabled or disabled in the design framework, though at least one is generally required to stabilise power in the system. The electrolyzer and HB synthesis capacities are denoted as E^{cap} and HB^{cap}, respectively. A buffer H_2 tank (T^{cap}) may also be enabled to stabilise the H_2 flowrate to the HB synthesis section, via charge ($F^{tank\ charge}$) or discharge ($F^{tank\ discharge}$) operations. A set of constraints may also be enabled to capture the availability (e.g., grid) or flexibility (e.g., HB synthesis) of all units in managing their loads, in accordance with industrial experience. System design consists of taking all requirements above and the complexity of managing this system over time to achieve the most economical NH_3 manufacturing cost.

However, a fully green route can only be achieved when all process equipment is powered by renewable energy sources, thereby minimizing direct and indirect CO_2 emissions. These processes, known as Power-to-Ammonia (P2A), are part of the broader Power-to-X class [6] and are schematically depicted in Figure 1.

Renewable sources, electrolysis, and HB synthesis are the core components of P2A systems. Collectively, they provide power for operation and enable a chemical route for producing ammonia from water (H_2O) and N_2. Multiple auxiliary services, including buffers (battery and H_2 storage tank), power curtailment, and grid transactions, may also be considered. Since renewable energy production is not constant, one or more services are generally required to stabilize energy and mass flows, and ensure that the core units operate within their safety specifications.

Moreover, the design of these systems is challenging because the fluctuating power profiles of renewables preclude the use of conventional methods tailored for full-load operation. While this approach would deliver the most cost-effective sizes for electrolysis and HB synthesis, it may require oversizing buffers and/or renewable-harvesting infrastructure (highlighted in blue in Figure 1), thereby increasing the costs of green NH_3 manufacturing.

Operating process units at variable loads can be advantageous in this context, provided time-varying operations in auxiliary units (highlighted in orange in Figure 1) are considered to achieve resilient, competitive project designs. Several contributions have been proposed in the last decade on this subject [3, 7, 8]. A review of design strategies for P2A systems is presented in [4].

This work presents the first steps towards a novel design methodology for P2A systems, informed by gaps identified in the scientific literature, as follows:

- Full system customization, including enabling/disabling process units and setting parameters to test and solve a wide range of process configurations, which is the main focus of this paper.
- Robust design by factoring uncertainty on renewable power, process costs, and key model parameters.
- Enhanced chemical process operations (e.g., electrolysis and/or HB synthesis startup/shutdown) for increased accuracy of system behaviour.
- Explore the potential of H_2 process loading/unloading for improved process flexibility and project economics.

A strong focus is placed on capturing the system's performance over a representative time interval, while high-level models are used to capture the behaviour of all the system's units. A design methodology based on Linear Programming (LP) tools is proposed. Its building blocks are presented in the next section, and its application is illustrated in the results section.

METHODOLOGY

Design and operation variables

The P2A superstructure used in this work is presented in Figure 1. It includes all the core and auxiliary units presented above, which may be enabled/disabled individually. For each of these units, a design variable representing their capacities is defined in the design problem (highlighted in blue in Figure 1, e.g., E^{cap} for the nominal electrolyzer capacity).

To capture the impact of short-term fluctuations and seasonal patterns in renewable energy harvesting on the operation of these systems, 1 year of operation, discretised in 1h intervals, is considered [4]. This amounts to a total of 8760h in the defined time-horizon, and as many variables in the design problem for each activated system operation (shown in orange in Figure 1, e.g., $P^{curtail}$ for power curtailment); the focus of the design problem is not on delivering the optimal values for this extended set of operation variables, but rather incorporating them on the design problem to more accurately capture the challenges of time-varying operation. This includes the variability of renewables and constraints on unit operations, to achieve a robust and economic system design.

P2A modelling

Renewable sources

Up to 5 independent renewable sources may be selectively enabled in the design framework. For all sources, a technical specification is selected, and the corresponding power profiles are obtained from historical data at the selected project location(s) consistently with the time structure presented above (e.g., from [9]. These are obtained and specified in the design problem as fractions of the renewable source capacities, such that, at all times in the time horizon, renewable power is given by the product of the corresponding source capacity and these fractions. For all sources, a constant energy price (€/MWh) is assumed.

Power curtailment is a mechanism by which the power generated from a renewable source may be reduced. Formally, this corresponds to adjusting the power from all sources individually; from a modelling perspective, a single variable per time interval is considered, bounded between 0 and the total renewable power.

Electrolyzer

Several technologies are available for water electrolysis [9]. Proton Exchange Membrane (PEM) electrolysis is considered, given the very low O_2 concentrations achieved in the H_2-rich stream, which acts as a catalyst poison in the HB synthesis. A PEM cell includes an anode and a cathode compartment, connected via a proton-exchange membrane and an external electron circuit as depicted in Figure 2.

An oxidation reaction (Equation 1) and a reduction reaction (Equation 2) occur at the electrolyzer's anode and cathode, respectively. This electrochemical reaction is driven by an externally applied voltage, in which H_2O is globally converted to H_2 and O_2, as shown in Equation 3.

$$H_2O \rightarrow 2H^+ + \frac{1}{2}O_2 + 2e^- \quad (1)$$

$$2H^+ + 2e^- \rightarrow H_2 \quad (2)$$

$$H_2O \rightarrow H_2 + \frac{1}{2}O_2, \Delta H^\circ = 241.93\ kJ/mol \quad (3)$$

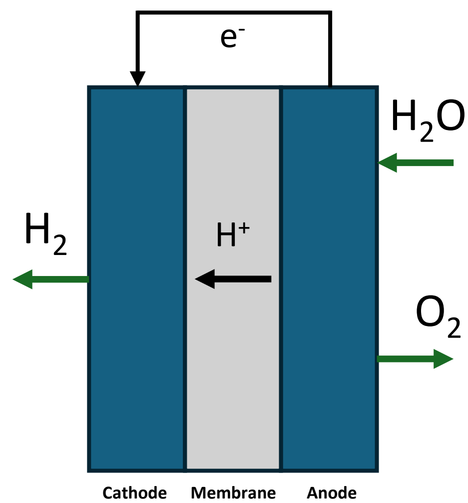

Figure 2. Schematic representation of a PEM cell.

A high-level model is used to capture system behaviour rather than to rigorously model all phenomena. The use of renewable energy to drive this reaction is the key focus, via the definition of a specific energy consumption – expressed in MWh / ton H_2 – where the reaction enthalpy in Equation 3 defines its lower bound. The output H_2 flowrate ($F^{H2\ elect}$) is then calculated as the product of this high-level parameter and the power input to the electrolyzer (P^{elect}).

H_2O is assumed to be available on demand, and O_2 is released from the P2A system (not sold). None is considered in the total cost of green NH_3 production, on the assumption that their prices would represent a small fraction of total manufacturing costs, and particularly the electrolyzer's operating costs.

HB synthesis

The process enables the conversion of a 3:1 molar mixture of H_2 and N_2 (syngas) to NH_3:

$$3H_2 + N_2 \rightleftarrows NH_3, \Delta H^{\circ} = -92.28\ kJ/mol \quad (4)$$

A simplified process layout is schematically depicted in Figure 3. The syngas is first compressed and fed to a converter, which typically includes 2 or 3 iron-based catalytic beds. Several designs for this converter have been proposed, in which the feed gas is conveniently distributed and preheated to sustain autothermal operation [2]. Conversions per pass of around 25% are commonly reported, which requires gas recycle to achieve high overall conversions. The mixture is then cooled to promote the condensation and removal of NH_3 from the process stream. A purge is commonly employed to remove inert components, such as Argon (Ar); in the SMR-based process, it also includes purging CH_4. The unreacted gas is compressed and mixed with the make-up gas, thus completing the synthesis loop. Operating pressures in the range 150-300 bar and temperatures 623-773 K have been reported for this process [10].

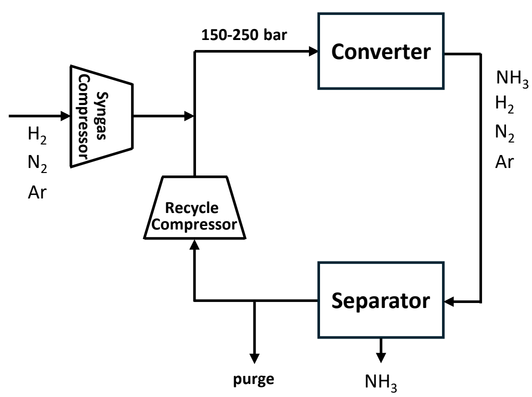

Figure 3. Schematic representation of the HB synthesis.

N_2 for the HB synthesis is supplied via an Air Separation Unit (ASU) or a Pressure Swing Adsorption (PSA) unit, depending on the scale of NH_3 production. It is assumed that the capital costs of the HB synthesis also include the ASU or PSA unit, and that the operational costs and operational constraints of this unit are not significant, in contrast with the operation of the electrolyzer and HB synthesis. Formally, the HB synthesis's compressors also require a power supply; some studies suggest this accounts for a small fraction of the electrolyzer's power demand and is not considered in this study.

The full conversion of the feed syngas is assumed, from which the NH_3 flowrate ($F^{NN3\ HB}$) is calculated directly from the stoichiometry in Equation 4.

Grid

Two 24h price profiles are assumed for: (i) energy bought from the grid, and (ii) energy sold to the grid. These profiles are repeated for the 365 days of the time horizon. The primary modelling consideration concerning grid interaction is setting the upper bounds of $P^{grid\ buy}$ and $P^{grid\ sell}$, which limit the extent of these operations.

Buffers

Battery and H_2 tank, if enabled, are modelled as conventional storage devices according to Equations 5 and 6, respectively:

$$C_{j+1} = C_j + \left(P_j^{batt\ charge} - P_j^{batt\ discharge}\right)\Delta t$$
$$j = 1, \dots, 8760 \quad (5)$$

$$H_{j+1} = H_j + \left(F_j^{tank\ charge} - F_j^{tank\ discharge}\right)\Delta t$$
$$j = 1, \dots, 8760 \quad (6)$$

where C_j and H_j denote the battery's energy charge and H_2 tank's holdup, respectively, at time j, and Δt = 1h. An initial condition for both buffers is also required.

Energy and mass balances

Energy and mass balances are defined at all nodes of the system, based on the associated power and flowrates in the system's main line. This includes the supply of renewable energy and interaction with auxiliary units. Power and flowrates are calculated for all streams over the 8760 h of the time horizon, assuming no power transmission losses occur.

From a modelling perspective, energy utilization in the electrolyzer to produce H_2 is the primary consideration; this is quantified by the electrolyzer's specific energy consumption. This is highlighted in Figure 1, where the modelling focus is on power/flowrate upstream/downstream of the electrolyzer, respectively. In the HB synthesis, H_2 is converted to NH_3 according to the stoichiometry in Equation 4.

Design problem via Linear Programming

The design problem must deliver the capacities of all hardware units (design variables) while minimizing ammonia production cost by fully articulating them with all operation variables. This problem is particularly well-suited to optimization, as it involves tens of thousands of process variables and operational constraints. This choice enables a systematic route to finding the best design via formal optimization principles. Since all model equations and inequations are expressed as linear functions of the design and operation variables, Linear Programming is a particularly suitable choice for the design problem.

Objective function

The objective function for the design problem, assuming all optional units are enabled, is shown below:

$$f = \left(E^{cap}k^E + HB^{cap}k^{HB} + B^{cap}k^B + T^{cap}k^T\right) + \sum_{i=1}^{5} RE_i^{cap}k_i^{RE} + \sum_{j=1}^{8760} P_j^{grid\ buy}k_j^{grid\ buy} - \sum_{j=1}^{8760} P_j^{grid\ buy}k_j^{grid\ buy}$$

(7)

The objective function comprises 3 types of costs. Firstly, the CAPEX and OPEX costs for all units enabled in the P2A design. All are expressed in the objective function as the product of a constant annualised cost factor (e.g., k^E in M€ / per unit of installed capacity – Table 1) with the corresponding design variable (e.g., E^{cap}). OPEX costs include maintenance and, in the case of the electrolyzer, exclude the power supply, which is accounted for through renewable power sources.

The second cost type relates to the total energy harnessed in 1 year of operation. For all enabled sources, this is calculated as the product of the selected source capacity (RE_i^{cap}, $i = 1, ..., 5$) with the sum of all load fractions (full year) and the corresponding energy price (k^{RE}).

The last cost component considers grid interaction. If buy from and/or sell to the grid service(s) are enabled, the costs are expressed in the objective for all hours in the time horizon as the product of $P^{grid\ buy}$ or $P^{grid\ sell}$, respectively, and the corresponding price vectors ($k^{grid\ buy}$ and $k^{grid\ sell}$). Note that for consistency, selling energy to the grid represents a monetary income, and the corresponding product in Equation 7 is multiplied by "-1".

Constraints

The design problem also includes several constraints. These relate mainly to the allowed flexibility in the operation of the core and buffer units as presented earlier. Two types of constraints may be imposed on electrolyzer operation, as follows:

- Power must be within a lower and an upper bound, defined as fractions of the nominal capacity.

$$E^{cap}\phi_{min}^{E} \leq P_j^{elect} \leq E^{cap}\phi_{max}^{E}, j = 1, \dots, 8760 \tag{8}$$

- Power change between consecutive time intervals must be within a lower and an upper bound, defined as fractions of its nominal capacity.

$$E^{cap}\mu_{min}^{E} \leq P_{j+1}^{elect} - P_j^{elect} \leq E^{cap}\mu_{max}^{E},$$

$$j = 2, \dots, 8760 \tag{9}$$

where $\phi_{min}{}^E$ and $\phi_{max}{}^E$ denote the minimum and maximum electrolyzer loads, expressed as a fraction of the electrolyzer capacity to enforce a valid power operating range. Equation 9 limits the extent of ramping power in this unit, by imposing a similar type of constraint via the difference of power between consecutive times, and where $\mu_{min}{}^E$ and $\mu_{max}{}^E$ enforce the corresponding limits.

A similar approach is adopted to HB synthesis operation via parameters $\phi_{min}{}^{HB}$, $\phi_{max}{}^{HB}$, $\mu_{min}{}^{HB}$ and $\mu_{max}{}^{HB}$:

$$HB^{cap}\phi_{min}^{HB} \leq F_j^{NH3\ HB} \leq HB^{cap}\phi_{max}^{HB},$$

$$j = 1, \dots, 8760 \tag{10}$$

$$HB^{cap}\mu_{min}^{HB} \leq F_{j+1}^{NH3\ HB} - F_j^{NH3\ HB} \leq HB^{cap}\mu_{max}^{HB},$$

$$j = 2, \dots, 8760 \tag{11}$$

System design also includes a key equality constraint that enforces that the sum of NH_3 manufactured across all time intervals matches a predefined target (M^{NH3}, in kt NH_3):

$$\sum_{j=1}^{8760} F_j^{NH3\ HB} \frac{\Delta t}{1000} = M^{NH3} \tag{12}$$

Global limits on the total energy bought from and sold to the grid annually may also be enabled to further constrain operations in line with local regulations, energy availability, and limits on green H_2 production. These are expressed as fractions of the total energy consumed in electrolyzer operation.

Additional constraints are also defined to ensure that the energy charge and H_2 mass holdup are within the minimum and maximum limits of the corresponding storage devices' capacities. The maximum discharge and charge rates are specified via the upper bounds on $P^{batt\ charge}$, $P^{batt\ discharge}$, $F^{tank\ charge,}$ and $F^{tank\ discharge}$.

Software/workflow

The design framework is implemented in Python. This includes calculating all matrices and vectors that define the design problem's objective function and constraints and using them to solve the corresponding LP problem. The numpy and scipy libraries [11, 12] deliver this functionality. All P2A plant specifications are imported to Python, and all LP matrices are automatically generated. At the end, the optimizer is returned, from which the design variables can be extracted, and some analyses of the system's performance may be performed.

Key unit specifications

A summary of the key parameters required for configuring P2A systems is presented in Table 1.

RESULTS AND DISCUSSION

To illustrate the application of the P2A design framework, 3 examples are configured based on the general superstructure presented in Figure 1 and solved via LP. A small-scale 10 kt NH_3/year production target is considered. The electrolyzer has a specific energy consumption of 50 MWh/tH_2 and is constrained to operate between 0% and 100% of the nominal load. Wind and solar sources are assumed to be available in Sines (Portugal) as the location for energy generation. Renewable harnessing data was collected for both sources from [9]; the average load factors for the solar and wind series are 0.189 and 0.447, respectively. Grid prices for a representative day of operation on an hourly basis are shown in Figure 4, and the remaining cost factors are estimated as listed in Table 2.

Table 1: Key user-defined parameters in the proposed

design framework for P2A systems.

Description	Units
Renewable energy prices (per source).	€/MWh
Renewables load fractions (per source, for all 8760 h in a year).	-
Grid buy and sell prices (24h series).	€/MWh
Electrolyzer specific energy consumption.	MWh/tH$_2$
Electrolyzer min and max loads[1].	-
Electrolyzer min and max load change[2].	-
HB synthesis min and max loads[1].	-
HB synthesis min and max load change[2]	-
CAPEX and OPEX cost factors (all units).	[3]
NH_3 target production.	kt NH_3

[1] – expressed as a fraction of the unit's capacity (ϕ_{min}^{E} and ϕ_{max}^{E}; ϕ_{min}^{HB}, ϕ_{max}^{HB}); [2] – same as [1] and referring to the load increments between consecutive hours (μ_{min}^{E} and μ_{max}^{E}; μ_{min}^{HB} and μ_{max}^{HB}); [3] – expressed in M€ per unit of installed capacity (annualised for a 30-year project duration).

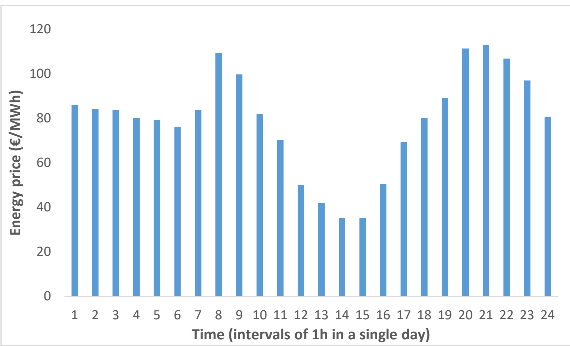

Figure 4. Grid prices for a representative day of operation, on an hourly basis.

Table 2: Infrastructure cost factors and renewable energy prices used in all scenarios.

Equipment	Cost factor	Units
Electrolyzer	$1.33*10^5$	€/MW
HB synthesis	$1.80*10^5$	€/(kt NH_3/y)
H_2 tank	$2.80*10^4$	€/t H_2
Solar source	40	€/MWh
Wind source	45	€/MWh

In the 3 illustrative examples presented in sequence, distinct auxiliary units and constraints are enabled. The key results for all scenarios are shown in Table 3.

Scenario 1: Full load P2A with grid

This design aims to reproduce the full-load operation of the classic HB process via SMR. This is achieved by enforcing the HB synthesis to operate at 100% of its nominal capacity for all hours of the time horizon. This scenario establishes a base case for comparison with the remaining P2A examples. Buying energy from the grid is enabled and subject to a 10% limit on the annual contribution of grid energy for green H_2 manufacture.

The design capacities and KPIs for all scenarios are listed in Table 3. The HB synthesis operates, as expected, at an average 100% load (always at full load), and the minimum installed capacity of 10 kt NH_3/y is achieved to deliver the target production. Since no buffer is active between the electrolyzer and the HB synthesis, the electrolyzer must also operate at 100%, thereby achieving the minimum costs for the core units. The 10% limit on grid energy utilization is active. The grid acts as an indispensable buffer to ensure full load requirements are met, particularly when renewable generation is low. The burden to deliver an optimal design under these conditions falls on the contracted power from renewables, which largely exceeds the actual system needs, as shown in the energy and cost shares in the second column of Table 3. Grid operation and curtail power for this scenario are illustrated in Figure 5.

A manufacturing cost of 1080 €/tNH_3 is achieved. If the 10% limit on grid usage is removed, the price would fall from 1080 to 841 €/tNH3, with 33.7% grid utilization.

Scenario 2: Flexible P2A with grid

In this and the next scenarios, the full-load requirement is relaxed, and instead, the HB synthesis is required to operate at 70%-100%, with load increments between consecutive hours limited to 10% of its nominal capacity. The same grid utilization conditions as defined in the first scenario are also considered.

From Table 3, the 10% grid utilization limit remains active. However, by adding flexibility to the HB synthesis, the design of the electrolyzer and HB synthesis are now slightly oversized, with an average load of 88.6%. These units contribute more significantly to overall costs but enable a significant reduction in the solar and wind contracted capacities from 17.9 MW to 13.6 MW and from 32.3 MW to 21.0 MW, respectively. Power curtailment is significantly reduced, and a much lower manufacturing cost of 894 €/tNH_3 is obtained. By further extending flexibility to 50-100% loads and a maximum of 20% loads' increment, the cost can be further reduced to 861 €/tNH_3.

Scenario 3: Flexible P2A with H_2 tank

An islanded system is considered, precluding the utilization of the grid to assist P2A system operation. An H_2 tank is considered to provide the necessary flexibility and meet the load requirements of HB synthesis operation as presented in scenario 2.

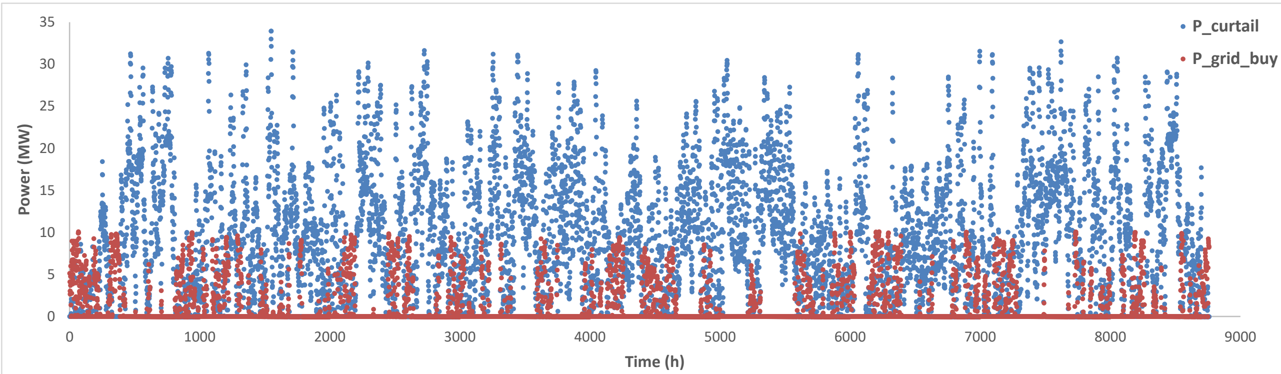

Figure 5. Curtailment and grid power bought from the grid over the full time-horizon in scenario 1.

The H_2 tank decouples the electrolyzer and HB synthesis operations: in the previous scenarios, there are no buffers between the two units, and their operating loads are always synchronized. Now, they are to some extent independent of one another, as confirmed by their average operating loads in Table 3. This change effectively enables full flexibility for the electrolyzer unit (0-100% load). A new energy mix is obtained, promoting the slightly cheaper solar source as listed in Table 2. Note that despite optimal capacities of 18.7 MW and 17.8 MW for solar and wind, respectively, wind power still dominates energy shares due to the higher load fractions in the corresponding renewables' series.

A 14.0 t H_2 tank capacity is delivered from the optimal design. This capacity would be sufficient to continuously supply the HB synthesis for 65 h at the nominal rate, with no H_2 supplied from the electrolyzer. The tank holdup is depicted in Figure 6, where several cycles between full charge and no charge are identified.

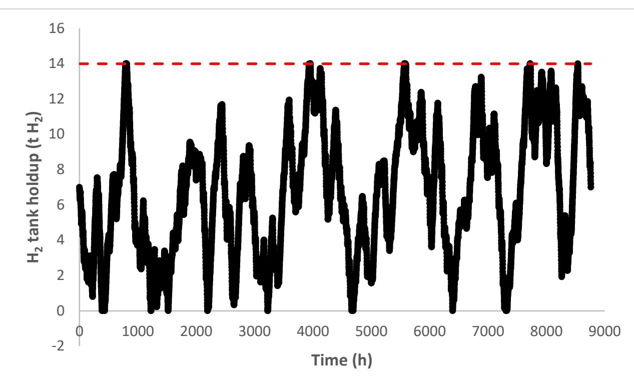

Figure 6. H_2 holdup over the time horizon for scenario 3.

A cost of 861 €/tNH_3 is achieved. While this is a small improvement over scenario 2, a fully green P2A system has been developed.

Design results

The design results and summary of the Key Performance Indicators (KPIs) in the 3 scenarios presented above are listed in Table 3.

Table 3: Summary of design results and KPIs for all scenarios presented earlier.

Design variables & KPIs		Scenario 1	Scenario 2	Scenario 3	Units
Design capacities	RE^{cap}_{solar}	17.9	13.6	18.7	MW
	RE^{cap}_{wind}	32.3	21.0	17.8	MW
	E^{cap}	10.1	11.4	15.0	MW
	HB^{cap}	10.0	11.3	10.6	kt NH_3/y
	T^{cap}	-	-	14.0	t H_2
KPIs	NH_3 cost	1080	894	868	€/tNH_3
	Elect load[1]	100	88.6	67.5	%
	HB load[1]	100	88.6	94.8	%
Energy shares	Solar	33.5	25.5	34.9	%
	Wind	142.4	92.7	78.7	%
	Grid	10	10	0	%
	Curtail	85.9	28.2	13.5	%
Cost shares	Renewables	63.6	51.5	50.5	%
	Electrolyzer	12.5	17.1	23.1	%
	H_2 tank	0	0	4.5	%
	Grid	7.2	8.7	0	%
	HB synthesis	16.7	22.7	21.9	%

[1] – average loads for 1 year of operation.

CONCLUSION AND FUTURE WORK

This work presents the key principles of a novel and fully customizable methodology for P2A design. It consists of a superstructure of core and auxiliary units, the latter of which may be enabled or disabled to test a multitude of P2A configurations. High-level models are defined for all units, and model complexity arises mainly from considering a full year of operation with hourly resolution. The design problem is formulated as an LP, containing both design and operation variables; while calculating the former is the main goal of the design problem, the full consideration of operation variables, and particularly their operation in the full time-horizon, is critical to achieve design results considering the full complexity of renewables' variability.

The initial results provide useful insights into how unit flexibility, renewable variability, buffers, and objective function definition affect unit capacities, thereby offering a systematic approach to optimal and robust P2A designs. While the initial results are promising, multiple key developments are desirable to enable a more detailed modelling and optimization of these systems. Several phenomena, including: (i) power transmission, (ii) reaction conversion in electrolyzer and HB synthesis, (iii) H_2O and N_2 supply, (iv) powering the HB synthesis' compressors from renewables, (v) neutrality conditions on buffers' operation, and (vi) setting multiple production objectives, will be considered in future work.

Furthermore, this framework enables more advanced utilization modes. For instance, assuming all design variables are set, the framework may be used in P2A systems to facilitate process management and articulation of all units to achieve the most economical manufacturing costs. One of the most critical elements in this framework is setting a priori load fractions for renewable sources based on historical data, as is common practice in the field. Understanding how the design methodology can be improved to deliver robust designs that operate efficiently across a broad range of meteorological conditions remains largely unexplored and may be explored in the future through this design framework.

Given the focus on design modularity presented in this design framework, it readily enables more advanced features than those captured in Figure 1. Work is ongoing to capture the impact of process shutdowns on P2A operation and economics. This is an important consideration because the HB synthesis may require maintenance for 10% of the total operation time [8]. To achieve better process economics and flexibility, buying/selling H_2 is also being developed as an optional feature to make the best use of the investments in renewable power and electrolyzer infrastructure.

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