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Multi-Objective Optimization for Sustainable Design of Power-to-Ammonia Plants

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ABSTRACT

This work addresses the process design of Power-to-Ammonia plants (*i.e.* ammonia from renewable-powered electrolysis) by a novel methodology based on the multi-objective optimization of the "Three pillars of sustainability": economic, environmental, and social. Specifically, we developed a tool estimating the installed capacities of every main process section typically featured by Power-to-Ammonia facilities (*e.g.*, the renewable power plant, the electrolyzer, energy and hydrogen storage systems, *etc.*) to maximize the plant's "Global Sustainability Score".

Keywords: Green ammonia, Decarbonization, Renewable energy, Power-to-X, Three pillars of sustainability

INTRODUCTION

In 2020, about 185 Mt/y of ammonia were produced worldwide, causing 1% of that year's global greenhouse gas (GHG) emissions [1]. Indeed, more than 96% of today's global hydrogen input for ammonia derives from fossil fuels. Specifically, the most common synthetic pathways for hydrogen feedstocks heading to Haber-Bosch reactors are (i) steam methane reforming, *i.e.* hydrogen from natural gas, accounting for about 70% of global sourcing and emitting from 2.5 to 3 t_{CO2eq}/t_{NH3}; (ii) coal gasification, providing 26% of hydrogen feedstocks and emitting ca. 5 t_{CO2eq}/t_{NH3}; (iii) partial oxidation of heavy oil, accounting for less than 1%; and (iv) hydrogen from electrolysis, currently representing few isolated cases [2]. The fossil-based routes are classified as "gray" ammonia if no carbon capture and storage (CCS) technologies are implemented or "blue" ammonia if featuring CCS. Conversely, employing hydrogen from electrolysis is defined as "green" ammonia if renewable energy is used to power the electrolyzer, ideally resulting in zero direct carbon emissions. That is why the optimal design of Power-to-Ammonia plants (*i.e.* facilities converting renewable power into green ammonia via water electrolysis) is a topic of significant interest in the recent scientific literature. In particular, the erratic trend of non-dispatchable renewable sources (*e.g.*, solar, wind, *etc.*) leads to several process complications in running (thus designing) such plants: above all, the need for dynamic operations instead of conventional steady-state ones and the demand for buffer mass and energy storage to mitigate the effects of oversupply or shortage occurrences in the renewable inputs. This paper introduces a methodology to optimally design Power-to-Ammonia plants according to the "Three pillars", *i.e.* economic, environmental, and social, "of sustainability". Precisely, the fundamentals of such an approach lie in the works of Scotti *et al.* (2017, 2018) [3,4], as they proposed a solution strategy for the multi-objective optimization (MOO) of sustainability in the conceptual design of conventional (*i.e.* fossil-based, thus operating in stationary conditions) chemical plants. Specifically, this work aims to enhance such an approach by extending it to the much more challenging green process field that calls for an intrinsically dynamic methodology to conceptual design.

METHODOLOGY

Figure 1 depicts the investigated Power-to-Ammonia plant's process sections and battery limits (*i.e.* the control volume of the present assessment). Specifically, to achieve an average productivity target of 100 t_{NH3}/d, such a facility features (a) a renewable (*i.e.* solar and wind) power plant; (b) an alkaline water electrolyzer; (c) an air separation unit, *i.e.* ASU; (d) a conventional ammonia synthesis loop (*i.e.* Haber-Bosch process); and both

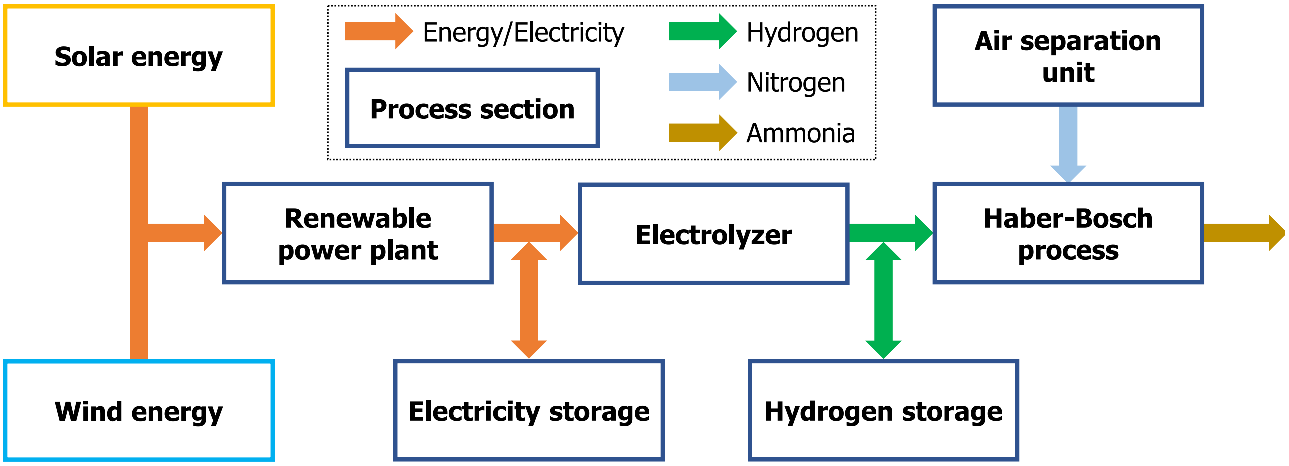


Figure 1: Block flow diagram of the assessed Power-to-Ammonia plant.

(e) energy and (f) mass buffer storages (namely, a lithium-ion battery amidst the power plant and the electrolyzer, and hydrogen pressurized tanks amid the electrolyzer and the ammonia plant) to dampen any process discontinuities introduced by solar and wind profiles. Furthermore, an auxiliary electricity supply from the power grid can be provided to meet the electric demand of the ASU, the Haber-Bosch process, and the multistage centrifugal compressors within the hydrogen storage section whenever the renewable electricity inputs exceeding the electrolysis demand are insufficient to power them. Both MATLAB™ R2024 (the power plant, electrolyzer, and storage systems) and UniSim® Design R492 (the ASU and Haber-Bosch process) were used to model the plant according to the renewable inputs, *i.e.* 2023 solar and wind profiles from CAISO (California Independent System Operator) [5], and the optimal policies for flexible mass and electricity storage discussed in Isella and Manca (2025a, 2025b) [6,7]. Accordingly, such process models provide the equation-oriented (in MATLAB™) and black-box (in UniSim®) equality constraints (*e.g.*, mass and energy balances) of the optimization problem. Moreover, the related degrees of freedom are the solar and wind installed capacities (*i.e.* the renewable power plant), determining the energy input to the electrolyzer (and the battery hold-up) and thus the hydrogen input to the ammonia synthesis loop (and the hydrogen storage size). Consequently, the resulting capacities for such process sections (conversely, both ASU and Haber-Bosch dimensions are already given according to the high technological maturity of small-scale gray ammonia plants) lead to a "global sustainability score" (GSS) that allows practical comparisons between multiple process configurations. Indeed, the present MOO problem has been approached by the scalarization technique, *i.e.* a solution method aggregating all the different objective functions (namely, the economic, the environmental, and the social ones) into a single one by a suitable scalarization function (in this specific case, their linear combination). Thus, the sustainability metrics formulated for each sustainability pillar are (1) the levelized cost of ammonia, *i.e.* LCOA, for the economic dimension; (2) the global warming potential, *i.e.* GWP, for the environmental dimension (as it counts the cradle-to-grave CO_2-equivalent emissions released per mass unit of ammonia product); and (3) the Fire and Explosion Index [8], *i.e.* FEI, for the social dimension. Then, to be scalarized (hence making them comparable with each other), these parameters need to be normalized first through "normalized sustainability indexes":

$$EcoSI_i = \frac{\max(LCOA) - LCOA_i}{\max(LCOA) - \min(LCOA)} \qquad (1)$$

$$EnvSI_i = \frac{\max(GWP) - GWP_i}{\max(GWP) - \min(GWP)} \qquad (2)$$

$$SocSI_i = \frac{\max(FEI) - FEI_i}{\max(FEI) - \min(FEI)} \qquad (3)$$

Where the i subscript denotes the i-th assessed process configuration within the decision space.

As evident from their formulation, all these indexes range from 0 (*i.e.* the least sustainable scenario) to 1 (*i.e.* the most sustainable scenario). Lastly, as mentioned above, the ultimate expression of the GSS (*i.e.* the objective function of the MOO problem, to be maximized) is the linear combination of such indexes, whose coefficients act as user-defined weighting factors for each sustainability pillar:

$$GSS = w_{ECO} \cdot EcoSI + w_{ENV} \cdot EnvSI + w_{SOC} \cdot SocSI \qquad (4)$$

Please note that the sum of the weighting factors must always be equal to 1 (*i.e.* 100%) and that, like the normalized sustainability indexes, even the GSS spans in the same sense from 0 to 1.

Table 1: Input data for the Power-to-Ammonia model [9].

DATASET			
	Location	California	
	Year	2023	
	Solar capacity factor	26.64%	[-]
	Wind capacity factor	29.66%	[-]
	Time discretization	1	[h]
TECHNO-ECONOMIC DATA			
Solar	Lifetime	25	[y]
	CAPEX	1119	[USD/kWe]
	OPEX	1.70%	[CAPEX/y]
	GWP	136.24	[kg_{CO2eq}/MWh]
Wind	Lifetime	25	[y]
	CAPEX	1285	[USD/kWe]
	OPEX	2%	[CAPEX/y]
	GWP	26.33	[kg_{CO2eq}/MWh]
Electricity storage	Lifetime	10	[y]
	CAPEX	310	[USD/kWe]
	OPEX	2%	[CAPEX/y]
	Charging efficiency	0.95	[-]
	Discharging efficiency	0.95	[-]
	Self-discharge rate	0.007%	[load/h]
	GWP	50	[kg_{CO2eq}/kWh]
Electrolyzer	Lifetime	10	[y]
	CAPEX	700	[USD/kWe]
	OPEX	2%	[CAPEX/y]
	Stack DC consumption	4.65	[kWh/Nm^3_{H2}]
	Maximum load flexibility	1	[nominal load]
	Minimum load flexibility	0.1	[nominal load]
	GWP	0.215	[kg_{CO2eq}/kg_{H2}]
Hydrogen storage	Lifetime	20	[y]
	CAPEX	1900	[USD/kg_{H2}]
	OPEX	1%	[CAPEX/y]
	P inlet (Electrolyzer)	30	[bar]
	P outlet (H_2 storage)	200	[bar]
	Electricity consumption	1.03	[MWh/t_{H2}]
	GWP	200	[$kgCO2eq/_{kgH2}$]
Air separation unit	Electricity consumption	0.08	[MWh/t_{N2}]
Haber-Bosch process	NH_3 target productivity	4.17	[t_{NH3}/h]
	H_2 target feed	0.78	[t_{H2}/h]
	Maximum ramp	100%	[load/h]
	Maximum load flexibility	110%	[nominal load]
	Minimum load flexibility	10%	[nominal load]
	Electricity consumption	0.59	[MWh/t_{NH3}]
Electric grid	Electricity cost	100	[USD/MWh]
	GWP	370	[kg_{CO2eq}/MWh]

RESULTS

The optimization problem, as defined in the previous section, is then applied to a Power-to-Ammonia plant showing the features reported in **Table 1**. Both degrees of freedom (*i.e.* the solar and wind installed capacities) are iteratively varied from 0 to 500 MW (according to a 10 MW step size) by a brute-force grid-search method. Multi-objective optimization always requires some human decision-making: in this particular case, such a feature lies in the weighting factors that the user must assign *a priori* (*i.e.* before the searching phase) according to the emphasis given to each sustainability pillar.

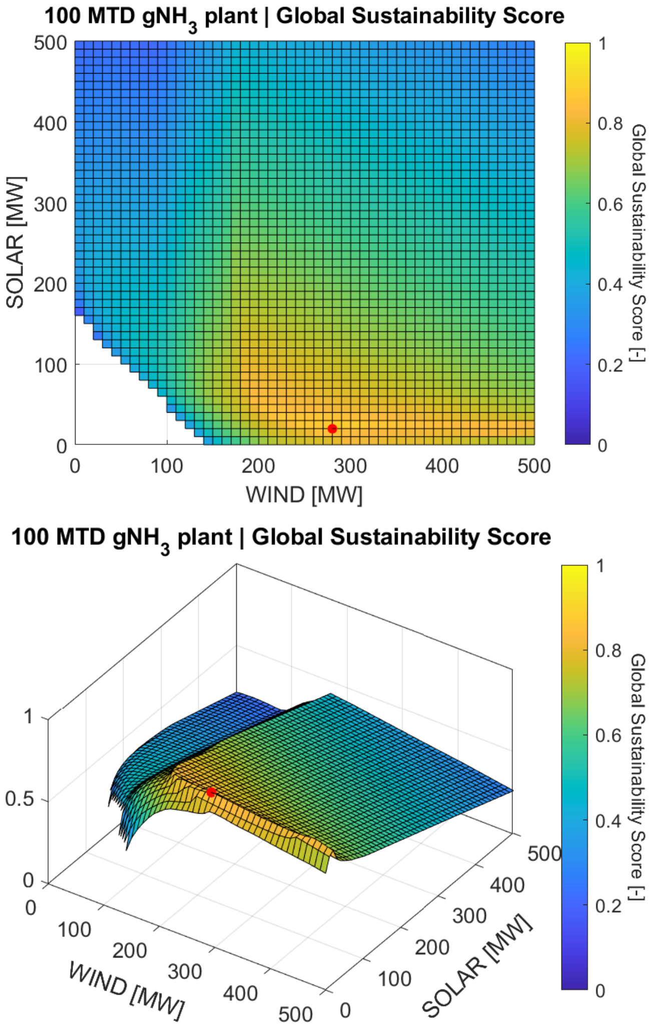


Figure 2: 2D (above) and 3D (below) diagrams of the GSS (the red dot corresponds to the maximum, *i.e.* 88.25%).

For example, let us assume: 50% economic; 25% environmental; and 25% social. **Figure 2** shows the two- and three-dimensional topologies of the resulting objective function, while the two panels of **Figure 3** return the main operating profiles of the optimal process configuration. Each pillar aims for a different solution: (A) economic sustainability typically results in a compromise solution on the installed capacity of the renewable power plant as lower ones would imply bigger electrolyzers and storage systems (to process, and mitigate, any energy input made available by the small power plant), and *vice versa*. Specifically, wind power is preferred to solar as its higher availability throughout the day reduces the storage systems' need (hence the size and total costs). (B) Environmental sustainability tends to minimize the renewable power plant sizes as they lead to far higher GWP values than the storage systems. However, the GWP associated with the electrolyzer (as, like its size, increases when the power plant size decreases) counterbalances such a trend, making the optimal power plant slightly more significant than the minimum allowable one. (C) Lastly, social sustainability pushes for huge renewable power plants as they minimize the electrolyzer and hydrogen storage sizes (hence the well-known hydrogen-related process hazards). Consequently, the resulting objective function (see **Figure 2**) displays all these features, though the corresponding weighting factors partially mitigate them. The corresponding optimal GSS is 88.25%, meaning the three sustainability pillars agreed fairly (although not entirely).

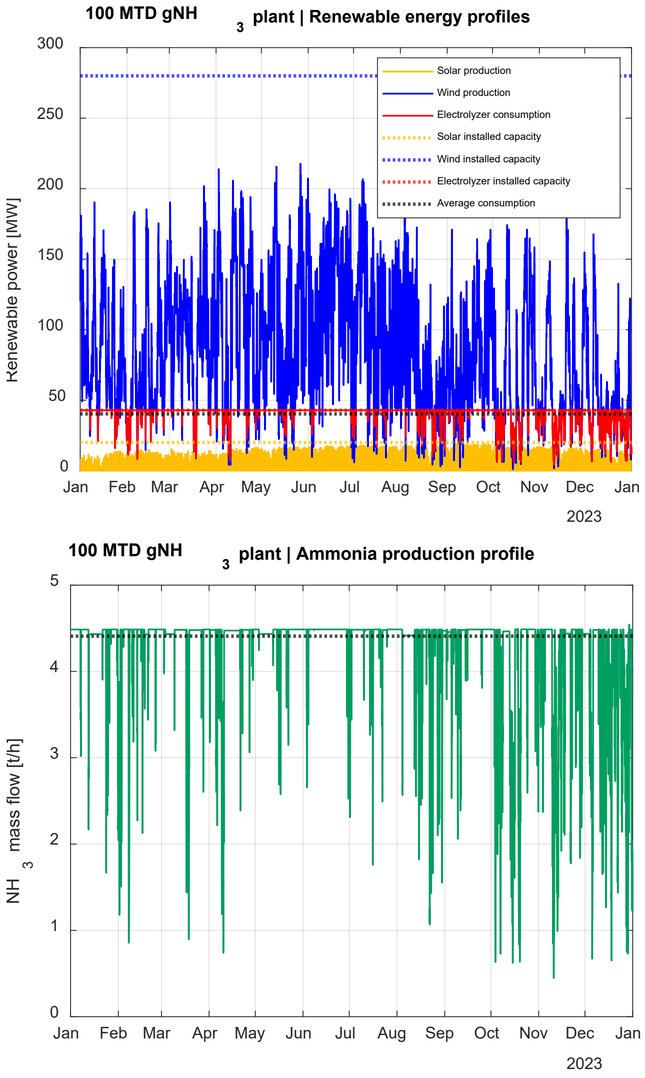
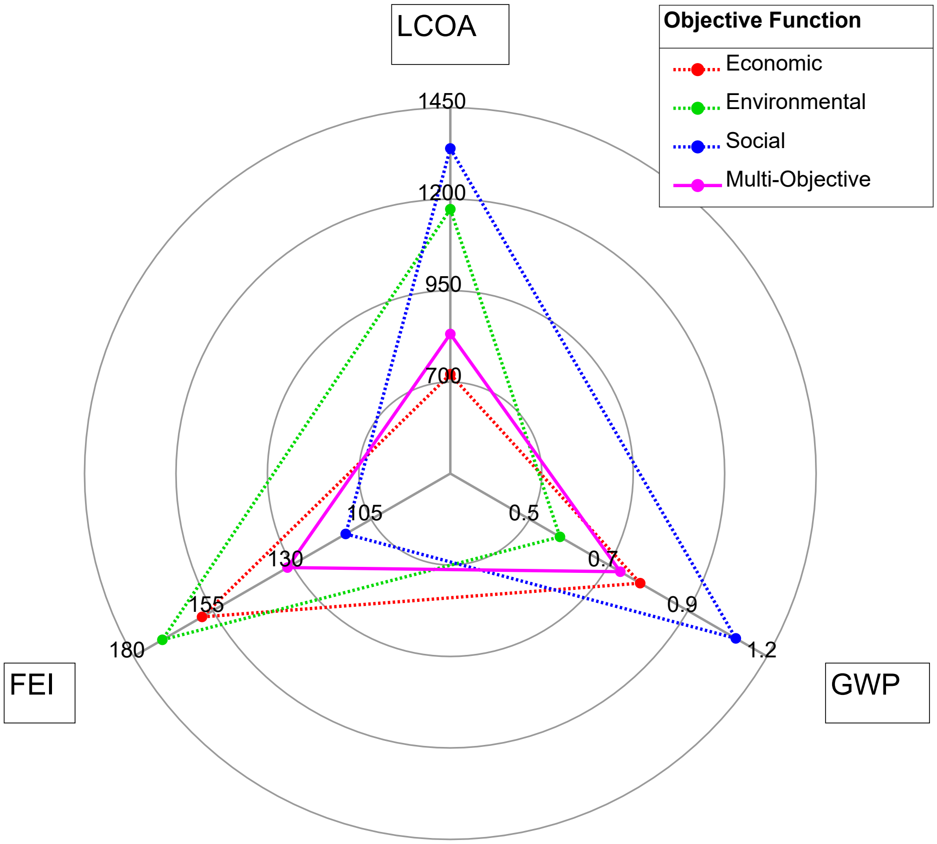


Figure 3: Renewable power generation vs. consumption (above) and ammonia production (below) profiles by the optimal Power-to-Ammonia plant process configuration.

Finally, **Table 2** summarizes the installed capacities and sustainability metrics resulting from the optimization

Table 2: Main results of the optimal process configuration.

Optimal process configuration: 50% economic + 25% environmental + 25% social		
Solar	20	[MW]
Wind	280	[MW]
Electrolyzer	42.87	[MW]
Electricity storage	2.29	[MWh]
Hydrogen storage	38.39	[kg$_{H2}$]
LCOA	871.86	[USD/t$_{NH3}$]
GWP	0.77	[t$_{CO2eq}$/t$_{NH3}$]
FEI	131.40	[-]
GSS	88.25%	[-]



problem. Specifically, the optimal process configuration features high wind-power installed capacities and negligible storage sizes (*i.e.* battery and tanks).

As evident from **Table 2**, compared to the economically optimal scenario (*i.e.* the single-objective optimization of the economic dimension only), both environmental and social sustainability improved (−3.5% in GWP and −17% in FEI, respectively) at the expense of the ammonia production cost (+21% in LCOA).

Please also note that solving the three single-objective optimization problems together (economic, environmental, and social) would allow visualizing the Pareto fronts, *i.e.* those points within the decision space whose corresponding objective function values cannot be concurrently improved. This is a traditional "*a posteriori*" technique (meaning that the decision process is postponed after the searching phase; thus, no preference criteria need to be provided "*a priori*"), giving interesting insights on the conciliation among every single objective function. However, the Pareto front approach may be unsatisfactory and confusing for many reasons. Above all, the somewhat chaotic representation of all the solutions explored and the high number of Pareto optimal points (60 out of 2601 process configurations investigated) still leaves too much space for the decision maker's discretion. That is why we opted for the scalarization method:

indeed, as an "*a priori*" technique, it provides the decision criterion (assuming a specific hierarchy of importance in the objective functions according to the weighting factors) before the searching phase, thus allowing for the examination of a unique solution.

CONCLUSIONS

This work presented a methodology to identify the process design of Power-to-Ammonia plants that best maximizes and harmonizes the three pillars of sustainability: economic, environmental, and social. Resorting to the scalarization method proved to be a successful approach to solving such a multi-objective optimization problem and allowing the users (*e.g.*, academic researchers and industrial stakeholders) to quickly compare the different results arising from the arbitrary choice of the three pillar-related weighting factors. Furthermore, this work stressed the importance of process flexibility in renewable-energy-powered chemical plants to adapt appropriately to the erratic nature of renewable energy sources. Indeed, the higher the process flexibility, the lower the required storage systems' capacities to mitigate the discontinuities in renewable power (hence, the lower the production costs).

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