Alternative Storage Of Hydrogen: Robust Design Optimization Of A Standalone Wind-powered Ammonia Plant

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Injecting renewables, like wind and solar power, in the electricity grid is quite a challenge due to their intermittent nature and inability to balance the grid without additional temporary storage facilities [1, 2]. The integration of these renewable sources is however advocated by the European Commission to reach the legislative goals of 2020 (each EU country needs to have an energy production share of 20% by renewables) [3]. Finding a perfect solution to this conundrum is challenging due to practical issues that sustainable carbon-free fuels (e.g. hydrogen and ammonia) possess, like storing and producing cheap renewable electrohydrogen, and efficient and flexible production of cheap, renewable electroammonia on small and medium scale [4, 5]. However, ammonia (NH_3) is still considered a practical solution for the next energy generation system in terms of energy transportation, storage and power generation [4, 6].

MODEL DEVELOPMENT AND OPTIMIZATION SETUP

Electroammonia is generally produced from nitrogen (extracted from air) and hydrogen (produced by electrolysis) in the Haber-Bosch process. This work describe a setup to accomplish an efficient and robust Haber-Bosch design. An Alkaline Water Electrolyzer (AWE), a Pressure Swing Adsorption (PSA) and a Haber-Bosch Synthesis (HBS) process were created in the Aspen Plus simulation software and a model of a Wind Turbine Generator (WTG) was developed in Python (Figure 1). A WTG model of the 3MW Vestas V112 to convert the wind speed in electric power is created in Python using the cut-in, rated and cut-out wind speed provided by the manufacturer [7]. The model to convert the hydrogen to NH_3 is based on a Aspen Plus model created by Frattini et al. and is validated according to their reported results

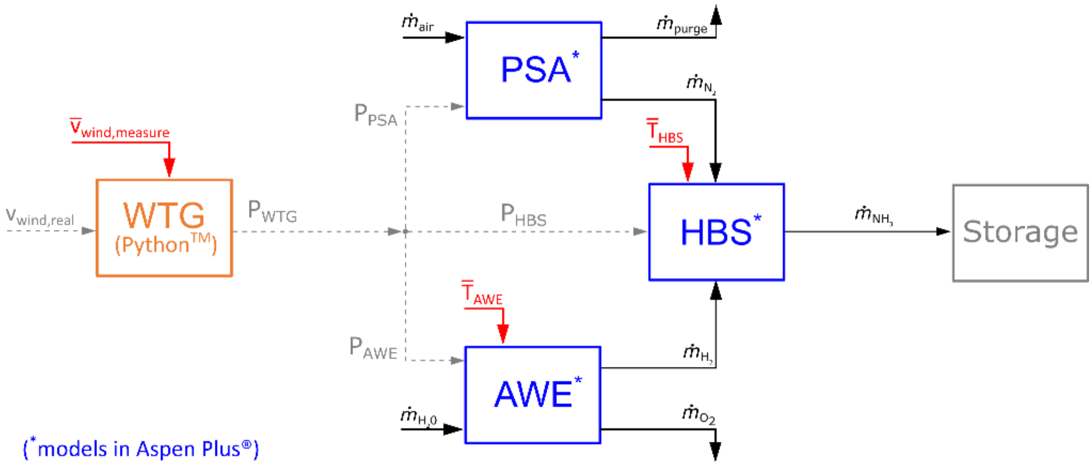

Figure 1: The Vestas V112 Wind Turbine Generator (WTG) model is used to power the NH_3 process plant which consists of an Alkaline Water Electrolyzer (AWE), Pressure Swing Adsorption (PSA) and Haber-Bosch Synthesis (HBS) loop process created in Aspen Plus.

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[8]. In this validation, the largest error that is observed is located on the result of the recycle ratio (the ratio of the recycled stream over the feed stream in mol/mol) where the relative error between these results is 1.87%. The model of the Phoebus alkaline electrolyzer, described by Ulleberg, is implemented in Aspen Plus using a Fortan script [9]. This AWE model is then successfully incorporated into the model of Frattini et al. [8].

The model undergoes a Deterministic Design Optimization (DDO) using a fast and elitist multi-objective genetic algorithm (NSGA-II) to optimize the model according to certain objectives. The DDO objectives are maximizing the production of NH_3 and the load factor of the plant by controlling four chosen design parameters. These design parameters and the search space of the optimization algorithm are defined as follows (Figure 2 as an example):

- $\%_{NH3} = P_{NH3}/P_{WTG}$: amount of power from the WTG (P_{WTG}) to the total process (P_{NH3}); $0 \leq \%_{NH3} \leq 100\%$; The unconsumed % of power coming from the WTG ($100\% - \%_{NH3}$) is considered to be supplied to an alternative storage system (e.g. battery, pumped hydro)
- n_{cells}: the number of electrolytic cells in series in the AWE stack; $1 \leq n_{cells} \leq 2600$ cells
- $\%_{AWE} = P_{AWE}/P_{NH3}$: amount of power provided to the electrolyzer stack (P_{AWE}); $90\% \leq \%_{AWE} \leq 97\%$
- $\%_{PSA} = P_{PSA}/P_{NH3}$: amount of power provided to the PSA (P_{PSA}); $0.5\% \leq \%_{PSA} \leq 3\%$

The residual power of the plant ($P_{NH3} - P_{AWE} - P_{PSA}$) is supplied to the compressor to pressurize the Haber-Bosch process (P_{HBS}).

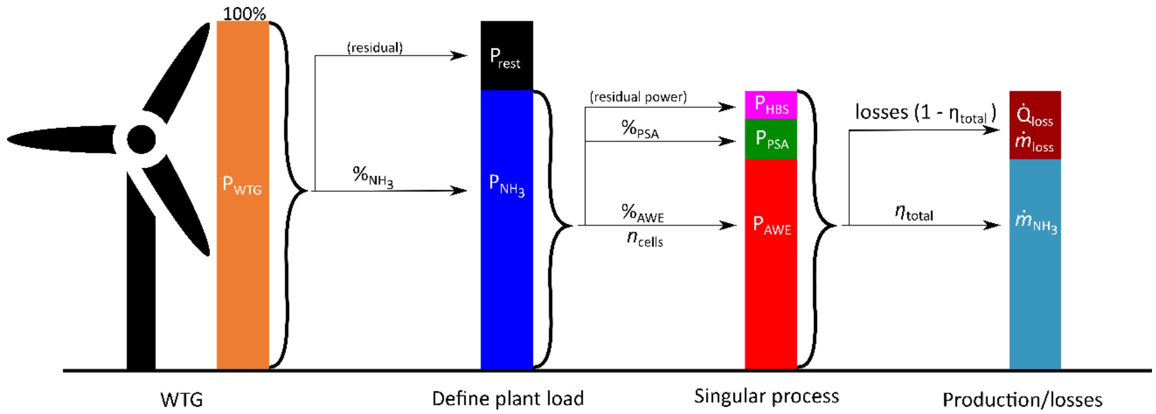

Figure 2: The optimization algorithm uses four design parameters ($\%_{NH3}$, $\%_{PSA}$, $\%_{AWE}$ and n_{cells}) to find a design that maximizes the NH_3 production ($\dot{m}_{NH3}$) and the load factor of the plant.

An Uncertainty Quantification (UQ) analysis, preformed on the basis of the Polynomial Chaos Expansion (PCE) theory, is completed to observe which integrated uncertain parameters have the biggest impact on the variation of the objectives. The wind speed measurement, the temperature of the electrolyzer and the NH_3 synthesis reactor are taken uncertain in this analysis (Figure 2). Finally, the NSGA-II and the PCE algorithm are combined in the Robust Design Optimization (RDO) process to find a design that is least sensitive to these uncertain parameters while maximizing the production of NH_3. The Coefficient of Variance (CoV) is used as a robustness indicator, where improving the robustness is accomplished by minimizing the CoV.

MAIN RESULTS OF UNCERTAINTY ANALYSIS AND DESIGN OPTIMIZATION

Wind measurements of a wind turbine park located in Lugo (Galacia), Spain are used as input to the model during the optimization [10]. The DDO delivers a trade-off between maximizing the NH_3 production and maximizing the load factor in the form of a Pareto front. The designer would have to choose between selecting a plant with a maximum load factor of 73.5% but an annual NH_3 production of 122 tonne, or a plant with a load factor of (maximum) 22.5% and a yearly production of 491 tonne of NH_3. In the "Most NH_3" case, this plant has the best performance at a wind speed of 6 m/s with an energy consumption of 47.1 MJ/kg$_{NH3}$. In the case of the "Best load factor" design, a constant energy consumption of 46.2 MJ/kg$_{NH3}$ is observed (which starts from a wind speed of 3.82 m/s until the cut-out wind speed of the WTG is reached).

The UQ analysis executed on these two designs shows that the wind speed measurement variations and the temperature fluctuation in the NH_3 synthesis reactor have the biggest impact on the overall performance of both designs. In order to reduce these influences, a RDO is executed. The result of this RDO shows a trade-off between the two objectives (production of NH_3 and its CoV) (Figure 3). One design is able to produce more NH_3 compared to the more robust NH_3 plant design. A UQ analysis of these two designs shows the dominating effect of the temperature variation of the NH_3 synthesis reactor on the "Robust design", while the "Productive design" is mainly influenced by the wind speed measurement error and this temperature variation in the synthesis reactor as was observed in the DDO analysis (Figure 4). Decreasing the influences even further could be achieved by including a more precise wind speed measurement device and a better control over the temperature fluctuation in the NH_3 reactor.

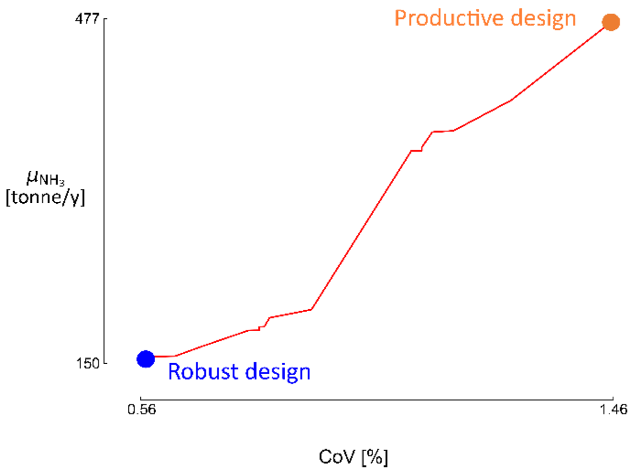

Figure 3: The RDO generates a trade-off between maximizing the yearly average NH_3 production (μ_{NH_3}) and minimizing the CoV as the objectives of the algorithm.

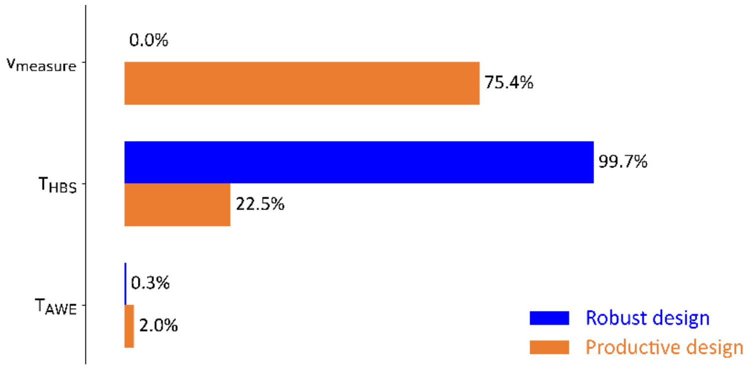

Figure 4: The Sobol' indices of the UQ analysis shows that the NH_3 production of the "Productive design" is influenced by the wind speed measurement variation and the temperature variation of the synthesis reactor. In the case of the "Robust design", the NH_3 production is dominated by the temperature fluctuation in the NH_3 synthesis reactor.

CONCLUSION

In order to find an alternative way to store hydrogen, the development of a robust full-electric NH_3 synthesis plant with its accessories (WTG, AWE, PSA and HBS) is created in Aspen Plus. The DDO analysis of this model provides a trade-off between maximizing the NH_3 production and maximizing the load factor. The results of the DDO provided two interesting sets of design parameters. One design can achieve a load factor of 73.5% and has a near constant energy efficiency of 46.2 MJ/kg_{NH3} but produces only 122 tonne NH_3 annually. The other DDO design can obtain however a load factor of 22.5% and an energy efficiency of 47.1 MJ/kg_{NH3} (at best) but features a yearly production of 491 tonne of NH_3. The RDO analysis executed on the Aspen Plus model provides a trade-off between maximizing the NH_3 production and minimizing the CoV which is done in order to reduce the influence of the uncertain parameters on the NH_3 production. A trade-off is obtained between a design with a large NH_3 production (477 tonne/year NH_3 on average) with a CoV of 1.46%, and a design with less NH_3 (150 tonne/year NH_3) but more robust to temperature fluctuations and wind speed variations (CoV of 0.56%). To minimize these influences on the CoV even further, a more accurate wind speed measurement device and a better control over the temperature fluctuation in the NH_3 reactor could be considered.

FUTURE WORK

As a future prospect, a more efficient NH_3 synthesis process should be considered in order to improve the energy consumption of the NH_3 production. In addition, an economical multi-objective robust design optimization will be looked upon in order to minimize the levelized cost of the electroammonia and maximize the NH_3 production.

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