Systems & Control Transactions

Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale, Monika E. Polańska, Filip Logist (Eds.)

PSE PRESS

Optimisation Under Uncertain Meteorology: Stochastic Modelling of Hydrogen Export Systems

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ABSTRACT

Deriving accurate cost projections associated with producing hydrogen within the context of an energy-export paradigm is a challenging feat due to non-deterministic nature of weather systems. Many research efforts employ deterministic models to estimate costs, which could be biased by the innate ability of these models to 'see the future'. To this end we present the findings of a multistage stochastic model of hydrogen production for energy export (using liquid hydrogen or ammonia as energy vectors), the findings of which are compared to that of a deterministic programme. Our modelling found that the deterministic model consistently underestimated the price relative to the non-deterministic approach by \$ 0.08 – 0.10 $kg^{-1}(H_2)$ (when exposed to the exact same amount of weather data) and saw a standard deviation 40% higher when modelling the same time horizon. In addition to comparing modelling paradigms, different grid-operating strategies were explored in their ability to mitigate three critical co-sensitive factors of the production facility: high-cost hydrogen storage, uncertainty in weather forecasting and sluggish production processes. We found that a 'grid-wheeling' strategy substantially reduces the production cost for a solar system (by 16% and 21% for LH_2 and NH_3, respectively) due to its ability to guarantee the return of energy borrowed overnight during the day, but was not effective for the wind system, due to the non-periodic nature of aeolian weather patterns.

Keywords: Hydrogen, Non-Deterministic Programming, Non-Convex Optimisation, Stochastic Modelling.

INTRODUCTION

The fervent interest in hydrogen's use as a decarbonisation tool has begun to show early signs of stagnation, primarily due to challenges associated with bridging its high production cost to that necessary to support its use in industry. However, in a net zero paradigm, many projections still see the deployment of the hydrogen economy as unavoidable, due to challenges associated with decarbonising specific 'hard-to-abate' sectors such as aviation, heavy industry and ammonia production.

Whilst technological innovations will substantially influence the prospects of the hydrogen economy, there is still a significant opportunity to reduce costs through optimal supply chain planning and design. This has led to hydrogen production within an export paradigm being a very active research area within the field of process systems engineering.

In order to design supply chains which operate at minimal cost, many research efforts employ deterministic optimisation with cost-minimising objectives. These supply chain models are unavoidably complex, due to the need to account for the dynamic nature of weather systems. There are numerous approaches available to account for the influence of weather system dynamics on the design of the hydrogen value chain. Some research efforts elect to use fixed capacity factors [1,2], a strategy which significantly simplifies the computational load, but is known to underpredict the cost of production by approximately 60% [3].

Other research efforts employ time-indexed Mixed-Integer-Programming, taking meteorological data at hourly intervals for a representative years' operation [4,5]. This modelling approach is, naturally, significantly more computationally demanding than employing fixed capacity factors, but in return cost estimates are more realistic. In order to mitigate this increase in complexity, some of these papers elect to cluster the meteorological time-series [5,6], employing different strategies to ensure time-critical decisions are still made accurately.

Stochastic optimisation allows for decisions to be made in stages, reflecting the influence of uncertainty on the optimal planning and operation of stochastic processes. This methodology offers numerous benefits as it is able to limit the foresight the optimisation model has, but does so with increased computational load. A further benefit of this methodology is that it allows for a better quantification of the cost-benefit yielded by operational strategies which aim to mitigate the cost of uncertainty in weather (such as having a grid connection).

Whilst some studies have used similar methodologies (i.e., those which quantify the influence of uncertainty) on liquid hydrogen or ammonia production systems [7,8,9], they have yet been used in a comparative context and to evaluate the cost-benefit yielded by specific operational strategies. As such, this research aims to do the following:

- Compare the cost estimates of a multistage stochastic model for hydrogen production, against those of a deterministic model.
- Quantify the cost-benefit of different grid operational strategies, such as grid wheeling (a strategy where energy can be 'borrowed' from the grid if it is returned within a fixed time period) and compare this benefit between LH_2 and NH_3.

METHODOLOGY

Model Description

This model is of a hydrogen production facility, for export and thus employs either liquefaction or Haber-Bosch synthesis to convert the hydrogen to a form that is suitable for long distance transportation. For the solar system, the facility is located in the north of Chile and the south of Chile for the wind system. A brief overview of the 'production model' is given, diagrammatically, in the centre of figure 1. The objective of this model was to minimise the levelised cost of hydrogen, the equation for which is shown below in equation 1.

$$\mathrm{LCOH} = \frac{\sum_{t=0}^{T_f}\left[\frac{C_{op}}{(1+r)^n}\right]+C_{cap}}{\sum_{t=0}^{T_f}\left[\frac{8760}{h_f(1+r)^n}\sum_{h=0}^{h_f}\dot{m}_{H_2}(h)\right]} \tag{1}$$

Where C_{op} is the annual operating cost of all equipment, r is the discount factor, C_{cap} is the capital cost of all equipment, h_f is the number of hours modelled (serially), T_f is the lifetime of the plant, $\dot{m}_{H_2}(h)$ is the hourly (mass) production of H_2.

The scale factor for this system is the number of parallel trains employed for the Haber-Bosch or Liquefaction process, with 5 and 12 trains used for each respectively. This enabled the hydrogen production to be a free variable, meaning the influence of weather variations manifested in the weekly production quantities of hydrogen.

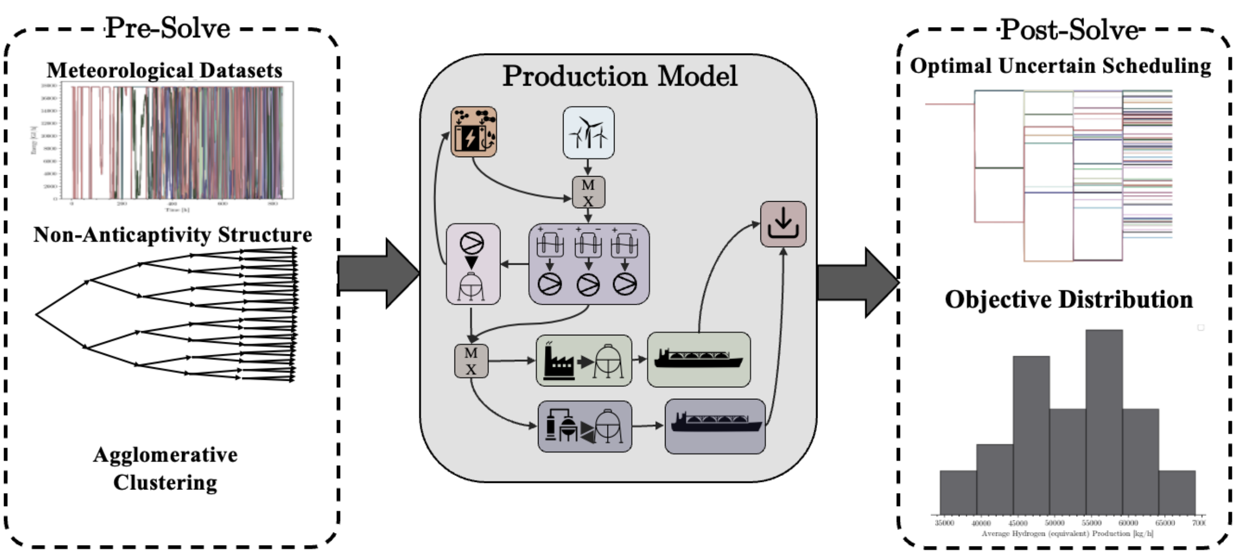

Figure 1: Diagram showing the modelling work flow for the stochastic systems modelling. During the pre-solve stages of the modelling, meteorological datasets are sampled and subsequently agglomeratively clustered using Ward's method [10]. Then, a non-anticipativity structure is produced using indexing rules in order to generate a contiguous time-series, which is sampled from the clustered weather dataset.

This, unavoidably so, results in the system being non-linear as both the system Net-Present-Cost (analogous the numerator of the LCOH quotient) and discounted lifetime hydrogen production (the denominator) were endogenous optimisation variables. The strategies involved in simplifying and solving this formulation are discussed in the forthcoming section.

Mathematical Formulation

The optimisation problem is formulated as a non-convex mixed integer quadratic programme, of structure that is shown below:

$$\min_{x,y} \; f(x,y) \cdot [g(x,y)]^{-1}$$

$$\text{s.t.} \qquad B\boldsymbol{x} + C\boldsymbol{y} \leq \boldsymbol{a}$$

$$0 \leq x \leq \boldsymbol{x^u}$$

$$0 \leq \boldsymbol{y} \leq \boldsymbol{y^U}$$

$$\boldsymbol{x} \in \mathbb{R}^n, y \in \mathbb{Z}^m$$

Where: $B \in \mathbb{R}^{n \times l}$, $C \in \mathbb{R}^{m \times l}$, $\boldsymbol{a} \in \mathbb{R}^l, \boldsymbol{x^u} \in \mathbb{R}^n$, $\boldsymbol{y^U} \in \mathbb{Z}^m$. This form of model can be solved iteratively using the Dinkelbach algorithm for fractional programming problems [10]. The solution approach involves replacing the objective with a linearised form (equation 2).

$$\lambda g(x,y) - f(x,y) \tag{2}$$

This modified sub-problem is subsequently solved iteratively, updating the value of $\lambda(\tilde{x},\tilde{y})$ in accordance with equation 3 after each iteration.

$$\lambda(\tilde{x},\tilde{y}) = f(\tilde{x},\tilde{y}) \cdot \; [g(\tilde{x},\tilde{y})]^{-1} \tag{3}$$

Where $\tilde{x}$, $\tilde{y}$ correspond to the optimal values from the previous solution. This means, given sufficient iterations, the value of the subproblem's objective will converge to 0 at $\tilde{x} = x^*$.

$$\lim_{(x,y)\to(x,y)^*} [f(x,y) - \lambda^* g(x,y)] \to 0 \tag{4}$$

In this case, this is iterated subject to the convergence condition shown in equation 5 (with $\varepsilon = 0.05$ used in these studies).

$$\lambda g(x^*,y^*) - f(x^*,y^*) \leq \varepsilon\, \lambda \tag{5}$$

Casting context to the system model at hand, the linearised equation is the Net-Present-Value (NPV) of the system, where λ is the sale price per kg of hydrogen. The LCOH is minimised when the NPV = 0, i.e. the sale price is equal to the unit production cost.

In order to simplify the computational complexity of this programme, as shown in figure 1, the model employs agglomerative clustering for the aeolian time series. This reduces the number of variables and equations in the model by clustering together identical values, thus improving tractability whilst minimising accuracy loss. For this model, Ward's method of agglomerative clustering was employed [11], with hierarchical grids to ensure key time-dependent decisions could still be made.

This clustering is performed as the initial pre-solve stage and influences the indexing of the stochastic programme's formulation. This is all handled by a standalone python module, called PyStochOpt, for which more information is given in the digital supplementary information.

Multistage Stochastic Programme

The objective of the stochastic programme was to model a months' operation of a hydrogen production facility (for export), using a *multistage* stochastic model in order to manifest the influence of non-deterministic weather forecasting on the optimal planning and operation of the facility. For this model, we take our meteorological system to be a stochastic process, $\{Z_n\}_{n \in N_s}$, defined on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Here, for each n, Z_n is defined to be a random vector consisting of 168 random variables.

In context of the above problem description, each random vector consists of a weeks' renewable energy production, with the index $h \in (1,2,\dots,168)$ enumerating a contiguous set of data. To reduce model complexity and size, this programme employs an inheritance-based indexing structure, rather than traditional non-anticaptivity constraints.

Specifically, for each $n \in (1,\dots,4)$, let $\mathcal{F}_n \coloneqq \sigma(Z_1, \dots Z_n)$ denote the σ-algebra generated by the random variables up until week n. Subsequently, the set of time-dependent decision variables: $\{x_t, y_t\}$ are enforced to be $\mathcal{F}_n$-measurable, where n is the current week of operation given hour t, and is determined in accordance with equation 6.

$$n \coloneqq \left\lfloor \frac{t}{168} \right\rfloor \tag{6}$$

This ensures that the model is not able to anticipate the future perfectly and can only make decisions based on the realised values of the stochastic process, up to week n. Regarding the equations used to model the system, equations 1-34 and 49-55 were taken from [5] and used in this study.

Single-Stage Deterministic Programme

For the counterfactual analysis, a deterministic analogue to the abovementioned stochastic programme was developed. In order to give consistency and comparability between the studies, the deterministic model uses the same formulation as the stochastic programme, but with a single stage.

The stochastic programme with three stages and three branches requires 40 distinct weeks weather data (27 + 9 + 3 + 1), in order to model the four weeks' operation. As such, in accordance with the first aim of this research, two deterministic models were developed: one with 4 weeks' data, and one with 40 weeks data.

Modelling Scenarios

In order to achieve the second and third aim of this research, a series of modelling scenarios in the form of Pareto optimal fronts, were developed. For each front, the analyses were repeated for both liquid-hydrogen and ammonia producing facilities, each employing both Solar and Wind power respectively (i.e., four different scenarios per front). These fronts studied the following operational strategies:

- Variations in hydrogen price. This was employed to study the behaviour of the abovementioned Dinkelbach algorithm. These price variations will also be used to study the behaviour of the deterministic model.
- Cost of employing a grid connection. Here, the grid energy cost, as a fraction of the levelised cost of power (for the wind or solar farm), was varied.
- The period at which the model may 'grid wheel'. As aforementioned, grid wheeling is an operational strategy allowed by some grid operators, such as in South Africa and Egypt.

RESULTS AND DISCUSSION

Dinkelbach Algorithm

Figure 2, below, shows the findings of employing the Dinkelbach algorithm for the wind production model. The findings of the solar model showed similar results and as such are not repeated here (but can be found in the digital supplementary information).

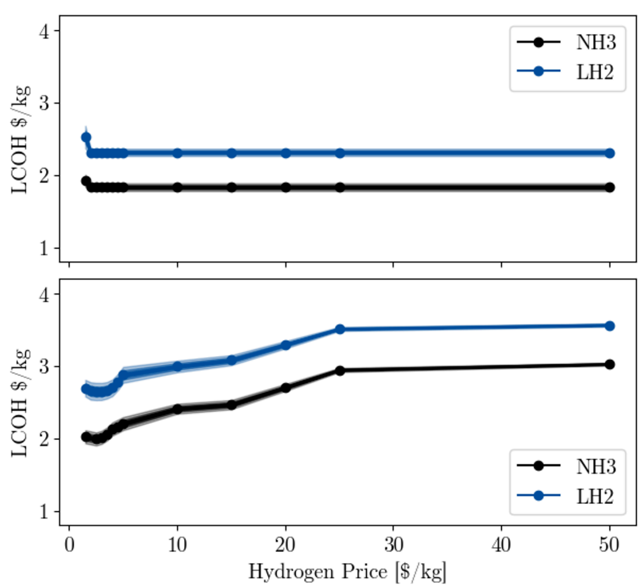

Figure 2: Pareto front for the grid connected (top) and islanded (bottom) Dinklebach algorithms. The shaded region represents the spread in LCOH from each of the leaf-nodes of the multistage stochastic model (27 total).

It is clear to see that the presence of the grid connection has a significant influence on the capacity of the production process to 'adapt' to different hydrogen prices. This manifests through varied investments in hydrogen storage. As such, when the hydrogen price is low, the model will elect to curtail excess energy.

In figure 3, below, we see the influence of employing the stochastic programme as opposed to the deterministic. In general, there is more 'noise' in the predictions as opposed to those shown in figure 2, and the deterministic model consistently *underpredicts* the cost of hydrogen production by an average of \$ 0.08 kg^{-1}(H_2) for LH_2. The case is similar for the NH_3 production model, but with a greater average under-prediction of \$ 0.10 kg^{-1}(H_2), which is proportionally more significant given the lower average production cost of NH_3. It is of note that both models are given the same amount of weather data and, as such, the difference in cost observed is due to the *overoptimised* nature of deterministic models.

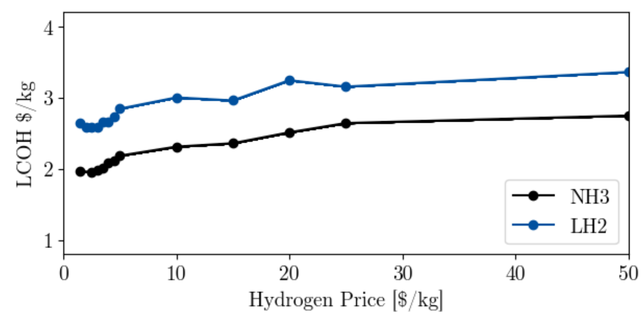

Figure 3: Pareto front showing an islanded Dinkelbach algorithm for a wind-powered deterministic model. This is for comparison to the bottom Pareto front of figure 2. This model employs a continuous series of 40 weeks weather data.

To understand the consistency of these models when modelling the same period (4 weeks), the models were solved numerous times whilst varying the random seed used in sampling the meteorological dataset. The deterministic model saw an average cost of \$2.80 kg^{-1}(H_2) with a standard deviation of \$ 0.25 kg^{-1}(H_2) for LH_2 and \$2.23 kg^{-1}(H_2) with a standard deviation of \$ 0.21 kg^{-1}(H_2) for NH_3 (for the islanded, wind powered systems). However, the stochastic model saw average production costs of \$2.92 kg^{-1}(H_2) with a lower standard deviation of \$ 0.16 kg^{-1}(H_2) for LH_2 and \$2.26 kg^{-1}(H_2) with a standard deviation of \$ 0.16 kg^{-1}(H_2) for NH_3. This finding serves to evidence the benefit of including non-determinism in cost estimates when modelling a short time period, as it enables much greater exposure of the model to a variety of weather patterns.

Grid Energy Cost

Figure 5 shows the influence of varying the cost of grid energy on the LCOH. An interesting observation is how the grid-energy ‘buffers out’ any uncertainty in weather energy, when it is available at a low cost. When the cost is high, the model elects to curtail more energy, meaning variations in weather have a more significant influence on the profitability of operation.

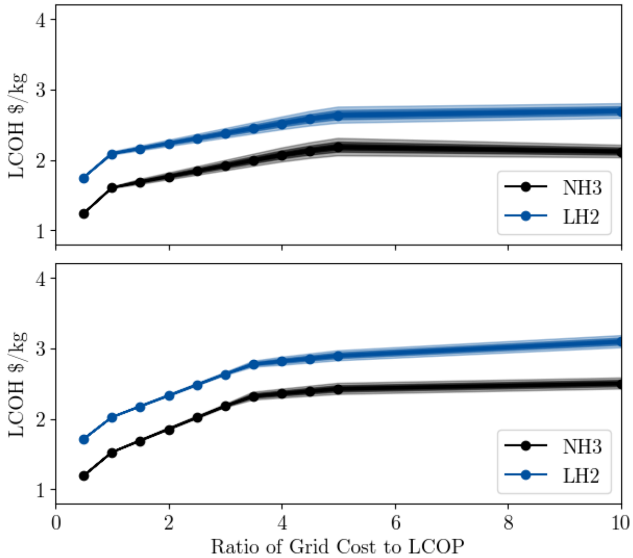

Figure 5: Pareto fronts for a grid-connected wind-powered system (top) and a grid-connected solar powered system (bottom). LCOP stands for levelised cost of power, referring to the cost of energy from the wind and solar farm, respectively.

Below a cost ratio of 1, the model will elect to not build a solar or wind farm as it is cheaper to use the grid energy directly. Above this ratio, the solar model uses the grid energy in lieu of storing or curtailing excess energy. The wind model, however, will use some grid energy, but will also begin curtailing energy and investing in storage (evidenced by the increased spread in LCOH values). This is because the capacity factor for the solar farm is lower than that of the wind, meaning the increase in output begotten when using grid energy warrants paying a high price for it, rather than using a curtailment strategy.

When the grid cost becomes excessively high, both models elect to employ storage and curtailment and do not use any grid energy. When not using grid energy the model is less able to ‘buffer out’ the variations in wind output and, as such, directly influences production quantities of hydrogen.

Grid Wheeling

The analysis of grid wheeling allowed for unlimited energy to be ‘borrowed’ within a given period (again, contingent on it being returned within the same period). The pareto fronts demonstrating the results of these analysis are shown in figure 6.

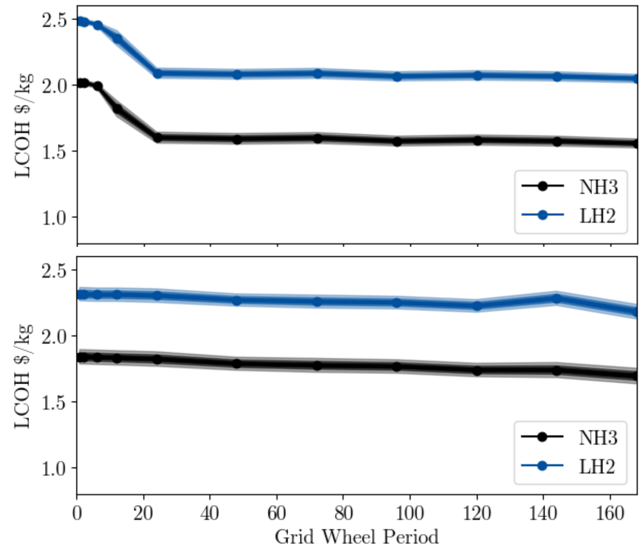

Figure 6: Pareto front for variations in the greed wheeling ‘period’ for the solar (top) and wind (bottom) system.

It is clear to see from figure 6 that enabling the system to grid-wheel offers a substantial benefit for the solar powered system when the wheeling period is above 24 hours, at which the model will wheel up to 42% of the solar farm’s capacity. This makes sense given the diurnality of solar production. For the wind system, the benefit is much less significant, which we hypothesise to be due to the more stochastic nature of aeolian weather patterns, meaning it is difficult to guarantee that any ‘borrowed energy’ can be returned in a singular fixed interval.

CONCLUSIONS

This research aimed to study the potential benefit yielded by employing a multistage deterministic model for hydrogen export systems and use it to study the cost-benefit yielded by different operational strategies. The stochastic model yielded some benefit over the deterministic system including highlighting the slight underestimation of the cost of hydrogen when compared to the deterministic model and the reduced standard deviation of LCOH prediction when modelling the same time period.

Another key benefit of the stochastic system is in its ability to model a solar system for a short time period. This is important as it is more challenging to cluster a solar time series than an aeolian, due to it being more continuously dynamic in nature. This challenge leads to many researchers using ‘representative days’ in order to model the solar time series, which assists in reducing computational load. Here, without clustering, the solar model was able to process 27 distinct 4-week weather patterns, giving a large exposure to different weather patterns whilst still solving in a reasonable time-frame.

Although the stochastic model offers slight improvements to the accuracy and repeatability of cost estimation, it is more computationally intense and scales geometrically with the number of decision-making stages, hence this analysis was limited to studying a months' operation. Whilst a month is a functional period to study in this context, it is insufficient when studying a full value chain which would include shipping between supply and demand regions.

Grid wheeling was found to be very effective in a solar system due to its ability to guarantee the return of energy in a given time period. There is a natural question as to the 'greenness' of wheeled energy, given on balance green energy is contributed to the grid and green energy is removed; but the energy used to produce the hydrogen when 'borrowing' may not be green itself.

Whilst the infrastructural requirements of endorsing a grid-wheeling approach would be significant, the potential economic remuneration associated with cutting hydrogen export costs by up to 20% would serve to stimulate interest in such strategies. As such, it is not untenable given the broad political interest in hydrogen export with certain nations. However, whilst this strategy shows promise, some nations have set limits on the amount of energy that can be wheeled, which could serve to limit the economic benefit of such an approach.

DIGITAL SUPPLEMENTARY MATERIAL

Digital supplementary material are available for this research and can be found at the following hyperlink: LAPSE:2025.0004.

ACKNOWLEDGEMENTS

The authors would like to acknowledge funding for this research through the UKRI Engineering and Physical Sciences Research Council via an iCASE studentship in partnership with Shell plc, and through HI-ACT (Hydrogen Integration for Accelerated Energy Transitions) (EP/X038823/2).

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