Modeling of hydrogen-based power-to-gas plant operation for evaluation of control strategies

Corey DUNCAN *, Samir JEMEI *, Robin ROCHE †, Marie-Cécile PERA *

* FEMTO-ST Institute, FCLAB, Univ. Bourgogne Franche-Comté, CNRS, Belfort, France
2 Rue Édouard Belin, 90000 Belfort

† FEMTO-ST Institute, FCLAB, Univ. Bourgogne Franche-Comté, CNRS, UTBM, Belfort, France
2 Rue Édouard Belin, 90000 Belfort

corey.duncan@univ-fcomte.fr

This paper presents a simulation model for operation of a power-to-gas plant for the purposes of project feasibility and control strategy analysis. The plant is translated into an optimization problem formulation using a modified unit commitment style technique. A pilot project in France is presented as a case study for simulation model application and results from running the simulation are presented. Using maximizing production and minimizing operational cost as two separate objective functions, the resulting output data are analysed. The results show the influence of wind power, natural gas grid availability and electricity prices on production, highlighting the importance of their inclusion in power-to-gas plant modeling, as well as the consideration of more realistic equipment modeling in feasibility studies.

MOTS-CLES - power-to-gas, optimization, system modeling, techno-economical analysis

1. Introduction

The first continent to make such a commitment, the European Council recently released the "Fit for 55 Package" which sets an ambitious goal for the European Union (EU) to reach carbon neutrality by 2050, with an initial reduction of 55% of greenhouse gas (GHG) emissions compared to 1990 levels by 2030 [1]. To reach carbon neutrality by mid-century, the International Energy Agency (IEA) estimates that global electricity demand will double by 2050, with renewable energy – namely variable renewable energy sources wind and solar – covering nearly 90% of total electricity generation [2]. For maximum utilization of these intermittent energy sources at such high penetration levels, flexible and adaptable energy networks must be implemented [3].

Coupling enables energy that may be curtailed or otherwise wasted to be fed into another energy network or sector through a mediary technology, decoupling the energy source generation from its direct energy consumption [4]. Hydrogen (H_2) has received increased attention in the past years as the mediary energy carrier as it allows for several sectors and energy networks to be coupled. This process is known as Power-to-Gas or PtG. PtG technologies also involve converting H_2 into methane – also known as synthetic natural gas or SNG when produced in this fashion – via methanation reactors for increased technology applicability and flexibility. Along with the IEA hydrogen tracking report [5] and their Net Zero study [2], many studies have been done that show the economical and energy efficiency benefits of including such technologies in future energy strategies [6], [7]. Further, Frischmuth and Härtel [7] demonstrated that a system consisting of both centralized and decentralized PtG systems show lower energy system costs and fewer power generation investments plus other flexibility options. However, designing and operating PtG systems is very complex as the flow of multiple energy vectors in the coupled system must be optimized such that they meet the design criteria as defined by the designer or operator. Further, how this design criteria – or optimization objective function – is evaluated depends upon the desired technique for formulating the optimization problem. The limitations of the equipment as well as internal system and external networks – also known as constraints – must also be considered during optimization. The influence of variable renewable energy, energy markets, energy loads, energy demands and other input data further add to the complexity of modeling a PtG system.

The objective of this paper is to present a PtG plant model which can be used to simulate operation over the project lifespan for ideal control strategy investigation and overall project feasibility analysis. A pilot plant will also be presented which is used as a case study of model application. The plant analysis is done by taking input parameters from the user based upon local conditions (i.e. electricity prices, feedstock limitations such as generation profiles), plant configuration (i.e. equipment to be used), end-use application(s) and simulation objective and converting the data into an optimization problem to be solved.

The structure of the rest of the paper will be as follows: a section discussing current state-of-the-art techniques used to model PtG plants will be presented with results of the simulation. Literature knowledge gaps will be shown and how they correlate to the scientific contribution of this work.

2. State-of-the-Art

McDonagh et al. [8] studied synthetic production as a transport fuel, calculating a cost of 107-143 €/MWh in 2020 when assuming an average electricity price of 35 €/MWh and 6,500 full-load operational hours. However, this study focuses on a national level (Ireland) and does not discuss cost reduction strategies for individual plants, nor does it use optimization techniques were used for simulation. Breyer et al. [9] modeled a PtG plant used on-site of a pulp mill in Finland with ancillary market participation and 4,000 full-load operational hours and found the business case to be profitable, with grid services representing 40% of total income. However, this model used an assumed fixed electricity price, did not consider limitations on local gas consumption, and simplified Excel® spreadsheets for economical calculations. Gorre et al. [10] performed an optimization analysis of production costs of SNG in terms of various electricity purchasing and gas selling strategies for a PtG plant in 2030 and 2050, comparing them to the expected SNG prices. The results showed that flexible operation in day-ahead markets with an average price of 30 €/MWh and 4,000 full-load operational hours can have a positive revenue by 2050. However, the study is generic to Europe and does not consider participation in ancillary services, local technical or physical limitations, governmental support schemes or specific country day-ahead electricity prices. Further the optimization method is not mentioned or presented. Abdelghany et al. [11] provide a mixed-integer linear programming method for optimizing energy management in a wind-powered PtG plant for power generation to meet an energy load. Their style includes equipment states and detailed operational constraints, however, its purpose is for real-time energy management not project lifespan analysis and thus uses very short time horizon without overall project feasibility analytics. Thus, from this brief literature review it can be seen that models which include plant operation are either very simplified, ignoring all possible limitations and opportunities of the system, or too detailed of minor plant dynamics and miss the overall picture of project feasibility. The model presented hopes to marry these differences into a model which captures major equipment dynamics, local feedstock or end-use constraints, and lifetime uncertainties to provide tangible results for project feasibility.

3. Plant Operation Simulation Model: An Optimization Problem

To simulate operation of a PtG plant over the project lifespan, the system can be converted into an optimization problem, using mathematical formulation to represent all the equipment, feedstock parameters, external system limitations, end-use applications and operational objectives. A unit commitment (UC) style model is used to form a mixed-integer linear optimization problem. There are several possible objective functions which can be maximized/minimized based upon simulation objectives. The formulated UC problem of the system is defined in Equations (1)-(3) and extracted from [12]:

$$min \sum_{g \in G} \sum_{t \in T} c_g(t) \tag{1}$$

s.t.

$$\sum_{g \in G} A_g(P_g, \overline{P}_g, \delta_g) + N(s) = L \tag{2}$$

$$(P_g, \overline{P}_g, c_g) \in \Pi_g \qquad \forall g \in G \tag{3}$$

where the objective function (1) is the minimization of the summation of the operational cost of each generator c_g at each time step t in the simulation period T. Other objective functions could be chosen but only minimization of operational cost is defined here. The Equation (2) matrix $A_g(P_g, \overline{P}_g, \delta_g)$ determine how the generators and interact with system requirements L while $N(s)$ refers to other potential decision variables involving operation of the system. P_g, $\overline{P}_g$ and δ_g represent the feasible power, maximum power and status of the generator, respectively. Finally, Equation (3) defines the feasible region for each generator and the cost associated to it, with the set Π_g representing the description of this feasible operational region for each generator. For reference, generators are defined as equipment which produce either final products or internal system feedstock i.e. electrolysers, reactors, and gas purification systems.

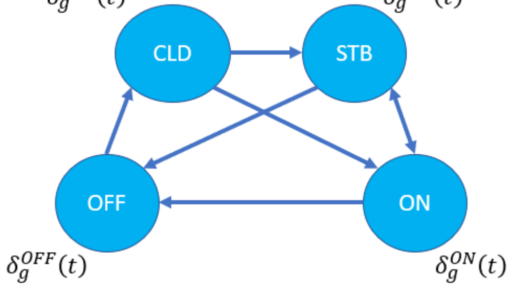

Figure 1: Generator operational states sequential graph. Modified from [11].

3.1 Critical Constraints

There are several constraints which are required to define Π_g and A_g, however, only the critical constraints which dominantly determine plant operation will be shown here. The proposed model goes beyond standard UC models such that extra operational states of the generators are included which consider startup and idle of the equipment – states which play an important role in real operation of the PtG plant. The modeling strategy presented by Abdelghany et al. [11] was modified and applied to a PtG UC model that can incorporate the "CLD" and "STB" states into the already defined "OFF" and "ON" states in the optimization problem formulation. The application of these states and possible transitions between them for plant generators is shown in a sequential graph in Figure 1. Once defined, these states are included in operational constraints to more accurately portray plant operation internally and with external systems.

Beyond internal constraints of equipment such as minimum and maximum production levels, ramping limitations and thermodynamic and kinetic processes, external systems have large governance over plant operation. If a PtG plant is producing hydrogen using exclusively wind farm power, the electrolyser must not consume more power than the farm produces at each time step in the simulation. This can be defined as shown in Equation (4):

$$P_{ez}(t) \leq P_{wind}(t) \qquad \forall t \in T \tag{4}$$

where $P_{ez}(t)$ is power consumption of the electrolyser at time step t and $P_{wind}(t)$ is the wind farm power generation. If the produced H_2 is being injected into the local NG grid or the H_2 is being further converted into SNG in a methanation reactor and and injected in the grid, any local grid capacity limitations must also be considered. This can be expressed as constraints as shown in Equations (5) and (6):

$$Q_{H_2}^{grid}(t) \leq d_{NG}^{H_2} Q_{NG,avail}(t) \qquad \forall t \in T \tag{5}$$

$$Q_{SNG}^{grid}(t) \leq Q_{NG,avail}(t) \qquad \forall t \in T \tag{6}$$

where $Q_{H_2}^{grid}(t)$ and $Q_{SNG}^{grid}(t)$ are the volumetric production of H_2 and SNG at time step t, respectively, $Q_{NG,avail}(t)$ is the volumetric availability in the NG grid at time step t and $d_{NG}^{H_2}$ is the volumetric ratio of H_2 accepted in the local NG grid. As operational cost is to be minimized and the cost of electrolysis is the majority of this cost [13], the price of electricity on the day-ahead market is of great interest. This price changes hourly and can have large variations depending upon the time of day, season or unforeseen events such as nuclear reactor shutdown. The cost of electrolyser operation is thus the most critical cost for simulation consideration and is summarized in Equation (7):

$$c_{ez}(t) = Q_{H_20}^{ez}(t) c_{H_20} + \frac{Q_{H_2}(t)}{\eta_{ez}} c_{el}(t) \tag{7}$$

where $c_{ez}(t)$ is the total operational cost of the electrolyser at time step t, $Q_{H_20}^{ez}(t)$ is the volume of water consumed at time step t, c_{H_20} is the cost of water, $Q_{H_2}(t)$ is the volumetric production of H_2 at time step t, η_{ez} is the efficiency of the electrolyser and $c_{el}(t)$ is the day-ahead market price of electricity at time step t.

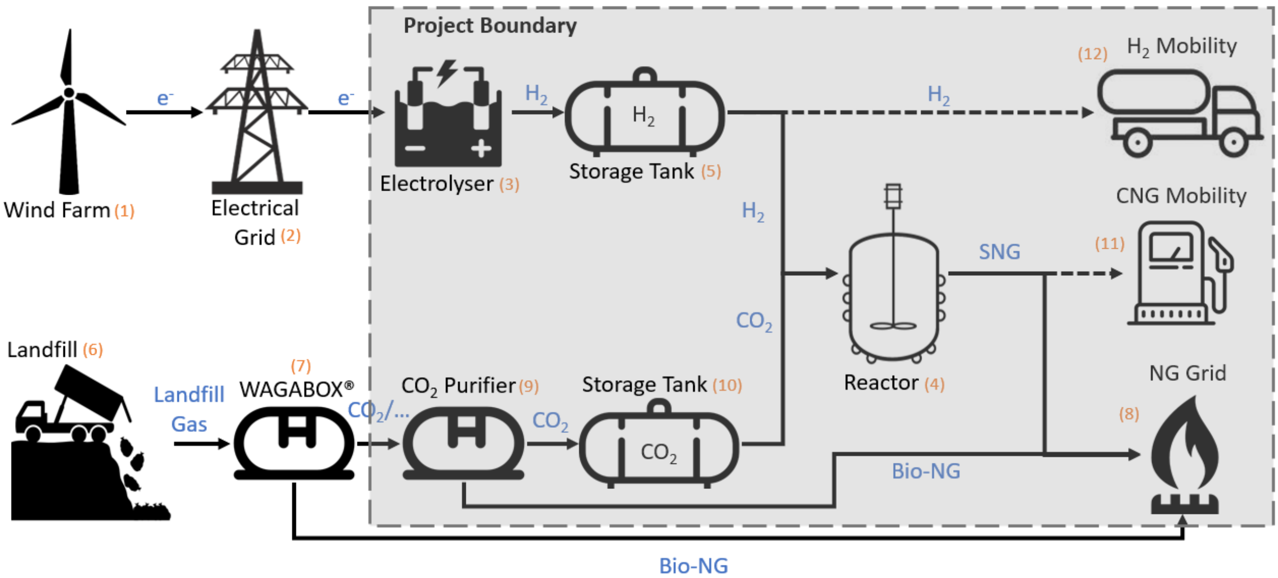

Figure 2: HYCAUNAIS project plant schematic and process flow.

4. Case Study

A PtG pilot plant named HYCAUNAIS has been used for a case study of the model. Located in Saint-Florentin, France the project is being led by Storengy and has several industrial and public partners [14]. A diagram of the HYCAUNAIS plant layout and possible configurations is shown in Figure 2. The plant will produce gases with a low environmental footprint for NG grid injection and possibly mobility. Following the combined power production signal of two existing wind farms (1) provided by the wind farm operator and sourcing the electricity via a grid connection (2), a 1 MW_{el} PEM electrolyser (3) will produce hydrogen for a 50 Nm^3/h biological methanation reactor (4), with intermediate H_2 storage (5) installed between the electrolyser and reactor. Currently, gas from the landfill (6) on-site is being upgraded by a WAGABOX® unit (7), recovering 90 vol% of the bio-CH_4 contained in it. This highly pure bio-CH_4 is being injected into the natural gas (NG) grid (8). The CO_2 stream (including some impurities) normally vented during upgrading will be utilized as the carbon source for methanation, which must be purified (9) prior to injection into the biological reactor. Intermediate storage of CO_2 (10) between the reactor and purifier is also used. Bio-NG captured during purification is combined with the produced SNG from the reactor and injected into the NG grid at the same existing site used by the WAGABOX® unit. Compressed natural gas (CNG) (11) and H_2 (12) mobility are also being investigated as secondary applications to improve operational hours of the plant and profitability while NG grid injection is seen as the primary application. In addition to these end-use applications, electrolyser participation in electricity grid ancillary services is also being investigated with the purpose of adding an additional revenue stream while only minorly effecting overall operation. The project boundary is input from the electrical grid and WAGABOX® effluent to output to NG grid injection as shown in Figure 2.

Based upon the plant description given above, the optimization model presented in section 3. can be used to simulate operation of the HYCAUNAIS pilot plant as a case study of model application.

5. Results

Case study results of model application will be presented using two objective functions: maximizing SNG production and minimizing operational cost. The objectives were modeled separately to analyse the production behaviour on the the electrolyser and reactor. The simulation was done over a week time horizon at time steps of one hour. Only NG grid injection has been considered in these results for end-use application; mobility is not included.

SNG production from the reactor is the primary end-use application of the plant and, hence, was chosen to be the technical objective to maximize. As the maximum operational output of the reactor is desired in this configuration, the only limitations on output gas flow is reactor rated capacity, ramping constraints, and NG grid capacity (referred to as NG consumption). These limitations are demonstrated in the top plot of Figure 3 and their effect on gas flow production in the bottom plot. When NG consumption is below reactor rated capacity, it means the NG grid cannot accept full gas output but only what is currently being consumed locally. Reactor production thus is forced to be limited and eventually terminated until consumption increases again. A similar effect on electrolyser operation can be seen with wind power: the electrolyser can only consume electrical power, and therefore produce H_2, up to what is available from the wind farm. Electrolyser operation is thus limited several times in the last third of the week. Due to the limited size of the H_2 storage – as seen as the orange dotted line in Figure 3, represented by internal gas pressure – the reactor cannot operate for long before the stock is depleted.

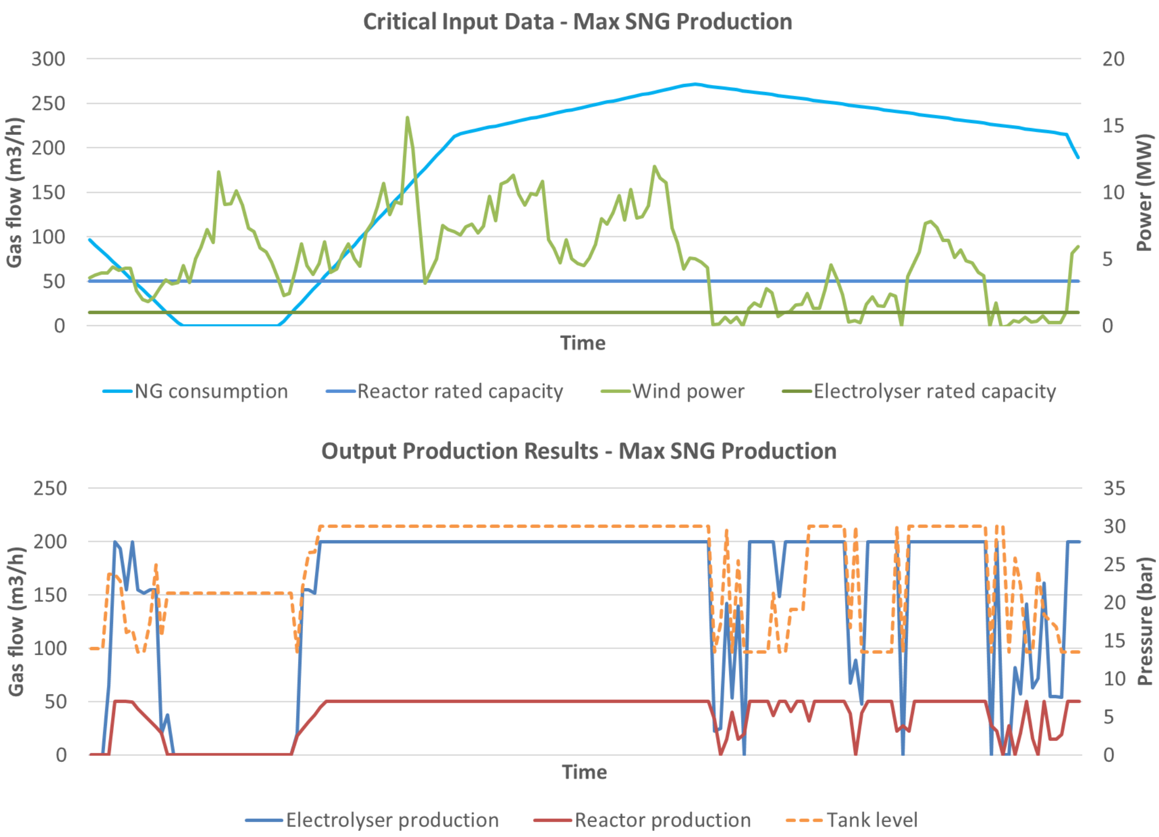

Figure 3: Critical input data (top) and out production results (bottom) are shown when maximizing SNG production is the objective function of simulation optimization. Simulation period is one week.

Figure 4 shows the critical input data and output production results when the objective function is changed to minimizing operational cost. As price of electricity is now a main concern for optimization (as price of electrolysis is most influential on cost of PtG plants [13]) and NG consumption limits reactor production for a short time, the former has been replaced with the latter in the parameters plot of Figure 4. Further, an additional constraint of 60% full-load operational hours of the reactor in the simulated horizon has been applied, forcing the solver to find the cheapest hours to operate for that minimum time. As the wind power limitations are still a factor in the later hours of the week, the equipment runs full-load during midweek and then chooses cheaper times to run at capacity while still considering wind power in the end of the week.

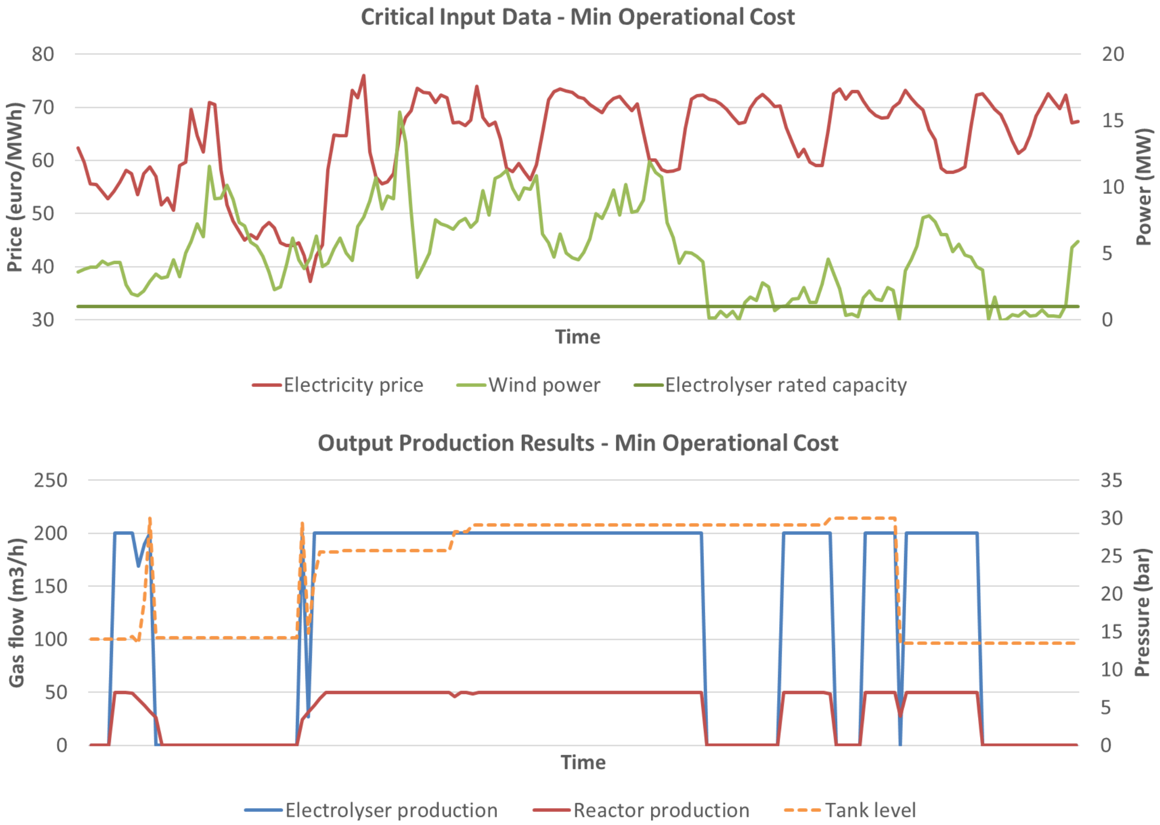

Figure 4: Critical input data (top) and output production results (bottom) are shown when minimizing operational cost is the objective function of simulation optimization. First segment of zero reactor production is due to no NG grid capacity available, which is not shown in the parameter plot to avoid figure clutter. It can be seen in Figure 3. Simulation period is one week.

As one could imagine, minimizing operational cost is a much more complex problem to solve when compared to maximizing SNG production as economics of operation increase considered constraints and decision variables. Indeed, solve runtime of maximizing SNG production for the 168 hour (7 days) horizon is 17.8 seconds while it took 6847 seconds (114 minutes) to solve minimizing operational cost, over 380 times slower.

6. Conclusion and Future Work

A power-to-gas plant operation simulation model has been proposed in this paper to be used for feasibility analysis of potential projects over their lifespan. The model uses optimization to achieve this by converting possible plant configurations into a mathematical problem formulation to be solved. A case study of a pilot plant under construction in France is presented to apply the model for demonstration. By implementing two objective functions separately (maximize reactor production and minimize operational cost), the influence of critical parameters on equipment output was shown to ultimately decide optimal values.

From the results shown, it can be seen that attempting to improve the solver runtime is of great interest in future work. Improving computational efficiency through other problem formulation methods or solvers will be investigated. Once the formulation method has been chosen, increasing applicability of the model to other PtG scenarios will be done, such as: CNG and H_2 mobility, ancillary services participation, multiple end-use applications, multiple objective functions and optimization of equipment sizing. Further, including forecasting models of variable renewable energy generation, energy markets and energy loads will improve accuracy of model results in future projects.

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