Techno-economic assessment of an industrial project towards carbon neutrality

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Abstract

This paper describes the application of the system simulation platform Modelon Impact for techno-economical assessment of energy projects towards carbon neutrality. The control co-design approach applied in the work allows for rapid assessment of various technology options without the need for deriving complex control laws for the considered assets. The approach is here applied on an industrial use case where the goal is to identify the technology options that minimize the total cost of ownership while achieving carbon neutrality.

Keywords: process design, controls, optimization, hybrid energy systems, renewables, hydrogen, energy storage systems

1   Introduction

Organizations have made a goal of significantly reducing CO_2 emissions to mitigate climate change. Not only governments and energy companies but also industries are now moving away from fossil fuels, investing in new technologies towards carbon neutrality. There are however many options, ranging from diverse renewable energy sources to carbon capture and utilization, hydrogen technologies and storage energy systems. The different alternatives vary significantly in terms of technical performance (efficiency, degradation, longevity) and in terms of economy (initial investment, operational cost, incentives). It is therefore not an easy task for the decision makers to efficiently explore the different paths and choose a cost-efficient implementation that meets the environmental targets (Venkatraman and Khaitan, 2015).

As shown in (Windahl *et al*, 2019) and (Fathima and Palanisamy, 2015), system simulation and optimization can efficiently help exploring and pruning the various options in a systematic way. The specificity of the approach proposed by the authors in (Velut *et al*, 2020) is twofold. It relies on the open modeling language Modelica and makes it thereby possible to model and simulate potentially any hybrid energy system. Secondly, the models can be used to formulate and solved dynamic optimization problems avoiding the need to derive & implement complex controllers for all considered configurations. Instead, optimal control and design problems can be setup to quickly assess the limits of performance and the cost of various alternatives.

The strategy has been applied in (Velut *et al*, 2020) for microgrid design and operation. In (Magnusson *et al*, 2021), the models have been further extended to include hydrogen components such as electrolyzer, fuel cell or hydrogen tanks. The current paper presents a major extension of the framework that is now able to assess the technical and economic feasibility of complex long term energy projects involving the production, conversion or supply of products like heat, electric power, hydrogen, synthetic methane or CO_2.

2   Framework

2.1   Tools and methods

Modelon Impact (Modelon, 2022) is used to model, simulate, and optimize the hybrid energy system in Modelica. Modelon Impact is a system modeling and simulation platform leveraging the benefits of web and open standard technologies. With openness at its core, Modelon Impact supports standards such as Modelica, FMI, Python and REST. The user-friendly browser interface provides modeling experts the tools they need to create, simulate, and experiment. The Modelon Impact API enables scripting of advanced analyses using Python through Jupyter notebooks. The optimization problem formulation has been written in

Optimica, a Modelica language extension (Åkesson, 2008). The API of Modelon Impact gives access to the Optimica Compiler Toolkit and its dynamic optimization framework (Magnusson *et al*, 2015), which is used to solve the dynamic optimization problem using direct collocation.

2.2 Physical modeling

A sketch of the system to be modeled and optimized is shown in Figure 1. The sketch represents a Honda-owned factory in the US that assembles cars.
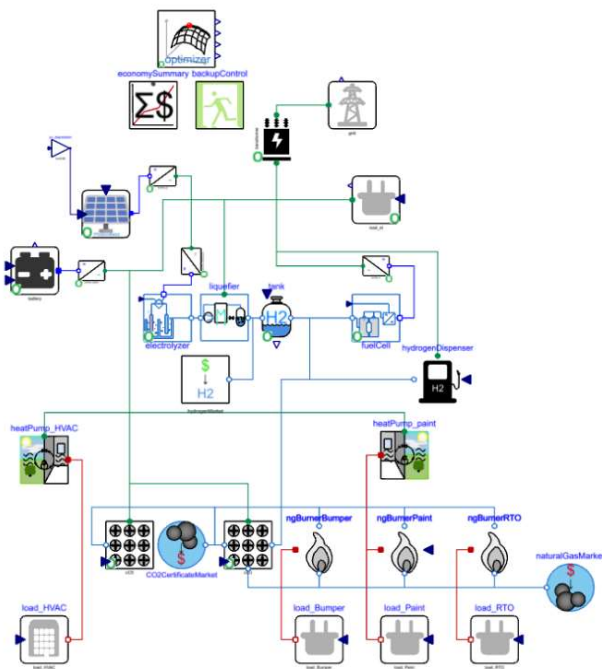

Figure 1 Overview of the system model

The plant model has been built by connecting component models from the Microgrid package in Thermal Power Library (Modelon, 2022). The Modelica package contains optimization-friendly models targeting optimal design and control. The models are typically static, semi-empirical and described by efficiency curves. Dynamics is mainly present in the storage components.

The plant consists of buildings, vehicle fleets, industrial equipment that can all be seen as some type of load:

- Electric loads for buildings' HVAC system, lighting, EV fleet, etc.
- Hydrogen loads for fuel cell-based transportation and logistics systems (forklifts, trucks, railroad)

- Thermal energy loads for heating and cooling in the buildings as well as industrial equipment such as burners

The goal of this work has been to assess different carbon neutral and sustainable options to satisfy the various loads. The model shown in Figure 1 represents a possible configuration where hydrogen technologies have replaced fossil fuel ones:

- Electrolyzer for onsite hydrogen production
- Hydrogen tank (for either gas or liquid hydrogen)
- Liquefaction plant
- Stationary fuel cell for power back-up or peak shaving
- Hydrogen dispenser

Compared with the work presented in (Magnusson *et al*, 2021), additional models have been derived:

- Heat pump, converting electric power to heat in buildings
- Burners to produce heat from the combustion of methane
- Carbon capture technologies to achieve carbon neutrality
  - A CCS block to capture the CO_2 produced in the combustion processes
  - A CCUS block for methane production from captured CO_2 and hydrogen
  - If CC(U)S is not applied, CO_2 is released to the ambient at a cost given by carbon taxes

Electric power, hydrogen and other fuels can also be imported using

- A power grid component acting as a voltage source
- A discrete delivery hydrogen market component that implements a controllable supply at a fixed frequency and the amount for every delivery being a degree of freedom in the optimization.
- A continuous fuel delivery, which can deliver methane (or other fuels) on demand, in case of pipeline delivery infrastructure.

Finally, energy can be stored either in batteries or as hydrogen to shave the power peaks and cope with the variations in renewable power. The goal is to assess the most economical alternative.

2.3 Economy modeling

2.3.1 Fixed and variable costs

The main goal of the work has been to perform a techno-economic analysis of the future plant. Economy information has therefore been added to every component to keep track of both the capital and operational cost of all equipment.

The considered time horizon for the optimization is the project lifetime T_{proj}, close to the components' lifespan.

The total cost of ownership of a component i has been divided into 2 parts:
- the fixed total cost $TCO_{fix,i}$, the sum of the capital cost and the fixed operational cost, i.e., due to maintenance
- the operational cost

If the fixed costs (capital cost and fixed operational cost) scale linearly with the assets size, the fixed cost can be computed using the following parameters:
- Lifetime L_i
- The specific capital expenditure CapEx C_i, i.e. normalized by the rated output or size $s_{opt,i}$
- The fixed yearly operational expenditure $o_{fix,i}$ (e.g. fixed maintenance cost) also normalized by the rated output or size $s_{opt,i}$

The fixed total cost component for component i over the project lifetime is then

$$TCO_{fix,i} = T_{proj} \cdot s_{opt,i} \left(\frac{C_i}{L_i} + o_{fix,i} \right)$$

The variable OpEx based on the usage of a component is typically computed by integrating the resource cost (power, fuel cost…) $o_{var,i}$ over time. Since this system has centralized energy markets, the variable OpEx is typically calculated on the respective markets. The project total cost of ownership of the system can be finally computed as:

$$TCO_{tot} = \sum \left[T_{proj} s_{opt,i} \left(\frac{C_i}{L_i} + o_{fix,i} \right) + \int_0^{T_{proj}} o_{var,i} dt \right]$$

The summation over the components is automatically done by aggregating all the costs in a single "Economy Summary", which makes it convenient and compact.

Any system configuration change does not require any manual update in the overall cost computation.

Although time-varying grid prices can be considered in the optimization, a fixed price was used to describe a virtual power purchase agreement.

2.3.2 Long term aspects: degradation and money value

While the data profiles used in the optimization only cover one year, to account for seasonal variations, the project lifetime is several decades. When considering such long periods, degradation of components as well as changes to the value of money need to be considered as well. Since the computational cost of dynamic grows superlinearly with the time horizon, optimization over the entire time horizon is computationally tractable. Two simplifications have been considered to account for these factors:

1. **Year separation**: By fixing the design and disregarding the storage between years, the TCO of each year can be calculated independently. By sampling the entire design space, the optimal design and control can be found.
2. **Mean year**: Lump degradation and NPV factors across all years to create a "Mean" year that allows simultaneous optimal design and control. This reduces the time horizon of the project optimization to a single year.

While the first approach is more accurate, it is still computationally expensive. It has been used to verify that the second approach yields satisfactory accuracy.

2.3.3 Demand charges and peak shaving

The objective of this model incorporates many aspects from previous projects that have been introduced and described in detail in (Velut *et al*, 2020) and (Magnusson *et al*, 2021). Similar to previous models, a form of peak shaving was being implemented. In this case, the utilities contract applied a demand charge on the maximum of the power demand from the grid during the summer months from June to September. The grid model has therefore been adapted to optimize the peak only during these months, so that both size and operation of relevant components results in an economically optimal peak shaving behavior.

The demand charge is a constant per-kW charge applied to the electricity grid and is being handled by use of a slack variable.

3 Optimization problem

As previously mentioned, the goal is to assess the technical and economic feasibility of the project of making the Honda-owned facility carbon neutral. For this purpose, some clean replacement technologies listed in Section 2.2 have been considered to meet the various needs in heat and power. Optimization will now be used to find the best options and size the equipment appropriately.

3.1 Objective function

The objective function is the total cost of ownership computed over the project lifetime T_{proj} as described in Section 2.3.1.

3.2 Discretization

The optimization problem is solved over a full calendar year. The sampling rate of the collocation algorithm is one hour (equal to the boundary conditions' sampling rate), which means that every control trajectory is described by 8760 degrees of freedom.

As the dynamics of the plant is relatively simple (integrators of the storage components), implicit Euler has been chosen in the collocation.

3.3 Co-design - simultaneous control and process design

The plant consists of many assets that interact with each other and some need to be controlled such as battery, electrolyzer, fuel cell. Instead of developing controllers for all these components, a control co-design approach has been chosen, where the optimizer operates the controllable assets at the same time as it sizes all equipment. If the design is solved for a specific control strategy, it leads to sub-optimal design, i.e. a higher total cost of ownership. By solving simultaneously for the assets' operation and their size, it is possible to minimize the asset's size and the overall cost. The strategy makes it also very convenient as no time is spent on deriving empirical controllers for all considered technologies and system configuration.

3.4 Degrees of freedom

The degrees of freedom in the co-design optimization problem are:
1. Parameters that define the size of the equipment (design problem)
2. Time trajectories for all control inputs of the controllable assets (control problem)

The list of degrees of freedom can be found in the tables below. Note that the discrete deliveries of hydrogen *hydrogenMarket.deliveries[i]* have been implemented as a vector of deliveries, the period being fixed to a week. All control signals have been normalized to operate between 0 (no output) to 1 (rated output).

With the chosen discretization level, the optimization problem contains **78905** degrees of freedom, 65 for the parameters and 78840 for the input trajectories (9 inputs and 8760 hourly values).

3.5 Constraints

Apart from the equality constraint of fulfilling the plant model equations, several inequality constraints have been considered in the formulation.

The first set concerns all degrees of freedom that need to lie within given bounds as shown in the previous section. Another set concerns the storage components (battery and tank) whose state of charge, eventually in terms of pressure or level, must be kept within reasonable limits. Export to the power grid was also prevented using an inequality constraint.

The last operational constraint that has been implemented ensures that power can be supplied in case of a full blackout. No black-out scenario is considered in our optimization and therefore we need to design and operate the system in a way energy is always available to handle that event. Since several backup solutions exist in the system, even a mix of technologies is conceivable. In this system, the backup power can be provided by either battery or fuel cell, i.e. the sum of rated output power P_{backup} should be greater than the minimum requirement for emergency power P_{backup}^0

$$P_{backup} \geq P_{backup}^0$$
$$P_{backup} = \Sigma P_{backupProvider}^i = P_{batt} + P_{fc}$$

This power needs to be available for a certain time t_{backup}^0:

$$t_{backup}(t) \geq t_{backup}^0 \quad \forall t$$

The back-up time is expressed in terms of the total energy stored in the back-up providers and the power level it needs to be provided at:

$$t_{backup}(t) = \frac{\Sigma(r^i * E_{store}^i(t))}{P_{backup}^0} > t_{backup}^0$$

Where r^i is a factor that accounts for the efficiency of the discharging process and the discharging power of the back-up assets. The constraint formulation has been generalized to allow for easy integration of alternative backup power solutions in case both battery and fuel cell turn out to be unfeasible.

3.6 Initialization

The solver for the nonlinear program needs reasonable initial guess of the solution for reliable convergence. This is typically generated by a dynamic simulation of the plant model where initial guesses for all degrees of freedom have been applied.

While the initial component size was typically constrained by simple physical considerations (available area for photovoltaics, yearly total energy demand, etc), the control signals' initial trajectories were derived using simple control laws. The battery charging and discharging rates were controlled by a PI controller driven by the renewable energy surplus. The electrolyzer was controlled using a PI controller to maintain a constant state of charge in the hydrogen tank. Concerning the other components, pre-defined trajectories were applied as initial guess.

4   Results

This optimization problem solves many tasks at the same time:
- It selects technology options (discrete choices)
- It sizes components (continuous choices)
- It operates assets to achieve the minimal total cost of ownership (continuous choices)
- It estimates the minimal total cost of ownership

In this paper, we review the results of a single optimization run. It is required in the future to perform a sensitivity analysis to assess the robustness of the

optimization results with respect to uncertainties in all forecasted data (prices, loads and weather).

4.1 Technology selection

In the plant configuration shown in Figure 1, all technology options to be assessed have been modeled. This means that there are redundancies in the way the loads can be met. If the optimization results in an asset of size zero, it means that the corresponding technology is neither technically nor economically viable. In some cases, the optimization finds it optimal to fulfill a need by investing in different technologies. Here are the technology options that have been investigated:

1. *Import versus on-site generation* for hydrogen and power
2. *Fuel cell versus battery* for backup-power and peak shaving
3. *CCS vs. CCUS vs. carbon tax* to deal with the emissions from the combustion processes
4. *Conventional burner versus heat pump* for paint drying

In the following sections, the technologies selected for the first 2 items will be presented and discussed.

4.1.1 Import versus onsite generation

With the given price structure for energy and the given CapEx and OpEx for electrolyzer and photovoltaic power plant, both hydrogen and electricity can economically be produced on-site to a significant amount. However, due to the different pricing of electricity in winter and summer, both technologies have been selected by the optimization:

1. While the CapEx cost for the electrolyzer and the required liquefier is rather high, and also the energy losses from well to wheel are considerable, electricity cost in this model is low enough to produce liquid hydrogen at a lower price than

Table 1 Optimizable parameters of the system

Parameter name	Min Value	Max Value	Unit
battery.capacity	0.01	2000	MWh
CCS.m_flow_rat	1e-5	1e5	kg/s
CCU.m_flow_rat	1e-5	1e5	kg/s
electrolyzer.n_cell	0.01	350	MW
fuelCell.n_cell	0.01	212	MW
grid.P_peak	0		MW
heatPump2.P_rat	1e-7	1e4	MW
hydrogenMarket.deliveries[i]	1e-7	1e4	MW
ngBurner2.P_rat	0.01	68.9	MW
photovoltaics.scale	0.1	1e06	m^3
tank.V	40	3e5	MW
transformer.P_max	0.01	2000	MWh

Table 2 Optimizable control signals of the system

Input name	Lower bound	Upper bound
I_electrolyzer__opt	0	1
I_fuelCell__opt	0	1
P_battery_charge__opt	0	1
P_battery_discharge__opt	0	1
P_processHeat__opt	0	1
m_flow_CCS__opt	0	1
m_flow_CCU__opt	0	1
ndot_H2_boiloff_vent	0	
pv_curtailment_opt	0	1

purchasing from an external supplier. In summer, the comparatively high peak demand charge means, that reducing the output of the electrolyzer is the most economical mode of operation. As a result, the optimizer determined that producing the hydrogen on-site and purchasing the hydrogen to almost equal parts is the most cost-effective option, see the Sankey diagram in Figure 2.

2. Photovoltaics cannot provide electric energy at a lower cost than the utility company with the available pricing structure and the given insolation profile for the plant location. But during peak-hours in the summer, photovoltaics can significantly reduce the demand charge, and drives the electrolyzer for a longer time at its rated power, decreasing the overall cost for hydrogen.

4.1.2 Fuel cell vs. battery

In this model, the fuel cell and the battery can fulfill similar tasks: both can provide power and lower the demand charge during peak hours. Both options can also both provide emergency power in case of a blackout in the grid.

The considered batteries are second-use and they come therefore with limited performance. Apart from a limitation on the usable SOC range, they cannot be fully discharged faster than 2 hours.

The optimization results show that the fuel cell is the far better alternative for both use cases. We attribute this to two main root causes:

1. While the price-per-kW of the battery is here lower than that of the fuel cell, the backup power time requirement t_{backup}^0 is much larger than 2h, meaning we will need to install several times as much power as P_{backup}^0 to achieve the required energy needs, which results in a battery that is more expensive than the fuel cell for this purpose.

2. Furthermore, the constraint on t_{backup}^0 means, that the battery needs to have enough energy stored to provide P_{backup}^0 for t_{backup}^0 at all times. A battery that is just big enough to fulfill the requirements for backup power needs to be kept completely charged and cannot be used for other purposes like peak-shaving without violating the backup power requirement.

While the fuel cell size is the significant parameter for the backup *power*, the time $t_{backup}(t)$ this power can be provided is largely determined by the available hydrogen in the tank, meaning that the tank will need to always retain t_{backup}^0 worth of hydrogen in the tank. In our model, hydrogen is delivered at fixed time intervals and the delivered amount is variable and optimal. At each delivery, the tank is filled just enough to have a sufficient backup of hydrogen in the tank before a new delivery arrives.

The investment cost (CapEx) for a fuel cell would be too high to justify its use as a peak-shaver. However, if the fuel cell doubles as emergency power provider, the operational cost make operation during peak hours economically viable. A detailed explanation of this behavior can be found in 4.3.
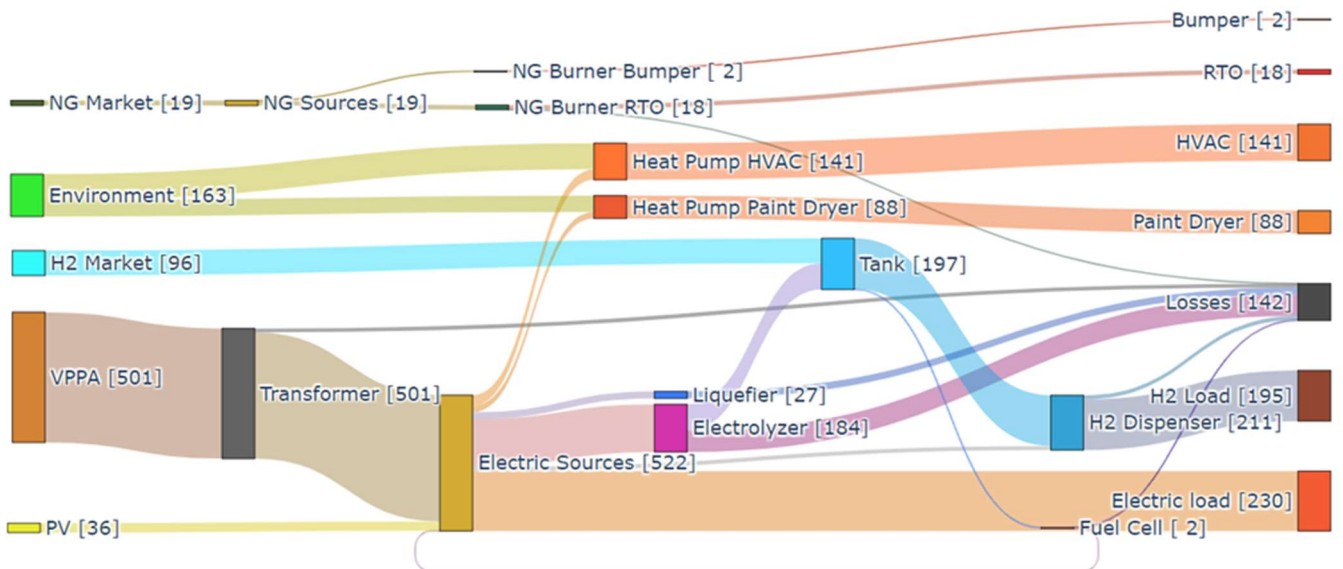

Figure 2 Sankey diagram of the energy flows [GWh] in the optimized system

Table 3 Optimized parameters

Parameter Name	Optimal size	Min	Max	Unit
battery.capacity	0.01	0.01	2000	MWh
cCS.m_flow_rat	1e-5	1e-5	1e5	kg/s
cCU.m_flow_rat	1e-5	1e-5	1e5	kg/s
electrolyzer.n_cell	22.6	0.01	350	MW
fuelCell.n_cell	3.1	0.01	212	MW
grid.P_peak	54.44	0		MW
heatPump2.P_rat	10.87	1e-7	1e4	MW
ngBurner2.P_rat	1e-7	1e-7	1e4	MW
photovoltaics.scale	22.26	0.01	68.9	MW
tank.V	1069	0.1	1e06	m³
transformer.P_max	92.73	40	3e5	MW

Figure 3 Optimal hydrogen deliveries over the course of a full year

The resulting fuel cell is just sized big enough to be the single provider of backup power P_{backup}^0 Since the battery does not provide any backup power, the hydrogen tank's level is directly proportional to the available emergency backup time t_{backup} (Figure 4)

4.2 Components' size

In this system, a total of 11 parameters have been optimized, most of them are related to the rated output or physical size of these components. Additionally, 53 weekly hydrogen deliveries have been computed (Figure 3). The results of the optimal sized components is shown in Table 3.
The following is worth to be noted:

- The resulting photovoltaics is not covering all the available area for the reasons previously exposed
- The fuel cell is sized mainly to match the backup power requirements.
- The battery capacity is minimal, reaching practical zero size
- Carbon taxes are more economical than carbon capture technologies

4.3 Optimal control

Interesting findings can be done by visualizing the control trajectories.

The state of charge of the tank is limited by the back-up requirements and not by its bound parameter, see Figure 4. The back-up requirements have therefore a direct impact on the amount of the weekly hydrogen delivery and the tank size.

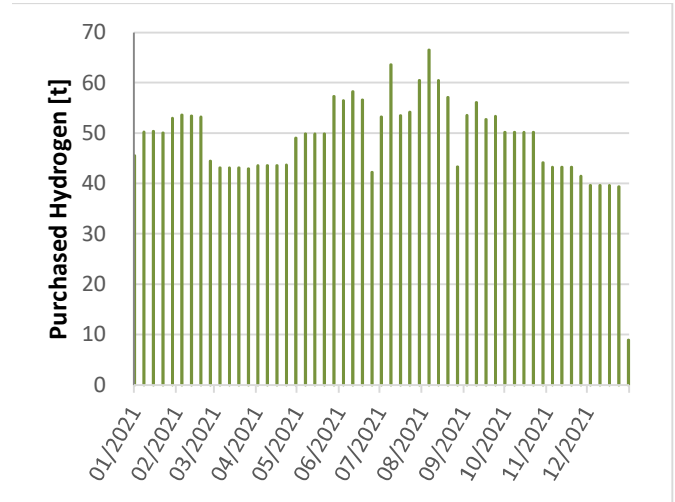The power from the photovoltaics is in principle never curtailed because the maximum output of the photovoltaic power plant is below the rated power input of the electrolyzer (Table 3), which means that the optimizer is always able to utilize the surplus energy either for the electricity load directly or for hydrogen production.

Peak shaving in the summer was mainly expected to be performed by engaging storage. As shown in Figure 5, the optimizer found that it is more cost effective to act on the significant controllable load that is the electrolyzer. Hydrogen is imported to a higher degree in the summer month when this happens, see Figure 3.
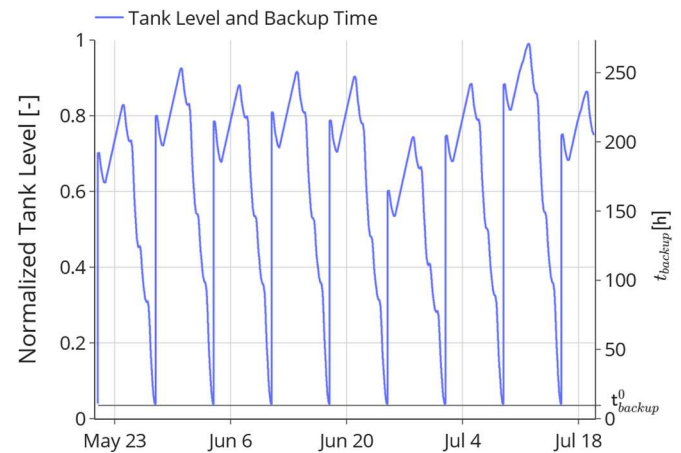

Figure 4 Backup reserve time t_{backup} and tank level (normalized)

The fuel cell is only used in 2 situations:

1. It takes over from the electrolyzer in its peak shaving activity when the electrolyzer power is completely shut down, see Figure 6. As explained in 4.1.2, due to its high CapEx, the fuel cell is sized to fulfill the backup requirements. Making thus up only roughly 15% of the electrolyzer's rated power demand, the impact on peak-shaving of the fuel cell is relatively small.

2. Besides its operation as peak shaver, the fuel cell converts the otherwise unused boil-off hydrogen into electricity. When demand for hydrogen becomes lower, the fraction of boil-off gas (BOG) at the tank outlet increases. During the weekends, the hydrogen-load is provided entirely as BOG (Figure 6). At the same time, the electrolyzer generates additional hydrogen, which results in a steady increase in the amount off boil-off hydrogen until the demand recovers during working hours at the plant.

   Reliquefying the hydrogen (zero boil-off) may be a more cost-effective option in such cases but is currently not supported in this model.

4.4 Performance

The optimization problem considered in the paper is complex and large-scale. Modelon's Thermal Power library, as well as the component models developed for this project, have been designed with dynamic optimization in mind. Thanks to a more efficient formulation and model improvements, it is now possible to solve the TCO optimization problem for a full year in a reasonable time. On an entry level PC (i3), initializing the problem takes about 5 minutes, with an additional 10 minutes to find a solution. Using parallelization, it is possible to run parameter sweeps in not more than 10 minutes.

5 Conclusion

In this paper, we have presented a framework that allows for the techno-economic assessment of complex hybrid energy projects. The benefit of the approach relies in the simultaneous design of the controls and the process, which lead to lower cost and a more systematic way of handling new configurations and technologies. The method has been applied on a car manufacturing plant to minimize the total cost of ownership of the transition towards carbon neutrality. The technique was able to estimate the overall cost and select the most viable technology options. S*ome* results are unexpected and cannot be found by considering a part of the system in isolation, but rather require a holistic system model.
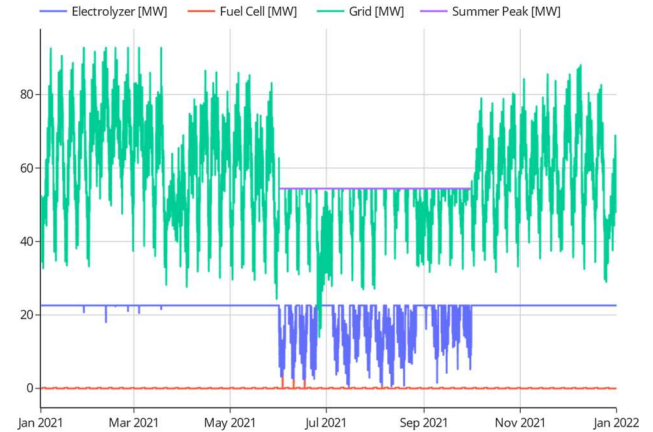

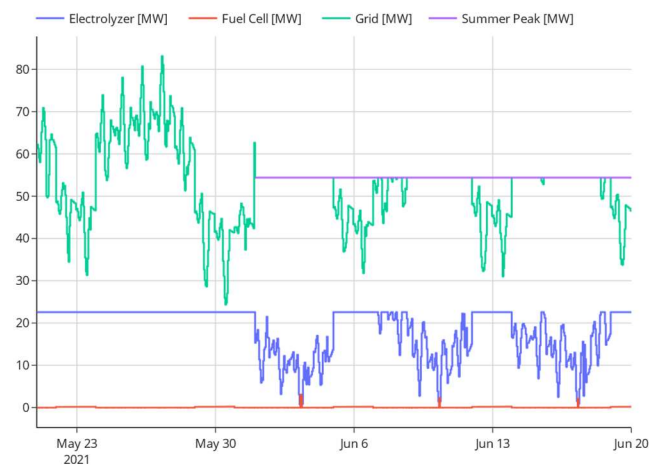**Figure 5 Demand reduction during summer months and peak shaving over the course of one year**
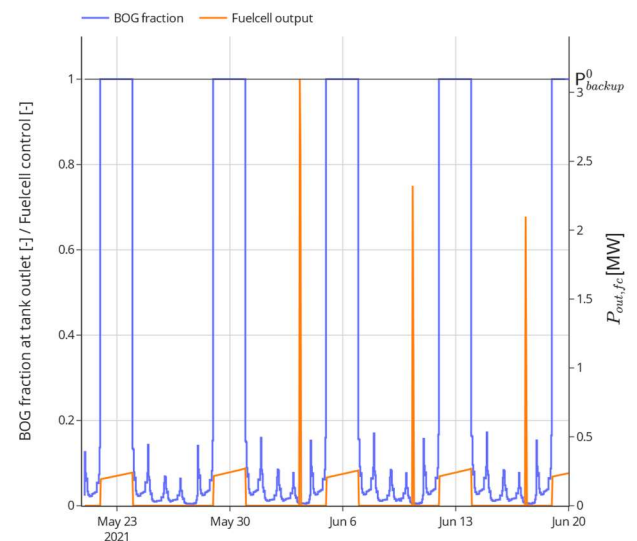

Figure 6 Demand reduction and peak shaving (detail)

Figure 7 Boil-off consumption and peak-shaving

Abbreviations

EV	Electric Vehicle
HVAC	Heating, Ventilation, Air-Conditioning
TCO	Total Cost of Ownership
BOG	Boil-off gas (hydrogen)
CapEx	Capital Expenditure
OpEx	Operational Expenditure
FC	Fuel cell
PV	Photovoltaic
CCS	Carbon Capture and Storage
CCUS	Carbon Capture, Utilization and Storage
NPV	Net Present Value
FMI	Functional Mock-up Interface

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