# HERA : Hydrogen Economics and Infrastructure Optimization Model

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RESEARCH

## HERA – HYDROGEN ECONOMICS AND INFRASTRUCTURE OPTIMIZATION MODEL

The article develops an optimization model of the whole hydrogen value chain, from the H2 production (including water electrolysis and steam reform with and without carbon capture) up to the H2 delivery to consumers via road transportation or pipelines.

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# HERA – Hydrogen Economics and infRAstructure optimization model

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## Abstract

Hydrogen from renewable sources has been discussed worldwide as a crucial energy carrier for climate change mitigation. It has multiple possibilities of production routes, as well as many current and potential applications. The objective of this research is to develop an optimization model for expanding and operating the hydrogen infrastructure for the promotion of hydrogen markets. The developed model can be applied for every location. It addresses the whole hydrogen value chain, from the $H_2$ production, including water electrolysis and steam reform with and without carbon capture, up to the $H_2$ delivery to consumers via road transportation or pipelines. The model was developed in GAMS language using Mixed Integer Linear Programming (MIP). Its objective function is to minimize the total cost of hydrogen supply, subject to demand, $CO_2$ emissions constraints, availability of resources and energy and mass balances of technologies. The model has an hourly discretization and includes options of hydrogen storage, electricity storage, grid electricity use, in addition to mixing different complementary resources and production technologies.

# Contents

## Introduction: objective of the modelling

This study presents the development of an optimization model for hydrogen infrastructure and is the result of a partnership between IFP School, in France, and the Federal University of Rio de Janeiro, in Brazil[1]. The theme is of interest both for France and Brazil, once hydrogen from renewable sources has been discussed worldwide as a crucial energy carrier for climate change mitigation (Ministerial Council on Renewable Energy, 2017; COAG Energy Council, 2019; MOTIE, 2019; República Portuguesa, 2020; Energy Ministry, 2020; European Commission, 2020; Federal Ministry for Economic Affairs and Energy, 2020; Gouvernement français, 2020; Ministry of Natural Resources Canada, 2020; DSI, 2021; MME, 2021).

Hydrogen has multiple possibilities of production routes, as well as many current and potential applications. Designing the optimal infrastructure for the hydrogen value chain, such as production and transport plants, is complicated since there are many variables involved. In addition, operational aspects related to the intermittency of renewable energy sources have great influence on the design of the infrastructure and need to be considered. Thus, the development of an optimization model for renewable hydrogen infrastructure tends to support the energy planning for the promotion of renewable hydrogen markets.

The model was developed in GAMS language using Mixed Integer Linear Programming (MIP) and can be applied for every location. The dynamic linear programming is appropriate to solve the optimization problem as the size of the model is not too large and is solved in a limited CPU (Central Processing Unit) time. The objective function is to minimize the total cost of hydrogen supply, subject to demand, $CO_2$ emissions constraints, availability of resources and energy and mass balances of technologies. The model contains equations and features of equipment for the whole value chain of hydrogen, from the production, including water electrolysis and steam reform with and without carbon capture, up to the delivery to consumers via road transportation or pipelines. The model includes hydrogen storage, electricity storage, grid electricity use, in addition to mixing different complementary resources and production technologies.

The Figure 1 shows a scheme of the model:

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[1] The study was carried out during the PhD visiting research of Gabriela Nascimento da Silva at the IFP School. This research was under the supervision of Professor Frédéric Lantz, from IFP School, Professor Alexandre Szklo and Professor Pedro Rochedo, from UFRJ.
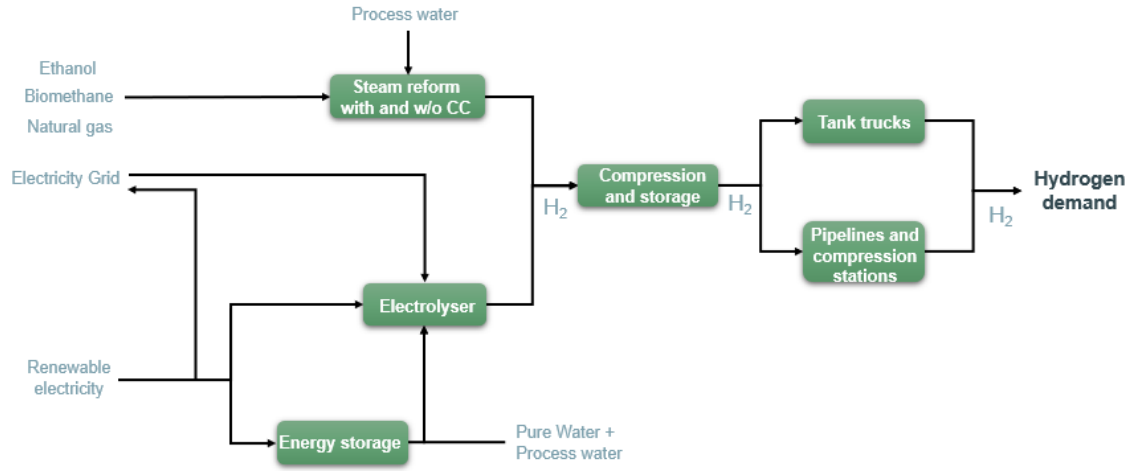
*Figure 1: Representative scheme for the hydrogen infrastructure model*

## 1. The components of the model

In this section, we present the main components of the hydrogen demand and supply.

### 1.1. Hydrogen demand

The demand for hydrogen is an exogenous variable, input by the user in an hourly scale. The hydrogen must be produced and transported to its destination, attending the hourly demand. Therefore, there are some constraints in the model for the attendance of the demand.

The input in an hourly scale allows the user to insert different demands over time, to represent a variation or seasonality. This may be interesting for specific applications such as transportation, for example.

After the user provides the demand data, the model calculates the maximum hydrogen demand per hour, for designing the pipelines and compression stations. The total demand for hydrogen for the time horizon is also calculated, for emission limit estimates.

Additionally, the model calculates the average daily demand for hydrogen, once the transportation via trucks is not able to deliver on an hourly scale, but rather in batches. Therefore, in this model we assumed that the trucks meet the average daily demand, delivering the amount the day before its use.

## 1.2. Resources and technologies availability

The user must also inform the model which resources and technologies are available to produce hydrogen. Binary variables are associated to each type of production technology, so, the result of the optimization may or may not include that form of production. More than one form of production can be associated together to produce hydrogen.

If the user wishes to choose the production technology in advance, before the optimization, it is possible to assign the number "1" to its binary variable and "0" to the others the user wants to exclude. In fact, this decreases the processing time since there will be fewer alternatives for the model to analyze during the optimization.

The main parts of the model include the production and the logistics of hydrogen.

### 1.2.1. Production of hydrogen

The Table 1 shows the options of hydrogen production technologies and the associated resources available in the model:

*Table 1: Options of hydrogen production technologies and resources*

| Production technologies | Resources |
|---|---|
| Steam reform with and w/o carbon capture | Hydrocarbons or alcohols (such as natural gas, light fractions of oil, bioethanol, biomethane etc.) |
| Electrolysis | Any kind of electricity (from wind, solar PV, hydro, curtailment, coal, nuclear etc.) |

The model accepts any kind of feedstock for the steam reform (hydrocarbon or alcohol), as the mains characteristics of the feedstock are parameters and can be input by the user (default values are available). The same applies for the electricity for the electrolysis. The electrolysis also considers two sources of electricity at the same time, which can benefit from temporal/spatial complementarity to smooth the variability. As they are associated to binary variables, if it is more convenient (cheaper), only one source of electricity can be used as well.

Batteries are available in the model. Typical sizes of batteries are input by the user (default values are available) and the model designs how many batteries are necessary for operating the electrolyser in the least costly solution. The same applies for electrolysers and steam reform units, typical sizes are input and the model returns with the number of units.

For the design of the solar PV and the wind plants, the model loops many possibilities of sizes for these plants and does the optimization inside the loopings: There are some default values for number of wind turbines and PV plants (Iw and Ipv), but the user can change it, as they are parameters. The optimization is executed inside the loop for every combination of Iw and Ipv and stops when all the possibilities were already calculated.

The final pressure of hydrogen is that for the storage and for transportation via trucks, defined by the user (default values are available). To reach this pressure, there is a compressor after the hydrogen production unit. If the transportation is made by pipelines, the pressure can be alleviated. The energy for the compressor comes from the same sources as that for the electrolyser: from energy plants, batteries and grid. For the compressor associated to the steam reform, the energy comes only from the grid.

The water required for the electrolyser is acquired from a desalination plant, transported from the coast until the electrolyser unit. Both ultrapure water and process water are used. For the steam reform only process water is used, but for this unit there are also costs associated to the fuel, electricity and catalyst in this plant.

1.2.2. Logistics of hydrogen delivery

The logistics part of the model allows to choose between different transportation technologies to take hydrogen to the demand. The choice is done by binary variables and only one modal is allowed. The transportation of hydrogen is in the compressed form. The two transportation modals available are:

- Pipelines
- Trucks

The transportation of electricity using the regional grid (to have the hydrogen production near the demand) is not considered in the model, as the rules for certification schemes of green hydrogen/low carbon hydrogen are not well established regarding the use of the grid. In addition, it would require further analysis of capacity of transmission lines and the expansion planning of the grid's transmission. Anyway, if the user wishes to evaluate this option, it is possible to include the cost of transmission into the cost of generation.

*Storage*

A hydrogen storage is available, which helps to regulate the production of hydrogen to attend the demand. Two virtual storages were modeled, one associated to pipelines and the other associated to trucks. This strategy was adopted once the demand constraints are different for each modal: while for pipelines the demand is attended hourly, for trucks we consider the daily delivery of hydrogen. Each virtual storage is associated to the binary variables of trucks and pipelines, so in practice there is only one storage being used.

The maximum initial amount of hydrogen in the storage is input by the user and the model determines the real quantity. The user can also input the fraction of cushion gas, important for maintaining the minimum pressure, especially for underground storage. As a result, the storage is designed and the model shows the operation (the amount of hydrogen input, output and accumulated for each hour). The kind of storage is not defined, but the costs can be input by the user.

*Pipelines*

The modelling of pipelines infrastructure is traditionally a non-linear problem. However, for this model, to have all equations linear, the possible sizes of the pipes follow standard diameters, which are selected according to binary variables. The user can choose five values for diameters to analyze and the respective thickness, but default values are available in the model. Binary variables are associated to each pipeline, so, as a result of the optimization, only one kind of pipeline, among the five options, will operate.

The flow of hydrogen as compressed gas inside the pipelines was modeled following the equations for incompressible fluids. This is recommended for gases with low speeds, in which Mach Number[2] is lower than 0.2 (Guerra e Gustafsson, 1986; Darbandi e Schneider, 1998). In this regard, we calculated the speed of the gas which corresponds to a Mach Number of 0.2 and the correspondent diameter, which was defined as the minimum diameter of the pipes.

To avoid land use constraints, we considered that the pipelines are built in parallel with the roadways, so further identification of protected areas is not in the scope of the model.

*Compression stations*

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[2] Mach Number refers to the ratio of the speed of the sound and the speed of the fluid.

The compression stations were modeled to compensate the pressure drop of hydrogen inside the pipes. For this, the user chooses the minimum pressure inside the pipelines and the compression stations are designed with the size of compressors and distance between each other along the pipelines. The electricity use of compression stations was calculated considering the higher speed of the hydrogen inside the pipeline. There is one last compression station, which aims to compress hydrogen to the pressure required by the final client and is different from the others. The required electricity for the compression stations comes from the grid, with the associated costs and $CO_2$ emissions.

*Transportation via trucks*

The transportation via trucks was modelled to attend the daily demand in the previous day. For example, the total demand of day one is attended in day zero. A tank truck is considered, with its main characteristics: capacity factor, fuel consumption, capacity of hydrogen transportation, lifetime (in km), refurbishment, fuel emissions etc. The salary of truck drivers and the cost of fuel are also considered as well as the average speed of trucks in roadways. They are parameters and input by the user (default values are available).

## 2. The static optimization model

The static model considers all the possibilities of technologies and resources presented in the previous sections and calculates, for the interval of one hour, the combinations that meet the constraints of the model, identifying the combination that minimizes the total cost of the project, the objective function.

## 2.1 The objective function

Like the traditional approach of optimization models, the objective function refers to cost minimization. The total cost for each equipment/plant is defined as follows:

$$Total\ cost = O\&M\ cost + K\ cost\ annualized + utilities\ cost + feedstock\ cost - revenues \tag{1}$$

$$K\ cost\ annualized = investment\ cost \times CRF \tag{2}$$

$$CRF = \frac{r \times (1+r)^n}{(1+r)^n - 1} \tag{3}$$

Where O&M cost is the annual operation and maintenance costs; CRF is the capital recovery factor; r is the discount rate; and n is the project's lifetime, in years. The costs to be considered regard feedstock, utilities, fuels, equipment for the production, compression, transportation, storage etc. In this model, we consider the O&M cost as a fraction of the CAPEX and can be defined by the user (default values are available).

The initial methodology considered to minimize the levelized cost of hydrogen (LCOH), which regards the total cost divided by the amount of hydrogen produced, but as the production of hydrogen is a variable, the resulting equation would be non-linear. So, to avoid the non-linear equations, not allowed in linear programming, the objective function regards the total cost of infrastructure. In practice, it means that the infrastructure is remunerated only by the defined demand, and some excess of hydrogen does not generate revenue for the project.

The LCOH is calculated after the optimization and its behavior does not necessarily follows the total cost's behavior, as the production of hydrogen is not necessarily equal to the demand. The operative constraints and the fixed costs associated can result in a hydrogen production greater than the demand.

## 2.2. The constraints

The constraints of the model are related to:

- Mass and energy balances
- Capacity/operation of the equipment
- The attendance of the demand
- $CO_2$ emissions limit
- Use of electricity from the grid
- Selling electricity to the grid

## 2.3. The formulation of the model

Based on the information described in the previous sections, it is possible to formulate the model as follows[3]:

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[3] The operational constraints are not in this formulation because they are particular from each equipment and cannot be generalized. Further information can be found in the Annex 1.

$$Min\left[\left(\sum_{i=1}^{n} C_{i,O\&M} + C_{i,K} + C_{i,utilities} + C_{i,feedstock} - R_i\right) + \tau_{CO2} * G_{CO2}\right] \qquad (4)$$

$$M_{H2Production} \geq M_{H2Demand} \qquad (5)$$

$$M_i = M_{i,input} - M_{i,output} + M_{i,accumulated} \qquad (6)$$

$$E_i = E_{i,input} - E_{i,output} + E_{i,accumulated} \qquad (7)$$

$$G_{CO2} \leq M_{H2Production} * l_{CO2} \qquad (8)$$

$$E_{grid} \leq l_{grid} \qquad (9)$$

$$E_{sell} \leq l_{sell} \qquad (10)$$

Where:

$C_{i,O\&M}$: Cost of Operation and Maintence of the plant/equipment i (in USD/year)

$C_{i,K}$: Annualized capital cost of plant/equipment i (in USD/year)

$C_{i,utilities}$: Utilities cost of plant/equipment i (in USD/year)

$R_i$: Revenues of the plant/equipment i (in USD/year)

$\tau_{CO2}$: $CO_2$ taxes (in USD/kg$CO_2$)

$G_{CO2}$: Total $CO_2$ emissions (in kg$CO_2$)

$M_{H2Production}$: Mass of hydrogen produced (in kg)

$M_{H2Demand}$: Mass of hydrogen demanded (in kg)

$M_i$: Mass of hydrogen in the equipment i (in kg)

$M_{i,input}$: Mass of hydrogen input in equipment i (in kg)

$M_{i,output}$: Mass of hydrogen output in equipment i (in kg)

$M_{i,accumulated}$: Mass of hydrogen already accumulated in equipment i (in kg)

$E_i$: Energy in the equipment i (in kWh)

$E_{i,input}$: Energy input in equipment i (in kWh)

$E_{i,output}$: Energy output in equipment i (in kWh)

$E_{i,accumulated}$: Energy already accumulated in equipment i (in kWh)

$l_{CO2}$: Limit of $CO_2$ emissions (in kg$CO_2$/kg$H_2$)

$E_{grid}$: Energy from the electricity grid for the electrolyser (in kWh)

$l_{grid}$: Limit of energy from the electricity grid for the electrolyser (in kWh)

$E_{sell}$: Energy sold to the electricity grid (in kWh)

$l_{sell}$: Limit of energy to be sold to the electricity grid (in kWh)

# 3. The dynamic linear programming model

The dynamic modelling of the infrastructure for hydrogen seeks to consider the variation of the parameters over time. Parameters such as resource availability, demand, costs, etc. are not necessarily constant and thus vary for different periods. Therefore, the result of the optimization and the behavior of the endogenous variables are affected.

The production framework of the model considers the availability of the resources hourly. The model was developed for two different time horizons, depending on the objective of the user: for 168 hours of one typical week; and for 8760 hours of one typical year. The main purpose of the version for the whole year regards the design of equipment, which need to consider the seasonality of the renewable resources. The version for one typical week is a zoom (shorter simulation), focusing on operational issues. The version for 8760 hours also details operational issues, but as it takes a very long computational time, it is indicated to be used only in very specific cases.

## 3.1. Economic function

For the dynamic model, the economic functions are affected by the endogenous variables. For example, utility costs depend on the variable related to hydrogen production, which varies over hours.

Binary variables also impact in the economic function since the fixed costs of a plant are "included" in the economic function only if its binary variables have the value 1. This occurs if the respective plant has been "chosen" in the optimization and thus it will come into operation. The opposite is true: if a plant is not chosen to operate, its production/use will be zero and thus its binary variable will also be zero.

The equation shows how the variables impacts in the economic function:

$$Min \sum_{t=0}^{8760} \left[ \left( \sum_{i=1}^{n} c_{i,O\&M} * Y_i + c_{i,K} * Y_i + c_{i,utilities} * M_i(h) + c_{i,feedstock} \right. \right.$$
$$\left. \left. * M_i(h) - r_i * M_i(h) \right) + \tau_{CO2} * g_{CO2} * M_i(h) \right] \qquad (11)$$

Where:

$c_{i,O\&M}$: Parameter for the cost of operation and maintenance of the plant/equipment i (in USD/year)

$c_{i,K}$: Parameter for the annualized capital cost of plant/equipment i (in USD/year)

$c_{i,utilities}$: Parameter for the utilities cost of plant/equipment i (in USD/year)

$r_i$: Parameter for the unit revenues of the plant/equipment i (in USD/(kg*year))

$\tau_{CO2}$: Parameter for the $CO_2$ taxes (in USD/kg$CO_2$)

$g_{CO2}$: Parameter for the unit $CO_2$ emissions of the i plant (in kg$CO_2$)

$Y_i$: Binary variable for the equipment i

$M_i(h)$: Variable for the mass of hydrogen produced in the equipment i (in kg/h)

This example serves for hydrogen production units but it can be easily adapted for energy plants, substituting Mi per Ei. The generic example also applies to other units, such as pipelines, compressors, storage etc. (the difference is that Mi is not the "Mass of hydrogen produced in the equipment i" but the "Mass of hydrogen used in the equipment i").

## 3.2. Supply and demand constraints

Like the economic function, the constraints related to supply and demand are affected by dynamic variables. In the dynamic model, production should not necessarily be equal to or greater than demand, as there is storage. Thus, for the dynamic model, the sum of the hydrogen produced in hour h and the output of the storage in the same hour must be equal to or greater than the demand.

$$M_{H2Production}(h) + M_{H2StorageOut}(h) \geq M_{H2Demand}(h) \qquad (12)$$

Where:

$M_{H2Production}(h)$: Mass of hydrogen produced (in kg/h)

$M_{H2Demand}(h)$: Mass of hydrogen demanded (in kg/h)

$M_{H2StorageOut}(h)$: Mass of hydrogen output from the storage (in kg/h)

## 3.3. Dynamic relationships between the periods

The connection between the static models for each period (in this case, hour) is made by equations. For the present model, its main links refer to the storage of energy and storage of hydrogen.

The equations of storage equipment inform the model that if there is an excess of resources, it is possible to save them for periods of absence. It also says that if there is no

availability of resources, it is possible to complement with the excess already stored and thus comply with the constraints of demand, during all periods.

## 4. Example of application

In this section we present a numerical example for the use of the model. This example point out how to optimize the design of the $H_2$ supply from renewable power taking into account the technical characteristics of $H_2$ electrolyser, the renewable power and the demand.

We developed the modelling using the GAMS language and platform. To use GAMS, it is necessary to define the indices (set), the parameters (exogenous variables), the variables (endogenous variables) and the equations of the model[4]. The description of these components is available in Annex 1.

The example refers to the city of São Gonçalo do Amarante, in Ceará, Brazil. The example considers an existing green hydrogen pilot plant[5]. The production capacity is 250 Nm$^3$/h of hydrogen, with a 3 MW solar PV plant and a PEM electrolyser. The data used for the example are described in the Annex 2. We considered that the hydrogen is transported to the demand in Fortaleza, the capital of Ceará, 63 km distance.

For this configuration, we considered the possibility to use or not the electricity from the grid to complement the solar PV electricity. For not allowing grid electricity, we must define the parameter "Limit of electricity from the Grid" as "0" and for allowing we can define this parameter as a very large number (such as "9999999999"), or a known limit, in kW.

For cases in which some plants are already defined, as the solar PV plant in the example, we need to define the binary variable for PV ("Ypv") as "1". The same applies for the variable of the design of the PV ("Ipv")[6] . The binary and design variables for other production units such as wind plant ("Yw"), steam reform with and without carbon capture ("Ysr" and "Ycc") must be defined as "0".

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[4] More information about GAMS can be found in <https://www.gams.com/latest/docs/UG_MAIN.html>

[5] More information in <https://www.complexodopecem.com.br/edp-produz-primeira-molecula-de-hidrogenio-verde-no-ceara/#:~:text=A%20produ%C3%A7%C3%A3o%20da%20mol%C3%A9cula%20%C3%A9,a%20primeira%20do%20Grupo%20EDP>

[6] The number "1" for the design varibale "Ipv" means that the model should use only one PV plant, with the size previous defined, in this case 3MW.

The data for the solar PV plant generation was obtained from the model System Advisor Model (SAM), for the 8760 hours of the year. We selected the typical weeks for each season (winter, spring, summer and autumn) using a clustering methodology which minimizes the Euclidean distance and run the model for the 4 typical weeks (672 hours).

The results of the optimization are shown in Table 2.

*Table 2: Results for the optimization of the example*

|  | **Without grid electricity** | **With grid electricity** |
|---|---|---|
| PEM Electrolyser (MW) | 1.15 | 1.18 |
| Solar PV (MW) | 3 | 3 |
| Batteries (MWh) | 6.22 | 4.85 |
| $H_2$ Storage capacity (kg) | 10240 | 1355 |
| Energy from the grid | - | 49.5% |
| Trucks (units of 885 kg) | 1 | 1 |
| Capacity factor of electrolyser | 49% | 92% |
| Average $CO_2$ emissions ($kgCO_2/kgH_2$) | 0.18 | 1.32 |
| Annualized cost (USD/year) | 2814574 | 1731727 |
| Total hydrogen production (kg/year) | 220573 | 185662 |
| LCOH (USD/kg) | 12.76 | 9.33 |

The table shows the optimized values for each unit, for example, 1.15 and 1.18 MW of electrolysers, 6.22 and 4.85 MWh of batteries and so on. It is possible to note the great difference of hydrogen storage capacity between the two rounds. This happens because the model allows to start the production with some hydrogen already in the storage (previous defined by the user, with its cost associated). As in the first round the electricity is provided only by solar PV plants, during the first hours, with no sun, the model uses the hydrogen in the storage to supply the demand. The results of the optimization also chose trucks instead of pipelines to transport the hydrogen to Fortaleza, due to the low demand.

In other cases where the production unit is not defined, the model also chooses and designs the production units and the electricity sources.

Some other examples of output are operational variables, such as the use of units hourly: input and output of storage, use of electrolysers, hydrogen production etc. The model also supplies the user with the cost per unit. The Figure 2 shows the impact of each unit in the LCOH for the example of São Gonçalo do Amarante.
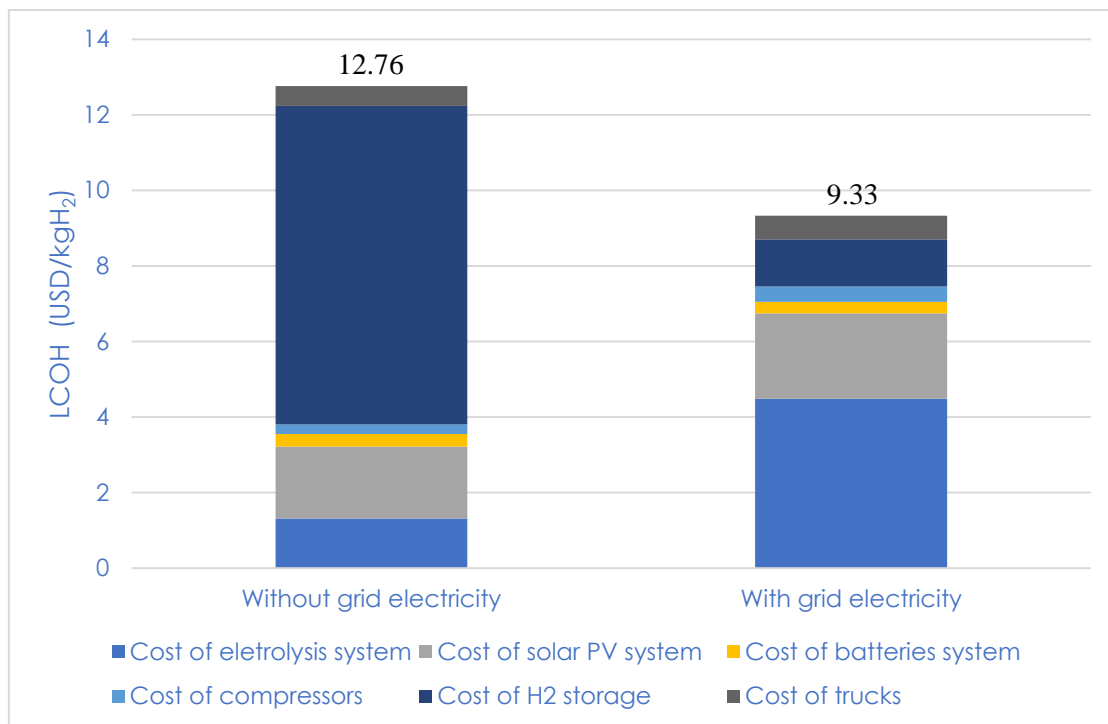
*Figure 2: Results for the costs of each unit of the example*

## 4. Discussion and conclusion

As more features are included in the model, more complex the model becomes. For models with discrete variables, integer or binary, the complexity is greater, once the group of solutions is lower. In these cases, the computational time can be very long, as the solver need a lot of effort to find the possible solutions. The time stamp also impacts on the complexity, for example, to analyze a typical year in hourly resolution, the computational time can become so long that that it hinders the progress of the study. In comparison, for daily resolution, it is simpler to execute the optimization, but we lose important details of the analysis, especially for electricity from renewable sources. For the hydrogen production via steam reform it is not an issue, as the resources do not necessarily vary along the time, but as renewable electricity like wind and solar depend on climate conditions, its intermittency impacts on the operation of the plants and on the equipment's design. For example, to operate a PEM electrolyser with i) 500 kW continuously for 24 hours, comparing to ii) receive 12 hours 0 kW + 12 hours 1000 kW. For the second case, if the design of the electrolyser is 1000 kW, there will be idle capacity during 12 hours. However, for a design lower than 1000 kW, there will be excess of electricity during 12 hours. So it is important to consider the intermittency of renewable energy in the model, as it impacts on the design of equipment and, consequently, in the total cost. Greater resolutions are even better, but it is important to reconcile resolution with reasonable computational time.

During the development of the present model, we ran some tests to assess the robustness of the sizing of the equipment according to the variability of the renewable electricity production. The optimization for 8760 hours for a typical year required more than one day of CPU time[7]. So, if the analyst needs to improve the computational time, we suggest some handling that can significantly reduce the effort of the computer:

- Reducing the number of integer variables: turning the integer variables related to the design of the equipment into real variables is an acceptable simplification.
- Instead of analyzing a typical year, run the model for typical weeks, considering the seasonality of the resources. For example, if the region has two seasons for wind and solar, it is possible to run the model for two consecutive weeks (336 hours), each one representing one season.

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[7] For a Dell computer with Windows 10, 16 GB RAM, processor Intel Core i7 and CPLEX solver.

- Optimization in two steps: it is possible to separate the logistics phase from the production phase and optimize the whole model in two steps.

Note that running this model with average values smooths the intermittency of renewable energy and result in underestimated investment costs optimizations.

The model is still under development and during the next months some improvements are suggested. For example, more production processes can be modelled, such as pyrolysis and gasification of biomass and fossil resources. We also intend to include in the model the infrastructure of transmission lines and substations to transport electricity instead of hydrogen, making available the option of producing hydrogen near the demand. Further improvements also include to add the operational constraints of electrolysers, such as partial load, ramp up, ramp down etc. The improvement of the design of steam reform units is also suggested, as it does not include economies of scale. Finally, another important issue is to estimate the land use, which depends on the technologies used.

Some other results were obtained with this model in a case study for Bahia, Brazil, and presented in the 3rd Momentom International Congress[8]. We point out that the results of the model are of the same order of magnitude found in the literature (International Energy Agency, 2022; Tozlu, 2022; Zhou, Searle e Baldino, 2022).

Therefore, using such modelling approach, plays crucial role to optimize the design of hydrogen production as supporting investors' decisions, for decision makers in the energy planning. The results help to understand how different taxes, subsidies, and specific policies can impact in the development of hydrogen markets and also for supporting the development of regulation for hydrogen markets.

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[8] https://momentom2023.sciencesconf.org/

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# Annex 1 – Parameters which are defined with some indices (sets), variables and equations of the model

<u>Sets</u>

<u>Hours</u>[9]

h 'hours of the week'

h0-h168

<u>Technology of the electrolyser</u>

itech 'kind of electrolyser'

PEM, ALC

<u>Fuels/feedstocks for the steam reform</u>[10]

fuel 'available fuels for SR'

NG, Eta, Bio

<u>Diameter of the pipeline</u>

pipe 'available diameters'

A,B,C,D,E

<u>Parameters (scalars)</u>

<u>General scalars:</u>

<u>Nhours</u> 'Total number of hours'

<u>LHV</u> 'Lower heating value for $H_2$, in kWh/$kgH_2$'

<u>PWP</u> 'Water process price, in USD/kg'

<u>WTdessa</u> 'Transportation of desalinated water to eletrolysis plant, in USD/$kgH_2$ for 100 km'

<u>$O_2P$</u> 'Oxygen price, in USD/$m^3$'

<u>$roO_2$</u> 'Density of Oxygen, in kg/$m^3$'

<u>dr</u> 'discount rate'

<u>liP</u> 'life of the project, in years'

<u>CarbonTa</u> 'Carbon tax, in USD/$kgCO_2$'

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[9] The equations in this document refer to 168 hours, but the model can be adapted to 8760 hours, representing one whole year.

[10] Natural gas, ethanol and biomethane.

limCO$_2$ 'Limit of CO$_2$ emissions, in kgCO$_2$/kgH$_2$'

limTr 'Limit of electricity from the Grid, in kW'

LimSell 'Limit of selling electricity to the Grid, in kWh/h'

efac 'emission factor of the grid, in kgCO$_2$/kWh'

Lenght 'Distance of the production site to the demand (straight), in m'

LenghtRoadway 'Distance of the production site to the demand via roadways, in m'


Scalars for electrolysis:

PTW 'Price of the water for the electrolyser (ultrapure water), in USD/kgH$_2$'

DTW 'Demand of water for the electrolyser (ultrapure water), in kg/kgH$_2$'

DPW 'Demand of cooling water for the electrolyser, in kg/kgH$_2$'

EleOMCostPerc 'O&M cost for electrolysers in %'


Scalars for wind energy

Iw 'Number of wind turbines'

WCapacity 'Capacity of wind turbine, in kW'

WCapCost 'Capital cost for the wind turbines, in USD/kW'

WOMcost 'O&M cost for the wind turbines, in USD/(kW*year)'


Scalars for solar PV energy

Ipv 'Number of solar PV farms'

PVCapacity 'Power of PV plant, in kW'

PVCapCost 'Capital cost of the PV plant, in USD/kW'

PVOMcost 'O&M cost of the PV plant, in USD/(kW*year)'


Scalars for battery

PVcostru 'running cost of operating solar PV, in USD/kWh'

lo 'Round-trip efficiency of the battery'

BatCapacity 'Capacity of the battery, in kWh'

limPbat 'Maximum power of the battery, in kW'

Bat0 'Maximum initial state of charge of battery'

BatCapCost 'Capital cost of the battery, in USD/kWh'

BatOMCost 'O&M cost of the battery, in USD/(kW*year)'

Batcostru 'running cost of discharging the battery, in USD/(KWh-cycle)'

Scalars for steam reform with and without carbon capture

CapH2SR 'Capacity of steam reform, in $kgH_2/h$'

OMSRcostperc 'O&M cost of steam reform in percentage'

WSR 'Process water consumption of steam reform, in $kg/kgH_2$'

eleSR 'Electricity consumption of steam reform, in $kWh/kgH_2$'

Pcat 'Price of catalyst for steam reform, in $USD/kgH_2$'

CapH2CC 'Capacity of steam reform with carbon capture, in $kgH_2/h$'

CCCapCost 'Capital cost for steam reform with carbon capture, in $USD/kgH_2$'

CCOMCostpercen 'O&M costs for steam reform with carbon capture, in percent'

WCC 'Process water consumption for steam reform with carbon capture, in $kg/kgH_2$'

CCcostru 'running cost of operating steam reform with carbon capture, in $USD/kgH_2$'

CCFuC 'Fuel consumption for steam reform with carbon capture (in $kg/kgH_2$ for liquids and $m^3/kgH_2$ for gases)'

eleSRCC 'Electricity consumption for steam reform with carbon capture (in $kWh/kgH_2$)'

CCCO2 '$CO_2$ emissions from steam reform with carbon capture, in $kgCO_2/kgH_2$'

CapCostCompSR 'Capital cost of the compressor for the SR w/o CCS, in $USD/(kgH_2/h)$'

OMCostCompSRperc 'O&M cost of the compressor for the SR w/o CCS, in percent'

eleCompSR 'Electricity consumption for the compressor for the SR w/o CCS, in $kWh/kgH_2$'


Scalars for hydrogen storage

StoCapa 'Capacity of each unit of storage, in $kgH_2$'

H2StoCapCost 'Capital cost of the hydrogen storage, in $USD/kgH_2$'

OMStorage 'O&M cost for storage, in percentage'

SH20 'Maximum initial mass of hydrogen in the storage, in percentage'

cushion 'Cushion gas, minimum volume of gas to keep the pressure, in percentage'

PH2 'Price of initial hydrogen in the storage in $USD/kgH_2$'


Scalars for pipelines

alfaPipe 'scale factor for pipelines'

PipeCostBasis 'Capital cost for a pipeline known in USD/m'

DiameterBasis 'Internal diameter of a pipe known in m'

OMPipe 'O&M cost for pipelines, percentage'

DenH2 'Density of hydrogen at 100 bar, in $kg/m^3$'

Mi 'Viscosity of hydrogen, in Pa*s'

epsilon 'Roughness of the pipelines, in m'

Ptarget 'Initial pressure inside the pipeline that should be maintained, in Pa'

Pmin 'Minimum pressure inside pipelines, in Pa'

liPPipe 'life of the pipelines, in years'


Scalars for compression stations

Z 'Compressibility factor'

R 'Gases constant, in kJ/(kg*K)'

T 'Inlet temperature, in K'

N 'Number of stages of compression'

NiIs 'Isentropic efficiency of compression'

k 'Ratio of specific heats'

efComp 'Efficiency of the compression stations'

OMCSta 'O&M cost for compression stations, in percentage'

alfaCS 'scale factor for compressors'

CompCostBasis 'Capital cost for a compressor known, in USD'

CompSizeBasis 'Power of a compressor known, in kW'


Scalars for trucks

Tload 'Time for loading and unloading the truck, in hours'

speedTruck 'Average speed for the truck, in km/h'

TruckSize 'Capacity of the truck, in $kgH_2$'

Salary 'Salary of truck drivers, in USD/hour'

TruckCapCost 'Capital cost of trucks for $H_2$ transportation, in USD/truck'

FuelTruck 'Fuel consumption (diesel) for trucks transporting hydrogen in km/L'

FuelPriTruck 'Price of the fuel (diesel) for transporting hydrogen, in USD/L'

TruckOM 'O&M cost for trucks, in percentage'

FCTruck 'Capacity factor of trucks'

MaxkmTruck 'Maximum distance for replacement, in km'

ReplacCost 'Replacement cost of trucks, in percentage of investment cost'

efacDiesel 'Average emission factor of diesel, in $kgCO_2/L$'


<div align="center">Parameters (related to sets)</div>

H2d(h) 'Hourly demand of hydrogen, in kg/h'

H2dMax 'Maximum demand of hydrogen in kg/h':

$$H2dMax = Max(H2d(h)) \qquad (13)$$

TH2d 'Total demand of hydrogen in kg/week':

$$TH2d = \sum H2d(h) \qquad (14)$$

p(itech) 'Capacity of electrolyser, in kW'

eff(itech) 'Efficiency of electrolyser'

Stack(itech) 'Stack cost, to be replaced every 7 years, in USD/kW'

ElecCapCost(itech) 'Capital cost of electrolyser, in USD/kW'

EleOMCost(itech) 'O&M cost of electrolyser, in USD/(kW*year)':

$$EleOMCost(itech) = ElecCapCost(itech) * EleOMCostPerc \qquad (15)$$

CapCostCompElec(itech) 'Capital cost of the compressor for the electrolyser, in USD/(kgH$_2$/h)'

OMCostCompElec(itech) 'O&M cost of the compressor for the electrolyser in USD/((kgH$_2$/h)*year)'

eleCompElec(itech) 'Electricity consumption for the compressor for electrolyser, in kWh/kgH$_2$'

CompElecostfi(itech) 'Fixed costs of electrolysers compressors':

$$
\begin{aligned}
CompElecostfi(itech) \\
= \left( \frac{dr * (1 + dr)^{liP}}{(1 + dr)^{liP} - 1} * CapCostCompElec(itech) + OMCostCompElec(itech) \right) \\
* \frac{p(itech) * eff(itech)}{LHV} * \frac{365}{7}
\end{aligned}
\qquad (16)
$$

techcostfi(itech) 'Fixed costs of electrolysers':

$$
\begin{aligned}
techcostfi(itech) = \left( \frac{dr * (1 + dr)^{liP}}{(1 + dr)^{liP} - 1} * ElecCapCost(itech) + \frac{Stack(itech)}{(1 + dr)^7} + \frac{Stack(itech)}{(1 + dr)^{14}} \right. \\
\left. + EleOMCost(itech) \right) * \frac{p(itech)}{365/7}
\end{aligned}
\qquad (17)
$$

techcostru(itech) 'Running cost of electrolyser, in USD/kgH$_2$'

Wcostfi 'Fixed costs of wind turbines':

$$Wcostfi = \left( \frac{dr * (1 + dr)^{liP}}{(1 + dr)^{liP} - 1} * WCapCost + WOMCost \right) * \frac{WCapacity}{365/7} \qquad (18)$$

PVcostfi 'Fixed costs of PV solar plants':

$$PVcostfi = \left(\frac{dr*(1+dr)^{liP}}{(1+dr)^{liP}-1}*PVCapCost + PVOMCost\right)*\frac{PVCapacity}{365/7} \qquad (10)$$

Batcostfi 'Fixed costs of batteries':

$$Batcostfi = \left(\frac{dr*(1+dr)^{liP}}{(1+dr)^{liP}-1}*BatCapCost + BatOMCost\right)*\frac{limPbat}{365/7} \qquad (19)$$

OMCostCompSR 'O&M cost of the compressor for the SR w/o CCS in USD/((kgH$_2$/h)*year)':

$$OMCostCompSR = OMCostCompSRperc * CapCostCompSR \qquad (20)$$

SRCapacity(fuel) 'Capacity of steam reform, in kgH$_2$/day'

SRCapCost(fuel) 'Capital cost of steam reform, in USD/kgH$_2$'

SROMCost(fuel) 'O&M costs of steam reform, in USD/(kgH$_2$*year)':

$$SROMCost(fuel) = SRCapCost(fuel) * OMSRcostperc \qquad (21)$$

CompSRcostfi(fuel) 'Fixed costs of SR w/o CCS compressors':

$$CompSRcostfi(fuel) = \left(\frac{dr*(1+dr)^{liP}}{(1+dr)^{liP}-1}*CapCostCompSR + OMCostCompSR\right)*\frac{SRCapacity(fuel)}{365/7} \qquad (22)$$

SRcostfi(fuel) 'Fixed costs of steam reform':

$$SRcostfi(fuel) = \left(\frac{dr*(1+dr)^{liP}}{(1+dr)^{liP}-1}*SRCapCost(fuel) + SROMCost(fuel)\right)*\frac{SRCapacity(fuel)}{365/7} \qquad (23)$$

SRcostru(fuel) 'running cost of operating steam reform, in USD/kgH$_2$'

FuC(fuel) 'Fuel consumption for the hydrogen production via steam reform (in kg/kgH$_2$ for liquids and m$^3$/kgH$_2$ for gases)'

FuP(fuel) 'Fuel price (in USD/kg for liquids and USD/m$^3$ for gases)'

SRCO2(fuel) 'CO$_2$ emissions from steam reform, in kgCO$_2$/kgH$_2$'

Parameters for steam reform with carbon capture

CCOMCost 'O&M costs of carbon capture for SR, in USD/(kgH$_2$*year)':

$$CCOMCost = CCOMCostpercen * CCCapCost$$

( 24)

CCcostfi 'Fixed costs of carbon capture in SR':

$$CCcostfi = \left(\frac{dr * (1 + dr)^{liP}}{(1 + dr)^{liP} - 1} * CCCapCost + CCOMCost\right) * \frac{CCCapacity}{365/7}$$

( 25)

Parameters for hydrogen storage

H2StoOMCost 'O&M cost of the hydrogen storage in USD/(kgH$_2$*year)':

$$H2StoOMCost = H2StoCapCost * OMStorage$$

( 26)

H2Stocostfi 'Fixed costs of the hydrogen storage, for one unit':

$$H2Stocostfi = \left(\frac{dr * (1 + dr)^{liP}}{(1 + dr)^{liP} - 1} * H2StoCapCost + H2StoOMCost\right) * \frac{StoCapa}{365/7}$$

( 27)

Parameters for Pipelines

NomDiameter(pipe) 'Diameter of the pipe, in in'

EspeP(pipe) 'Thickness of the pipe, in m'

diameter(pipe) 'Internal diameter of the pipe, in m':

$$diameter(pipe) = \frac{NomDiameter(pipe) * 2.54}{100} - 2 * EspeP(pipe)$$

( 28)

PipeCapCost(pipe) 'Capital cost of the pipe, in USD/m':

$$PipeCapCost(pipe) = PipeCostBasis * \left(\frac{diameter(pipe)}{DiameterBasis}\right)^{alfaPipe}$$

( 29)

PipeOMCost(pipe) 'O&M cost of the pipe, in USD/(m*year)':

$$PipeOMCost(pipe) = PipeCapCost(pipe) * OMPipe$$

( 30)

H2FlowH 'Maximum flow of hydrogen in pipelines, in m$^3$/h':

$$H2FlowH = \frac{H2dMax}{DenH2} \qquad (31)$$

H2FlowSec 'Maximum flow of hydrogen in pipelines, in m$^3$/s':

$$H2FlowSec = \frac{H2FlowH}{3600} \qquad (32)$$

Area(pipe) 'Area of the transversal section of the pipe, in m$^2$':

$$Area(pipe) = 3.14159 * \frac{diameter^2(pipe)}{4} \qquad (33)$$

MaxSpeed(pipe) 'Maximum speed of H$_2$ in the pipelines, in m/s':

$$MaxSpeed(pipe) = \frac{H2FlowSec}{Area(pipe)} \qquad (34)$$

Re(pipe) 'Reynolds Number':

$$Re(pipe) = \frac{diameter(pipe) * MaxSpeed(pipe) * DenH2}{Mi} \qquad (35)$$

fad(pipe) 'Friction factor':

$$fad(pipe) = \left( \frac{-1}{1.8 * \log_{10} \left[ \left( \left( \frac{\frac{epsilon}{diameter(pipe)}}{3.7} \right)^{1.11} + \frac{6.9}{Re(pipe)} \right) \right]} \right)^2 \qquad (36)$$

DP(pipe) 'Pressure drop, in Pa/m':

$$DP(pipe) = \frac{8 * fad(pipe) * H2FlowSec^2 * DenH2}{3.14159^2 * diameter^5(pipe)} \qquad (37)$$

TDP 'Total pressure drop, in Pa':

$$TDP = Ptarget - Pmin \qquad (38)$$

LenghtCS(pipe) 'Distance between compression stations, in m':

$$LenghtCS(pipe) = \frac{TDP}{DP(pipe)} \qquad (39)$$

Pipecostfi(pipe) 'Fixed costs of pipelines':

$$Pipecostfi(pipe) = \left( \frac{dr * (1 + dr)^{liP}}{(1 + dr)^{liP} - 1} * PipeCapCost(pipe) + PipeOMCost(pipe) \right) * \frac{LenghtRoadway}{365/7} \qquad (40)$$

Parameters for compression stations

NCS(pipe) 'Number of compression stations, integer number':

$$NCS(pipe) = Rounddown \left( \frac{LenghtRoadway}{LenghtCS(pipe)} \right) \qquad (41)$$

TECompStation 'Energy required in the compression stations, in kWh/week':

$$TECompStation = Z * R * T * N * \frac{1}{NiIs} * \frac{k}{k - 1} * \left[ \left( \frac{Ptarget}{Pmin} \right)^{\frac{k-1}{N*k}} - 1 \right] * 0.000277778 * TH2d \qquad (42)$$

SizeCompStation 'Power of the compressor for compression stations in kW':

$$SizeCompStation = \frac{TECompStation}{Nhours * EfComp} \qquad (43)$$

LenghtFinal(pipe) 'Distance between the last compression station and the demand, in m':

$$LenghtFinal(pipe) = LenghtRoadway - NCS(pipe) * LenghtCS(pipe) \qquad (44)$$

Plast(pipe) 'Pressure at the end of the pipelines before arriving at the demand, in Pa':

$$Plast(pipe) = Ptarget - DP(pipe) * LenghtFinal(pipe) \qquad (45)$$

ELastCS(pipe) 'Total energy required in the LAST compression station, in kWh/four weeks':

$$ELastCS(pipe) = Z * R * T * N * \frac{1}{NiIs} * \frac{k}{k-1} * \left[ \left( \frac{Ptarget}{Plast(pipe)} \right)^{\frac{k-1}{N*k}} - 1 \right] * 0.000277778 * TH2d \quad (46)$$

SizeLastCS(pipe) 'Power of the compressor for the LAST compression station in kW':

$$SizeLastCS(pipe) = \frac{ELastCS(pipe)}{Nhours * EfComp} \quad (47)$$

CompSCapCost 'Capital cost of the compressor, in USD':

$$CompSCapCost = CompCostBasis * \left( \frac{SizeCompStation}{CompSizeBasis} \right)^{alfaCS} \quad (48)$$

CompSOMCost 'O&M cost of the compression stations, in USD/year':

$$CompSOMCost = CompSCapCost * OMCSta \quad (49)$$

LastCSCapCost(pipe) 'Capital cost of the LAST compressor, in USD':

$$LastCSCapCost(pipe) = CompCostBasis * \left( \frac{SizeLastCS(pipe)}{CompSizeBasis} \right)^{alfaCS} \quad (50)$$

LastCSOMCost(pipe) 'O&M cost of the last compression station, in USD/year':

$$LastCSOMCost(pipe) = LastCSCapCost(pipe) * OMCSta \quad (51)$$

CompScostfi 'Fixed costs of the compression stations in USD/week':

$$CompScostfi = \left( \frac{dr * (1+dr)^{liP}}{(1+dr)^{liP} - 1} * CompSCapCost + CompSOMCost \right) * \frac{7}{365} \quad (52)$$

LastCScostfi(pipe) 'Fixed costs of the LAST compression stations in USD/week':

$$LastCScostfi(pipe) = \left(\frac{dr * (1 + dr)^{liP}}{(1 + dr)^{liP} - 1} * LastCSCapCost(pipe) + LastCSOMCost(pipe)\right) * \frac{7}{365} \qquad (53)$$

Parameters for trucks

DH2d 'average daily demand in kgH$_2$/day':

$$DH2d = \frac{TH2d}{\frac{Nhours}{24}} \qquad (54)$$

TruckOMCost 'O&M cost of trucks for H$_2$ transportation, in USD/(truck*year)':

$$TruckOMCost = TruckOM * TruckCapCost \qquad (55)$$

TimeTravel 'Time the truck takes for 1 round trip, in hours':

$$TimeTravel = \left(\frac{2 * \frac{LenghtRoadway}{1000}}{speedTruck}\right) + 2 * Tload \qquad (56)$$

Rh 'Total number of hours the truck drivers work per day, integer number':

$$Nh = Roundup\left(\left(\frac{DH2d}{TruckSize}\right) * TimeTravel\right) \qquad (57)$$

Nvt 'Number of travels per truck per day, integer number':

$$Nvt = Rounddown\left(\frac{24}{TimeTravel}\right) \qquad (58)$$

Nt 'Number of trucks, integer number':

$$Nt = Roundup\left(\frac{DH2d}{Nvt * TruckSize * FCTruck}\right) \qquad (59)$$

Tokm 'Total distance each truck runs per day, in m':

$$Tokm = \left(2 * \frac{LenghtRoadway}{1000}\right) * Nvt \qquad (60)$$

LiPTruck 'Time of life for the truck, in years':

$$LiPTruck = \frac{MaxkmTruck}{Tokm * 365 * FCTruck} \qquad (61)$$

NTiRepl 'Times of replacement the truck, integer number':

$$RTiRepl = Rounddown\left(\frac{LiP}{LiPTRuck}\right) \qquad (62)$$

ReplaAnnu 'Total cost with replacement of trucks':

ni 'Parameter to drive the loop, from 0 to LiPTruck, considering the whole lifetime of the project':

$$ReplaAnnu = ReplaAnnu + \left(\frac{ReplacCost * TruckCapCost}{(1 + dr)^{ni}}\right) \qquad (63)$$

Truckcostfi 'Fixed costs for trucks in USD/week':

$$Truckcostfi = \left(\frac{dr * (1 + dr)^{liP}}{(1 + dr)^{liP} - 1} * (TruckCapCost + ReplaAnnu) + TruckOMCost\right) * \frac{Nt}{365/7} \qquad (64)$$

TruckcostFuel 'Fuel costs for trucks, in USD/week':

$$TruckcostFuel = 7 * Tokm * Nt * FCTruck * \left(\frac{FuelPriTruck}{FuelTruck}\right) \qquad (65)$$

CostSal 'Cost with salaries of the truck drivers, in USD/week':

$$CostSal = Salary * Nh * 7 \qquad (66)$$

CO2Truck 'Total $CO_2$ emissions from truck transport in $kgCO_2$':

$$CO2Truck = 7 * Tokm * Nt * FCTruck * \left(\frac{efacDiesel}{FuelTruck}\right) \qquad (67)$$

CostTrucks 'Total cost of transportation via trucks in USD/week':

$$CostTrucks = Truckcostfi + TruckcostFuel + CostSal \qquad (68)$$

Parameters for electricity

WGEN(h) 'Wind turbine generation, in kWh'

SolPVGen(h) 'Solar PV generation, from a given plant, in kWh'

ep(h) 'electricity price in USD/kWh for off peak and peak hours'

avgElecGri 'Average cost of grid electricity':

$$avgElecGri = \frac{\sum ep(h)}{Nhours} \qquad (69)$$

sell(h) 'selling price for electricity to the grid, in USD/kWh'

## Variables

Positive variables

   capa(itech) 'Capacity of electrolysers, in kW'

   CO2 'Total $CO_2$ emissions, in $tCO_2$/week'

   CO2CS 'Total emissions from compression stations, in $tCO_2$/week"

   CostBat 'Total cost of batteries system, in USD/week'

   CostCCSR 'Total cost of steam reform with carbon capture, in USD/week'

   CostCompE 'Total cost of compressors for electrolysers, in USD/week'

   CostEleSys 'Total cost of water electrolysis, in USD/week'

   CostH2SR 'Total cost of steam reform, in USD/week'

   CostPV 'Total cost of solar PV plant, in USD/week'

   CostW 'Total cost of wind plant, in USD/week'

   CStaCost 'Total cost of compression stations, in USD/week'

   ECpv(h) 'Electricity for the compressor that comes from the solar PV plants, in kWh/h'

   ECw(h) 'Electricity for the compressor that comes from the wind turbines, in kWh/h'

   EElecUsed 'Total electricity used by the electrolyser, in kWh/h'

   ENpv(h) 'Electrolyser energy input from the solar PV, in kWh/h'

   ENw(h) 'Electrolyser energy input from the wind turbines, in kWh/h'

   Gri(h) 'Electricity purchased from the grid, in kWh/h'

   GriC(h) 'Electricity purchased from the grid that goes to the compressor, in kWh/h'

   GriE(h) 'Electricity purchased from the grid that goes to the electrolyser, in kWh/h'

H2SR(h,fuel) 'Hydrogen production via steam reform per fuel, in kg/h'

H2CC(h) 'Hydrogen production via steam reform with carbon capture, in $kgH_2/h$'

H2elec(h,itech) 'Hydrogen production via electrolysis per technology, in $kgH_2/h$'

H2H(h) 'Total hydrogen production, in $kgH_2/h$'

H2Pipe(h) '$H_2$ that goes directly to pipelines, in $kgH_2/h$'

H2S(hplus) '$H_2$ accumulated in the storage associated to pipelines, in $kgH_2/h$'

H2S2(hplus) '$H_2$ accumulated in the storage associated to trucks, in $kgH_2/h$'

H2So(hplus) '$H_2$ that leaves the storage associated to pipelines, in $kgH_2/h$'

H2So2(hplus) '$H_2$ that leaves the storage associated to trucks, in $kgH_2/h$'

H2Ss(hplus) '$H_2$ that goes into the storage associated to pipelines, in $kgH_2/h$'

H2Ss2(hplus) '$H_2$ that goes into the storage associated to trucks, in $kgH_2/h$'

H2Tpipe(h) 'Total $H_2$ going to the pipelines, in $kgH_2/h$'

PipeCost 'Total cost of pipelines and compression stations, in USD/week'

PVEWast(h) 'Solar PV energy that is wasted, not used, in kWh/h'

RPVGEN(h) 'PV generation if the model chooses to use solar PV, in kWh/h'

RWGEN(h) 'Wind generation if the model chooses to use wind turbine, in kWh/h'

S(h) 'energy accumulated in the batteries, in kWh/h'

Sc(h) 'Total electricity surplus that is commercialized, in kWh/h'

Scpv(h) 'Solar PV electricity surplus that is commercialized, in kWh/h'

Scw(h) 'Wind electricity surplus that is commercialized, in kWh/h'

So(hplus) 'Batteries output, in kWh/h'

SoC(h) 'Batteries output that goes to the compressor, in kWh/h'

SoE(h) 'Batteries output that goes to the electrolyser, in kWh/h'

Speed(pipe) 'Speed of hydrogen flowing in the pipe, in m/s'

Ss(hplus) 'Total electricity surplus that is stored, in kWh/h'

Sspv(h) 'Solar PV electricity surplus that is stored, in kWh/h'

Ssw(h) 'Wind electricity surplus that is stored, in kWh/h'

StoCost 'Total cost of storage, in USD/week'

Su(h) 'Total electricity surplus, in kWh/h'

Supv(h) 'Solar PV electricity surplus, in kWh/h'

Suw(h) 'Wind electricity surplus, in kWh/h'

TH2 'Total production of hydrogen in one week, in $kgH_2/week$'

TH2CC 'Total $H_2$ production via SR with carbon capture in one week, in $kgH_2/week$'

TH2elec 'Total $H_2$ production via eletrolysis in one week, in $kgH_2/week$'

TH2SR 'Total $H_2$ production via SR in one week, in $kgH_2/week$'

WEWast(h) 'Wind energy that is wasted, not used, in kWh/h'

Integer variables

    Ialc 'Integer for Alkaline electrolyser'

    Icc 'Integer for steam reform with carbon capture'

    Inb 'Integer for battery'

    Ipem 'Integer for PEM electrolyser'

    Isr 'Integer for steam reform'

    Nsto 'Integer variable for $H_2$ storage associated to pipelines'

    Nsto2 'Integer variable for $H_2$ storage associated to trucks'

Binary variables

    Yalc 'Binary for alkaline electrolyser'

    Yelec 'Binary for electrolyser'

    Yh2in(h) 'Binary for H2 going into the storage'

    Yh2out(h) 'Binary for H2 leaving the storage'

    Yin(h) 'Binary for charging the battery'

    Yout(h)'Binary for discharging the battery'

    Ypem 'Binary for PEM electrolyser'

    Ypipe 'Binary for pipelines'

    Ytruck 'Binary for trucks'

    Ypv 'Binary for solar PV'

    Ywin 'Binary for wind turbines'

Free variable

    Zed 'Total cost of the project'

<div align="center">Equations</div>

The first equation aims to associate the parameter $WGEN(h)$ with a variable, $RWGEN(h)$, multiplied by the integer variable $Iw$, which represents the number of wind turbines. This equation aims to give the model the option to use or not the wind turbines:

$$RWGEN(h) \leq Iw * WGEN(h) \qquad (70)$$

The equation below aims to limit the energy from the wind turbine that goes directly to the electrolyser, $ENw(h)$, and to the compressor, $ECw(h)$:

$$ENw(h) + ECw(h) \leq RWGEN(h) \qquad (71)$$

The equation below describes the electricity that is wasted, $WEWast(h)$, as the difference between the total electricity that could be provided by the wind turbine minus the total electricity generated by the wind turbine:

$$WEWast(h) = Iw * WGEN(h) - RWGEN(h) \qquad (72)$$

The equation below describes the wind electricity surplus, $Suw(h)$, the difference between the total electricity generated by the wind turbine and the wind energy which goes directly to the electrolyser and to the compressor:

$$Suw(h) = RWGEN(h) - ENw(h) - ECw(h) \qquad (73)$$

The part of the wind energy surplus which is commercialized, $Scw(h)$:

$$Scw(h) \leq Suw(h) \qquad (74)$$

The part of the wind energy surplus which is stored in batteries, $Ssw(h)$:

$$Ssw(h) = Suw(h) - Scw(h) \qquad (75)$$

The equations for energy from solar PV are similar to those for wind turbines:

$$RPVGEN(h) \leq Ipv * SolPVGEN(h) \qquad (76)$$

$$ENpv(h) + ECpv(h) \leq RPVGEN(h) \qquad (77)$$

$$PVEWast(h) = Ipv * SolPVGEN(h) - RPVGEN(h) \qquad (78)$$

$$Supv(h) = RPVGEN(h) - ENpv(h) - ECpv(h) \qquad (79)$$

$$Scpv(h) \leq Supv(h) \qquad (80)$$

$$Sspv(h) = Supv(h) - Scpv(h) \qquad (81)$$

The constraint for commercializing electricity to the grid:

$$Scw(h) + Scpv(h) \leq LimSell \qquad (82)$$

The total electricity surplus:

$$Su(h) = Suw(h) + Supv(h) \qquad (83)$$

The total electricity that is commercialized:

$$Sc(h) = Scw(h) + Scpv(h) \tag{84}$$

The total electricity that is stored in batteries:

$$Ss(h) = Ssw(h) + Sspv(h) \tag{85}$$

The energy required for compressor comes from wind turbines, solar PV, batteries and from the electricity grid:

$$H2elec(h, itech) * eleCompElec(itech) \leq ECw(h) + ECpv(h) + SoC(h) + GriC(h) \tag{86}$$

At the hour 0, the total energy available in batteries is limited by the initial charge, $Bat0$, multiplied by the integer variable which represents the number of batteries, $Inb$:

$$S(h0) \leq Inb * Bat0 \tag{87}$$

At the hour zero, the energy that goes to the batteries, $Ss(h)$, is zero. At the hour zero and the first hour, the energy that leaves the batteries is zero as well:

$$Ss(h0) = 0 \tag{88}$$

$$So(h0) = 0 \tag{89}$$

$$So(h1) = 0 \tag{90}$$

The balance for the energy accumulated in the batteries is the surplus which is stored, minus the energy that leaves the batteries plus the energy that was already stored in the previous hour:

$$S(h) = Ss(h) - So(h) + S(h-1) \tag{91}$$

The energy that leaves the batteries is limited by the energy that was already stored in the previous hour:

$$So(h) \leq S(h-1) \tag{92}$$

The energy that leaves the batteries goes to the electrolyser and to the compressors, considering the parameter which defines the efficiency of the battery, $lo$:

$$So(h) * lo = SoE(h) + SoC(h) \tag{93}$$

The three equations below mean that at the same hour, the storage cannot charge and discharge:

$$So(h) \leq Yout(h) * 9999999999 \tag{94}$$

$$Ss(h) \leq Yin(h) * 9999999999 \tag{95}$$

$$Yin(h) + Yout(h) \leq 1 \tag{96}$$

The strategy adopted in the above equations regards defining constraints with an upper bound (for example, Vmax = 9999999999), to select a value 0 or 1. It means that when the real variable on the left side of the equation is positive, then the integer variable is equal to 1.

The equations below mean that the model should choose only one technology for the electrolyser (itech, which refers to ALC or PEM):

$$H2elec(h, itech) \leq \left(\frac{eff(itech)}{LHV}\right) * capa(itech) \tag{97}$$

$$capa(ALC) \leq Ialc * p(ALC) \tag{98}$$

$$capa(PEM) \leq Ipem * p(PEM) \tag{99}$$

$$Ialc \leq Yalc * 9999999 \tag{100}$$

$$Ipem \leq Ypem * 9999999 \tag{101}$$

$$Yalc + Ypem \leq Yelec \tag{102}$$

The production of hydrogen, $H2elec(h, itech)$, is limited by the ratio of the parameters efficiency of electrolyser and the lower heating value multiplied by sum of the four "sources" of energy: the one which comes directly from the wind, the other comes directly from the solar PV, plus the energy stored in batteries plus some electricity from the grid:

$$H2elec(h, itech) \leq (\frac{eff(itech)}{LHV}) * (ENw(h) + ENpv(h) + SoE(h) + GriE(h)) \tag{103}$$

The total electricity that goes to the electrolyser is limited by the capacity of the electrolyser, $p(ALC)\ or\ p(PEM)$. The integer variables $Ialc$ and $Ipem$ represent the number of modules of eletrolysers for each technology (alkaline or PEM, respectively):

$$ENw(h) + ENpv(h) + SoE(h) + GriE(h) \leq p(ALC) * Ialc + p(PEM) * Ipem \tag{104}$$

The electricity purchased from the grid is limited by the parameter defined by the user:

$$Gri(h) \leq limTr \tag{105}$$

The total electricity from the grid which is used for the electrolyser and for the compressor:

$$Gri(h) = GriC(h) + GriE(h) \tag{106}$$

The equations below are constraints for the capacity of batteries (power and energy) and also aim to determine the number of batteries requested, represented by the integer variable $Inb$:

$$So(h) \leq Inb * limPbat \tag{107}$$

$$Ss(h) \leq Inb * limPbat \qquad (108)$$

$$S(h) \leq Inb * BatCapacity \qquad (109)$$

The total production of hydrogen by the electrolyser, $TH2elec$:

$$TH2elec = \sum H2elec\,(h, itech) \qquad (110)$$

As the steam reform does not depend on weather conditions, the equations for this technology are simpler. The hydrogen production via steam reform is limited by the capacity of the plant, parameter defined by the user ($CapH2SR$) multiplied by the number of plants, represented by the integer variable $Isr$:

$$H2SR(h, fuel) \leq Isr * CapH2SR \qquad (111)$$

The total production of hydrogen by the steam reform, $TH2SR$:

$$TH2SR = \sum H2SR\,(h, fuel) \qquad (112)$$

The same applies to steam reform with carbon capture:

$$H2CC(h, fuel) \leq Icc * CapH2CC \qquad (113)$$

$$TH2CC = \sum H2CC\,(h, fuel) \qquad (114)$$

The hydrogen production, hourly:

$$H2H(h) = \; H2elec(h, ALC) + H2elec(h, PEM) + H2SR(h, GN) + H2CC(h) \qquad (115)$$

The total hydrogen amount that goes to the demand includes also the hydrogen that was already available in the hydrogen storage at hour 0:

$$TH2 = TH2elec + TH2SR + TH2CC + H2S(h0) + H2S2(h0) \qquad (116)$$

Total CO$_2$ emissions:

$$CO2 = \sum Gri(h) * efac + \sum H2SR(h, fuel) * SRCO2(fuel) + \sum H2CC(h, fuel) * CCCO2(fuel) \qquad (117)$$
$$+ +CO2CS + CO2TRuck$$

Constraints for CO$_2$ emissions:

$$CO2 \leq limCO2 * TH2 \qquad (118)$$

The equations below aim to inform the model that if it does not choose the respective technology, it must not include the fixed costs of the technology in the total cost of the project:

$$\sum RWGEN(h) \leq Ywin * 99999999 \tag{119}$$

$$\sum RPVGEN(h) \leq Ypv * 99999999 \tag{120}$$

$$Ypv + Ywin \leq Yelec * 99999999 \tag{121}$$

$$\sum S(h) \leq Inb * 99999999 \tag{122}$$

$$\sum H2SR(h, fuel) \leq Isr * 99999999 \tag{123}$$

$$\sum H2CC(h, fuel) \leq Icc * 99999999 \tag{124}$$

$$\sum H2elec(h, itech) \leq Yelec * 99999999 \tag{125}$$

Total energy used by the electrolyser, calculated for further estimates of capacity factor of electrolyser:

$$EElecUsed = \sum ENw(h) + \sum ENpv(h) + \sum SoE(h) + \sum GriE(h) \tag{126}$$

For the logistics of hydrogen, the main variables are exogenous, defined as parameters. Then the optimization defines whether to use trucks or pipelines and the diameter of pipelines, according to five values for diameters, previously defined by the user (or default).

The equations below aim to associate a binary value with the activity of each option of diameter for the pipeline. So, in practice, only one kind of pipeline, among the five options, will operate.

$$Speed(A) = Ya * MaxSpeed(A) \tag{127}$$

$$Speed(B) = Yb * MaxSpeed(B) \tag{128}$$

$$Speed(C) = Yc * MaxSpeed(C) \tag{129}$$

$$Speed(D) = Yd * MaxSpeed(D) \tag{130}$$

$$Speed(E) = Ye * MaxSpeed(E) \tag{131}$$

$$Ya + Yb + Yc + Yd + Ye = Ypipe \tag{132}$$

The following equations regard the hydrogen storage associated to pipelines. The first equation defines the initial amount of hydrogen in the storage, which is proportional to the number of storages (the integer variable $Nsto$), the capacity of each storage unit (parameter $StoCapa$) and the maximum fraction of storage initially filled with hydrogen (the parameter $SH20$).

$$H2S(h0) \leq Nsto * StoCapa * SH20 \qquad (133)$$

The parameter cushion regards the minimum fraction of gas to keep the minimum pressure of the storage:

$$H2S(h) \geq Nsto * StoCapa * cushion \qquad (134)$$

The following equations mean that at hour 0 there is no inlet neither outlet to the hydrogen storage:

$$H2Ss(h0) = 0 \qquad (135)$$

$$H2So(h0) = 0 \qquad (136)$$

The equation bellow regards the mass balance for the hydrogen storage: the amount of hydrogen accumulated, $H2S(h)$, is equal to the input, $H2Ss(h)$, minus the output, $H2So(h)$, in addition to the mass that was already accumulated in the previous hour, $H2S(h-1)$:

$$H2S(h) = H2Ss(h) - H2So(h) + H2S(h-1) \qquad (137)$$

The output of hydrogen is limited by the mass that was accumulated in the previous hour:

$$H2So(h) \leq H2S(h-1) \qquad (138)$$

The amount of hydrogen that goes to the pipelines, $H2Tpipe(h)$, must attend the hourly demand, $H2d(h)$, a parameter defined by the user. The binary variable $Ypipe$ helps the model to choose or not pipelines for transporting hydrogen:

$$H2Tpipe(h) \geq Ypipe * H2d(h) \qquad (139)$$

The equations below also regard the mass balance for hydrogen storage. The first one regards the total amount of hydrogen which goes to pipelines to attend the demand, $H2Tpipe(h)$, and the second one regards the amount of hydrogen coming from the production, $H2H(h)$, and going to the storage, $H2Ss(h)$, or directly to pipelines, $H2Pipe(h)$ .

$$H2Tpipe(h) \geq H2So(h) + H2Pipe(h) \qquad (140)$$

$$H2H(h) \geq H2Pipe(h) + H2Ss(h) \qquad (141)$$

The equation below aims to design the number of storages required:

$$H2S(h) \leq Nsto * StoCapa \qquad (142)$$

The equations below mean that the storage for hydrogen cannot load and unload at the same hour:

$$H2So(h) \leq Yh2out(h) * 9999999999999 \qquad (143)$$

$$H2Ss(h) \leq Yh2in(h) * 9999999999999 \tag{144}$$

$$Yh2out(h) + Yh2in(h) \leq 1 \tag{145}$$

$$Nsto \leq Ypipe * 9999999999999999 \tag{146}$$

The following equations regard the hydrogen storage associated to trucks. They are similar to the equations of the storage associated to pipelines, with the main difference of the constraint for the demand: while for pipelines the modelling regards an hourly demand, for the delivery by trucks, we consider the daily demand.

$$H2S2(h0) \leq Nsto2 * StoCapa * SH20 \tag{147}$$

$$H2S2(h) \geq Nsto2 * StoCapa * cushion \tag{148}$$

$$H2Ss2(h0) = 0 \tag{149}$$

$$H2So2(h0) = 0 \tag{150}$$

$$H2S2(h) = H2Ss2(h) - H2So2(h) + H2S2(h-1) \tag{151}$$

$$H2So2(h) \leq H2S2(h-1) \tag{152}$$

$$H2S2(h) \leq Nsto2 * StoCapa \tag{153}$$

$$Nsto2 \leq Ytruck * 9999999999999999 \tag{154}$$

We consider that the loading of trucks with hydrogen is realized through the storage, so there is no bypass and all hydrogen molecules must pass through the storage.

As the model is in hourly discretization, the demand constraints for trucks are defined for the end of the previous day:

$$H2So2(24 * (d-1)) \geq Ytruck * DH2d \tag{155}$$

Where $d$ is the day on which the demand should be met.

The total emissions from the compression stations:

$$CO2CS = (NCS(pipe) * Ypipe * TECompStation + Ypipe * ELastCS(pipe)) * efac \tag{156}$$

The binary variables, to inform the model to choose to use or trucks or pipelines to transport hydrogen:

$$Ytruck + Ypipe = 1 \tag{157}$$

The following equations regard the costs of the units.

The cost of the hydrogen storage, which is the sum of the fixed costs of the storage, *H2Stocostfi,* an exogenous variable, multiplied by the number of storages, *Nsto* or *Nsto2* in addition to the cost of the initial amount of hydrogen in the storage.

$$StoCost = (Nsto * H2Stocostfi) + (PH2 * H2S(h0)) + (Nsto2 * H2Stocostfi) + (PH2 * H2S2(h0))$$

(158)

The cost of pipelines regards the fixed costs of each pipeline (A, B, C, D and E) multiplied by its respective binary variable (Ya,Yb,Yc,Yd,Ye):

$$PipeCost = Ypipe * Pipecostfi(pipe)$$

(159)

The cost of compression stations is the sum of the fixed costs of the compression stations and the energy used by its compressors:

$$CStaCost = Ypipe * \left(NCS(pipe) * CompScostfi + LastCScostfi(pipe)\right) + NCS(pipe) * Ypipe * TECompStation + Ypipe * ELastCS(pipe) * avgElecGri$$

(160)

The total cost of logistics for hydrogen:

$$LogiCost = StoCost + PipeCost + CStaCost + (Ytruck * CostTrucks)$$

(161)

The total cost for steam reform:

$$CostH2SR = TH2SR * (FuC(fuel) * FuP(fuel) + WSR * PWP + Pcat + SRcostru(fuel)) + \sum\left(H2SR(h, fuel) * eleSR * ep(h) +\right) + Isr * SRcostfi(fuel)$$

(162)

The total cost for steam reform with carbon capture:

$$CostH2CC = TH2CC * (CCFuC(fuel) * FuP(fuel) + WCC * PWP + Pcat + CCcostru(fuel)) + \sum\left(H2CC(h, fuel) * eleSRCC * ep(h) +\right) + Icc * CCcostfi(fuel)$$

(163)

The total cost for wind turbines:

$$CostW = Iw * \left(Ywin * Wcostfi + \sum RWGEN(h) * Wcostru\right)$$

(164)

The total cost for solar PV:

$$CostPV = Ipv * \left(Ypv * PVcostfi + \sum RPVGEN(h) * PVcostru\right)$$

(165)

The total cost for batteries:

$$CostBat = Inb * (Batcostfi) + S(h0) * ep(h1) + BatCapacity * \frac{\sum So(h)}{limPbat*168} * Batcostru$$

(166)

The total cost for compressors (after hydrogen production), which addresses both fixed costs and costs with energy use from the electricity grid:

$$
\begin{aligned}
CostCompE = &\ Ialc * CompElecostfi(ALC) + \sum (H2elec(h, ALC) \\
& * eleCompElec(ALC) * ep(h)) + Ipem * CompElecostfi(PEM) \\
& + \sum (H2elec(h, PEM) * eleCompElec(PEM) * ep(h)) + Isr \\
& * CompSRcostfi(fuel) + \sum (H2SR(h, fuel) * eleCompSR * ep(h)) \\
& + Icc * CompCCcostfi(fuel) + \sum (H2CC(h, fuel) * eleCompSR \\
& * ep(h))
\end{aligned}
\qquad (167)
$$

The total cost for the electrolysis system:

$$
\begin{aligned}
CostEleSys = &\ \sum (GriE(h) * ep(h)) + TH2elec * techcostru(itech) + Itech * \\
& techcostfi(itech) + PTW * DTW * TH2elec + PWP * DPW * TH2elec + \\
& \frac{WTdessa * TH2elec * LenghtRoadway}{100000} - \sum \big(Scw(h) + Scpv(h)\big) * sell - \Big(\frac{TH2elec * 8 * O2P}{roO2}\Big)
\end{aligned}
\qquad (168)
$$

Total cost (objective function):

$$
\begin{aligned}
Zed = &\ CostH2SR + CostCCSR + CostEleSys + CostCompE + CostBat + \\
& CostW + CostPV + LogiCost + CarbonTa * CO2
\end{aligned}
\qquad (169)
$$

After the optimization, we created a loop for defining the optimal design of wind plants and solar PV plants. The loop tests several numbers of wind turbines, $Iw$, and solar PV plants, $Ipv$, executes the above optimization inside it, and gives the least costly solution.

# Annex 2 – Data for the numerical example

| Unit | Parameter | Value | Source |
|---|---|---|---|
| | | | **Economic parameters** |
| **Project** | Exchange rate (R\$/USD) | 5.16 (average for 2022) | https://www.bcb.gov.br/estabilidadefinanceira/historicocotacoes |
| | Discount rate | 0.085 | https://www.gov.br/economia/pt-br/centrais-de-conteudo/publicacoes/notas-tecnicas/2020/nt_taxa-social_vf.pdf/@@download/file/NT_Taxa%20Social_VF.pdf |
| | Lifetime of the project, in years | 20 | - |
| | Energy tariff for industrial consumers in Ceará | Hourly data | https://www.enel.com.br/pt-ceara/Tarifas_Enel.html |
| **Electrolysis** | Price of the water for the electrolyser (treated water), in USD/kgH$_2$ | 0.01323 | https://www.sciencedirect.com/science/article/abs/pii/S0011916422004040 |
| | Price of water transport, to take desalinated water until the plant, in USD/(kgH$_2$*100 km) | 0.05-0.06 | https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2004WR003749 |
| | Limit of CO2 emissions, in kgCO2/kgH$_2$ | 4.368 | https://www.certifhy.eu/go-labels/ |
| | O&M cost for electrolysers in % | 3% | https://theicct.org/wp-content/uploads/2022/02/fuels-eu-cost-renew-H-produced-onsite-H-refueling-stations-europe-feb22.pdf |
| | Capital cost of electrolyser, in USD/kW | PEM 1770 | https://www.iea.org/reports/global-hydrogen-review-2022 |
| | | Alkaline 1400 | |
| | Stack cost, to be substituted every 7 years, in USD/kW | PEM 580 | https://www.lazard.com/media/451922/lazards-levelized-cost-of-hydrogen-analysis-version-20-vf.pdf |
| | | Alkaline 345 | |
| | Capital cost of the compressor for the electrolyser, in USD/(kgH$_2$/h) | PEM 14118 | https://www.sciencedirect.com/science/article/pii/S0360319920325842 |
| | | Alkaline 16807 | |
| | O&M cost of the compressor for the electrolyser in USD/((kgH$_2$/h)*year) | PEM 282 | https://www.sciencedirect.com/science/article/pii/S0360319920325842 |
| | | Alkaline 336 | |
| **Solar PV** | Capital cost of the PV plant, in USD/kW | 788 | https://www.epe.gov.br/sites-pt/publicacoes-dados-abertos/publicacoes/PublicacoesArquivos/publicacao-490/topico-522/Caderno%20de%20Par%C3%A2metros%20de%25 |
| | O&M cost of the PV plant, in USD/(kW*year) | 10 | |
| **Batteries** | Capital cost of the battery, in USD/kWh | 150 | https://www.sciencedirect.com/science/article/pii/S2542435119305392?via%3Dihub#mmc2, no material suplementar |

| | | | |
|---|---|---|---|
| | O&M cost of the battery, in USD/(kW*year) | 30 | https://www.sciencedirect.com/science/article/pii/S2542435119305392?via%3Dihub#mmc2, no material suplementar |
| | Running cost of discharging the battery, in USD/(KWh-cycle) | 0.00085 | https://www.sciencedirect.com/science/article/pii/S2542435119305392?via%3Dihub#mmc2, no material suplementar |
| **Hydrogen storage** | Capital cost of the hydrogen storage, in USD/kg | 723 | https://theses.hal.science/tel-03506254/document |
| | O&M cost for storage, percentage | 3% | https://theses.hal.science/tel-03506254/document |
| | Price of initial hydrogen in the storage in USD/kg | 6.5 (average for solar PV) | https://www.iea.org/reports/global-hydrogen-review-2022 |
| **Pipelines and compression stations** | Scale factor for pipelines | 0.9 | https://theses.hal.science/tel-03506254/document |
| | Capital cost for a pipeline known in USD/m | 376 | https://transitionaccelerator.ca/wp-content/uploads/2021/12/Hydrogen-Pipelines-_30Nov2021-PUBLISH-V2.0-1-Dec-2021.pdf |
| | Internal diameter of a pipe known in m | 0.07 | https://transitionaccelerator.ca/wp-content/uploads/2021/12/Hydrogen-Pipelines-_30Nov2021-PUBLISH-V2.0-1-Dec-2021.pdf |
| | O&M cost for pipelines, percentage | 3% | https://transitionaccelerator.ca/wp-content/uploads/2021/12/Hydrogen-Pipelines-_30Nov2021-PUBLISH-V2.0-1-Dec-2021.pdf |
| | life of the pipelines, in years | 50 | https://transitionaccelerator.ca/wp-content/uploads/2021/12/Hydrogen-Pipelines-_30Nov2021-PUBLISH-V2.0-1-Dec-2021.pdf |
| | O&M cost for compression stations, percentage | 3% | https://theses.hal.science/tel-03506254/document |
| | Scale factor for compressors | 0.8 | https://theses.hal.science/tel-03506254/document |
| | Capital cost for a compressor known in USD | 4656000 | https://theses.hal.science/tel-03506254/document |
| | Power of a compressor known in kW | 4000 | https://theses.hal.science/tel-03506254/document |
| **Trucks** | Salary of truck drivers in USD/hour | 10 | - |
| | Capital cost of trucks for $H_2$ transportation, in USD/truck | 736230 | https://theses.hal.science/tel-03506254/document |
| | Price of the fuel (diesel) for transporting hydrogen, in USD/L | 1.11 | https://g1.globo.com/ce/ceara/noticia/2023/02/18/fortaleza-tem-a-gasolina-comum-mais-cara-do-pais-diz-pesquisa-da-anp.ghtml |
| | O&M cost for trucks in percentage of investment | 3% | https://theses.hal.science/tel-03506254/document |
| | Replacement cost of trucks in percantage of investment cost | 30% | - |
| **Technical parameters** | | | |
| **Electrolysis** | Demand of water for the electrolyser (ultrapurewater), in kg/kgH$_2$ | 9 | https://www.eurowater.com/en/hydrogen-production |

| | | | |
|---|---|---|---|
| | DPW 'Demand of cooling water for the electrolyser, in kg/kgH$_2$ | 18 | https://www.eurowater.com/en/hydrogen-production |
| | Lower heating value for H2, in kWh/kg | 33.324 | https://theicct.org/wp-content/uploads/2022/02/fuels-eu-cost-renew-H-produced-onsite-H-refueling-stations-europe-feb22.pdf |
| | Oxygen price, in USD/m$^3$ | 0.13 | https://theicct.org/wp-content/uploads/2022/02/fuels-eu-cost-renew-H-produced-onsite-H-refueling-stations-europe-feb22.pdf |
| | Capacity of electrolyser, in kW | PEM 1000 | https://theicct.org/wp-content/uploads/2022/02/fuels-eu-cost-renew-H-produced-onsite-H-refueling-stations-europe-feb22.pdf |
| | | Alkaline 20000 | |
| | Electrolyser efficicency, regarding LHV | PEM 0.6 | https://theicct.org/wp-content/uploads/2022/02/fuels-eu-cost-renew-H-produced-onsite-H-refueling-stations-europe-feb22.pdf |
| | | Alkaline 0.7 | |
| | Electricity consumption for the compressor for electrolyser, in kWh/kgH | PEM 1.6 | https://www.sciencedirect.com/science/article/pii/S095965261832170X?via%3Dihub |
| | | Alkaline 2.2 | |
| **Batteries** | Round-trip efficiency of the battery | 0.7 | https://www.sciencedirect.com/science/article/pii/S2542435119305392?via%3Dihub#mmc2, no material suplementar |
| | Capacity of the battery, in kWh | 3700 | https://www.ge.com/renewableenergy/sites/default/files/related_documents/Reservoir%20Solutions%20Product%20Specification%20Sheets.pdf |
| | Maximum power of the battery, in kW | 960 | https://www.ge.com/renewableenergy/sites/default/files/related_documents/Reservoir%20Solutions%20Product%20Specification%20Sheets.pdf |
| | Initial state of charge of battery | 100% | - |
| **Hydrogen storage** | Capacity of each unit of storage, in kg | 500 | - |
| | Initial mass of hydrogen in the storage in percentage | 1 | - |
| | Cushion gas, minimum volume of gas to keep pressure | 0.3 | https://www.sciencedirect.com/science/article/abs/pii/B9780444626165000097 |
| **Pipelines and compression stations** | Density of hydrogen at 100 bar, in kg/m$^3$ | 7.8 | https://h2tools.org/hyarc/hydrogen-properties?f%5B0%5D=hydrogen_properties_keywords%3A271 |
| | Viscosity of hydrogen, in Pa*s | 9.1533E-06 | https://h2tools.org/hyarc/hydrogen-data/hydrogen-viscosity-different-temperatures-and-pressures |
| | Roughness of the pipelines, in m | 0.0000178 | https://transitionaccelerator.ca/wp-content/uploads/2021/12/Hydrogen-Pipelines-_30Nov2021-PUBLISH-V2.0-1-Dec-2021.pdf |
| | Initial pressure inside the pipeline that should be maintained, in Pa | 10000000 | https://transitionaccelerator.ca/wp-content/uploads/2021/12/Hydrogen-Pipelines-_30Nov2021-PUBLISH-V2.0-1-Dec-2021.pdf |
| | Minimum pressure inside pipelines, in Pa | 7000000 | https://transitionaccelerator.ca/wp-content/uploads/2021/12/Hydrogen-Pipelines-_30Nov2021-PUBLISH-V2.0-1-Dec-2021.pdf |
| | Diameter of the pipe, in in | A 3.0 | https://www.octalsteel.com/steel-pipe-dimensions-sizes |
| | | B 3.5 | https://www.octalsteel.com/steel-pipe-dimensions-sizes |
| | | C 4.0 | https://www.octalsteel.com/steel-pipe-dimensions-sizes |

| | | | |
|---|---|---|---|
| | | D 5.0 | https://www.octalsteel.com/steel-pipe-dimensions-sizes |
| | | E 6.0 | https://www.octalsteel.com/steel-pipe-dimensions-sizes |
| | | A 0.00549 | https://www.octalsteel.com/steel-pipe-dimensions-sizes |
| | | B 0.00574 | https://www.octalsteel.com/steel-pipe-dimensions-sizes |
| | Thickness of the pipe, in m | C 0.00602 | https://www.octalsteel.com/steel-pipe-dimensions-sizes |
| | | D 0.00655 | https://www.octalsteel.com/steel-pipe-dimensions-sizes |
| | | E 0.00711 | https://www.octalsteel.com/steel-pipe-dimensions-sizes |
| | Compressibility factor, dimensionless | 1.027 | https://transitionaccelerator.ca/wp-content/uploads/2021/12/Hydrogen-Pipelines-_30Nov2021-PUBLISH-V2.0-1-Dec-2021.pdf |
| | Gases constant, in kJ/(kg*K) | 4.12 | https://transitionaccelerator.ca/wp-content/uploads/2021/12/Hydrogen-Pipelines-_30Nov2021-PUBLISH-V2.0-1-Dec-2021.pdf |
| | Inlet temperature, in K | 293 | - |
| | Number of stages of compression | 3 | https://transitionaccelerator.ca/wp-content/uploads/2021/12/Hydrogen-Pipelines-_30Nov2021-PUBLISH-V2.0-1-Dec-2021.pdf |
| | Isentropic efficiency of compression | 0.8 | https://transitionaccelerator.ca/wp-content/uploads/2021/12/Hydrogen-Pipelines-_30Nov2021-PUBLISH-V2.0-1-Dec-2021.pdf |
| | Ratio of specific heats | 1.41 | https://transitionaccelerator.ca/wp-content/uploads/2021/12/Hydrogen-Pipelines-_30Nov2021-PUBLISH-V2.0-1-Dec-2021.pdf |
| | Efficiency of the compression stations | 0.95 | https://transitionaccelerator.ca/wp-content/uploads/2021/12/Hydrogen-Pipelines-_30Nov2021-PUBLISH-V2.0-1-Dec-2021.pdf |
| **Trucks** | Time for loading and unloading the truck, in hours | 1 | https://theses.hal.science/tel-03506254/document |
| | Average Speed for the truck, in km/h | 60 | - |
| | Capacity of the truck in kgH$_2$ per travel | 885 | https://theses.hal.science/tel-03506254/document |
| | Fuel consumption (diesel) for trucks transporting hydrogen in km/L | 2.86 | https://www.epe.gov.br/sites-pt/publicacoes-dados-abertos/publicacoes/PublicacoesArquivos/publicacao-626/IEA-EPE_Brazilian_Road_Freight_Transport_Benchmarking-2021.09.09%20[PT].pdf |
| | Capacity factor of trucks | 90% | https://theses.hal.science/tel-03506254/document |
| | Maximum distance for replacement of engine/truck in km | 500000 | - |
| | Average emission factor of diesel, in kgCO$_2$/L | 2.70 | https://www.epa.gov/sites/default/files/2018-03/documents/emission-factors_mar_2018_0.pdf |
| **Solar PV** | Data for hourly solar PV generation | Hourly data | System Advisor Model (SAM) - https://sam.nrel.gov/ |

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