Economic Optimization of the Hydrogen Demand in a Hard-To-Abate Industrial Sector

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***Abstract*—Hydrogen is a zero-emission fuel that, if produced from renewable sources (so-called green hydrogen), can provide a significant contribution in the decarbonization of several sectors. The main drawback that still hinders its deployment is its high cost, as well as critical operational issues related to the entire supply chain, both for safety and efficiency reasons. Incentives and certification schemes are needed to support the green hydrogen. In this paper, with the aim to identify the green hydrogen supply chain and associated costs, an energy hub with electricity and hydrogen demands has been studied comparing the centralized green hydrogen production and distribution via trucks, against the installation of an on-site green hydrogen production plant made up of renewable power generation, an electricity storage system, and an electrolyzer. The problem was modeled and solved as a MILP optimization in MATLAB environment. Furthermore, a sensitivity analysis on the cost was carried out, which showed that even if the truck transportation cost for hydrogen is set at 0 €/kg, it is still more cost-effective to install an on-site electrolyzer to produce the required hydrogen.**

Keywords — Green hydrogen, energy hub, optimization, decarbonization

I. INTRODUCTION

The energy transition, i.e. the shift from fossil fuels to renewable energy sources, is vital to combat climate change. According to data provided by scientists at NASA's Goddard Institute for Space Studies (GISS) in [1] and shown in Fig. 1, the average global temperature in 2020 was 1.02°C (1.84° F) higher than it was in the period 1951-1980 (the U.S. National Weather Service uses a three-decade period to define "normal" or average temperature).

Such temperature increase is due mainly to the use of fossil fuels whose use has increased by 5 percent per year in the postwar period [2]. This has caused and continues to cause melting of glaciers, rise of sea levels, desertification, and increased extreme phenomena including hurricanes, floods, and wildfires.

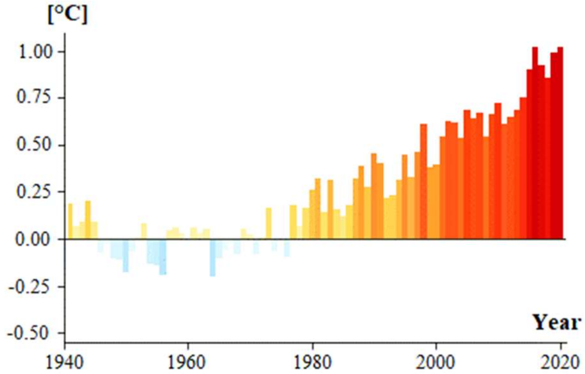

Fig. 1. Trend of global average temperature increase compared to the 1951-1980 average [1]

In this context, hydrogen, along with renewable sources, can play a key role. In detail, hydrogen can be used as an alternative fuel in the chemical and steel industries, where it is necessary to reach high temperatures that cannot be achieved through electrification, or in the heavy transport sector, where the generation of electricity directly on board the vehicle, via hydrogen-fueled fuel cells, allows for a number

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of advantages over the use of Battery Electric Vehicles, such as longer travel range and shorter refueling time [3].

In addition to being used as a fuel, hydrogen can also be used as a chemical process element, such as instead of coke in iron oxide reduction reactions for the production of pig iron. The strengths of hydrogen are:

- high mass energy density (120 MJ/kg) [4];
- great availability (hydrogen is the most abundant element in the universe);
- its combustion produces no CO_2 or other greenhouse gas emissions, but simply water ($2H_2 + O_2 \rightarrow 2H_2O$).

On the other hand, however, some critical issues along the supply chain of this fuel are briefly discussed in Section II.

In the present paper, an optimization study for the proposal of the integration of hydrogen for the decarbonization of industrial final users is described. In detail, Section III illustrates the Mixed-Integer Linear Programming (MILP) energy hub model developed for the economic optimization of hydrogen production and supply, aimed at evaluating the convenience of producing the hydrogen on-site, via an electrolyzer, or purchasing it and transporting it via tank trucks. Section IV illustrates the results of the simulations developed for a base case and a sensitivity analysis of the most critical parameters while Section V discusses the results and shows the main conclusions.

II. HYDROGEN-RELATED ISSUES

A. *Hydrogen Production*

Hydrogen, while the most abundant element in the universe, is not a primary source but must be produced by consuming energy because it is found bound to other elements.

Hydrogen is commonly extracted from fossil fuels by hydrocarbon reforming, which is divided into three categories: steam reforming, partial oxidation, and autothermal reforming [5]. Among them, steam methane reforming is the most developed and widely used technology in industry [6]. Its advantages are the high efficiency (about 70-85% for process on an industrial scale) and the low operational and production costs. The disadvantage is the high production of CO2, that is around 7.05 kg CO_2/kg H_2 [7].

The only truly sustainable type of hydrogen, with almost no impact on the environment, is the green hydrogen, which is produced from renewable electricity used to power electrolyzers that break down the water molecule into hydrogen and oxygen.

The main drawback of this process is the high cost, which is why about 96% of hydrogen is still globally produced from fossil sources, while hydrogen produced from renewable sources by electrolysis constitutes only 0.04% of world production [8].

There are many reasons for the high costs. Despite the great progress achieved by this technology in recent years, in fact, the process itself still faces some inherent limitations. The first is the need for a minimum thermodynamic potential difference of 1.23 V; the latter value must still be exceeded to overcome the kinetic dissipations. Another big limitation is the need to operate with distilled water, free of impurities or salts. Finally, some electrolyzers' technologies rely on catalysts made of precious metals, such as platinum and iridium.

A different approach recently proposed in [9] is the use of biocatalysts, i.e., natural enzymes such as bacterial hydrogenase, which can offer negligible overpotential, high specificity and complete biodegradability. On paper, enzymes can catalyze high-throughput chemical reactions in a scalable and cost-effective manner. Research is also moving forward to try to produce hydrogen using seawater directly and not necessarily distilled water [10]. Another possible form of renewable hydrogen is that obtained by gasification of biomass; these, when preheated, produce coal with a high carbon content through which synthesis gas is produced, providing further heat, until temperatures reach about 800°C. Hydrogen is then extracted from this gas by means of a water-gas-shift reaction, similar to what happens in hydrogen production by steam methane reforming. Again, therefore, considerable amounts of heat must be provided, with a thermal efficiency between 35 and 50%, thus much lower than the efficiency of methane reforming, which can be as high as 85%, as written earlier. In addition, biomass has a fairly modest calorific value, which implies the need to use large-volume plants [5].

To ensure stability in the supply of hydrogen, however, it would be better not to rely on a single production technology, but to create a mix of sources that combine the advantages of the various technologies while reducing the environmental impact as much as possible.

In [11], for example, an integrated system is proposed that combines electrolysis with biomass gasification and methane reforming. In this way, the oxygen produced during electrolysis can be used to make gasification and reforming while also the heat produced from the gases obtained from biomass is used to provide thermal energy for methane reforming. With this system, an increase in efficiency of almost 10% has been estimated compared to the value when hydrogen is produced using only one form of energy, with a reduction in carbon emissions of about 67%.

B. *Hydrogen Storage And Transportation*

While hydrogen has a good energy density by weight, it also has a low density in terms of energy per unit volume, which is why, in order to facilitate its transport and storage, its physical state must be altered by resorting to one of the following processes: compression, liquefaction, physical or chemical storage in hydrides [4].

The simplest and cheapest way to store hydrogen is under the form of compressed gas, avoiding the costs and evaporation losses of liquefaction, the conversion losses of synthetic fuels such as ethanol, and the technological immaturity of hydrogen carriers such as hydrides [12]. In particular, liquefaction would require a huge expenditure of energy, as hydrogen would need to be brought to -253°C, requiring special tanks. As written earlier, evaporation of liquid hydrogen is also a factor to be considered: according to the study conducted in [13] , evaporation from cryogenic tanks is estimated at about 0.4% per day; this means that after 4 months the energy content carried would be halved. This would result in the inability to make the best use of hydrogen as a form of seasonal storage of renewable electricity.

Also important is the pressure to which the hydrogen gas is brought. For hydrogen vehicles, for example, the gas must be compressed to very high pressures to reduce the space occupied by the tanks on board the vehicle and thus enable FCEVs (Fuel Cell Electric Vehicles) to achieve characteristics similar to those of conventional vehicles. Buses currently use hydrogen at 350 bar as they have more on-board storage space, but most passenger cars use 700 bar [12].

Once compressed, hydrogen can be transported via pipelines or through tank trucks. However, the pipelines must be made of a particularly strong structure that does not allow the hydrogen molecules, which are very small and very light, to "escape" (remember, in fact, that hydrogen is the first element in the periodic table and is, therefore, the lightest). In addition, due to the low molar mass of hydrogen and the higher volumetric flow, about 3 times more compression power is required to transport pure hydrogen than in normal methane pipelines in order to achieve the same capacity in terms of energy flow [13].

Road transportation, on the other hand, which can also be done for fuel in liquid form, requires 8 kg of hydrogen per 100 km if zero environmental impact is to be achieved on transportation using a fuel cell truck, or 270 kWh of electricity [13].

III. ENERGY HUB WITH HYDROGEN MODELLING

An energy hub is a centralized unit in which different forms of energy are transformed, converted and stored; thus, an energy hub represents the coupling of flows on different networks (gas/electricity/heat) with the aim of achieving a number of benefits.

First, reliability of supply can be increased because it is no longer completely dependent on a single grid. Second, such a system allows for supply optimization; energy carriers offered at the hub entrance can be characterized according to their cost, relative emissions, availability, and other criteria [14]. Another advantage is to facilitate the integration of renewable energy sources through storage and conversion systems, reducing the risk of grid congestion and energy losses [15].

The energy hub model studied in this paper is shown below, in Fig.2.

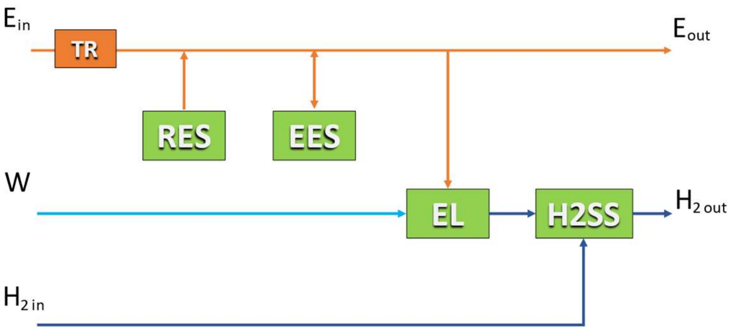

Fig. 2. Energy hub model of the case study

Inputs to the system are electricity from the grid (E_{in}), water needed to power the electrolyzer (W), and hydrogen transported by road via tank trucks ($H_{2\,in}$).

System's outputs are the demands for electricity (E_{out}) and hydrogen ($H_{2\,out}$).

Within the hub, there are five components, i.e. the transformer interfacing the industry to the main grid and the four components to be sized in the optimization process, namely a renewable energy source (RES) generation plant, an electric energy storage system (EES), an electrolyzer (EL), and a hydrogen storage system (H2SS).

A linear optimization algorithm based on mass balance equations and energy flows was developed for such an energy hub in the MATLAB environment, according to an approach similar to previous works of some of the authors [16], [17].

The aim of the model is to minimize costs and evaluate, therefore, the convenience of relying on an external hydrogen supply carried by truck against the local green hydrogen production through the installation of the various necessary components and determining the relative sizes.

The objective function of the optimization problem, namely the annual cost function, is shown in Eq. (1). The latter was written assuming that the demands of the industrial facility are constant over the year and well represented by the standard day assessed in this study.

$$365\,[\,C_{opex,E}\,E_{in}(t) + C_{opex,W}\,W(t) + C_{opex,H2}\,H_{2\,in}(t)\,] + C_{capex,RES}\,CRF_{RES}\,S_{RES} + C_{capex,EES}\,CRF_{EES}\,S_{EES} + C_{capex,EL}\,CRF_{EL}\,S_{EL} + C_{capex,H2SS}\,CRF_{H2SS}\,S_{H2SS} + z_{RES}\,C_{capex,RES(0)}\,CRF_{RES} + z_{EES}\,C_{capex,EES(0)}\,CRF_{EES} + z_{EL}\,C_{capex,EL(0)}\,CRF_{EL} + z_{H2SS}\,C_{capex,H2SS(0)}\,CRF_{H2SS} \tag{1}$$

The equality and inequality constraints for the optimization problem, are illustrated here below. Eq. (2) is the electricity flows balance equation, Eq. (3) is the EES balance equation, and Eq. (4) is the H2SS balance equation.

$$E_{in}(t)\,K_{TR} - E_{EES,ch}(t) + E_{EES,disch}(t) - E_{EL}(t) + E_{RES}(t) = E_{out}(t) \qquad \forall t \in T \tag{2}$$

where $K_{TR} = 0.99$ [18] is the transformer efficiency, $E_{EES,ch}(t)$ and $E_{EES,disch}(t)$ are respectively the electricity flows during the charge and discharge phases of the electrical storage, $E_{EL}(t)$ is the energy absorbed by the electrolyzer and $E_{RES}(t)$ is the energy coming from the renewable source plant;

$$SOC_{EES}(t+1) - SOC_{EES}(t)\cdot(1 - E_{EES,loss}) - E_{EES,ch}(t+1)\cdot K_{EES,ch} + E_{EES,disch}(t+1) / K_{EES,disch} = 0 \qquad \forall t \in T \tag{3}$$

in which SOC_{EES} is the state of charge of the electric energy storage system, $E_{EES,loss} = 0.01$ [17] is a coefficient that takes into account the losses, $K_{EES,ch}$ and $K_{EES,dich}$ are respectively the charge and discharge efficiencies of EES and are equal to 0.97 [18];

$$SOC_{H2SS}(t+1) - SOC_{H2SS}(t)\cdot(1 - H_{2\,SS,loss}) - [E_{EL}(t+1)\cdot K_{EL\;eh2} + H_{2\,in}(t+1)]\cdot K_{SS,ch} + H_{2\,out}(t+1) / K_{SS,disch} = 0 \qquad \forall t \in T \tag{4}$$

where SOC_{H2SS} is the state of charge of the hydrogen storage system, $H_{2SS,loss} = 0.02$ [17] is a coefficient that takes into account the losses, $K_{SS,ch}$ and $K_{SS,dich}$ are respectively the charge and discharge efficiencies of H2SS and are equal to 1 [17].

In this study, a photovoltaic system is considered as a renewable energy source, so it is necessary to write Eq. (5) for the photovoltaic production:

$$E_{RES}(t) - A_{PV} \cdot K_{PV} \cdot I_{sun}(t) \cdot S_{RES}/S_{PVm} = 0 \tag{5}$$

where $A_{PV} = 1.64$ m^2 is the PV module surface area, $K_{PV} = 0.16$ is the PV radiation to electricity efficiency, I_{sun} is the solar irradiance of the selected location, whose data were gathered from the PV-GIS online database, and S_{RES} is the size of photovoltaic plant; $S_{PVm} = 0.4$ kW is the rated power of the individual photovoltaic module.

$$SOC_{EES}(1) - SOC_{EES}(T) = 0 \tag{6}$$

$$SOC_{H2SS}(1) - SOC_{H2SS}(T) = 0 \tag{7}$$

The equations (6) and (7) are used to equalize the state of charge of the storages of the first and last hour of the time interval considered, in order to let the system repeat the cycling every day.

In addition to the equations just seen, inequality constraints have also been written for the various components, starting with the electrical energy storage system for which the following inequalities are valid:

$$E_{EES,ch}(t) \leq \delta_{EES,ch}(t) \cdot Q \tag{8}$$

$$E_{EES,disch}(t) \leq \delta_{EES,disch}(t) \cdot Q \tag{9}$$

$$\delta_{EES,ch}(t) + \delta_{EES,disch}(t) \leq 1 \tag{10}$$

$$DoD_{EES} \cdot S_{EES} \leq SOC_{EES}(t) \tag{11}$$

$$SOC_{EES}(t) \leq S_{EES} \tag{12}$$

$$E_{EES,ch}(t) \leq S_{EES} \cdot (1 - DoD_{EES}) \tag{13}$$

$$E_{EES,disch}(t) \leq S_{EES} \cdot (1 - DoD_{EES}) \tag{14}$$

where $\delta_{EES,ch}(t)$ and $\delta_{EES,disch}(t)$ are boolean variables, Q is a very large number that is used to give an upper limit to the energy that can be charged or discharged, while $DoD_{EES} = 0.2$ [18] and S_{EES} are the depth of discharge and the size of the storage system, respectively.

Similar inequalities have been written for hydrogen storage:

$$E_{EL}(t) \cdot K_{EL\ eh2} + H_{2\ in}(t) \leq \delta_{TK,ch}(t) \cdot Q \tag{15}$$

$$H_{2\ out}(t) \leq \delta_{TK,disch}(t) \cdot Q \tag{16}$$

$$SOC_{H2SS}(t) \leq S_{H2SS} \tag{17}$$

$$DoD_{H2}\ S_{H2SS} \leq SOC_{H2SS}(t) \tag{18}$$

$$E_{EL}(t) \cdot K_{EL\ eh2} + H_{2\ in}(t) \leq S_{H2SS}\ (1\text{-}DoD_{H2SS}) \tag{19}$$

$$H_{2\ out}(t) \leq S_{H2SS}\ (1\text{-}DoD_{H2SS}) \tag{20}$$

in which, also in this case, $\delta_{TK,ch}(t)$ and $\delta_{TK,disch}(t)$ are boolean variables, $DoD_{H2SS} = 0.1$ is the depth of discharge of the hydrogen storage system and S_{H2SS} is its size.

The following inequality capacity constraints were added:

$$E_{EL}(t) \leq S_{EL} \tag{21}$$

$$E_{RES}(t) \leq S_{RES} \tag{22}$$

$$S_{EES} \leq z_{EES} \cdot Q \tag{23}$$

$$S_{H2SS} \leq z_{H2SS} \cdot Q \tag{24}$$

$$S_{EL} \leq z_{EL} \cdot Q \tag{25}$$

$$S_{RES} \leq z_{RES} \cdot Q \tag{26}$$

where S_{EL} and S_{RES} are the sizes of the electrolyzer and renewable power generation plant, while the various z are Boolean variables that will take value 0 if it is not convenient to install the relevant component, 1 if it is.

As a result, the optimization variables are collected in the vector $\boldsymbol{x}$ whose entries are both real values and Boolean values.

$$\boldsymbol{x} = [E_{in}(t), E_{EES,ch}(t), E_{EES,disch}(t), E_{EL}(t), E_{RES}(t), H_{2\,in}(t), SOC_{EES}(t), SOC_{H2SS}(t), \delta_{EES,ch}(t), \delta_{EES,disch}(t), \delta_{TK,ch}(t), \delta_{TK,disch}(t), S_{EES}, S_{H2SS}, S_{EL}, S_{RES}, z_{EES}, z_{H2SS}, z_{EL}, z_{RES}] \tag{27}$$

All equations and inequalities in the model were written in matrix form in the MATLAB script, and two vectors containing lower and upper bounds were defined for the different variables in the problem; in particular, the lower bounds were set equal to 0, and the upper bounds equal to infinity, except for the Boolean variables for which, of course, the upper bound is unit.

A vector was also written containing the coefficients of the function to be minimized, namely, the cost function. The values of the coefficients are given in TABLE I:

TABLE I. COEFFICIENTS OF THE COST FUNCTION

Coefficient	Meaning	Value	Unit Of Measure
$C_{opex,\,E}$	Electricity cost	0.32	€/kWh
$C_{opex,\,W}$	Water cost	4.16 [19]	€/m^3
$C_{opex,\,H2}$	Cost of purchased hydrogen	12.89	€/kg
$C_{capex,\,RES}$	Term of the Investment cost for RES depending on the size	786.59 [20]	€/kW
$C_{capex,\,RES(0)}$	Term of the Investment cost for RES independent of the size	0	€
CRF_{RES}	Capital Recovery Factor of the investment for RES	7.24%	
$C_{capex,\,EES}$	Term of the Investment cost for EES depending on the size	1200	€/kWh
$C_{capex,\,EES(0)}$	Term of the Investment cost for EES independent of the size	0	€
CRF_{EES}	Capital Recovery Factor of the investment for EES	13.08%	
$C_{capex,\,EL}$	Term of the Investment cost for EL depending on the size	666.14	€/kW
$C_{capex,\,EL(0)}$	Term of the Investment cost for EL independent of the size	5000000	€
CRF_{EL}	Capital Recovery Factor of the investment for EL	9.76%	
$C_{capex,\,H2SS}$	Term of the Investment cost for H2SS depending on the size	171.33	€/kgH2
$C_{capex,\,H2SS(0)}$	Term of the Investment cost for H2SS independent of the size	716859	€
CRF_{H2SS}	Capital Recovery Factor of the investment for H2SS	11.41%	

For the electricity price, the average value for 2022 in Italy was calculated from the six-month values provided in the eurostat database in [21].

The cost of purchased hydrogen was calculated by summing green hydrogen production price in Italy, compression cost and transportation cost, respectively equal to

- 8 €/kg [22]
- 1-1.5 $/kg [23]
- 1.8 $/kg [24]

by making the appropriate dollar-euro conversions, considering the average value of 1.25 \$/kg for the compression cost, and increasing the total by 20 percent to account for the profit for the hydrogen distributor.

The various CRF terms, on the other hand, are the Capital Recovery Factors of the investment, i.e., coefficients that are used to allocate investments on an annual basis, and were calculated, for each component, according to Eq. (28):

$$\mathrm{CRF}=i\cdot(1+i)^{\wedge}n/[(1+i)^{\wedge}n-1] \tag{28}$$

where i is the interest rate, assumed to be 5.2% for Electricity Distribution and Metering [25], and n is the lifetime of the individual components.

The terms of investment C_{capex} and $C_{capex(0)}$ shown in TABLE I for each component were derived from a linear regression conducted on average market values.

For this study, an electricity hourly demand of 500 MWh and a hydrogen demand of 7212.33 kg/h were considered as energy hub outputs. The latter was calculated by considering an Italian company's annual steel production of 1,018,211 tons [26], which was divided by 300 operating days (a value chosen to take into account plant downtime for maintenance) and by 24 in order to trace the hourly production.

The value obtained was then multiplied by 51 because about 51 kg of hydrogen is needed to produce one ton of steel [27]. Power and hydrogen demands were assumed constant over time.

IV. RESULTS

A. *Reference Case*

The results obtained from solving the optimization problem in MATLAB for the energy hub model described above, assuming a 24-hour time step to simulate a typical day, are summarized in the following graphs and TABLE II.

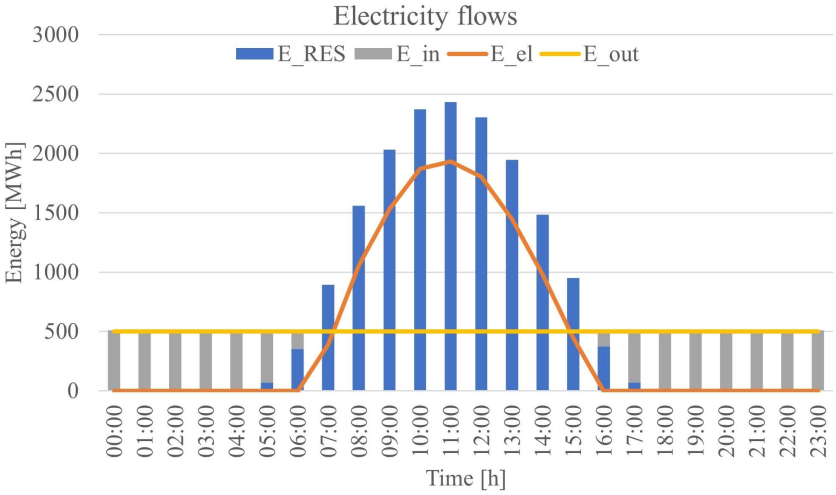

Fig. 3. Electricity flows in the reference case

As can be seen in Fig. 3, electricity demand is fully met by the grid from midnight until 5 a.m., when the PV system starts producing. From 7 a.m. to 3 p.m., the renewable electricity is used both to meet electricity demand and for on-site production of green hydrogen, which follows the production curve of the PV plant. From 4 p.m. onward it will again be necessary to purchase energy from the grid.

The results of the optimization problem do not include the presence of electrical storage.

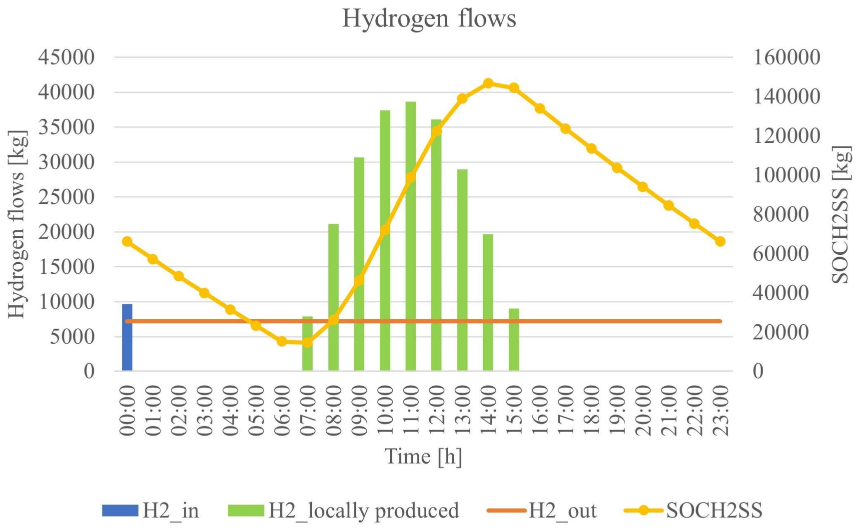

Fig. 4. Hydrogen flows in the reference case

As for the demand for hydrogen, in order to meet it, it is necessary to purchase hydrogen transported by tanks for only one hour per day (Fig. 4). Almost all the demand is covered by the green hydrogen produced on-site by the electrolyzer powered by the PV plant.

The excess production that occurs from 7 a.m. to 3 p.m. is, in fact, accumulated in the tank, which begins to empty soon afterwards covering the hydrogen demand during the hours when there is neither local production nor hydrogen purchase and transportation.

TABLE II. SIZES OF COMPONENTS

Component	Size	Unit Of Measure
RES	4713.50	MW
EES	0	kWh
EL	1932.85	MW
H2SS	146667	kg

The minimum value found for the annual cost function is 1.084 billion euros.

By setting 0 as the upper limit for H_{2in} (t), so as to consider the case where all the hydrogen needed to meet demand is produced on-site through the electrolyzer, the annual cost becomes 1.094 billion euros; however, if 0 is set as the upper limit for E_{EL} (t), so as to consider the case where all the hydrogen needed to meet demand is purchased and transported on road, the cost rises to 1.66 billions.

B. *Sensitivity Analysis*

Relative to hydrogen flows, the factors influencing the optimization results are the cost of imported hydrogen and demand. Leaving the latter unchanged and gradually increasing the cost of hydrogen to be transported locally, starting at 0 €/kg, it was seen that even setting the cost of imported hydrogen equal to zero, the solution to the optimization problem still involves installing the electrolyzer, even if it only produces for five hours a day (Fig. 5). In this case, it is as if the electrolyzer replaces electric storage, the installation of which continues to be uneconomical.

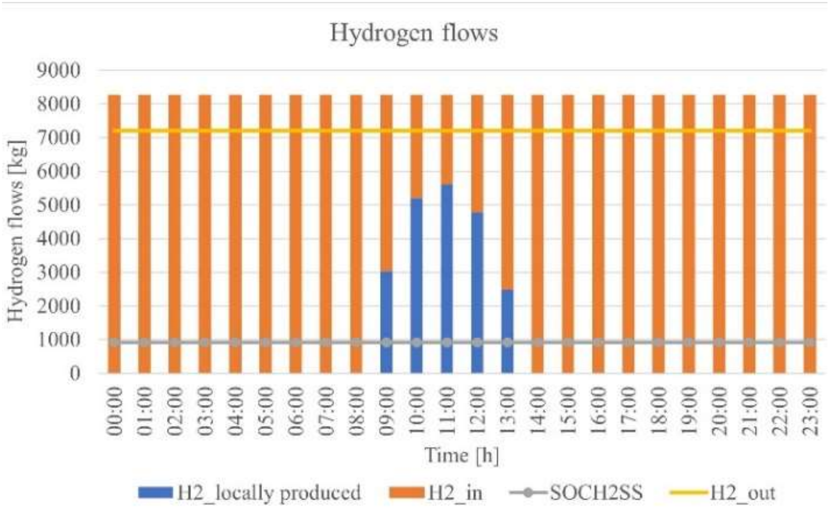

Fig. 5. Hydrogen flows for cost of imported hydrogen equal to 0 €/kg

In this limiting case, where the cost of hydrogen transported is zero, the costs are distributed according to the breakdown shown in Fig. 6, totalling 0.85 billion euros.

In particular, the consumption of electricity purchased from the grid accounts for 88% of annual costs, the photovoltaic system for 10%, and the electrolyzer for 2%, while water consumption for the electrolyzer and hydrogen storage have a negligible impact.

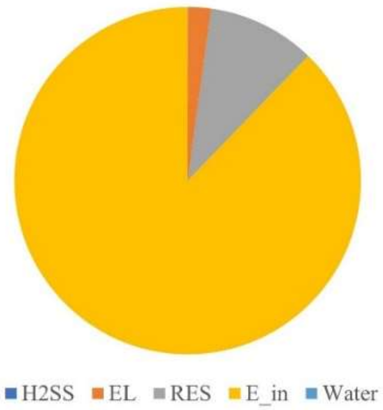

Fig. 6. Allocation of annual costs in the limiting case with cost of transported hydrogen equal to 0 €/kg

V. CONCLUSIONS

Decarbonization of so-called hard-to-abate sectors, such as the chemical and steel industries, is a hot topic in the fight against climate change. Green hydrogen can be of great help in achieving this goal, but its cost hinders its deployment. A hydrogen demand optimization work in an industrial energy hub for steel production was described in this paper. In particular, the cost-effectiveness of on-site production of the required hydrogen versus its purchase and transport by tanker was determined, finally performing a sensitivity analysis on the costs of transported hydrogen. The results showed that the installation of an electrolyzer for on-site production of hydrogen is always cost-effective, even in the ideal case of zero cost of imported hydrogen.

Further work on this topic will be directed toward evaluating other scenarios, with different means of hydrogen transport (pipelines, ammonia, hydrides etc.) and with different types of renewable energy for on-site production. Emission optimization through a multi-objective approach will also be evaluated.

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