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Exploring the Role of Hydrogen to Achieve the Italian Decarbonization Targets Using an Open-Source Energy System Optimization Model

A. Balbo, G. Colucci, M. Nicoli, L. Savoldi

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***Abstract*—**Hydrogen is expected to become an undisputed player in the ecological transition throughout the next decades. The decarbonization potential offered by this energy vector provides various opportunities for the so-called "hard-to-abate" sectors, including industrial production of iron and steel, glass, refineries and the heavy-duty transport. In this regard, Italy, in the framework of decarbonization plans for the whole European Union, has been considering a wider use of hydrogen to provide an alternative to fossil fuels in hard-to-abate sectors. This work aims to assess and compare different options concerning the pathway to be followed in the development of the future Italian energy system in order to meet decarbonization targets as established by the Paris Agreement and by the European Green Deal, and to infer a techno-economic analysis of the required asset alternatives to be used in that perspective. To accomplish this objective, the Energy System Optimization Model TEMOA-Italy is used, based on the open-source platform TEMOA and developed at PoliTo as a tool to be used for technology assessment and energy scenario analysis. The adopted assessment strategy includes two different scenarios to be compared with a business-as-usual one, which considers the application of current policies in a time horizon up to 2050. The studied scenarios are based on the up-to-date hydrogen-related targets and planned investments included in the National Hydrogen Strategy and in the Italian National Recovery and Resilience Plan, with the purpose of providing a critical assessment of what they propose. One scenario imposes decarbonization objectives for the years 2030, 2040 and 2050, without any other specific target. The second one (inspired to the national objectives on the development of the sector) promotes the deployment of the hydrogen value-chain. These scenarios provide feedback about the applications hydrogen could have in the Italian energy system, including transport, industry and synfuels production. Furthermore, the decarbonization scenario where hydrogen production is not imposed, will make use of this energy vector as well, showing the necessity of its exploitation in order to meet pledged targets by 2050. The distance of the planned policies from the optimal conditions for the achievement of Italian objectives is clarified, revealing possible improvements of various steps of the decarbonization pathway, which seems to have as a fundamental element Carbon Capture and Utilization technologies for its accomplishment. In line with the European Commission open science guidelines, the transparency and the robustness of the presented results are ensured by the adoption of the open-source open-data model such as the TEMOA-Italy.

***Keywords*—**Decarbonization, energy system optimization models, hydrogen, open-source modeling, TEMOA.

ACRONYMS

AR6	Sixth Assessment Report
BAU	Business As Usual
CapEx	Capital Expenditure
CCUS	Carbon Capture Utilization and Storage
CHP	Combined Heat and Power
DRI	Direct Reduced Iron
ESOM	Energy System Optimization Model
ESR	Effort Sharing Regulation
ETS	Emissions Trading System
GDP	Gross Domestic Product
GHG	Green House Gas
IPCC	Intergovernmental Panel on Climate Change
MAHTEP	Modeling of Advanced Heat Transfer and Energy Problems
NGA	Natural Gas
LCV	Light Commercial Vehicle
LTS	Long Term Strategy (for GHG emissions reductions in Italy)
LULUCF	Land Use, Land Use Change and Forestry
OF	Objective Function
PA	Paris Agreement
PJ	Petajoule
PNIEC	National Integrated Plan for Energy and Climate
PNRR	National Recovery and Resilience Plan
RES	Reference Energy System
TEMOA	Tools for Energy Model Optimization and Analysis
WEM	World Energy Model

I. INTRODUCTION

HYDROGEN represents a promising energy vector for the decarbonization of each country's energy system, and the objectives that Europe imposes for its share are ambitious and wide. Nevertheless, the path to be travelled is still long and not as straightforward as it could seem. In fact, at the European level, hydrogen (in the following also "H_2") covers less than 2% of energy consumption with a demand of 8.4 million tons per year, being mainly used in refineries (49%), ammonia (31%) and methanol (5%) production [1]. On the other hand, it is produced almost completely from steam methane reforming processes accounting for a total amount of 10.5 million tons per year [1]. Nevertheless, the possible uses of this energy vector spread extensively beyond the current exploitation, covering a wide range of different purposes and sectors. Among these, it can be used directly in electrolytic cells, especially for heavy transport and non-road categories, it can be exploited for long-term energy storage and carrier or for high temperature industrial production processes and several other purposes

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including residential and commercial heat and power production and electricity generation [2]. However, even though positive signals are coming from worldwide and European H_2 applications, current pace in its value-chain development is not sufficient to be on track for meeting net zero emissions targets in 2050 [3]. Specifically, H_2 demand is estimated [4] to reach up to 115 million tons by 2030 from the current 94 million tons world-based value (in 2021), but with barely 2 million tons employed for new uses. In comparison, to simply meet currently announced pledges that amount should grow up to 130 million tons by 2030, with a 25% coming from new uses, and to meet decarbonization targets in 2050 this should be additionally raised up to 200 million tons by 2030 [4]. Italy is the fifth country in Europe for hydrogen consumption, with a current demand of about 0.6 million tons per year, 70% of which is destined to refinery, and the remaining to chemical production. The amount of resource needed for refineries and ammonia production is in total 0.51 million tons per year and is currently satisfied through grey hydrogen supply. In order to replace only this amount with low-carbon H_2, the additional renewable source required would be of about 104 PJ [1], corresponding to 22% more than solar resource consumed to produce electricity in Italy in 2020 [5]. Moreover, a possible refurbishment with the addition of carbon capture technologies for fossil fuel produced H_2 would imply new possibilities for the production of synfuels and lower carbon intensity propellants [6], but also significant reductions in the efficiency of hydrogen synthesis and a cost for prevented CO_2 emissions of about 100-111€ per ton of carbon dioxide, depending on the capturing efficiency, with a CO_2 cost of 90€ per ton on the ETS market (in 2022) [1]. Furthermore, in the case of green H_2, the prevented carbon dioxide cost would grow to an unbearable 900€ per ton [1].

Among the alternative tools available for the study of the future energy mix, ESOMs aim to evaluate the optimal configuration of the modeled energy system, usually according to an economic optimization paradigm, which in the current formulation corresponds to the minimization of the total cost of the system. Their usefulness lies in the technologically explicit description of the system which allows to provide an exhaustive set of technological alternatives among which the model can choose in order to fit the best configuration for the required constraints. Moreover, the possibility to compare results corresponding to different scenarios is provided by simple modification of the input database for the addition or removal of constraints or parameters, allowing a complete control on the model.

Aim of the Work

The purpose of this paper is to assess the decarbonization potential hydrogen can have in the Italian energy system, along with the possible extent of its deployment in the same framework in the perspective of meeting decarbonization targets imposed by the Paris Agreement and with the path established by the more recent Green Deal and its included law-binding document, Fit for 55 [7]. The decarbonization potential of hydrogen was estimated implementing a multi-scenario analysis using an open-source bottom-up ESOM, namely, the existing TEMOA-Italy model [8], [9].

II. Hydrogen Module

The hydrogen module was implemented in the existing TEMOA-Italy, in order to accomplish the objectives of the study. This procedure followed the four steps of the H_2 value-chain represented inFig. 1: production, storage, delivery and consumption. The implementation phase of the production side followed a logic of size definition and location detail. This means that different plant sizes are distinguished in small, medium and large. This distinction is implemented with different costs and lifetimes, in order to realistically represent the possible infrastructure to be chosen by the optimization process. Furthermore, the location of the plant has been identified with two different possibilities, namely: centralized and decentralized. This associates or neglects, respectively, transportation-related costs and commodities consumption for H_2 dispatchment, increasing the variability of possible combinations for H_2 production configuration at system scale.

It is relevant to underline that blue hydrogen production technologies, hence, deriving from fossil fuels production coupled with carbon capture technologies, are formally implemented in the model in another module, called CCUS, (Carbon Capture Utilization and Storage), and described in the following paragraph. This one contains a duplication of H_2 production technologies through fossil fuels, namely, grey hydrogen production technologies, which are associated with capture technologies, in such a way that their activities are tied together. The blue-hydrogen production technologies have different costs, efficiency and in general a different set of techno-economic parameters according to the existing or under development technologies.

Note that the model has not the possibility to retrofit or refurbish existing grey-hydrogen production plants (or any other) with the integration of carbon capture technologies, transforming them into blue hydrogen production facilities. It can only install brand new blue (or grey, as green, namely, low-carbon) hydrogen production plants. Clearly, this is a noticeable simplification when studying H_2 development in general, since the costs associated to new installations compared to refurbishing ones have a much different impact on sector economy and refurbishing strategies implementation could be one of the next future refinements of the current model. Nevertheless, being the model optimized with a perfect foresight approach, this would have an impact only on technologies that are already existing in the first year, while all the new instalments would be chosen to best fit the system's requirements, hence, being H_2-related installed capacity very low in the first year, this approximation does not lead to relevant changes in the model behavior.

Storage system is defined by three different technologies depending on the kind of H_2 produced, namely: centralized tank-allocated, decentralized tank-allocated or centralized underground-allocated hydrogen.

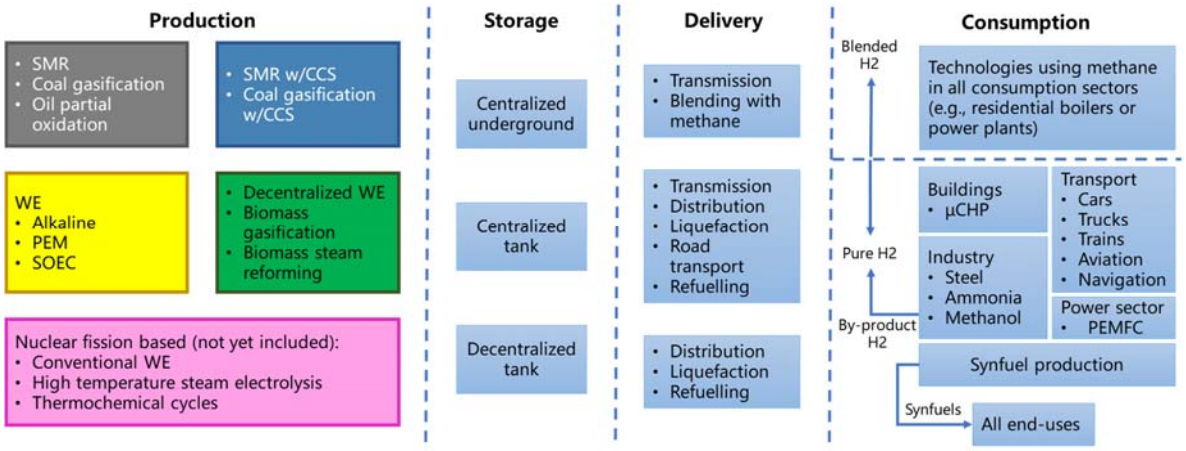

Fig. 1 High level representation of hydrogen value-chain, distinguishing among different qualities of H_2 based on the typology of production [15]

The distribution phase is used in the model to define the use of H_2 by sector, since each of them is going to be accounted for with diverse combination of techno-economic factors. Alternatively, hydrogen can directly enter the production of synfuels without any delivery process to be accounted for, since the assumption for these facilities is that synfuels are produced in situ where hydrogen is extracted. The distribution step also includes H_2 transformation for blending use: this specific utilization is modeled with a mixing limit in order to respect actual natural gas infrastructure constraint, and it does not imply additional costs for H_2 presence in the natural gas grid, although costs are included for the technology which allows hydrogen to be used for blending purposes, modeled as a previous step in the value-chain. In this case, where blending is considered and used in the system, the emission computation takes into account the reduction provided by hydrogen contribution in natural gas consumption [10]. A specific distribution process exists for industry, though fictitious in the case of ammonia and methanol, due to the fact that in this case the two processes (H_2 production, in particular from decentralized electrolysis, and ammonia or methanol manufacture) take place in the same facility, hence, without generating any transportation cost. Another peculiarity of industrial sector is related to the H_2 production, in fact there are various processes which have hydrogen as a side-product, namely, chlorine production through membrane, diaphragm and mercury cells. This hydrogen amount is usually negligible and does not appear in the final accounting analysis due to the extremely low volume produced, furthermore, it can be exploited exclusively in the same sector in which it is produced, namely, industry.

End use technologies constitute the main structure of the consumption phase of H_2, although also other technologies belonging to secondary transformation are included in this group.

Consumption side includes all the economic sectors of the system as hydrogen can be exploited in each of them in different forms:

- Commercial and residential: CHP systems for electricity and heat production
- Industry: iron production through direct reduction
- Power sector: electricity production through fuel cells
- Transport: gaseous and liquid hydrogen for road and non-road transport categories
- Upstream: hydrogen combined with captured CO_2 for synfuels production
- Blending: mixing with natural gas for all the sectors which use it.

Also, a summary containing the main sources of the structure and technologies belonging to the hydrogen value-chain is represented in Table I.

TABLE I
SUMMARY OF SOURCES FOR HYDROGEN VALUE-CHAIN TECHNOLOGIES

Value Chain step	Typology/Sector	Source
Production	Fossil	JRC, JRC-EU-TIMES Hydrogen Module, 2019
	Electrolysis	IEA, The future of hydrogen, 2019 - IRENA, Green Hydrogen Cost, 2020
	Biomass w/ CCS	
Secondary transformation Storage Distribution End uses		JRC, JRC-EU-TIMES Hydrogen Module, 2018 [11]

III. Carbon Capture Utilization and Storage Module

In order to obtain a complete overview on the hydrogen value-chain as implemented in the model, it is also necessary to describe the CCUS module, which contains carbon capture technologies, blue hydrogen production technologies and synfuels production technologies, some of which exploit also hydrogen in the process. Fig. 2 represents a simplified scheme of the CCUS module, highlighting synfuels production and carbon capture connections with other sectors, reproducing the same structure of the model itself. Hence, if the model chooses to produce blue H_2, CCUS techs are recruited including CO_2 capture activities. Blue hydrogen technologies have an

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emission factor which corresponds to the one of grey hydrogen production ones, minus the average of the captured CO_2 in the correspondent process. CO_2 storage technologies for sinks are than exploited as deposit. Alternatively, captured carbon dioxide can enter the synfuels production chain.

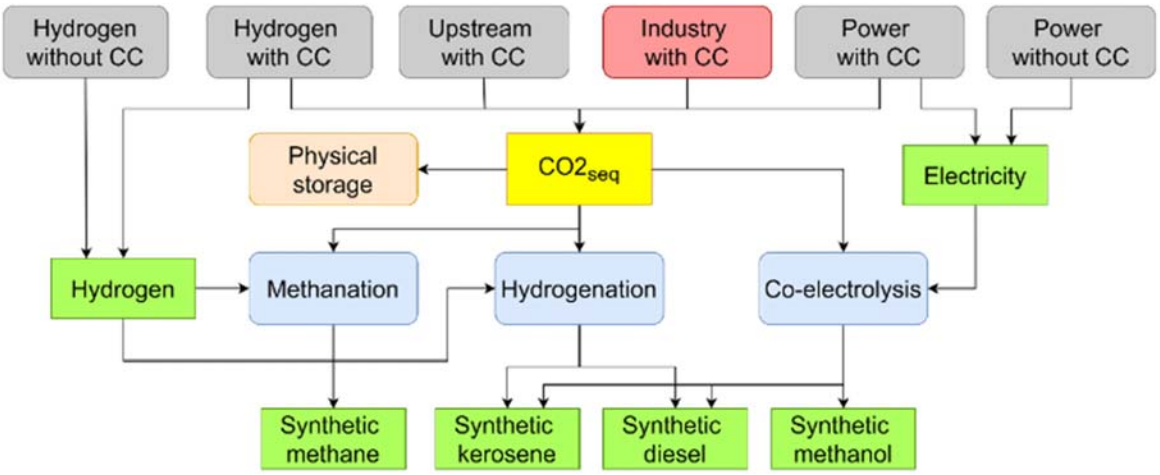

Fig. 2 Simplified representation of the Carbon Capture Utilization and Storage module, including technologies for hydrogen synthesis [10]

In general, synfuels are produced from previously captured CO_2 and an energy commodity, such as electricity or hydrogen. In TEMOA-Italy, three processes producing CO_2-based synfuels were modeled:

1. Methanation: It is a process used to produce synthetic natural gas, (syn-)NGA, from captured carbon dioxide and hydrogen
2. Hydrogenation: in this case same components are combined to produce different synfuels, like synthetic kerosene or synthetic diesel
3. Co-electrolysis: captured CO_2 is combined with electricity to obtain same products of step 2 or synthetic methanol.

Synfuels, either produced from H_2 or not, enter end-uses phase themselves to satisfy corresponding demands in various sectors: they can be consumed in blending with the corresponding fossil fuels, hence in the existing end-use technologies (e.g., synthetic kerosene and fossil kerosene in jet kerosene-based airplanes), or they can be also consumed as pure in innovative technologies (e.g., synthetic methanol in ships).

IV. Scenario Analysis

After integrating the whole hydrogen value-chain in the model, the next step is to design two different scenarios to be compared with a baseline – a Business-As-Usual (BAU) one – that should represent possible pathways for both decarbonization and hydrogen penetration in the energy system. Considered the aim of the work, scenarios should be representative of a decarbonization pathway which can or not include hydrogen technology uses, in order to compare their convenience with respect to the model unconstrained choices.

Provided the high level of complexity that a set of constraints which precisely reflects the PNRR-related H_2 development would have involved, and the lack of precise values from this plan, it was decided to implement a simpler version of constraining parameters, in order to better interpret results of the model. It is necessary to underline that increasing the number of constraints acting on the model, the optimization process possibility to provide a robust and reliable result decreases proportionally. If many strong assumptions were needed to apply these constraints in order to adhere to PNRR precise projections, further weakening the robustness and reliability of the results would have followed, ultimately undermining the usefulness of present analysis. For this reason, the path of minimum constraint was chosen for the scenario definition, using the following configuration of three scenarios in total; in particular: a BAU scenario based on the currently implemented policies [11], a decarbonization scenario based on the Italian decarbonization targets (Net Zero Emissions, NZE) [12] and a scenario with the same decarbonization targets combined with a minimum H_2 consumption (NZE w/H_2). The results about the hydrogen supply and consumption were also compared to the up-to-date Italian policies, in order to critically oversee current Italian policies for hydrogen-related technologies development and dedicated funds relevance [12]-[14]. The definition of these scenarios is represented in Table II.

Note that the final values used in the model as constraints are somewhat approximations. This is due to various factors that influence the functioning of the model itself and a compromise was needed between the desired constraints and the feasible ones. Considering H_2 production values, for example, the ambitions reported in the Italian hydrogen strategy were taken as a reference [14], applying the targets of covering the 2% and the 20% of the final energy demand to the years 2030 and 2050, respectively. Nevertheless, the model resulted in an unfeasible solution and the system could not be solved, so that the constraints were attenuated to the largest feasible value of 600 PJ. A similar procedure was followed also for the total carbon dioxide emissions constraint. The established constraints were applied as follows:

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- Carbon dioxide emission limit: it represents the net emission of aggregated carbon dioxide coming from all the sectors included in the model, where CCUS technologies provide negative output amounts. Hence, these facilities can be used in order to respect the limit imposed by the constraint.

TABLE II
SUMMARY OF CONSTRAINTS FOR SCENARIO DEFINITION WITH CARBON DIOXIDE EMISSIONS LIMIT AND MINIMUM CONSUMPTION OF HYDROGEN FOR CORRESPONDING SCENARIO

			BAU	NZE	NZE w/H_2	Sources
Constraints	Total CO_2 [kton]	2030	-	114000	114000	Least reasonably achievable
		2040	-	85000	85000	Interpolated value
		2050	-	45000	45000	Maximum LULUCF absorption capacity according to LTS
	Hydrogen production [PJ]	2030	-	-	88	2% of BAU final energy demand in 2030
		2040	-	-	489	Interpolated value (with respect to 890 PJ in 2050)
		2050	-	-	600	Starting from 890 PJ (20% of BAU final energy demand in 2050), reduced until a solution could be found

- Hydrogen production limit: this constraint is applied in such a way that it does not force any specific hydrogen related technology, instead it requires the system to produce (and consequently consume) a specified amount of H_2, identified by an energy amount, corresponding to the related percentage of final energy demand as previously described. In order to apply this generic constraint, a group of technologies was created in the database of the model, including all those technologies that transform produced hydrogen in sector-specific hydrogen, and this group was later constrained to have the established activity, meaning that the output energy, provided to final demands, corresponded to the desired amount. The list of technologies belonging to this group and, in general, the modification applied to the TEMOA-Italy database are reported in Appendix.

V. RESULTS

This section presents all the relevant results obtained from the three analyzed scenarios, comparing the possible evolution of the Italian energy system respecting the related constraints. In all the presented cases the structure of the analysis will be the following, with minor deviations:

- In general, for each kind of result three graphs are presented, one for each scenario, directly comparing different relevant features of the energy system and the most considerable differences will be underlined and justified.
- Where needed, further analysis with a focus on the comparison of just two of the studied scenarios is performed, to highlight important differences in the obtained profiles.
- Usually, a time step of five years is represented in Figs. 3-13 and in Figs. 15, 17 and 18 in the sake of clarity and conciseness. For what is represented as years 2035 and 2045, linearly interpolated values are shown.

The presentation of results starts with a general description of the obtained evolution of the energy demand for end uses and power production in all three cases, and proceeds with the details of the hydrogen production and consumption configuration, underlining where constraints are set and where they are not, and the model is freely choosing to recruit different technologies.

A. End Uses

Fig. 3 reports results obtained for BAU, showing the evolution of the final energy demand from 2010 to 2050, in terms of the bulk energy demand used to satisfy final energy consumption, including services from agriculture, commercial, residential, transport and industry. It is possible to observe how the system undergoes a slight efficiency increase, diminishing the total amount of required energy in the first represented decade. It must be considered that this trend reflects the historical evolution of the demand which is the same throughout the different scenarios.

Concerning the commodities consumption, it can be noticed how the increase in the efficiency of the system represented a decrease in the oil and natural gas consumption, while electricity uses slightly increased in the time horizon. In the meanwhile, coal consumption remained almost constant and some other energy sources entered the system with a share accounting for less than 1% each, falling in the "OTHER" category. This includes in particular renewable energy sources other than biomass, namely, solar, synfuels, geothermal and hydrogen which reasonably do not reach a high share in a BAU scenario.

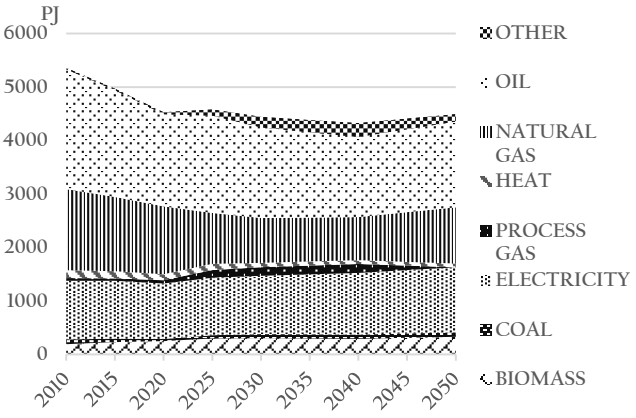

Fig. 3 Final energy consumption for the BAU scenario

The configuration of the system varies considerably in the NZE scenario reported in Fig. 4. A remarkable variation occurs

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especially in later years, as expected, where oil and natural gas shares drop consistently starting from 2030, with a progressive substitution obtained through synfuels use. Also, a higher efficiency increase can be highlighted for this scenario, with a total amount of end uses demand which is much closer to 4000 PJ with respect to the previous case and achieving a reduction of 8% in 2050 with respect to BAU. Synfuels share is going to be deeper analyzed in the following, but it is important to take into account what explained in previous chapters about the functioning of the CCUS module. This includes the synfuels production through the use of captured CO_2, a combination of technologies that appears to be as convenient in a scenario where constraints on total emissions are imposed. Additionally, a more intense electrification process is occurring for this and the following scenarios, increasing the share of this commodity use on the total demand and reaching a value of 32% and 30% in 2050, respectively, with respect to 27% in BAU.

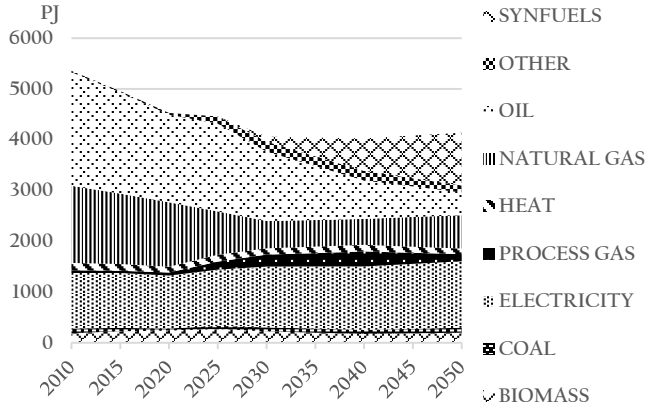

Fig. 4 Final energy consumption in the NZE scenario

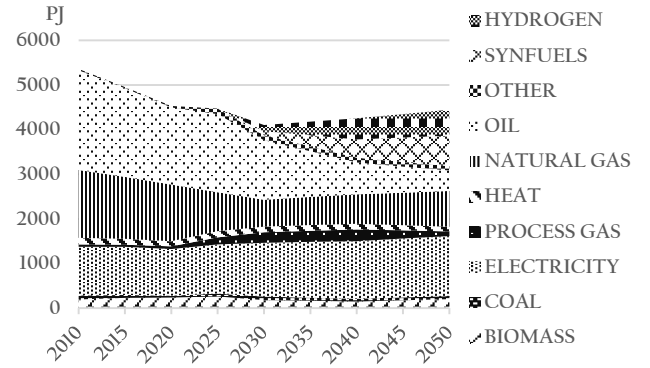

Fig. 5 Final energy consumption in the NZE w/H_2 scenario

A very similar outcome results from the NZE w/H_2 scenario, and this is represented in Fig. 5, for which same consideration as the previous ones can be done. Additionally, the expected introduction of H_2 use is noticeable in this scenario, and a slightly higher total energy demand, especially after 2040, is reported, but still 2% lower with respect to BAU. However, the same decreasing trend for oil and natural gas is provided by this optimization, which is reasonable considering that emissions constraints hold for this one as well.

A quite remarkable absence of renewable sources other than biomass can be noticed in all these results, but it must be emphasized that primary energy consumption for electricity production is not yet considered so far.

B. Hydrogen Production

H_2 production is one of the most important results to be analyzed in this work, since the aim is focused on this specific energy vector and most of the conclusion should be supplied by these and the following results. Fig. 6 reports a particular outcome of the model for the ABU scenario. In fact, being this scenario unconstrained, it was not expected to freely choose blue-hydrogen production, since this technology represents a higher cost with respect to the grey counterpart. However, it must be underlined that this scenario already contains some of the implementation deriving from PNIEC national plan, extended until 2050 and it must be considered the very low share that hydrogen represents with respect to energy demand, reported in TABLE III.

Additionally, as it is going to be displayed in further paragraphs, the hydrogen hereby produced is partially used for synfuels production, for which carbon capture is required; for this reason, the model could only choose of installing a blue-hydrogen technology to provide both supplies, instead of a grey-hydrogen technology plus a carbon capture technology for CO_2 provision. On this specific outcome, however, further studies shall be performed in order to obtain exhaustive explanation of this unexpected choice.

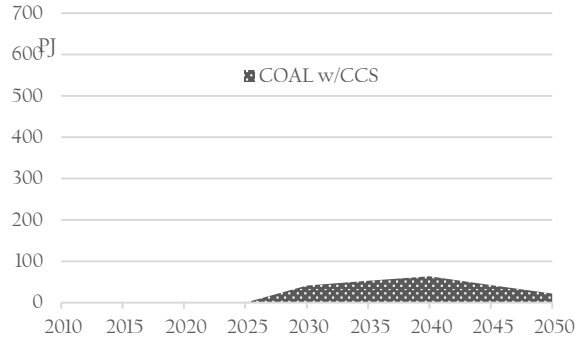

Fig. 6 Hydrogen production in the BAU scenario by technology

Fig. 7 represents the production of hydrogen for the NZE scenario, in which the model freely chooses to include this energy vector in the system, in particular producing it through solid biomass gasification.

Considering it is unconstrained, the amount of H_2 produced is remarkable and this evidence strongly suggests that the energy vector is to be included consistently in the energy system framework in order to obtain a complete decarbonization of the economy and to put the country on track with emissions targets for 2050. Since the optimization process is obtained through a least-cost optimization, the inclusion of hydrogen technologies marks them as belonging to the convenient options needed for a NZE pathway. In the following

section the use of H_2 is going to be studied more in detail, and the share of H_2 consumption on the total energy demand is also reported (see Table III).

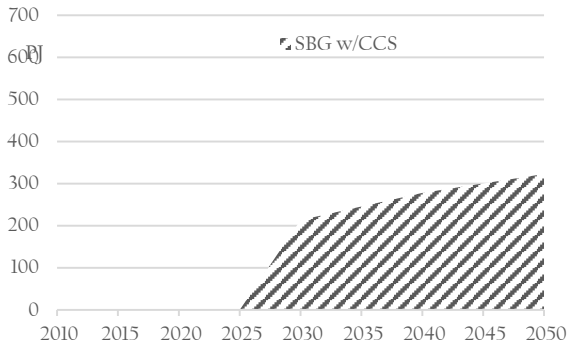

Fig. 7 Hydrogen production in the NZE scenario by technology

Fig. 8 shows hydrogen production technologies configuration in the case of a production constraints (NZE w/H_2 scenario), exceeding the amount spontaneously produced by the model and represented in Fig. 7. Looking at Figs. 7 and 8 from NZE and NZE w/H_2 scenarios, it could be noticed how the activity related to solid biomass gasification is preserved from the unconstrained to the constrained scenario, with the further addition of other technologies to meet the imposed limit. A combination of four H_2 production technologies is chosen in the NZE w/H_2 scenario, including one for grey hydrogen, one for blue hydrogen and two for green hydrogen, namely, steam methane reforming, steam methane reforming with CCS, solid biomass gasification with CCS and AEM cells for water electrolysis, the latter intervening after 2040. Grey-H_2 production technology seems to be needed in order to accomplish the required production in 2040, being considered also in a decarbonization scenario, where the model considers more convenient to emit in the upstream sector instead of in the demand side one. Also, in this case the share of H_2 over the total energy consumption is reported in Table III. This can also be used to verify that the constraint foreseen of 20% of share of total demand satisfied with the use of hydrogen could not be respected, as previously stated and explained.

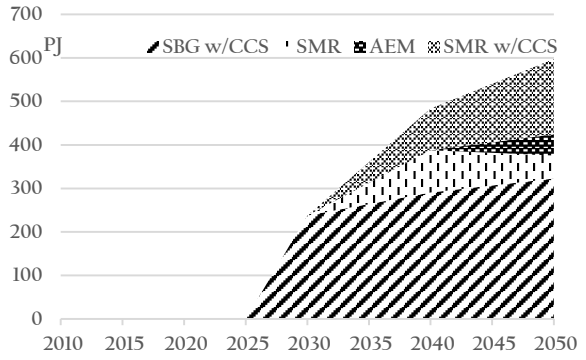

Fig. 8 Hydrogen production in the NZE w/H_2 scenario by technology

TABLE III
HYDROGEN CONSUMPTION SHARE IN THE ENERGY DEMAND FOR THE STUDIED SCENARIOS

		2030	2035	2040	2045	2050
% gross energy demand	BAU	0.67%	0.87%	1.06%	0.70%	0.35%
	NZE	3.53%	4.03%	4.53%	4.67%	4.80%
	NZE w/H_2	3.89%	5.77%	7.56%	8.05%	8.49%
% end uses	BAU	0.94%	1.20%	1.48%	0.97%	0.49%
	NZE	5.26%	6.08%	6.90%	7.36%	7.81%
	NZE w/H_2	5.79%	8.63%	11.37%	12.42%	13.44%

C. Hydrogen Consumption

The use of H_2 in the BAU scenario shows more than half of the share deployed in synfuels production in 2030, and all the rest destined to blending uses, with an evolving distribution along the time horizon as depicted in Fig. 9, reporting the share of consumption by sector. This blending follows the rules previously described for mixing limit due to restrictions of the infrastructure and can be used in all the sectors of the system to contribute to natural gas consumption decreasing the associated emissions. However, the represented amount of hydrogen produced is quite low and can be considered almost negligible with respect to the following scenarios.

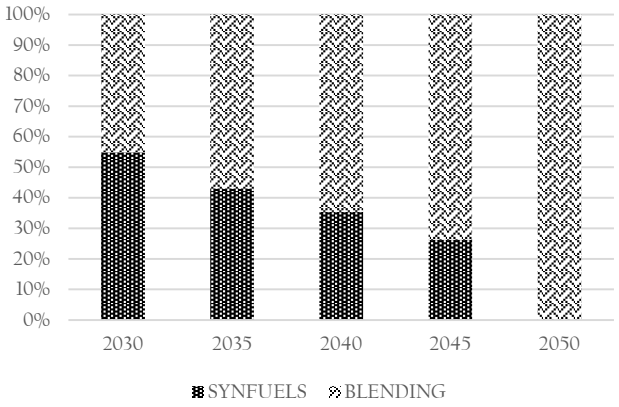

Fig. 9 Share of hydrogen consumption by sector in the BAU scenario

As far as NZE scenario results are concerned, the share of the hydrogen consumption is heavily unbalanced towards synfuels production, as Fig. 10 is clearly showing. This choice made by the model is sided by the use of blending, and slight other uses including commercial sector and industry. The development of this consumption configuration also explains the rationale of having a H_2 production with CCS, allowing to install a single technology and simultaneously obtaining captured carbon dioxide and hydrogen from it, two fundamental ingredients needed for synfuels production.

The results obtained from the NZE scenario can be already compared to the choices made by the model optimization for the NZE w/H_2 scenario in Fig. 11, where an extensively different configuration for the hydrogen consumption is shown, heavily including transport and industry sectors in hydrogen end uses. This behavior of the system closely reflects what is foreseen in the PNRR projection, since hydrogen would have the major role of decarbonizing hard-to-abate emissions in

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industry, especially in iron and steel production, as it does in this case, and contributing to decarbonizing transportation technologies, especially in the case of heavy-duty freight transport and non-road categories. In particular, from these results hydrogen is extensively used in transport for both domestic and international aviation purposes, reflecting long-term projects and technology development in this field. However, this specific result requires further analyses and developments regarding the aviation sector modeling (also integrating proper constraints due to infrastructural prospects) to be solidly supported.

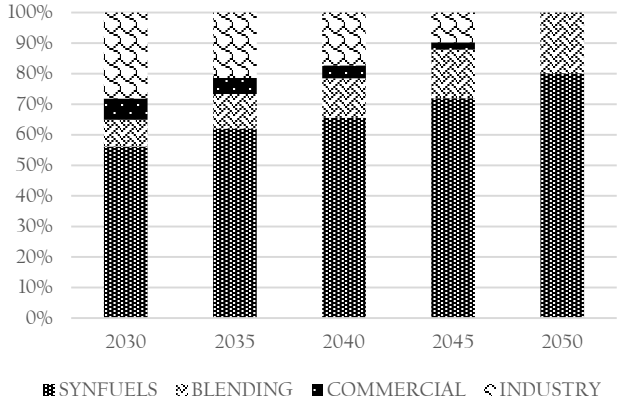

Fig. 10 Share of hydrogen consumption by sector in the NZE scenario

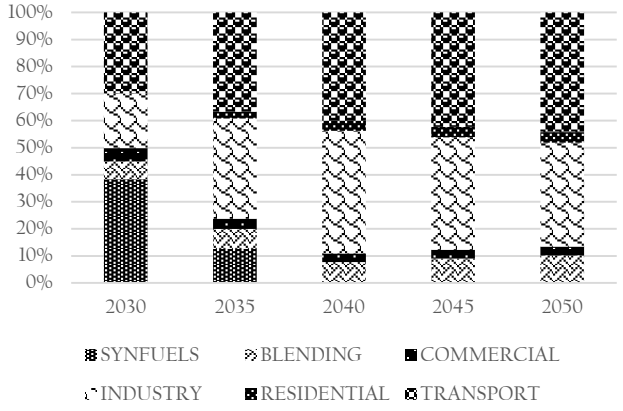

Fig. 11 Share of hydrogen consumption by sector in the NZE w/H_2 scenario

On the other hand, the results from NZE w/H_2 scenario show a limitation in synfuels production strictly between 2025 and 2035. This specific characteristic seems to be in contrast with what expected in hydrogen developing pathway, where early blending and industry utilizations should enable the enhancement of a wider market for H_2 deployment, in order to achieve a consistent share of synfuels and abating fossil fuels emission on long-term horizon. Obviously, synfuels consumption has the same emission factor of traditional fuels, but they present the great advantage of being produced through captured carbon dioxide, hence removing it from the atmosphere, and not introducing additional amounts of CO_2 in the system. Conversely, what represented in Fig. *11* seems to sustain an opposite process, in which early usage of synfuels should foster later spreading of hydrogen in other sectors of the economic system. Furthermore, if compared with the results deriving from the NZE scenario, where hydrogen utilization was unconstrained, the constraint on H_2 production in NZE w/H_2 seems to prevent the model to get closer to the optimum to which it would seem to tend, since in the NZE scenario, wherehydrogen was not constrained, was produced anyway but used mainly for synfuels production. For this reason, a modification of the NZE w/H_2 scenario was made, consisting of the addition of the technology that allows the use of hydrogen for synfuels production in the group which is constrained by the limit of minimum activity imposed. Previously, synfuels could be produced anyway (and it happens in NZE w/H_2 scenario), but as an additional amount freely chosen by the optimization process, standing outside the constraint. Conversely, including possible synfuels production in the restricting value, this activity is used by the model to satisfy that same limitation. The results of this modified scenario are reported in Fig. 12. What were already stated about expectations in H_2 development pathway are not met here, since synfuels production occupy a consistent share of hydrogen use since 2030, and industry remains a secondary consumption purpose, while pure hydrogen does not appear in transport (as direct consumption) at all. However, in order to better clarify what happens in consumptions steps which are closer to final demand, the NZE scenario is compared together with the latter in the following section to perform a deeper analysis on the use of synfuels.

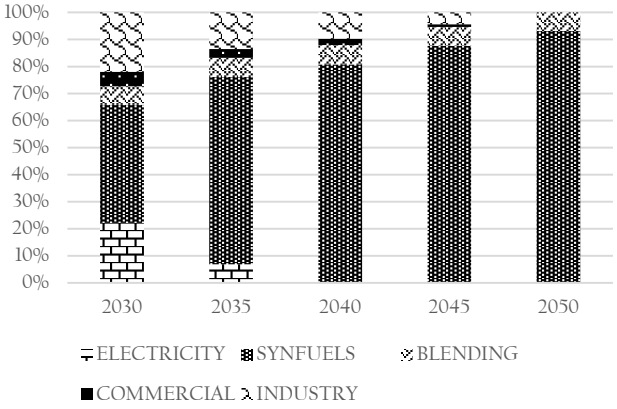

Fig. 12 Share of hydrogen consumption by sector in the alternative NZE w/H_2 scenario

D.Synfuels

In order to compare synfuels utilization, only the NZE and the alternative scenario for hydrogen constraint are considered; these being the scenarios within which a considerable amount of synfuels production, making the analysis consistent and useful for drawing conclusions. Starting with the NZE scenario,Fig. 13 illustrates the production of synfuels provided without constraints on H_2 utilization; it can be noticed how faster this production increases for those fuels that do not require H_2 use. Instead, captured carbon dioxide and electricity

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are necessary for these processes, corresponding to the grey area, justifying the choice of blue hydrogen production technology use in the NZE scenario.

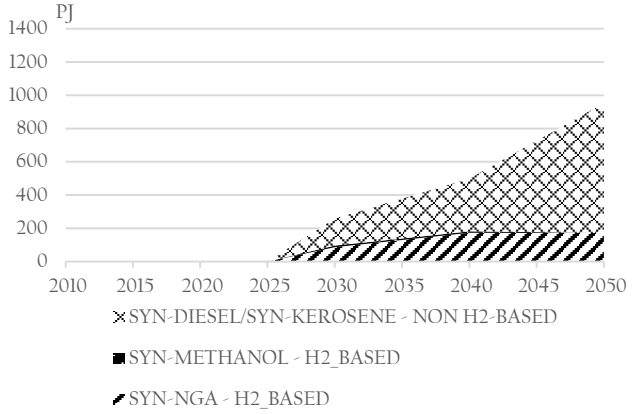

Fig. 13 Synfuels production, both H_2 and non- H_2 based, in the NZE scenario

Furthermore,Fig. 14 reports the share of the synfuels consumption sector-by-sector, showing percentages corresponding to the fraction of each of the synfuel for each of the end uses demands, accounting for the cumulative amount of synfuel along the entire time horizon. This choice was made in order to prevent analysis of possibly biased data produced by single year considerations. Syn-diesel and syn-kerosene, which are produced without the use of hydrogen, are mainly consumed by agriculture and commercial sector, with former using the 12% of the total amount of syn-diesel produced and the 91% of the total amount of syn-kerosene, and the latter almost all of the remainder of the two fuels (but for 1% of the syn-diesel being consumed in residential sector). Syn-methanol is almost completely consumed in the residential sector (96%) but it must be underlined that the total amount of this propellant is almost negligible. Synthetic natural gas, which covers the large majority of the hydrogen-based synfuel production, is mainly used in the residential sector to contribute to space heating and cooking purposes (57%), equally consumed in commercial and industrial sectors (16% for each one of them), and the remainder subdivided between electricity production (9%) and agriculture (1%).

The same kind of analysis was performed for the second scenario considered in this section, with results reported in Fig. 15. The considerations previously explained can be applied for this case also, whereas the share of hydrogen-based synfuels is much higher than before, due to the H_2 constraint on the system. Syn-methanol, as in the former analysis, accounts for an almost negligible amount of total synfuels production. Considering the increase of blue hydrogen production, the system has at its disposal a higher captured CO_2 stock, hence, also non-hydrogen based synfuels production raised with respect to the previous case.

Concerning synfuels end uses, almost same configuration as the one already described is displayed inFig. 16, with some differences to be underlined only for syn-NGA, here being consumed for 61% in residential sector and for 33% in industry, and the remainder sectors accounting for less than 5% each.

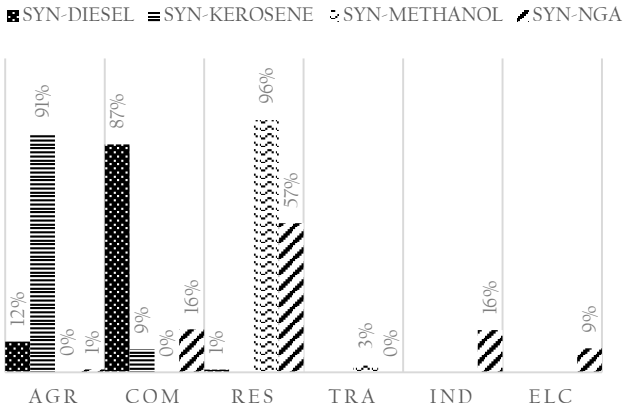

Fig. 14 Share in the use of synfuels by sector for the NZE scenario: The percentage is computed with respect to the cumulative amount of synfuels along the entire time horizon in order to prevent possible bias referred to single years

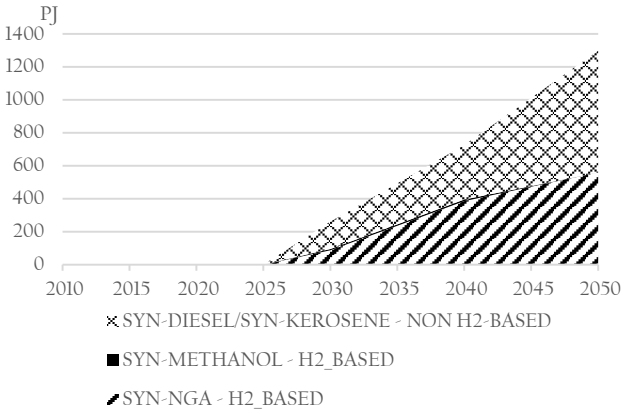

Fig. 15 Synfuels production, both hydrogen and non-hydrogen based, in the alternative NZE w/H_2 scenario

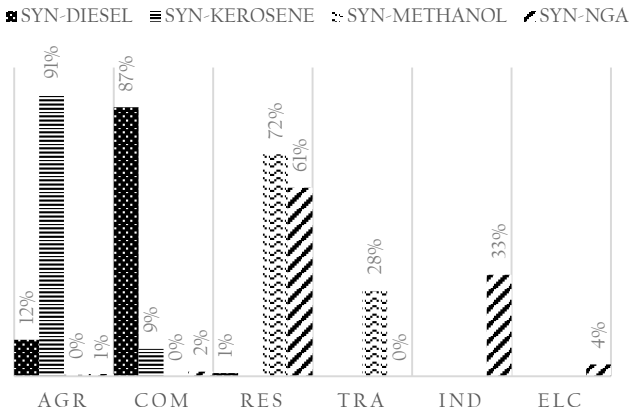

Fig. 16 Share in the use of synfuels by sector for the alternative NZE w/H_2 scenario: The percentage is computed with respect to the cumulative amount of synfuels along the entire time horizon in order to prevent possible bias referred to single

E. Sector-Specific Hydrogen Consumption

In order to analyze the uses of hydrogen for the NZE w/H_2 scenario, since the two most relevant contributions to this

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energy vector consumption were provided by industry and transport sector by far, these sectors where further studied to obtain the configuration of the produced end uses. Fig. 17 reports the amount of consumed resource for the manufacture of ammonia, steel, and methanol, where the latter accounts for negligible amount and was included for completeness. Steel is produced through direct reduction processes, and the activity hereby shown covers more than 80% of the total domestic production, a remarkable result considering the PNRR and the National Hydrogen Strategy objectives, according to which this manufacture typology is one of the most promising for H_2 usage and emissions abatement. In parallel, ammonia-related activities reach a coverage of 100% of ammonia production from 2040, being also this amount halved with respect to previous years. These results clearly introduce a promising framework for further hydrogen penetration analysis, since its potential lies mainly in the decarbonization power for these kinds of industrial processes.

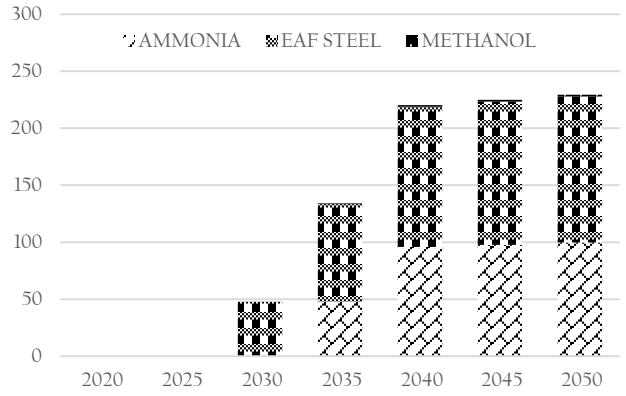

Fig. 17 Hydrogen consumption in industrial sector by final product in the NZE w/H_2 scenario

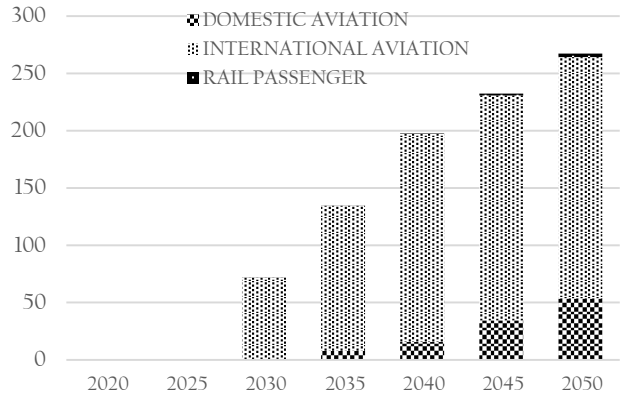

Fig. 18 Hydrogen consumption in transport sector by final product in the NZE w/H_2 scenario

Additionally, transport sector presents equally encouraging results, even though exclusively limited to the aviation category, as reported in Fig. 18, with an increasingly important intervention of hydrogen-based mobility for this fraction of the sector, which achieves an outstanding 95% of the total domestic aviation demand and over 85% of the international one. This remarkable outcome brings further encouragement for hydrogen technologies development including also the transport sector. However, the downside note is that these are the only hydrogen technologies related to mobility which were taken into consideration by the model, but for a negligible amount of rail passenger transport. This is also possibly related to high costs of hydrogen-based road transports, a factor which heavily affects results in such an optimization type model. Nevertheless, the real economic system presents a similar behavior with respect to prices, favoring least-cost technology diffusion rather than other qualities, which is also the reason why these models can reliably be used for real-system applications and interpretations. It must also be underlined that non-road transports are defined in order to satisfy a demand which is expressed in PJ, while the most obvious unit of measurement for this sector would be billion vehicles per kilometer, which would also take into account the efficiency of the used fuel. This improvement in the model is already under development but was not ready at the time of this study. The outcomes of this refinement should however additionally favor H_2 uses in the transport sector, being this energy vector more efficient than others.

F. Emission Analysis

Finally, a deep overview of emissions configuration by sector is provided, in order to understand the decarbonization strategy put in place by the optimization processes.

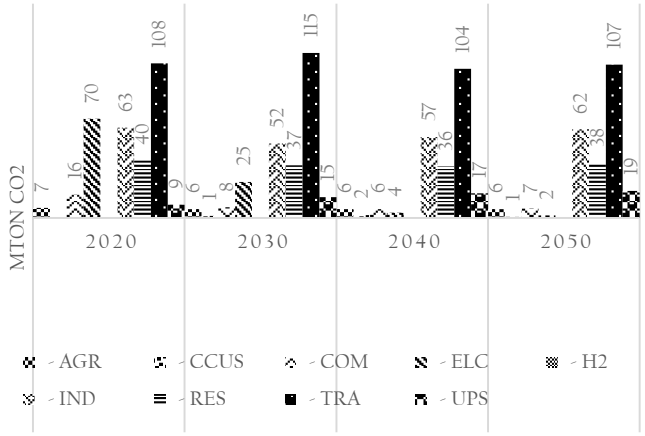

Fig. 19 Total CO_2 emissions by sector, BAU scenario: AGR – Agriculture, CCUS – Carbon Capture Utilization and Storage, COM – Commercial, ELC – Power sector, H_2 – Hydrogen, IND – Industry, RES – Residential, TRA – Transport, UPS – Upstream

Firstly, the BAU scenario results are reported inFig. 19, indicating value labels in million tons of CO_2 per sector, and it is noticeable how some sectors, as the electricity production and, more slightly, residential ones, undergo even in this scenario a decarbonization process. Specifically, in the former this phenomenon is heavily marked, in fact only a minor residual amount of natural gas is consumed for power production, with all the other inputs being zero-emissive energy

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sources. Conversely, other sectors like transport and industry face a much slighter decarbonization process, remaining the two most carbon dioxide emissions intense fractions of the system. This is due to the lack of emissions constraints in the model and the difficulty in abating such sectors.

The picture drastically changes for the NZE scenario, inFig. 20, reporting different relevant changes with respect to the previous case. Almost all the sectors, in this scenario, undergo a heavy decarbonization process, with transport remaining the highest emissive one in 2050. Nevertheless, also this sector diminishes its emissions by a gross 35% along the entire time horizon, representing an extensive improvement of the system. However, the most relevant characteristic of the described decarbonization pathway is the appearance of negative carbon dioxide emissions, representing a direct CO_2 capture from atmosphere. In fact, recalling Fig. 7, hydrogen production was provided through solid biomass gasification with CCS. This technology is in truth emitting carbon dioxide during use phase; hence, the capturing of the CO_2 should barely compensate this emission instead of accounting for a negative amount. Nevertheless, the assumption made in this model is that biomass use is always sustained with new biomass supply, compensating emissions with increasing natural carbon sinks and therefore not introducing new fossil CO_2 in the atmosphere, instead recirculating it. This is obviously a strong assumption, yet, included in the perspective of sustainable development.

Results provided for the NZE w/H_2 scenario, asFig. 21 shows, represent a completely similar configuration, with slightly less biomass-based CCUS activity as well as a more intense decarbonization pathway for transport sector, probably associated to what seen in the previous paragraph with the extensive use of hydrogen in aviation, which reaches a 46% reduction in total emissions.

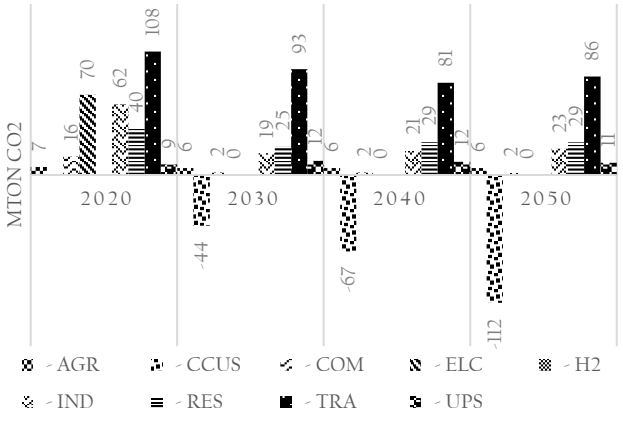

Fig. 20 Total CO_2 emissions by sector, NZE scenario: AGR – Agriculture, CCUS – Carbon Capture Utilization and Storage, COM – Commercial, ELC – Power sector, H_2 – Hydrogen, IND – Industry, RES – Residential, TRA – Transport, UPS – Upstream

In general, what emerges from the two decarbonization scenarios, is that a pathway for meeting 2050 targets is not only possible but is presumably achievable through the intense use of combined CCUS with other technologies, like blue-hydrogen and synfuels production, rather than through a complete abatement of sectorial emissions, and since the complete abatement of these residual emissions seems to be unfeasible, CCUS applications reveal to be not only useful, but necessary. This result is extremely relevant for strategic planning of energy system evolution dynamics and with further improvement of the tool hereby utilized even more accurate and reliable optimization can be provided, to work as a robust pillar for policy making in Italy.

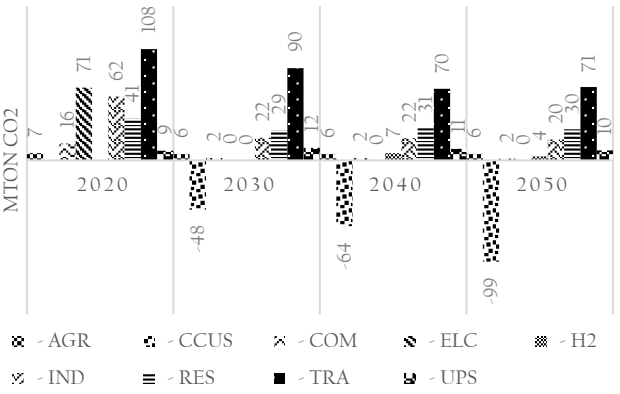

Fig. 21 Total CO_2 emissions by sector, alternative NZE w/H_2 scenario: AGR – Agriculture, CCUS – Carbon Capture Utilization and Storage, COM – Commercial, ELC – Power sector, H_2 – Hydrogen, IND – Industry, RES – Residential, TRA – Transport, UPS – Upstream

VI. Conclusions

This work presented an assessment of the possible future role of hydrogen in pursuing the Italian decarbonization objectives. The current national hydrogen-related policies have been critically analyzed, highlighting that:

a. Hydrogen may play a key role in decarbonizing the energy system. More specifically, combined with the activity of carbon capture technologies it appears to be crucial to enable the production of synfuels, selected as the most economically convenient low carbon fuel for the end-uses decarbonization.
b. The penetration of synfuels in the final energy consumption is preferred with respect to the direct consumption of H_2 in the demand sectors. This appears in contrast with the national strategies, that aim to firstly develop hydrogen value chain in the industrial system and secondly to exploit the production capacity to produce synfuels.
c. While the optimization process seems to give credits to what is included in the national hydrogen plans in transport and industry, other sectors completely miss. The optimal configuration of the system found here differs from the proposals included in national strategies for hydrogen development.

The conclusion hereby included need to be put in the context of the model limitation as of today. The various assumptions, described in the different chapters, are clearly playing an

important role in the optimization process and their effects on the final result can be possibly measured only when they will be removed, where needed and possible. The most critical aspects can be summarized as follows:

a. The transport sector could present different results once the described improvements are applied, also further favoring hydrogen use in both road and non-road categories.
b. Input data clearly make a wide difference on results obtained. For this reason, a sensitivity analysis would be needed for applying reasonable and robust techno-economic ranges to these data, especially on newer and future technologies like hydrogen- and synfuels-related ones, providing unexpected results in this study.
c. The applied constraints are extensively simplified and limited only to a general use of hydrogen in the system. A more accurate policy framework definition would foster highly more detailed studies and corresponding more robust outcomes.
d. Finally, ESOMs have anyway intrinsic limitations in capturing the involvements of the broader context in which the energy system is included, neglecting factors which do not directly influence or act on it, and this remains an open matter in the modeling community for the improvements of these tools.

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