A dynamic accounting method for CO2 emissions to assess the penetration of low-carbon fuels: application to the TEMOA-Italy energy system optimization model

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A dynamic accounting method for CO2 emissions to assess the penetration of low-carbon fuels: application to the TEMOA-Italy energy system optimization model ☆

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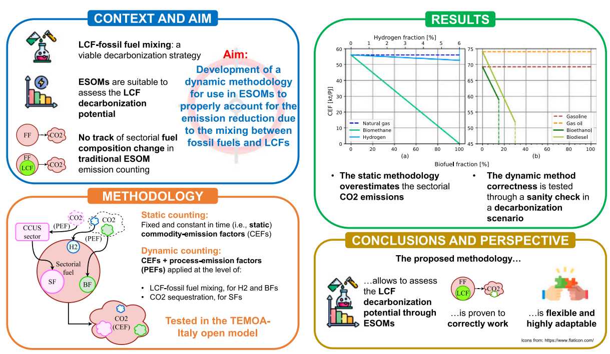
HIGHLIGHTS

- A new dynamic CO2 emission accounting method for energy system models is presented.
- The method is suitable to assess the decarbonization potential of low-carbon fuels.
- The method is tested in the TEMOA-Italy open Energy System Optimization Model.
- The method is producing the expected results in base and decarbonization scenarios.
- The flexibility and adaptability of the method allow its use in other ESOMs.

GRAPHICAL ABSTRACT



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ABSTRACT

A correct counting of greenhouse gas emissions, mainly CO2, is crucial in energy system optimization models, widely used to assess the effectiveness of decarbonization strategies. Sectorial emissions are typically computed at each modeled time period using commodity-specific factors based on a given static fuel composition. For fuels generated by combining fossil and low-carbon commodities, however, the share of the low-carbon component may change over time. Under certain fractions, the blending with hydrogen, biofuels, and synfuels, constitutes a viable decarbonization alternative, without the need for retrofitting the existing infrastructure. This work proposes a dynamic accounting method for the avoided emissions thanks to blending low-carbon fuels with fossil fuels as an alternative to the traditional static evaluation in energy system models. The proposed methodology is based on the application of negative process-specific factors to account for avoided emissions. This new scheme is integrated and tested in the TEMOA-Italy open model. The dynamic methodology is first compared to the static one, showing that the latter provides an overestimation of the emission levels. Then, it is proven to work properly in a very stringent decarbonization scenario for a large range of blending fractions. Finally, the results of the decarbonization scenario are deeply analyzed to provide valuable insights for future policy-relevant assessments. Even if the high penetration of blended low-carbon fuels in the energy mix quantitatively differs from the

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evolution foreseen by national, European, and global energy policies, such penetration reflects the crucial role of hydrogen, biofuels, and synfuels depicted in those policies, to fulfill the intermediate and long-term emission reduction targets.

Nomenclature

Acronym

AFOLU	Agriculture, Forestry, and Other Land Use
BECCS	Bioenergy with carbon capture and storage
CCUS	Carbon capture utilization and storage
CEF	Commodity emission factor
CHP	Combined heat and power
DAC	Direct air capture
ESOM	Energy system optimization model
EU	European Union
FIXOM	Fixed operation and maintenance costs
GHG	Greenhouse gas
HEV	Hybrid electric vehicles
ICE	Internal combustion engine
IEA	International Energy Agency
IPCC	Intergovernmental Panel on Climate Change
LCF	Low-carbon fuel
NET	Negative emission technologies
PEF	Process emission factor
PHEV	Plug-in hybrid electric vehicles
RES	Reference Energy System
TEMOA	Tools for Energy Model Optimization and Analysis
VAROM	Variable operation and maintenance costs

Symbol

act	Activity
bio, dyn, st	Indices for biofuel commodities, dynamic emission factor, static emission factor
CEF	Parameter/variable for commodity emission factors
$CO2_{seq}$	Variable for sequestrated CO2
cons, mix, net	Indices for end-use consumption, mix of fossil fuels and low-carbon fuels, net sectorial CO2 emissions
CR	Parameter for CO2 capture ratio from CO2 sequestration processes
$Emission_i$	Variable for global emission from a technology of an emission commodity associated with an input commodity
energy cons	Consumed energy commodity
f_{BF}	Variable for share of biofuels in the optimal blend of fossil fuels and low-carbon fuels
f_{H2}	Variable for share of hydrogen in the optimal blend of fossil fuels and low-carbon fuels
Flow	Variable for commodity consumption/production
$H2, BF, SF, FF$	Variables for hydrogen, biofuels, synfuels, fossil fuels
kt	Kilotons
LCF	Variable for the sum of all the low-carbon fuels mixed in a fuel technology
M€	Millions of Euros
$mass_{GHG}$	Unit mass of the emitted emission of a certain greenhouse ga
Mt	Millions of tons
PEF	Parameter for process-based emission factors of the CO2 sequestration processes
PJ	Petajoule
SECTCO2	Variable for emission at the end-use consumption level
SECTF	Variable for sectorial fuel
seq	Index for process-based emission factors of CO2 sequestration processes
t, in, out, i, o	Indices for technology, input, output, input commodity, output commodity
η_{FT}	Parameter for efficiency of a fuel technology

1. Introduction

Energy system optimization models (ESOMs) are tools customarily used to analyze the effectiveness of possible energy policies in pursuing declared environmental targets [1]. An ESOM framework typically relies on the description of the different interconnected sectors of the Reference Energy System (RES) through a technology-rich database. The match between commodities produced in the supply side and the end-use demands is computed according to a minimum cost paradigm, subject to a set of constraints depending on the analyzed scenario, over a medium-to-long-term time scale and a (possibly) multiregional spatial scale. Among the results of the optimization, the CO2 emissions corresponding to the energy system evolution are typically computed.

While demand-side sectors (transport, buildings, industry) consume fuels to meet the final energy service demands in the region under exam, the supply side (upstream and power sector) of the RES is devoted to the production of intermediate energy commodities (such as fossil fuels, electricity, renewables, etc.) at levels that must be sufficient to meet the requirements of the demand side. To separately track fuel consumption, sector-specific technologies, referred to as fuel technologies (FTs), can be adopted, allowing to assess the sectorial contribution to the modeled decarbonization scenarios and strategies [2,3]. The FTs are then fictitious technologies used to transform generic commodities, produced by the supply-side, into sector-specific commodities, consumed by demand technologies. Besides allowing to account for the efficiency and costs of the distribution network, FTs are particularly useful to model the mix between two or more fuels (as shown in Fig. 1 for a FT producing sectorial natural gas) occurring within the distribution infrastructure before the demand-side consumption. In this regard, the mix between fossil fuels and alternative low-carbon fuels (LCFs) provides a viable alternative to decarbonize some sectors, e.g. the transport one, without deep changes in the currently existing infrastructure [4,5]. For instance, the injection of hydrogen in the existing methane pipelines can be a transitionary solution to trigger the initial development of low-carbon hydrogen, until its devoted distribution chain is built [6]. In this regard, the feasibility of such an injection in the methane distribution grid tests is being tested through several projects worldwide, especially in Europe [7], where the European Union (EU) is planning to support the blending of hydrogen in the existing methane infrastructure [8]. Moreover, renewable transport fuels, such as biofuels and synfuels, are considered necessary to decarbonize the transport sector in the short and medium terms: however, since dedicated transport technologies are not yet widely commercialized globally, these fuels can be used in blends with the more common refined oil products [5]. In this context, many countries require biofuel blending mandates in the transport sector, with the majority of biofuels consumed today in low-percentage blending rates [9]: instead, the existing infrastructure can be exploited with much higher blending rates for some synthetic fuels (from now on called synfuels) such as synmethane, syndiesel, and synkerosene [10].

As far as the computation of emissions in ESOMs is concerned, that is performed considering both commodity emission factors (CEFs) and process-specific emission factors (PEFs), as shown in Fig. 2 [11,12]. CEFs are generally used to evaluate emissions related to combustion processes and are expressed in units of $\frac{\text{mass}_{\text{GHG}}}{\text{energy cons.}}$, where mass_{GHG} represents the unitary emitted mass of a certain greenhouse gas (GHG), typically CO2, CH4, N2O, or SOx, associated to the combustion of a certain fuel, while energy cons. is the specific consumption of the burned fuel. While a CEF just depends on the chemical composition of the burned fuel, PEFs represent additional contributions to GHG emissions from particular technologies from different sources than fuel combustion, e.g., emissions from calcination in cement plants [13]. PEFs result then in additional contributions to total emissions from specific technologies. Moreover, it is important to point out that such a computation of emissions, and more in general the approach adopted in ESOMs, does not involve any life-cycle assessment-related approach. Indeed, CEFs and PEFs only consider direct emissions occurring at the level of each modeled technology. On the other hand, the emissions associated with the life cycle (i. e., from manufacturing to end-of-life) of the technologies are not considered.

The application of CEFs to the sector-specific commodities produced by the FTs allows tracking the emissions at the level of the consumption technologies separately for each modeled sector (e.g., natural gas-based power plants or gasoline cars) [12]. However, the CEFs are fixed parameters provided a priori as input to the model, that do not consider the possible changes in the sector-specific fuel composition as in [3,14]. This static approach does not correctly consider the emission reduction induced by the possible blending of fossil fuels with alternative LCFs, which can also vary in time. A partial solution to this static nature is provided in [15] for the transport sector: in the case of mixing between fossil fuels and biofuels, CO2-related CEFs are applied only to generic fossil commodities (e.g., gasoline). While this strategy only allows to account for fossil-generated CO2, it does not allow to evaluate the emissions of the end-use transport technologies (e.g., gasoline cars), unless other CO2-related CEFs are also applied to the sectorial commodities (e.g., transport gasoline), leading to two parallel CO2 counts.

Instead, this work aims to provide a proper methodology to account for the emission reduction associated with the penetration of blended LCFs in the consumption sectors, evaluating at the same time their environmental benefits accurately by assessing the emissions at the end-use technology level. The proposed methodology, developed for CO2 emission, is dynamic in the sense that it depends on the fuel composition, which can vary throughout the ESOM time horizon. The methodology is here applied to the case study of the open-source model TEMOA-Italy [16,17], developed as an instance of the Tools for Energy Modeling Optimization and Analysis (TEMOA) framework.

Section 2 describes the proposed dynamic methodology, providing the rationale and mathematics behind its use when modeling the LCFs in ESOMs, with details on the related value chains modeled in the TEMOA-Italy model. In Section 3, the results from the application of this methodology to the TEMOA-Italy model are presented and discussed, while Section 4 concludes the work, with insights for future perspectives.

2. Methodology

In this section, the idea behind the dynamic CO2 emission counting is first presented in Section 2.1, while the associated equations are shown in Section 2.2. Section 2.3 provides an overview of the LCF value chains modeled in the TEMOA-Italy model, the ESOM instance to which the methodology is applied. Finally, the scenarios used to check its correctness are described in Section 2.4.

2.1. The avoided CO2 emissions from low-carbon fuels

The dynamic CO2 emissions accounting method is used to properly represent the effect of mixing fossil fuels and LCFs. In general, the latter refers to those fuels the consumption of which would contribute to satisfy a GHG emission reduction threshold (for example, at least 70% in the EU framework [18]), if compared to fossil alternatives. In this analysis, the combustion of LCFs is deemed not to affect the CO2 atmospheric concentration. That is the case of hydrogen, biofuels, and CO2-based synfuels and in particular:

- Hydrogen does not contain any carbon atoms, independently on how it is produced (indeed, possible CO2 emissions related to hydrogen production, e.g., through natural gas-based steam reforming processes, are accounted for at the level of the hydrogen production technologies).
- Biofuel combustion is assumed to emit the same amount of CO2 previously directly absorbed by the feedstock growth from which the BFs are produced: this emission is referred to as biogenic CO2 [19] and it is generally considered with a null climate change potential [20].
- Synfuels are produced starting from the CO2 previously captured in other processes (such as power plants with CO2 sequestration systems) [21], and their combustion emits the same amount of CO2 needed to produce them [15].

As described in Section 1, the mix between fossil fuels and LCFs can be modeled in ESOMs through the so-called FTs. When this mix occurs, the CO2 emissions due to the consumption of the sector-specific commodities produced by the FTs are lower than in the case of pure sectorial fossil fuel, for the reasons just described. While this cannot be accounted for in a static emission computation scheme, which is based on fixed and constant CEFs (see Fig. 3a), the dynamic methodology proposed in this work is capable to consider the avoided CO2 emissions from LCFs. The logic behind it is sketched in Fig. 3b. One energy unit of mixed hydrogen or biofuels avoids net CO2 emissions due to the consumption of one energy unit of the sector-specific commodity made of both the fossil and the low-carbon components. Note that the energy commodities entering the fuel technology are in turn produced by specific processes in the supply-side sector, here omitted except for the CO2 used for the synfuel production in the Carbon Capture Utilization and Storage (CCUS) sector. Indeed, the synfuels fraction eventually mixed would produce an amount of CO2 equal to the one used to produce those fuels, namely "Input CO2 for synfuel" in Fig. 3.

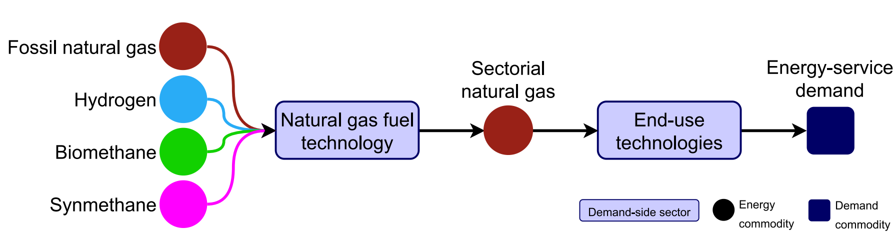

Fig. 1. Example of fuel technology for the production of a sectorial natural gas commodity from a mix of fossil natural gas, synthetic methane, biomethane and hydrogen in the natural gas network. The energy commodities entering the natural gas fuel technology are in turn produced by specific processes in the supply-side sector, here omitted.

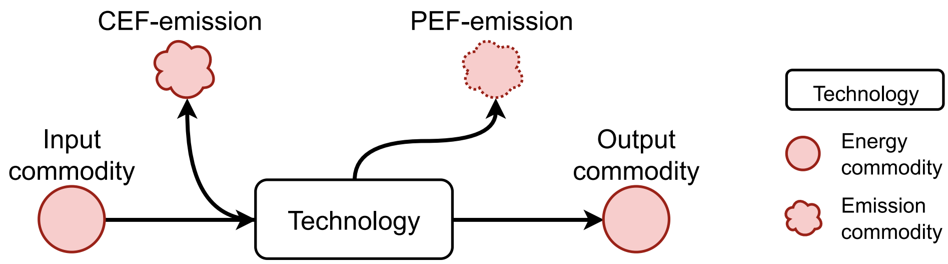

Fig. 2. Application of process-specific emission factor PEF (cloud with dashed line) and commodity emission factor CEF (cloud with solid line) to a generic technology and its input energy commodity.

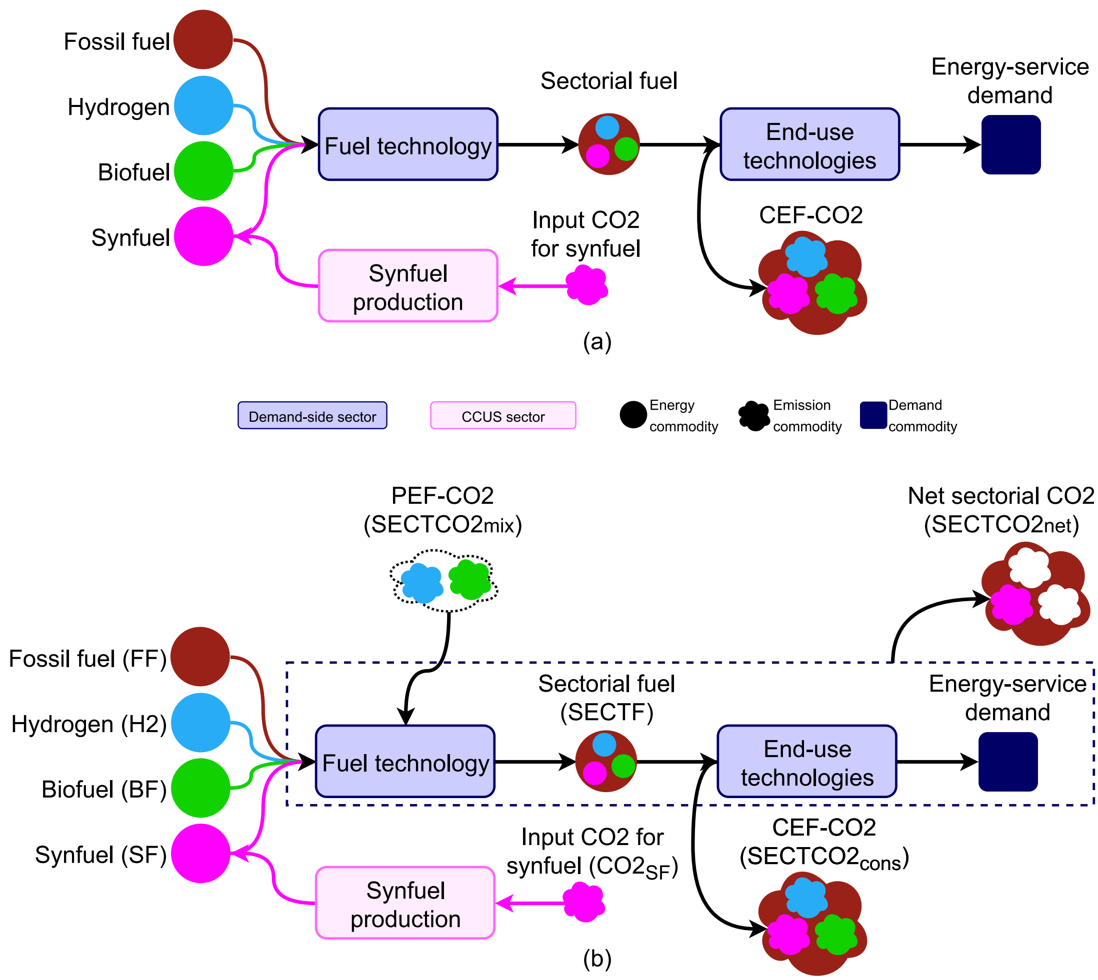

Fig. 3. Sketch of the application of commodity emission factors (CEFs) and process emission factors (PEFs) to a generic fuel technology producing a sectorial fuel from fossil fuels, hydrogen, biofuel and synfuel, for both the (a) static and (b) dynamic accounting methods. The brown cloud depicts the CO2 emissions from the consumption of the sectorial fuel, while the smaller clouds represent the CO2 fractions associated to the low-carbon fuels (with corresponding colors). In (b), the generic demand-side sector borders are depicted with a blue dashed box, while the nomenclature adopted in the equations used to describe the dynamic methodology are put in parentheses. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

2.2. The dynamic CO2 emission accounting method

In a static emission accounting approach, CEFs and PEFs are combined to obtain the overall emission level for technology according to Eq. (1), where: $Emission_{e,t,i,o}$ represents the global emission from technology t of the emission commodity e associated to the input commodity i and output commodity o; $Flow^{in}_{t,i,o}$ and $Flow^{out}_{t,i,o}$ are the consumption of the commodity i by technology t producing commodity o and the production of commodity o by technology t consuming commodity i, respectively. The following equations are valid for a technology t consuming and producing only one commodity i and o, respectively: in case of more than one input/output commodity, the sum of both the CEF and PEF contributions would be needed for each commodity flow.

$$Emission_{e,t,i,o}[kt] = CEF_{e,i}\left[\frac{kt}{PJ}\right] \cdot Flow^{in}_{t,i,o}[PJ] + PEF_{e,t,i,o}\left[\frac{kt}{act}\right] \bullet Flow^{out}_{t,i,o}[act] \tag{1}$$

The dynamic accounting method proposed here accounts for LCFs mixing contribution to CO2 emissions reduction, envisaging the addition of PEFs assigned to sectorial FTs. Fig. 3 shows the accounting of CO2 emissions in a generic demand-side sector due to the consumption of a sectorial fuel, resulting from the mix between fossil fuel and LCFs. Note that the CO2 emissions produced in the supply-side sectors are here omitted, since they are useless for the methodology description The following equations describe the same dynamic accounting method.

The total net sectorial CO_2 emissions $SECTCO2_{net}$ due to the consumption of the sectorial fuel *SECTF* is shown in Eq. (2):

$$SECTCO2_{net}[kt] = SECTCO2_{cons}[kt] + SECTCO2_{mix}[kt] \tag{2}$$

Two terms contribute to $SECTCO2_{net}$:

I. The emission at end-use consumption level $SECTCO2_{cons}$ (see Eq. (3)), corresponding to the emissions due to combustion processes, proportional to *SECTF* consumption through its commodity emission factor CEF_{st}, provided a priori as model input. Indeed, that $SECTCO2_{cons}$ would be the only contribution to $SECTCO2_{net}$ in the case of static emission accounting.

$$SECTCO2_{cons}[kt] = SECTF[PJ]\cdot CEF_{st}\left[\frac{kt}{PJ}\right] \tag{3}$$

II. The emissions resulting from the mix of fossil fuels and LCFs, namely $SECTCO2_{mix}$ (see Eq. (4)), to account for the avoided emissions due to, and proportional to, the consumption of hydrogen H2 and biofuels BFs. A PEF equal and opposite to CEF_{st} is here imputed to the FT producing *SECTF* (indeed, the arrow verse $SECTCO2_{mix}$ in Fig. 3 is entering the FT): since the PEF refer to the output of a technology (see Eq. (1)), the efficiency η_{FT} of the FT is included to account for possible transmission and distribution losses in the FT itself.

$$ECTCO2_{mix}[kt] = \eta_{FT}[-]\cdot\left(-CEF_{st}\left[\frac{kt}{PJ}\right]\right)\cdot(BF[PJ]) \tag{4}$$

E The definition of η_{FT} is shown in Eq. (5), where the term *LCF* represents the sum of all the LCFs mixed in the FT (namely H2, BF, and SF).

$$\eta_{FT}[-] = \frac{SECTF[PJ]}{(FF[PJ] + LCF[PJ])} \tag{5}$$

Based on Eqs. (3)–(5), $SECTCO2_{net}$ can be rewritten as in Eq. (6), where the CEF_{st} is associated only to the portion of fossil fuel *FF* and synthetic fuel *SF* mixed in the specific sectorial fuel *SECTF*. Hence, the dynamic methodology allows to account for the avoided CO2 emissions due to the mixing of hydrogen and biofuels: as already described in Section 2.1, the fraction of CO2 associated to the mixed synfuel equals the amount of CO2 needed to produce the synfuel itself (see Eq. (7)).

$$SECTCO2_{net}[kt] = \eta_{FT}[-]\cdot CEF_{st}\left[\frac{kt}{PJ}\right]\cdot(FF[PJ] + SF[PJ]) \tag{6}$$

$$CO2_{SF}[kt] = \eta_{FT}[-]\cdot CEF_{st}\left[\frac{kt}{PJ}\right]\cdot SF[PJ] \tag{7}$$

Finally, a dynamic emission factor CEF_{dyn} associated to the sectorial fuel can be defined from the ratio between $SECTCO2_{net}$ and *SECTF*, resulting in Eq. (8).

$$CEF_{dyn}\left[\frac{kt}{PJ}\right] = CEF_{st}\left[\frac{kt}{PJ}\right]\cdot(1 - f_{H2} - f_{BF}) \tag{8}$$

In the case of hydrogen and biofuel mix, the value of CEF_{dyn}, computed according to the proposed dynamic accounting methodology is lower than the corresponding static emission factor by the terms f_{H2} and f_{BF}. The latter are the shares of H2 and BF in the fuel mix that produces *SECTF*, resulting from the optimization process. Hence, using Eq. (8) allows to establish the potential emission reduction due to the possible blending of a certain fraction of hydrogen and/or biofuel a priori (i.e., without running the model to which the methodology is applied), as performed in Section 3.1.

The technical limitations on the possible share of LCFs to contribute to the generation of specific commodities are accounted for in the ESOM framework in the form of suitable constraints. According to [6], the existing methane transmission and distribution networks can accept hydrogen injection in pipelines up to $10\%_{vol}$ and $20\%_{vol}$, respectively, without the need to be retrofitted. Instead, no technical limitations exist for the possible mixing of biomethane and synthetic methane, since they are chemically equivalent to fossil methane [22]. Considering the blending of gasoline with alternative fuels for car fueling, currently, a maximum of $10\%_{vol}$ and $3\%_{vol}$ of bioethanol and methanol (that can be CO_2-based synthetic), respectively, can be managed by conventional gasoline engines in the EU [23,24].

Note that, since the emission factors implemented in ESOMs only represent direct emissions (as already stated in Section 1), the proposed methodology is not intended to be compliant with any Life Cycle Assessment standard ([25–27]), nor Dynamic Life Cycle Assessment [28], nor to represent life-cycle emissions of energy commodities and/or technologies. Indeed, ESOMs evaluate energy system emissions within a very specific time interval, whereas a Life Cycle Assessment aggregates emissions occurring at different phases: production, operation, end of life. To the best of the authors' knowledge, the dynamic methodology presented in this work is a novelty for energy system model instances that account for emissions through commodity and/or process emission factors (a feature shared by most of the available tools for energy system optimization, as discussed in Section 1).

2.3. Low-carbon fuels in the TEMOA-Italy model

The methodology presented above is applied to the TEMOA-Italy [16,17] open-source model, based in turn on the well-consolidated TIMES-Italy model [14,17]. TEMOA-Italy relies on an extended version [29] (in terms of available parameters and constraints) of Tools for Energy Modeling Optimization and Analysis (TEMOA) [30,31], and it is currently used with a capacity expansion approach. The technology-rich database of the TEMOA-Italy model includes also a wide spectrum of technologies belonging to the hydrogen, biofuel, and synfuel value chains: they are integrated within an interconnected multi-sectorial RES, as shown in Fig. 4. The specific version used for this work (both for input data and results from the model) corresponds to the Release 2.0 of TEMOA-Italy [32]. The technology modules for LCFs related to the dynamic methodology presented in this paper are described below.

Fig. 5 shows an overview of the value chain of the hydrogen. It can be produced from fossil fuels, using technologies with or without CO2 sequestration (in the figure referred to as CCS), from biomass and through electrolysis. Also, different storage and delivery options are included, before end-use consumption. Furthermore, the sector coupling potential is considered by modeling the hydrogen-based electricity production, and most importantly for this work, the injection within the current existing methane transmission and distribution infrastructure before the consumption, and the production of CO2-based synfuels. The techno-economic characterization of the hydrogen production, storage, and delivery steps is provided in Appendix A-Techno-economic characterization of the hydrogen, synfuel, and biofuel value chains, in Table A1 and Table A2 [33], while the complete database as implemented in the TEMOA-Italy model is available at [32].

The production of synfuels from hydrogen is the linking point in the energy system between the hydrogen module and the so-called Carbon Capture Utilization and Storage (CCUS) module, to which the synfuel value chain belongs. This module is depicted in Fig. 6. The sequestration of CO2 can occur in refineries (Upstream sector), in some hydrogen production processes and power plants (in the figure referred to as "CCS"), and within some industry sub-sectors, such as chemical, iron and steel and non-metallic mineral productions. Moreover, atmospheric CO2 can be directly captured through direct air capture (DAC), a system that leads to negative net emissions [32,34,35]. Once the CO2 is sequestrated, two possibilities arise: storage in depleted gas fields, or utilization to produce synfuels. Then, synmethane, syndiesel, and

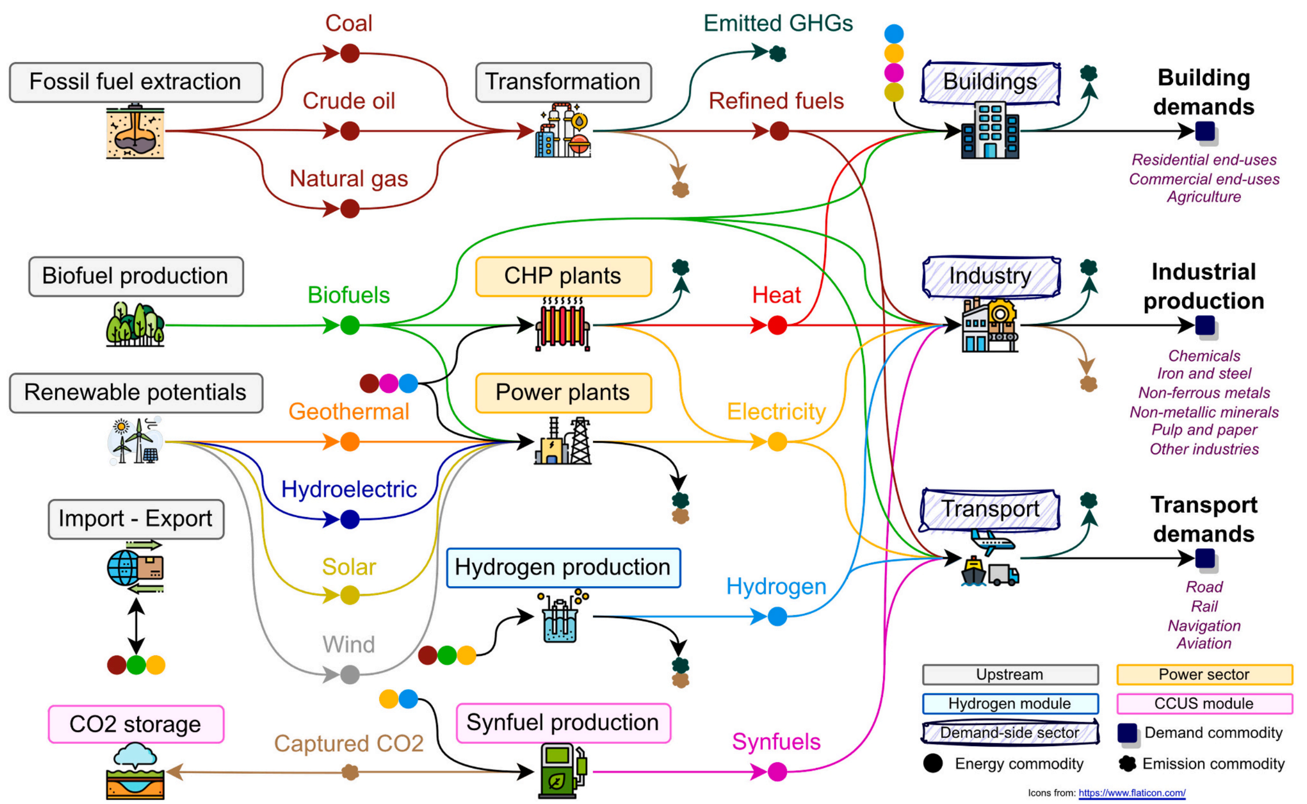

Fig. 4. Reference energy system of the TEMOA-Italy model [16]. The interconnection between the upstream, transformation and demand-side sectors is visualized through energy commodities and arrows which represent the direction of the energy flows. Moreover, the greenhouse gas (GHG) emissions and the Carbon Capture Utilization and Storage (CCUS) module are represented. To make the figure more readable, commodity names are displayed just once and the detail about all the modeled technologies and the end-use demands is omitted.

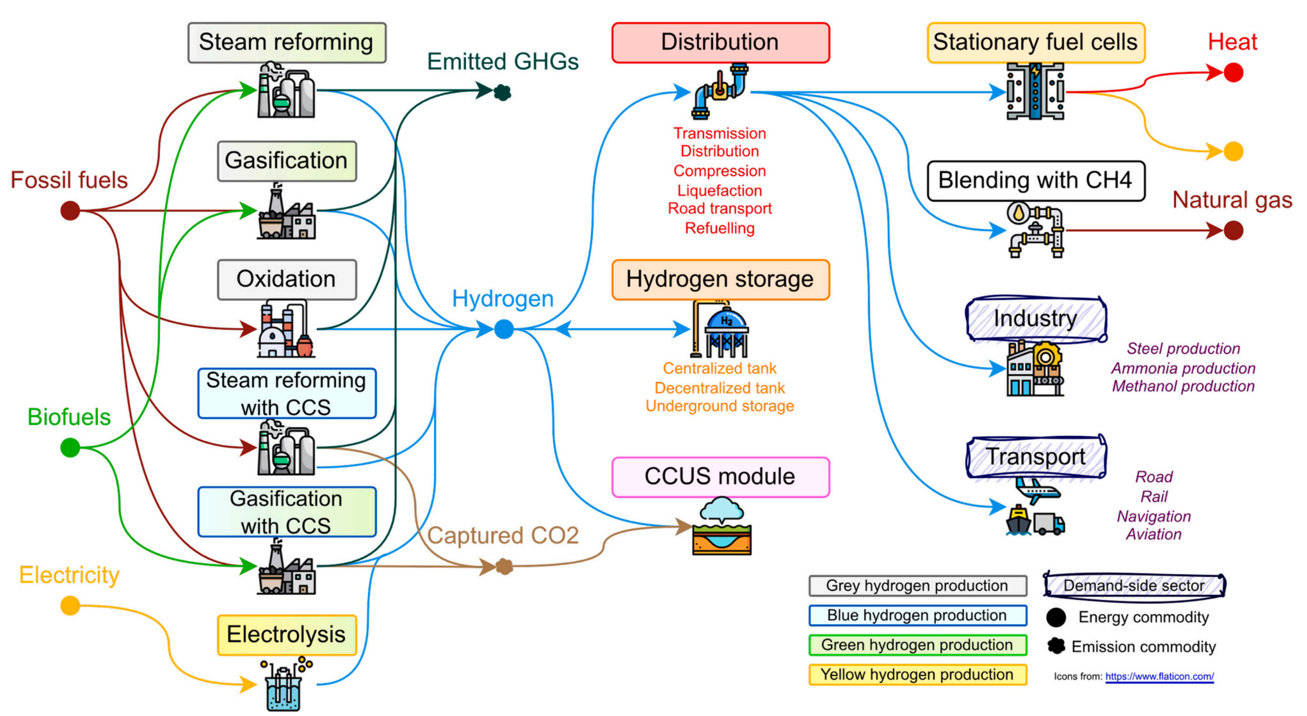

Fig. 5. Hydrogen value chain as modeled in the TEMOA-Italy model [16]. The interconnection between all the steps of the value chain is visualized through energy commodities and arrows which represent the direction of the energy flows. Moreover, the emissions and CO2 capture are represented.

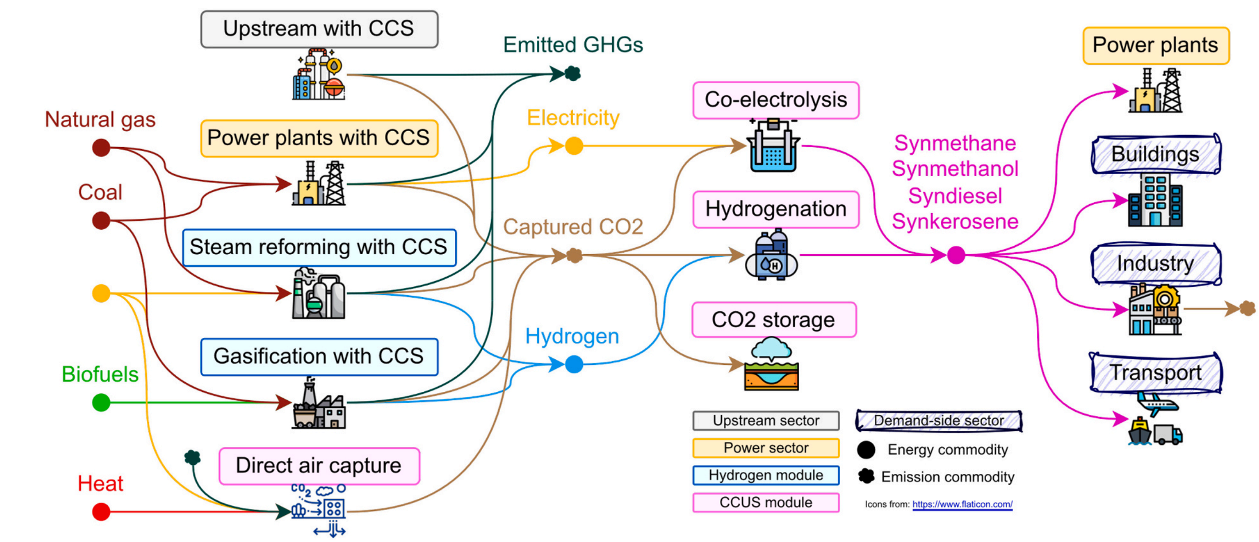

Fig. 6. Carbon Capture Utilization and Storage (CCUS) module of the TEMOA-Italy model [16]. The interconnection between all the steps of the value chain is visualized through energy and emission commodities, and arrows which represent the direction of the commodity flows.

synkerosene can be mixed with the corresponding fossil counterpart, while synmethanol can be used in blends with gasoline. The techno-economic characterization of the SF production technologies is provided in Appendix A-Techno-economic characterization of the hydrogen, synfuel, and biofuel value chains in Table A3 [33], while the complete database as implemented in the TEMOA-Italy model is available at [32].

All the activities related to the so-called Agriculture, Forestry, and Other Land Use (AFOLU) sector with a significant potential of reducing GHGs anthropogenic emissions [36] are currently missing in the carbon sequestration module: that is the case of reducing deforestation, carbon sequestration in agriculture and afforestation [36], considered crucial also in national decarbonization strategies to meet emission reduction targets in the medium-to-long term [37,38]. According to the guidelines of the Intergovernmental Panel on Climate Change (IPCC), CO2 emissions and removals related to biomass value chain processes should be included in the AFOLU sector in national GHG inventories [39]: in the TEMOA-Italy model null CO2-related CEFs are assigned to sectorial BFs, as described in Section 2.1, and this leads to two levels of simplification. First, biomass is considered carbon neutral, even though in recent years there is a rising awareness that biogenic CO2 might have a climate change impact [20,40,41]. Then, being the AFOLU sector is not directly modeled in TEMOA-Italy, there is no distinction between sustainable and unsustainable feedstock management. Another relevant feature of the biogenic CO2 modeling in the model instance concerns the biofuel-based processes with sequestration (also known as Bioenergy with carbon capture and storage (BECCS) [42]), namely solid biomass gasification for hydrogen production (see Table A1) and biomass-based clinkers in the non-metallic mineral sub-sector of the industry. In this regard, in the CCUS sector there is no distinction between fossil and biogenic CO2, according to the IPCC guidelines [39]: hence, being the biomass carbon-neutral, the sequestration of biogenic CO2 leads to negative net emissions, similarly to DAC. Indeed, BECCS and DAC technologies are usually referred to as negative emission technologies (NETs) in many works (e.g., [42–44]). As for the avoided emissions due to hydrogen and biofuel blending, also CO2 sequestration is modeled by applying negative PEFs to the technologies that represent the processes where the capture occurs. Fig. 7a and Fig. 7b show, respectively, the emission modeling rationale for technologies equipped with CO2 sequestration systems (in the figure referred to as *CCS*) excluding BECCS, and for NETs. Considering a technology with a commodity consumption $Flow_{in}$ and a commodity production $Flow_{out}$, three cases can be distinguished:

I. CO2 sequestration, excluding biofuel-based processes (see Eq. (9)): the assigned $PEF_{seq,CCS}$ accounts for only a fraction (i.e., the capture ratio CR) of the CEF-emission, the latter computed through the static CEF_{st} assigned to the input commodity. Then, being the PEFs related to commodity production (see Eq. (1)), the inverse of the technology efficiency is included in the calculation.

$$PEF_{seq,CCS}\left[\frac{kt}{act}\right] = -CEF_{st}\left[\frac{kt}{PJ}\right]\cdot\frac{Flow_{in}}{Flow_{out}}\left[\frac{PJ}{act}\right]\cdot CR\,[-] \tag{9}$$

II. CO2 sequestration through BECCS (see Eq. (10)): the rationale is the same as above, with the difference that in this case no CEF is assigned

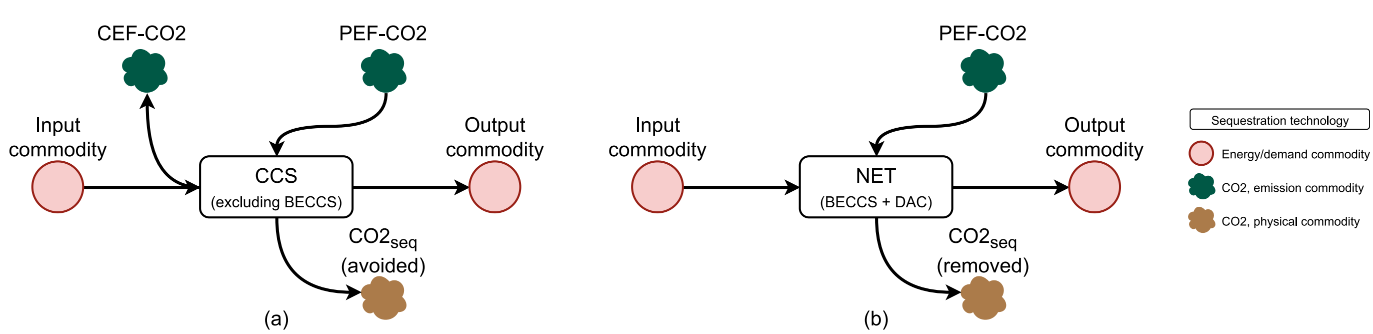

Fig. 7. Modeling of CO2 sequestration in the TEMOA-Italy model [16], through the application of process-specific emission factor PEF and commodity emission factor CEF. The captured $CO2_{seq}$ (where seq stands for sequestration) is the commodity that can be then permanently stored or used to produce synfuels.

to the input commodity, being the latter a biofuel. However, to account for the capture, hence for the negative emission, an emission factor CEF_{bio} is considered only for the calculation of $PEF_{seq,BECCS}$. In particular, in the TEMOA-Italy model CEF_{bio} is assumed to be $112\left[\frac{kt_{CO2}}{PJ}\right]$ according to [39].

$$PEF_{seq,BECCS}\left[\frac{kt}{act}\right] = -CEF_{bio}\left[\frac{kt}{PJ}\right]\cdot\frac{Flow_{in}}{Flow_{out}}\left[\frac{PJ}{act}\right]\cdot CR\,[-] \tag{10}$$

III. CO2 sequestration through DAC (see Eq. (11)): in this case, the PEF indicates the amount of CO2 needed to produce the Flow_{out}, which can be a synfuel production or only CO2. In the latter, the $\mathrm{PEF}_{seq,DAC}$ would be unitary (that is the case of DAC systems without a CO2 onsite utilization).

$$PEF_{seq,DAC}\left[\frac{kt}{act}\right] = -\frac{Flow_{in}}{Flow_{out}}\left[\frac{kt}{act}\right] \tag{11}$$

In all cases I-III, the captured CO2 becomes the physical flow $CO2_{seq}$ (see (12)), which can be stored or used to produce synfuels. The CO2 sequestration modeling approach with CEFs and PEFs and the BECCS negative emission accounting are also used in other energy system models, such as [2,3,45,46].

$$CO2_{seq}[kt] = -PEF_{seq}\left[\frac{kt}{act}\right]\cdot Flow_{out}[act] \tag{12}$$

The biofuel value chain of the model instance is simpler than the hydrogen and synfuel ones, and it is depicted in Fig. 8. Five types of biofuels can be internally produced: solid biomass, industrial and municipal waste, biogas, biodiesel, and bioethanol (techno-economic data from [14,47]). The last two, together with solid biomass, can also be traded (market prices from [2,48]). There is only a primary production step for all biofuels, except for biogas, that can also be upgraded into biomethane, through a process in which CO2 is separated (techno-economic data from [49]). Finally, biofuels can be consumed as pure fuels (e.g., biogas power plants, biomass boilers), or mixed with fossil fuels in the latter case, it is assumed that biomethane, bioethanol, and biodiesel can be blended with natural gas, gasoline, and gas oil, respectively.

Table 1 shows which LCF can be mixed for each sector and fossil fuel modeled in the TEMOA-Italy model. Besides all the demand-side sectors, also the power production sector – including combined heat and power (CHP) plants – which is a supply-side sector, is involved in the dynamic accounting (as far as the natural gas chain is concerned). Furthermore, only natural gas, transport gas oil, and gasoline can be mixed with at least one among hydrogen and biofuels, leading to a dynamic CEF (see Eq. (8)) in case of an actual mixing. The choice of the mixing alternatives is taken from [2,3,45].

2.4. Definition of the analyzed scenarios

The dynamic methodology is tested in the TEMOA-Italy model [32] with two different approaches, corresponding to two different energy scenarios. First, the static and dynamic emission accounting schemes are compared in a base scenario [17], that is meant to assess a possible business-as-usual evolution of the Italian energy system, without any emission reduction constraint. For this reason, the optimization process is not affected by the dynamic methodology: in this regard, while the results on energy consumption should be the same for both the static and dynamic counting, on the other hand, an overestimation of the emission by the static methodology in case of LCF blending can be expected. This comparison is presented in Section 3.2. The second test aims to prove the correctness of the dynamic methodology in a situation where it is likely to be “stressed” much more than in a base scenario. For this purpose, a scenario with very stringent CO2 emission limits, namely a decarbonization scenario, is considered: in this case, the optimization process would be highly influenceable by the dynamic scheme, since the LCF blending represents a valuable decarbonization strategy and their potential could be fully exploited. The proper functioning of the methodology is checked in Section 3.3.

The assumptions behind the base scenario are described in [17], while the decarbonization scenario differs only for the emission constraints, as described in the following. They are built in the framework of the Fit for 55 package of the European Commission [50], and of the long-term Italian strategy on GHG emission reduction [37]: in particular, the former provides for a 55% reduction of net GHG emission by 2030, concerning the 1990 levels, while the latter aims to reach a net zero GHG emission target by 2050. For the work, the constraints to the TEMOA-Italy model were considered only for the CO2 emissions, and the adopted values were obtained starting from the national emission inventory provided by the Italian government agency ISPRA [51]. Indeed, the time horizon of the TEMOA-Italy model starts in 2007, while the Fit-for-55 target refers to the 1990 levels: hence, the 2030 target referred to the 1990 ISPRA data was computed (applying the 55% reduction), and then, the difference between the obtained 2030 ISPRA target and the 2007 ISPRA data was applied to the 2007 TEMOA-Italy model result of the base scenario, to get the 2030 model target, that is 194,208 kt. The same rationale was applied to compute the 2050 model target, but

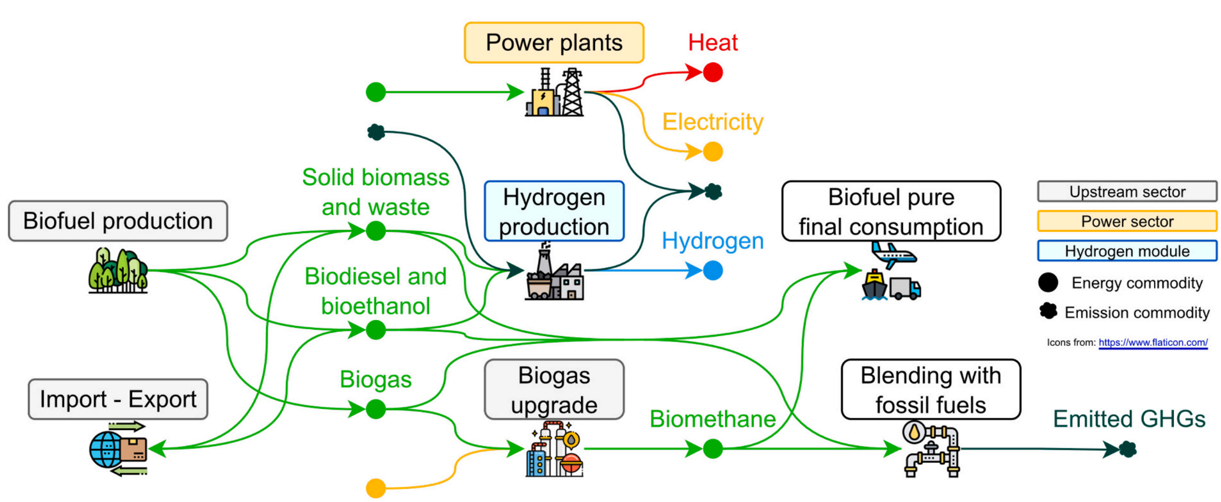

Fig. 8. Biofuel value chain modeled in the TEMOA-Italy model [16]. The interconnection between all the steps of the value chain is visualized through energy commodities and arrows which represent the direction of the energy flows.

Table 1
Qualitative description of the mixable low-carbon fuels with fossil fuels by sector and by fuel in the TEMOA-Italy model instance [32].

Sector	Fossil fuel	Mixable low-carbon fuels							
		Hydrogen	Biomethane	Biodiesel	Bioethanol	Synmethane	Syndiesel	Synkerosene	Synmethanol
	Natural gas	X	X			X			
Agriculture	Gas oil						X		
	Gasoline								X
Commercial	Natural gas	X	X			X			
Residential	Natural gas	X	X			X			
	Natural gas	X	X			X			
	Gas oil			X			X		
Transport	Gasoline				X				X
	Aviation Gasoline								X
	Jet kerosene							X	
	Natural gas	X	X			X			
Industry	Oil						X	X	
	Naphtha								X
Power production	Natural gas	X	X			X			

considering instead the national emission reduction strategy [37]: in this case, the 2007–2050 emission reduction trend of [37] (about 94%), was applied to the 2007 model instance result of the base scenario, to get the 2050 model target, that is 28,742 kt. In accordance with [37], this value is not null, since it is assumed that these residual emissions can be compensated by the removals of the AFOLU sector, which is not currently modeled in TEMOA-Italy, as described in Section 2.3. Fig. 9 shows the CO2 emissions resulting from the base and the decarbonization scenario, the latter referred to as Fit55-Net0, recalling the rationale behind its implementation. The results are the same for the past years, between 2007 and 2022, thanks to the model calibration carried out against the historical energy consumption, with a tolerance of ±5%. Then, since 2025, the effect of the imposed constraints arises: the latter were put only for 2030 and 2050, while for the years in between the values are linearly interpolated by the model. As expected, for the involved years, the results are equal to the imposed constraints. Moreover, the historical data from ISPRA [51] were plotted, too, showing almost a perfect overlapping with the model results, unless for almost 5% differences in the period 2014–2018: this is another indication of the effectiveness of the calibration performed on TEMOA-Italy.

In the definition of the above-described energy scenarios, the modeling approach for the maximum blending rates consists of gradually increasing shares, starting from the present situation (being the model calibrated against historical data until 2020) up to the end of the time horizon, that is 2050 in the TEMOA-Italy model, to avoid possible

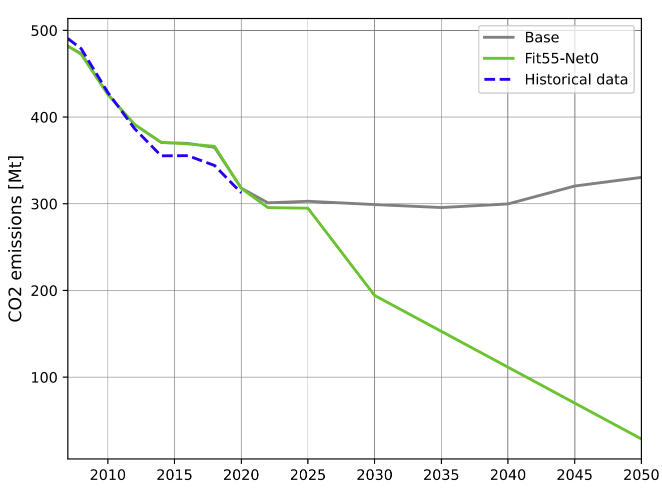

Fig. 9. Comparison between the CO2 emission results in the base and decarbonization (namely Fit55-Net0) scenarios implemented in the TEMOA-Italy model [32], and the historical data from ISPRA [51].

Table 2
Constraints on maximum blending share (in energy terms) of low-carbon fuels applied in the TEMOA-Italy model [32].

Low-carbon fuels	Maximum share			
	2020	2025	2030	2050
Hydrogen	1%	2%	6%	6%
Biomethane	0.2%	1%	5%	100%
Biodiesel	7%	–	–	30%
Bioethanol	7%	–	–	15%
Synmethanol	0%	0%	3%	3%
Other synfuels	0%	0%	5%	100%

unrealistic and sudden mixing, remaining compliant with the blending limitations in the existing infrastructures. In this regard, the values and trends from 2020 to 2030 are shown in Table 2, and they are assumed based on the present penetration of these LCFs and the middle-term perspectives. Hydrogen blending into natural gas existing infrastructure is currently tested through spatially limited demonstration projects from 5% up to 20% in volume [7]: as an example, in 2019 Italy tested from 5% to 10% in volume in a very small city in the southern country, while other projects are in the pipeline for the coming decade [7,52]. For this reason, maximum energy limits of 1% in 2020 and 2% in 2025 are assumed to be realistic constraints, while the maximum content of hydrogen is fixed at 6% in energy terms from 2030, corresponding to about 20% in volume [53] (the conversion from volume to energy units is performed according to [2]), as already explained in Section 2.2. The limits adopted for biomethane were chosen according to the following assumptions. Currently, the fraction blended with methane is about 0.2% of the total natural gas consumption in Italy [54]. Then, in a recent analysis carried out by the Italian Transmission system operator TERNA and the main Italian gas transport and storage operator SNAM, biomethane and hydrogen would contribute up to about 11% of gas demand in 2030, while meeting the Fit-for-55 European carbon emission reduction targets [55]. Instead, the maximum possible content of biomethane in the natural gas distribution network is assumed to be 100%, being its molecule chemically equal to the fossil methane ones, as discussed in Section 2.2. The maximum limits for biodiesel and bioethanol are assumed considering the European quality of petrol and diesel fuels used for road transport in recent years [56], and the future regulatory indications [57–59] (the conversion from volume to energy units has been performed according to [60]). Furthermore, also minimum constraints are imposed, based on the Italian present penetration of these biofuels into transport fuel blends [54], and on the minimum legislative requirements [59]: for biodiesel, the minimum limits are 6.5% in 2022 and 10% in 2050; for bioethanol, the minimum limits are 0.3% in 2022 and 3% in 2050. According to the JRC modeling in [2], synfuel production technologies would start to be commercial by the end of this decade, with the European and Italian targets aligned for the long-term [8,61]: accordingly, the maximum imposed share for synfuels is 5% in 2030, while 0% before. Synmethanol represents an exception, as already described in Section 2.2. The constraints on maximum and minimum blending shares just described, are only put for some reference year and then linearly interpolated.

3. Results and discussion

The results of the application to the TEMOA-Italy model of the CO2 emission dynamic accounting methodology are presented as follows. First, the static and dynamic methodologies are compared in terms of CEFs in Section 3.1 and in a base scenario in Section 3.2. Then, the correctness of the dynamic accounting scheme is assessed in Section 3.3 in a decarbonization scenario. The latter results are deepened in Section 3.4, providing insights about the possible decarbonization role of low-carbon fuel blending. Finally, the relevance of the results is discussed in Section 3.5.

3.1. Potential emission reductions from low-carbon fuel blending

This section compares the dynamic CEFs for natural gas, gas oil, and gasoline associated with different percentages of biofuels and hydrogen (the latter in the case of blending with natural gas) against the static CEFs, being those fossil fuels the only ones with dynamic CEF, as shown in Table 1 and according to Eq. (8). As explained in Section 1, the static CEFs are strictly dependent on the carbon content of fuels. The CO2 static emission factors are taken from [39] and are 56.10$\left[\frac{\text{kt}}{\text{PJ}}\right]$ for natural gas, 74.07 $\left[\frac{\text{kt}}{\text{PJ}}\right]$ for gas oil, and 69.03 $\left[\frac{\text{kt}}{\text{PJ}}\right]$ for gasoline.

Even if the dynamic CEFs are not known a priori, since they are not inputs to the model, but dependent on the optimization process, the comparison can be carried out without running the model thanks to Eq. (8). Indeed, according to mixing share constraints applied to hydrogen and biofuels, it is possible to know to which extent these LCFs can contribute to the reduction of the CO2, as described in the following.

Fig. 10a shows the resulting dynamic emission factor associated with natural gas, by varying the percentage content of biomethane or hydrogen, against the constant in-time static CEF. As expected, the dynamic emission factor is linearly decreasing with increasing contents of biomethane and hydrogen. Considering the assumed maximum mixing shares (shown in Table 2) the CO2 emission reduction potential of injecting H2 into methane pipelines appears to be very low compared to the biomethane one. However, the optimal mixing of these LCFs is affected by their entire value chains structure, and not only by the share constraints: for example, hydrogen can be used to produce synthetic methane, that can be mixed with fossil methane without any limitations [62]; then, biomethane potential depends on the biomass resource availability (e.g., organic fraction of the municipal solid waste [63]) and the biogas upgrading plants, but only a small fraction of this potential is currently exploited [64].

Fig. 10b shows the static CEFs for gas oil and gasoline, and the dynamic CEFs for different percentages of biodiesel in gas oil and bioethanol in gasoline, up to 30% and 15% in energy, respectively. These maximum limits are based on the current and future European regulatory indications, as described in Section 2.4: the maximum share of biodiesel allows to have lower CO2 emissions per energy unit in gas oil vehicles compared to the ones fueled by gasoline blended with bioethanol.

3.2. Comparison between static and dynamic emission accounting in a base scenario

The static and dynamic methodologies are here compared analyzing the net CO2 emissions resulting from the consumption of gas oil in the Italian transport system in 2030, shown in Fig. 11, and computed using the model instance, in a base scenario [17]. Focusing on the gas oil consumption in the transport end-use sector, the biodiesel fraction in gas oil blends is 7.5% in 2030 (about 66 PJ), which is equal to the minimum constraint for biodiesel (interpolating between the constraints above-discussed of 6.5% in 2020 and 10% in 2050), and it is a value slightly higher than the current blending fraction of about 6% [54], in accordance to the business-as-usual evolution expected in a base scenario. As anticipated in Section 2.4, the expectations on the results are met here: while the results about energy consumption are the same applying both the static and dynamic methodology, the ones on CO2 emissions are different, Indeed, the CO2 emissions are allocated both to the fossil component (orange bar) and the low-carbon component (green bar) when considering static CEFs. Instead, by applying the dynamic counting, biodiesel contribution to the composition of transport gas oil reduces total CO2 emissions coming from gas oil consumption in the

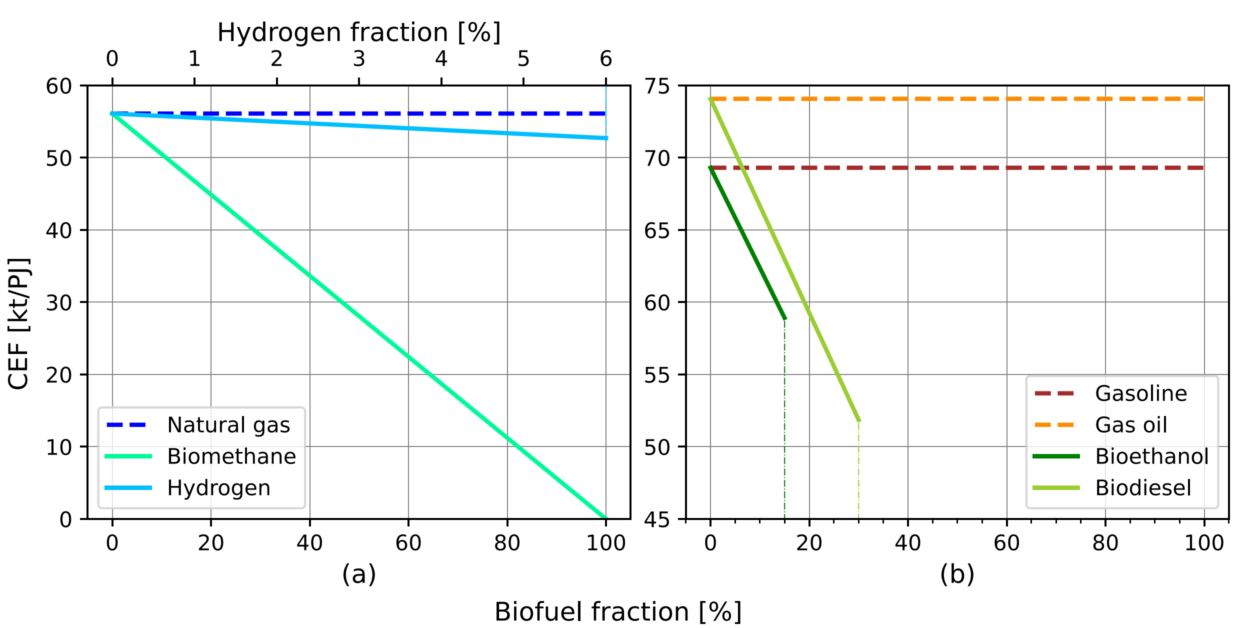

Fig. 10. Static (dashed line) and dynamic (solid lines) commodity emission factor (CEF) for natural gas (a) and gas oil and gasoline (b) associated to different percentage contents of low carbon fuels.

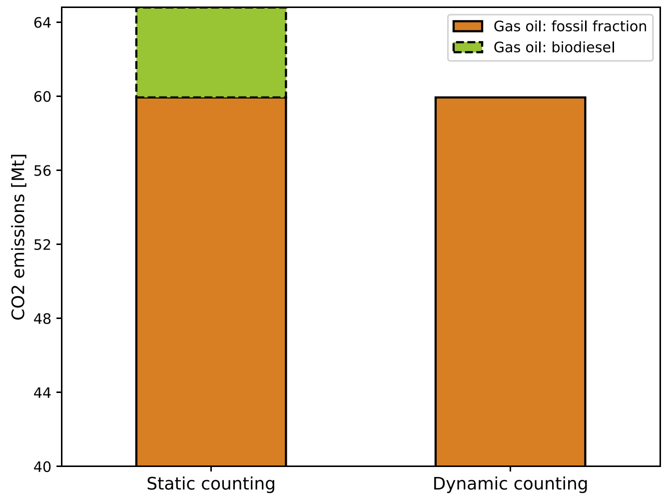

Fig. 11. Comparison between static and dynamic accounting of net CO2 emissions for gas oil consumption in the Italian transport sector in 2030, in a base scenario [17] studied through TEMOA-Italy [32].

transport sector by 7.5% (almost 5 Mt), a value equal to the share of biodiesel in gas oil: this result demonstrates how the static counting methodology leads to overestimation in the calculation of sectorial CO2 emissions, and hence of the total net CO2, being them the sum of all the sectoral emissions. When LCF penetrates in the energy mix through blending, the static accounting scheme provides wrong results in terms of emission balance, directly affecting the optimization problem in case of constraints on CO2 emissions (e.g., reduction targets, carbon tax). From this perspective, it can be stated that a dynamic counting is necessary in ESOMs when modeling the blending of LCFs.

3.3. Assessment of the dynamic accounting method in a decarbonization scenario

The decarbonization scenario described in Section 2.4 is used to check the correctness of the dynamic accounting methodology. For this purpose, as a sanity check, the results on CO2 emissions (a direct result of the emission levels performed by the model) should equal the expected outcomes of the dynamic methodology, manually computing the emissions through the energy results and the dynamic methodology equations described in Section 2.2. This assessment is performed looking separately at hydrogen and biofuels, and synfuels. Indeed, while the contribution to the CO2 emissions of blending hydrogen and biofuels is directly accounted for at the sectorial level (as described in Section 2.2), the contribution of blending the synfuels is accounted for at the overall system level, with sequestration of the CO2 eventually used to produce them, that can occur in different sectors (as described in Sections 2.2 and 2.3).

For hydrogen and biofuels, the dynamic accounting method properly works if the dynamic CEF associated with certain sectorial fuel and computed through Eq. (8) (from now on referred to as CEF_{dyn} from methodology, i.e., the expected outcome of the methodology) equals the ratio between the CO2 emissions associated to the consumption of the sectorial fuel and the consumption of the sectorial fuel itself (from now referred to as CEF_{dyn} from results, i.e., the direct result of the emission counting performed by the model). For the above-described reasons behind the separate checks between hydrogen and biofuels from one side, and synfuels from the other one, the CO2 emissions from the sectorial fuel are gross with respect to eventual consumption in processes with sequestration, that is the case of natural gas for the industry and power sectors. The sectorial fuels considered here are the ones in which blending with hydrogen and/or biofuels can occur, according to Table 1: they are transport gas oil, transport gasoline, and natural gas consumed in all the demand-side sectors and for power production. The results of the check are summarized in Table 3 and Table 4 for natural gas, and transport gas oil and gasoline, respectively. It is shown that the dynamic methodology correctly works for all involved sectorial fuels, and along the whole time horizon, for all the modeled time periods (also known as "milestone years"), since the dynamic CEF directly computed from results (i.e., the row "$CEF_{dyn}\left[\frac{kt}{PJ}\right]$ from results"in Table 3 and Table 4) is exactly equal to the one expected by manually computing dynamic from static CEF with Eq. (8) (i.e., the row "$CEF_{dyn}\left[\frac{kt}{PJ}\right]$ from methodology" in Table 3 and Table 4). Moreover, the tables show the consumption of the sectorial fuels and the CO2 emissions associated with its consumption (net for what concern the blending of hydrogen and biofuels, gross for what concern the eventual subsequent CO2 sequestration), that are used to compute the CEF_{dyn} from results, and the eventually blended LCFs in absolute and share terms, the latter used to compute the CEF_{dyn} from methodology.

In general, biofuel blending starts already in the past years, reflecting the behavior of the historical period, thanks to the energy consumption calibration: then, in future years, the minimum constraints discussed in Section 2.4 are respected. Instead, hydrogen is mixed with natural gas since 2030, even if it can be produced starting from 2020, while synfuels are mixed since 2030, according to the maximum constraints reported in Table 2. About constraints, hydrogen and synmethanol are the only LCFs that reach the maximum allowable blending shares of 6% and 3%, respectively. Among the others, biodiesel and syndiesel represent about 25% and 75% of the transport gas oil since 2045, completely decarbonizing it, while biomethane is the main LCF mixed with natural gas, reaching almost 40% in 2050, followed by about 12% of synmethane. Finally, transport gasoline is the least decarbonized sectorial fuel, with only about 5% of bioethanol (compared to a maximum constraint of 15%) and 3% of synmethanol. Overall, the increasing blending of hydrogen and biofuels along the time horizon leads to the reduction of the commodity emission factors of natural gas, transport gas oil, and

Table 3
Comparison in a TEMOA-Italy [32] Fit55-Net0 scenario between the dynamic commodity emission factor CEF_{dyn} of the sectorial natural gas, directly obtained from results, and the expected one computed by paper-and-pencil from the proposed methodology.

Milestone year	2016	2018	2020	2022	2025	2030	2035	2040	2045	2050
CO2 emissions [kt]	136,411	138,031	124,222	102,969	94,431	68,564	48,648	34,485	27,383	26,650
Natural gas consumption [PJ]	2434	2463	2219	1842	1690	1373	1174	938	834	851
$CEF_{dyn}\left[\frac{kt}{PJ}\right]$ from results	56.1	56.0	56.0	55.9	55.9	49.9	41.4	36.8	32.8	31.3
Hydrogen [PJ]	–	–	–	–	–	82	70	56	50	51
Biomethane [PJ]	2	2	4	6	6	69	236	267	296	325
Synmethane [PJ]	–	–	–	–	–	3	32	49	59	106
Hydrogen fraction [%]	–	–	–	–	–	6.0%	6.0%	6.0%	6.0%	6.0%
Biomethane fraction [%]	0.1%	0.1%	0.2%	0.3%	0.4%	5.0%	20.1%	28.5%	35.5%	38.2%
Synmethane fraction [%]	–	–	–	–		0.2%	2.7%	5.2%	7.1%	12.4%
$CEF_{dyn}\left[\frac{kt}{PJ}\right]$ from the methodology	56.1	56.0	56.0	55.9	55.9	49.9	41.4	36.8	32.8	31.3

Table 4
Comparison in the TEMOA-Italy [32] Fit55-Net0 scenario between the dynamic commodity emission factor CEF_{dyn} of transport gas oil and gasoline, computed from results, and the one computed by paper-and-pencil from the methodology.

Milestone year		2007	2008	2010	2012	2014	2016	2018	2020	2022	2025	2030	2035	2040	2045	2050
Transport gas oil	CO2 emission [kt]	74,932	73,083	75,233	65,715	68,047	71,115	72,465	65,907	65,307	66,220	53,783	47,863	42,374	38,067	46,416
	Final consumption [PJ]	1016	999	1052	956	968	1005	1027	931	943	960	900	828	760	693	832
	$CEF_{dyn}\left[\frac{kt}{PJ}\right]$ from results	73.8	73.2	71.5	68.8	70.3	70.8	70.5	70.8	69.3	69.0	59.8	57.8	55.8	54.9	55.8
	Biodiesel [PJ]	4	12	37	68	50	45	49	41	61	66	174	182	188	179	205
	Syndiesel [PJ]	–	–	–	–	–	–	–	–	–	–	45	162	399	514	627
	Biodiesel fraction [%]	0.4%	1.2%	3.5%	7.1%	5.1%	4.5%	4.8%	4.4%	6.5%	6.9%	19.3%	22.0%	24.7%	25.9%	24.7%
	Syndiesel fraction [%]	–	–	–	–	–	–	–	–	–	–	5.0%	19.6%	52.5%	74.1%	75.3%
	$CEF_{dyn}\left[\frac{kt}{PJ}\right]$ from the methodology	73.8	73.2	71.5	68.8	70.3	70.8	70.5	70.8	69.3	69.0	59.8	57.8	55.8	54.9	55.8
Transport gasoline	CO2 emission [kt]	36,868	35,630	31,060	26,149	25,291	22,922	23,360	16,746	27,511	33,345	36,540	39,084	43,242	45,788	30,388
	Final consumption [PJ]	532	516	452	381	368	333	339	243	399	485	535	576	639	679	461
	$CEF_{dyn}\left[\frac{kt}{PJ}\right]$ from results	69.3	69.1	68.8	68.6	68.8	68.8	68.9	69.0	69.0	68.7	68.3	67.9	67.7	67.4	66.0
	Bioethanol [PJ]	–	2	3	4	3	2	2	1	2	4	8	12	15	19	22
	Synmethanol [PJ]	–	–	–	–	–	–	–	–	–	–	16	16	16	20	14
	Bioethanol fraction [%]	–	0.4%	0.8%	1.0%	0.7%	0.7%	0.5%	0.4%	0.5%	0.8%	1.5%	2.0%	2.4%	2.7%	4.8%
	Synmethanol fraction [%]	–	–	–	–	–	–	–	–	–	–	3.0%	2.8%	2.5%	3.0%	3.0%
	$CEF_{dyn}\left[\frac{kt}{PJ}\right]$ from the methodology	69.3	69.1	68.8	68.6	68.8	68.8	68.9	69.0	69.0	68.7	68.3	67.9	67.7	67.4	66.0

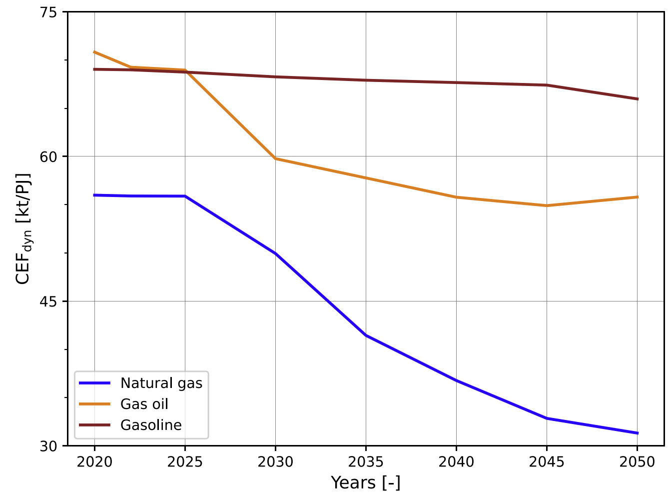

Fig. 12. Evolution of the dynamic commodity emission factor CEF_{dyn} of natural gas, transport gas oil and transport gasoline in the Fit55-Net0 decarbonization scenario studied through TEMOA-Italy [32].

transport gasoline, as shown in Fig. 12. The CEF is almost constant from 2020 to 2025 when the blending shares of LCFs are very low (see Table 3 and Table 4). Then, the largest reduction occurs for natural gas, with about 44%, corresponding to the blended fractions of hydrogen and biomethane: the trend is almost linear, with a slightly decreasing rate of reduction. Instead, transport gas oil is fully decarbonized since 2045, with the highest contribution coming from syndiesel: however, the majority of the CEF reduction occurs between 2025 and 2035, when the biodiesel fraction is still higher than the syndiesel one. As expected, transport gasoline has the lowest CEF reduction, due to the very small fraction of blended bioethanol.

The remaining emissions associated with the consumption of natural gas, transport gas oil, and gasoline are associated both with the fossil component and the synfuel one. However, as explained in Section 2.2 and Section 2.3, the latter fraction is compensated at the production level. For synfuels, the dynamic methodology is considered to be correct if Eq. (7) is satisfied at the system level, hence if the CO2 fraction associated with the blended synfuels (from now on referred to as $CO2_{SF}$ from methodology, i.e., the expected outcome of the methodology) is equal to the CO2 consumed to produce the synfuels (from now on referred to as $CO2_{SF}$ from results, i.e., the direct result of the emission counting performed by the model). Besides the consumption of synmethane in natural gas, syndiesel in transport gas oil, and synmethanol in transport gasoline, the other blending occurs in gas oil agriculture (syndiesel) and industrial oil refined products (syndiesel, synkerosene, and synmethanol). As for hydrogen and biofuels, the methodology is proven to correctly work also for synfuel, as summarized in Table 5. It

Table 5
Comparison in the TEMOA-Italy [32] Fit55-Net0 scenario between the $CO2_{SF}$ from results, disaggregated distinguishing among the different production routes, and $CO2_{SF}$ from methodology, disaggregated distinguishing among the different blending possibilities and referred to as avoided CO2.

Milestone year	2030	2035	2040	2045	2050
CO2 for hydrogenation [kt]	4858	14,991	10,667	6127	5704
CO2 for methanation [kt]	181	1790	2734	3307	5935
CO2 for co-electrolysis	–	–	23,513	38,762	48,274
$CO2_{SF}$ [kt] from results	5039	16,781	36,914	48,196	59,913
Avoided CO2, synmethane [kt]	181	1790	2734	3307	5933
Avoided CO2, syndiesel [kt]	3670	13,802	32,991	43,100	53,020
Avoided CO2, synkerosene [kt]	61	61	61	292	–
Avoided CO2, synmethanol [kt]	1127	1127	1127	1496	958
$CO2_{SF}$ [kt] from the methodology	5039	16,780	36,913	48,195	59,913

shows that $CO2_{SF}$ from results (i.e., the row "$CO2_{SF}$ [kt] from results" in Table 5), disaggregated distinguishing among the different production routes (for more details see Table A3), is the same as $CO2_{SF}$ from methodology (i.e., the row "$CO2_{SF}$ [kt] from methodology" in Table 5), disaggregated distinguishing among the different blending possibilities and referred to as *avoided CO2*. There is a very small difference between the two $CO2_{SF}$ calculation, in the order of 10^{-3}%, hence negligible. This is because the static CEFs associated with the industrial refined oil products and industrial naphtha are slightly different compared to the CO2 needed to produce one unit of syndiesel and synkerosene, which can be mixed with the former, and of synmethanol, that can be mixed with the latter. Indeed, apart from the synfuel fraction, industrial refined oil products are a mix of different fossil fuels, and the related static CEF is computed as an average of the specific fuel CEFs. Then, naphtha and synmethanol are different substances, but they can be mixed according to [2]. In general, from 2030 to 2050 the production of synfuels increases by almost 11 times, and this is reflected also in the CO2 used to produce them, with co-electrolysis as the main production process at the end of the time horizon. Moreover, syndiesel is the most produced synfuel, being also the only one consumed in three different end-use sectors, namely transport, agriculture, and industry. More details on these and other results of the decarbonization scenario are provided in Section 3.4.

3.4. The potential of low-carbon fuels blending in a decarbonization scenario

The results of the Fit55-Net0 scenario are now analyzed in more detail. It is important to highlight that the decarbonization scenario under investigation here is considered a suitable case study to check the functioning of the dynamic CO2 emission accounting methodology, as pointed out in Section 2.4 and Section 3.3, without aiming to address any policy assessment. Hence, by analyzing the potential of LCF blending in decarbonizing the Italian energy system, the following result focus is meant not to derive specific results, but rather to provide possible insights for future ESOM-based policy-relevant studies, that can be carried out thanks to the application of a dynamic emission counting such as the one proposed in this work. The complete set of results is available at [65].

Fig. 13 compares the final energy consumption by commodity of the Base and the Fit55-Net0 scenarios, in the period 2020–2050: the mixing between fossil fuels and LCFs (the latter indicated with (bl) in the legend) is depicted using different filling patterns. In particular, from now on, gaseous fossil fuels, biomethane, and hydrogen will be referred to as gaseous fuel blends, while liquid fossil fuels, liquid biofuels, and liquid synfuels as liquid fuel blends. It is important to highlight that the final energy consumption accounts for the energy consumption in the demand-side sectors, namely agriculture, commercial, residential, transport, and industry sectors (see Fig. 4). The total final energy consumed slightly increases in the Base scenario, from about 4602 PJ to about 4855 PJ, while slightly decreases in the decarbonization one, in which in 2050 the final energy consumption of about 4195 is <8% and < 14% compared to the Fit55-Net0 2020 and the Base 2050, respectively. The latter can be considered a small energy saving result if compared with the EU target of 13% in 2030 compared to a baseline scenario, proposed by the European Commission in the context of the REPowerEU plan [66]. Comparing the energy mixes, while heat and biomass consumptions are almost identical, the following differences arise. In the base scenario, as expected, the current trend is kept almost constant in the future, unless for natural gas, whose consumption decreases between 2020 and 2025, due to the high natural gas prices caused by the Russia-Ukraine conflict. Instead, in the decarbonization scenario, fossil fuel consumption starts to decrease in 2025 in favor of blending with low-carbon fuels. In particular, hydrogen and biomethane fractions reach about 45% of gaseous fuel blend final consumption in 2050, while liquid synfuels and biofuels overcome the fossil fraction with ~67% of liquid fuel blend final consumption in 2050 (with about more than half contribution coming from synfuels). As an overall result, looking at 2050, while in the Base scenario, the gaseous and liquid fuel blends are almost entirely fossil-based, with a 66% share of the final energy consumption, in the decarbonization the share is reduced to 52%, but with the LCF fraction increasing to 60%. Besides LCF blending, fossil fuel final consumption is substituted in the Fit55-Net0 scenario with increasing electrification and the consumption of pure hydrogen. The latter, together with the blended hydrogen, reach a final consumption share of about 7% in 2050, which is quite lower compared to the European and Italian targets of about 14% and 20% in the respective hydrogen strategies [8,61].

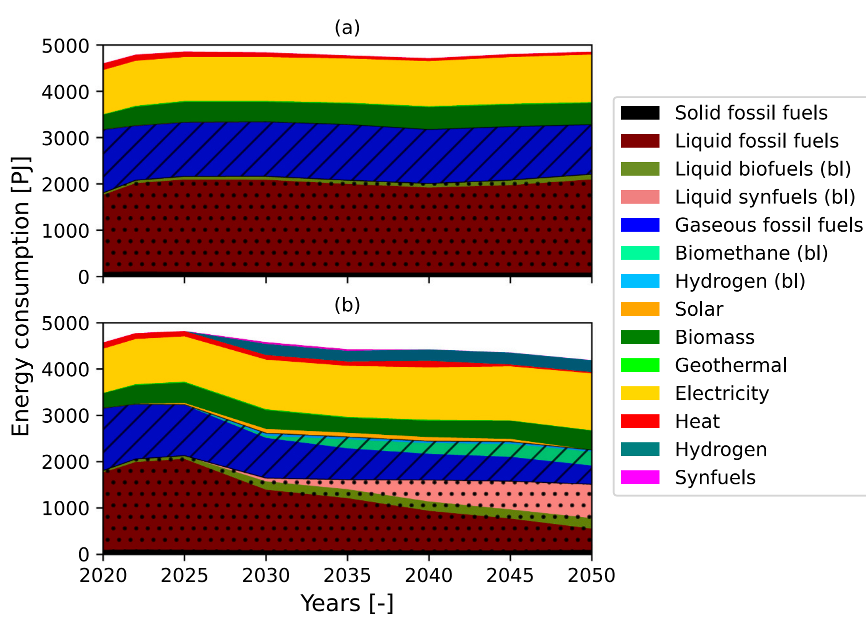

Fig. 13. Evolution of the final energy consumption by commodity in the TEMOA-Italy [32] Base scenario (a) and the Fit55-Net0 decarbonization one (b). The blended low-carbon fuels are referred to as (bl) in the legend. Their mixing with the fossil fuels is visualized through a specific filling pattern (gaseous fuels with diagonal hatches, liquid fuels with point hatches). The complete set of results is available at [65].

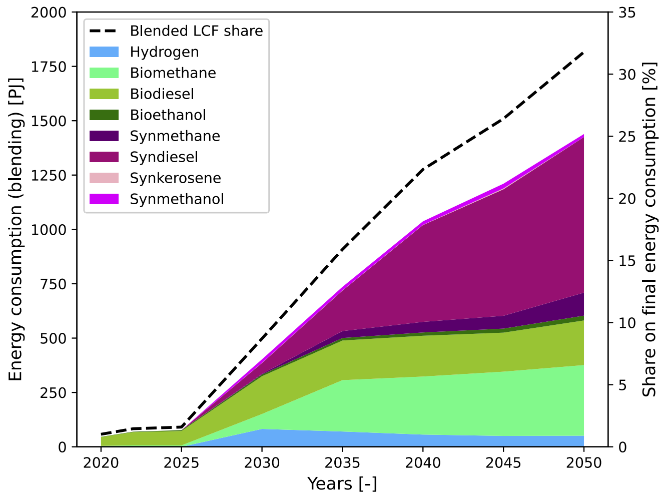

Fig. 14. Evolution of the blended low-carbon fuels (LCFs) in the TEMOA-Italy [32] Fit55-Net0 decarbonization scenario. Both the energy consumption and the overall blended LCF share on the final energy consumption are shown. The complete set of results is available at [65].

The evolution of the blended LCF consumption is shown in Fig. 14: apart from the small consumption of biodiesel and the negligible amounts of bioethanol and biomethane (see Table 3 and Table 4 for more details) between 2020 and 2025, the blending of LCF explodes reaching a share on final energy consumption of, respectively, almost 9% in 2030 and 32% in 2050. In particular, hydrogen blending increases until 2030, and then decreases: this is in accordance with the decreasing gaseous fuel blend consumption depicted in Fig. 13b (the fossil fraction is almost entirely natural gas) and the maximum allowable share of 6% reached by hydrogen in the natural gas blend, as reported in Table 3. Instead, the blended biofuel consumption increases almost six times in the period 2025–2035, passing from 77 PJ to 430 PJ, while increasing less until 2050, up to 552 PJ: the majority of this consumption is biomethane, followed by biodiesel and a marginal fraction of bioethanol. Finally, the blended synfuels experience the largest increases, reaching about 835 PJ in 2050, which corresponds to almost 60% of all the blended LCFs. The most consumed blended synfuel is syndiesel, followed by synmethane and very small fractions of synmethanol and synkerosene. It is important to recall that the blended LCF share does not include the synmethane fraction, since it is mixed with natural gas consumed in the power sector, which belongs to the supply-side sectors of the model instance, and produces electricity and heat, the latter instead included in the final energy consumption results. Overall, the trends of the final blended LCF consumption and the blended LCF share on final consumption are quite similar, since the total final energy consumption does not change a lot in the period 2020–2050, as previously described.

Despite the small improvement in energy savings and the still-present final consumption of fossil fuels, very stringent emission reduction targets are met in the Fit55-Net0 scenario mainly thanks to CCUS and the LCF blending, as depicted in Fig. 15. The picture compares the total CO2 emissions in the Base scenario (Fig. 15a) and in the decarbonization scenario (Fig. 15b), showing also the contribution to the emission reduction of hydrogen and biofuel blending and CO2 storage and utilization. According to Fig. 9, total CO2 emissions are almost identical among the scenarios between 2020 and 2025. Then, the emission constraints discussed in Section 2.4 come into play in 2030, when also the effect of LCF blending, mainly of biofuels, arises, with an emission reduction that is about 14% of the total emitted CO2. That emission reduction contribution linearly increases (in absolute terms) until 2050: the evolution of the different contributions of synfuels, biofuels, and hydrogen reflects their evolution in energy terms shown in Fig. 14, with the hydrogen blending fraction almost negligible if compared to the other contributions. In 2040, the emission reduction due to CCUS (mainly synfuel production) overcomes the contribution of hydrogen and biofuel blending, with the effect of synfuel blending indirectly considered in synfuel production. Then, in 2045, the emission

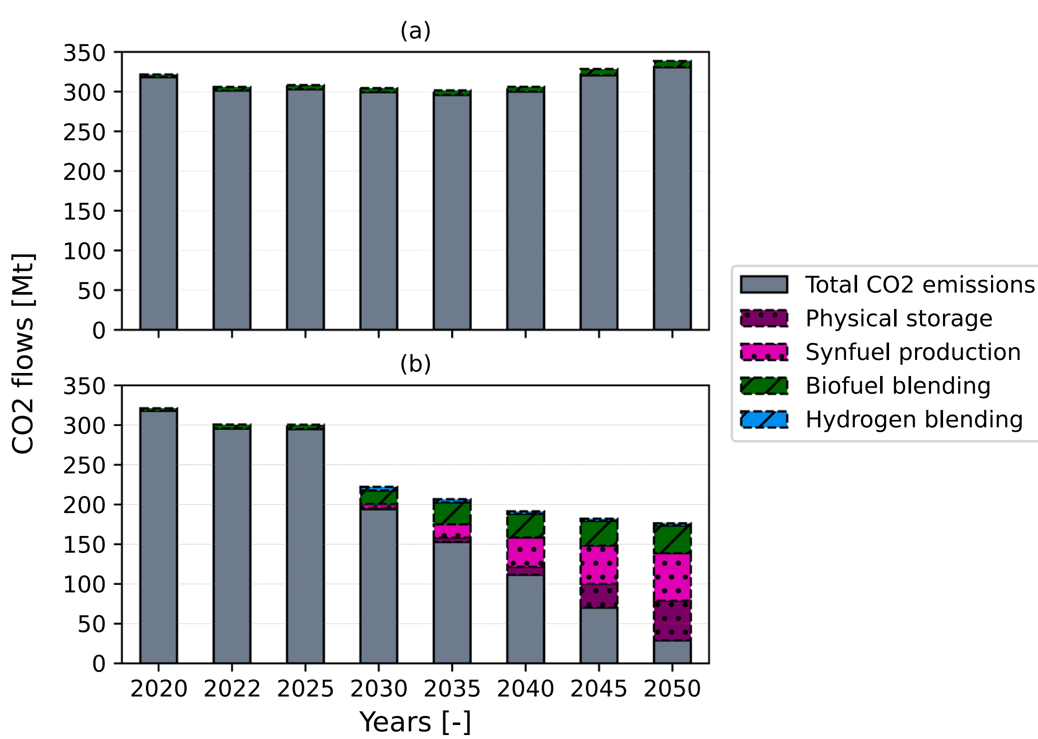

Fig. 15. Total CO2 emissions in the TEMOA-Italy [32] Base scenario (a) and the Fit55-Net0 decarbonization one (b). Moreover, the figure shows the avoided emissions due to biofuel and hydrogen blending (colored bars with diagonal hatches), and the stored and used CO2 amounts (colored bars with point hatches). The complete set of results is available at [65].

reduction becomes higher than the actual CO2 emissions, reaching about 5 times the 28,742 Mt. emitted in 2050: in particular, the CO2 storage and utilization contribute to about 74% of emission reduction. In this regard, the contribution from synfuel production is slightly higher than the one from physical storage.

The CO2 balance is shown from a different perspective in Fig. 16, for the decarbonization scenario. Differently from Fig. 15, the emissions are represented by sector. Furthermore, the CCUS contribution to emission reduction is here depicted distinguishing among the avoided and removed emissions, according to the distinction discussed in Section 2.3. In this regard, the emissions are avoided through capture, excluding BECCS, while they are removed through NETs, namely DAC, and the BECCS processes in the industry (biomass-based clinkers) and upstream (biomass gasification for hydrogen production) sectors. Hence, the balance between the emissions by sector and the removals provides the total CO2 emissions of Fig. 15: then, as highlighted in Section 2.4, the remaining emissions in 2050 are supposed to be compensated through the AFALU sector, reaching net zero emissions in accordance with [37]. Overall, looking at the gross sectorial emissions, namely the total CO2 emissions without considering the removals, the reduction in the period 2020–2050 is about 58% (that is almost equal to the reduction in 2050 comparing the decarbonization scenario with the Base one). However, the reduction does not occur at the same rate during this period. The higher reduction concerns the decade 2020–2030 and is about 39%: in this period, synfuels are not available and the maximum allowable blending shares for hydrogen and biofuels are still low until 2030, according to Table 2. Then, a smaller reduction of 31% occurs in the longer period 2030–2050, when the maximum allowed blending share increases and the synfuels start to be produced. In this regard, the main contribution to emission reduction comes from CCUS, in particular from the NETs. Their role becomes relevant in 2040, in accordance with the International Energy Agency (IEA) Net zero scenario [67]: the CO2 removal allows to still have sectorial emissions in 2050. Indeed the only sector in which an almost complete decarbonization occurs is the commercial one, while for the others there is a partial decarbonization. The power and industry sectors experience the second and third largest emission reduction, respectively, with about −85% and − 80% compared to 2020. Then, the industry and upstream sectors reach a similar emission reduction, without considering the removals: the former, about 53%, the latter about 56%. However, considering also the effect of BECCS, emission reduction slightly increases up to 56% for the industry sector, while negative net emissions are reached in the upstream sector, with about −13 Mt., even if about 6.5 Mt. of CO2 are emitted in 2050. The least decarbonized sectors are agriculture, with a 21% reduction, and transport, with a 28% reduction.

The presence of sectorial CO2 emissions in 2050 is mainly possible thanks to the presence of NETs: indeed, despite the net zero decarbonization target, the remaining CO2 emissions are removed through DAC and BECCS processes. This is in accordance with other decarbonization scenarios [37,67] at least qualitatively. However, compared to the latter, the role of CCUS is much more important in the Fit55-Net0 scenario implemented in the model instance. As a comparison, the emission reduction associated with the CCUS is almost 110 Mt. (see Fig. 15), a result to be further investigated if assessing a policy-relevant study, since that number is more than double if compared to the maximum expected by the Italian decarbonization strategy [37]. Then, all the sectors reach >90% of decarbonization compared to actual levels in the IEA scenario [67], while a lower emission reduction is accomplished in the decarbonization scenario discussed in this section (see Fig. 16). Besides synfuels, also hydrogen and biofuel blending role is important for the emission reduction, with a contribution of about 26% (see Fig. 15). Hence, LCF blending plays a crucial role in reaching the decarbonization targets imposed for the Fit55-Net0 scenario under analysis. In particular, Fig. 17 shows the CO2 emission reduction by blended LCF and by sector. Hydrogen, in Fig. 17a, has the lowest absolute contribution, decreasing from about 4.6 Mt. in 2030 and almost 3 Mt. in 2050. This behavior is in accordance with the energy results shown in Table 3: natural gas consumption decreases along the time horizon, as well as the blended hydrogen fraction, however, is mixed up to the maximum allowable share. Overall, the mainly decarbonized sector is the residential one, where the blend, with those hydrogen shares, can be used in traditional natural gas boilers. Compared to hydrogen, the biofuel contribution, depicted in Fig. 17b, is one order of magnitude higher and increases from 2020 to 2050. According to the results shown in Table 4, almost all the emission reduction occurs in the transport sector until 2030, mainly due to biodiesel blending with gas oil. Then, in 2030 the reduction triples, in connection to the Fit55 target, and the contribution of biomethane starts to become relevant, until

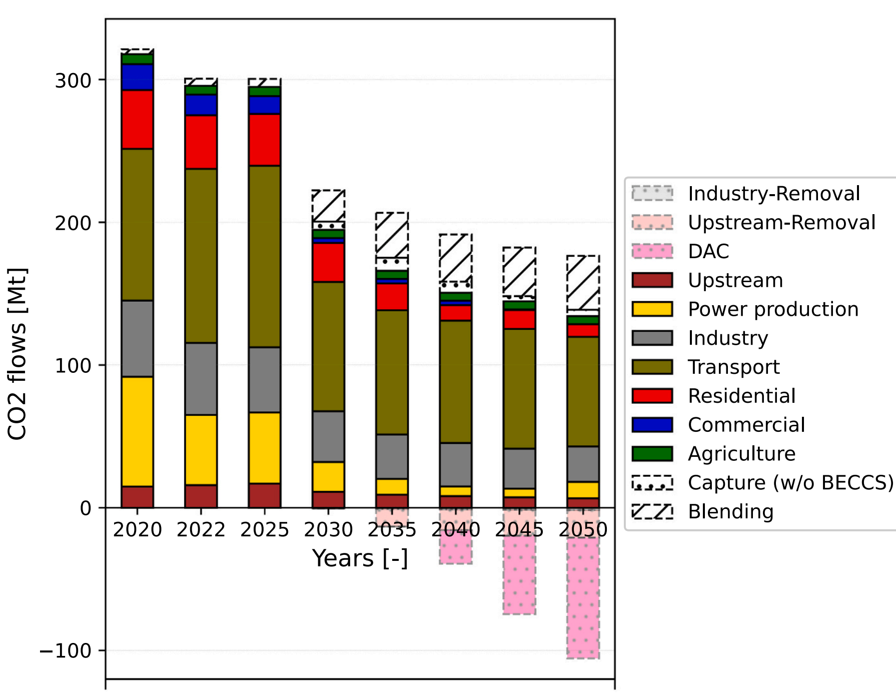

Fig. 16. Actual CO2 emissions by sector in the TEMOA-Italy [32] Fit55-Net0 scenario. Moreover, the figure shows: the avoided emissions due to biofuel and hydrogen blending (white bars with diagonal hatches), and the ones due to capture (white bars with point hatches), the latter excluding biomass-based processes with capture (BECCS); the emission removals through negative emission technologies, hence direct air capture (DAC) and BECCS in industry and upstream sectors (light colored bars with point hatches). The complete set of results is available at [65].

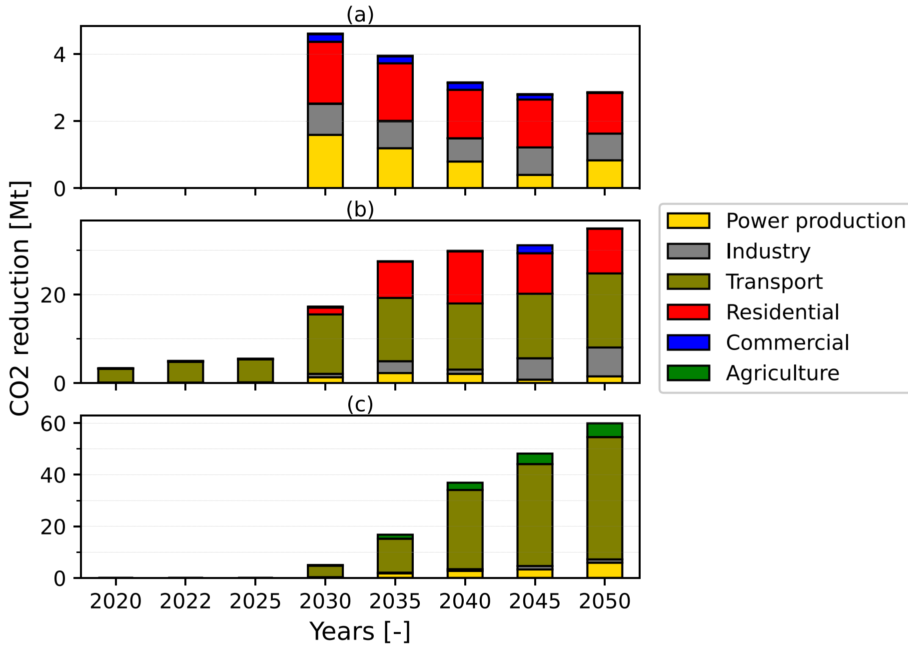

Fig. 17. Evolution by sector in the TEMOA-Italy [32] decarbonization scenario of the avoided CO2 emissions due to hydrogen (a) and biofuels (b), and of the CO2 fraction related to synfuels in blends with fossil fuels (c). The complete set of results is available at [65].

2050 when represents slightly >50% of biofuel contribution to emission reduction. This is due to the higher consumption of biomethane than the other biofuels, in particular almost 60% of the total blended biofuels: the blending contribution is higher than the emission reduction one, due to the higher static CEFs of gas oil and gasoline, respectively 32% and 24% higher than the natural gas one. Moreover, this is reflected in the fact that the most decarbonized sector is the transport one. That is also the case of synfuels in Fig. 17b, for which the highest emission reduction occurs for transport CO2 from 2030 up to 2050, with respectively 90% and 80% of the total reduction due to synfuel blending. The increasing trend of CO2 reduction is perfectly in line with the synfuel blending evolution shown in Fig. 14, dominated by syndiesel, which contributes to the decarbonization of transport and agriculture sectors, and by synmethane, that instead is mixed with natural gas consumed in the power sector.

Transport and agriculture are the sectors in which there is the higher penetration of blended synfuels in the energy mix, following the fact that those sectors are the least decarbonized ones between 2020 and 2050, as discussed before (see Fig. 16). In particular, the agriculture energy mix remains the same from the Base to the Fit55-Net0 scenario, both quantitatively and qualitatively. In the period 2020–2050, the gas oil share decreases from 75% to 69%, almost all compensated by electricity, which increases from 18% to 22%: while in the Base scenario, pure fossil gas oil is consumed, in the decarbonization scenario the latter is

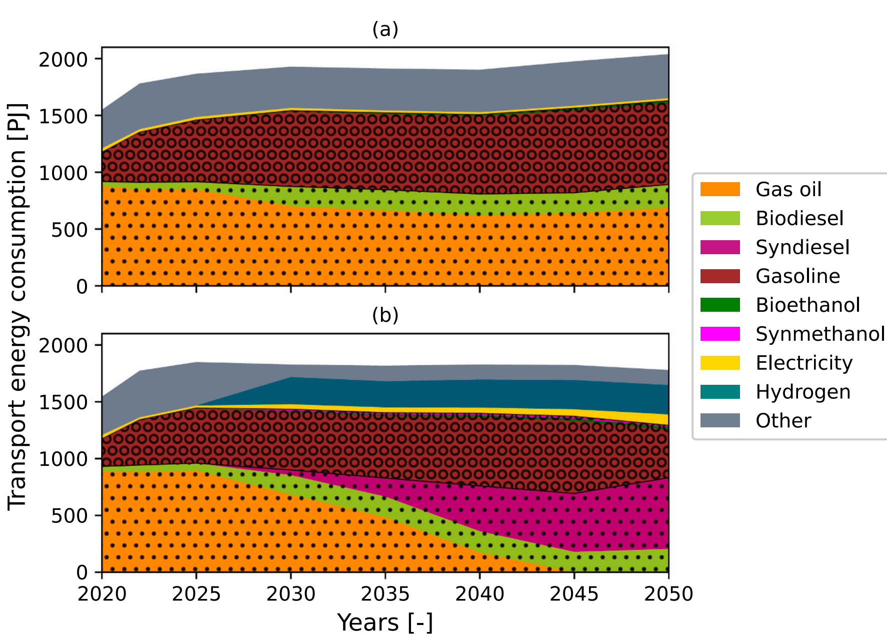

Fig. 18. Evolution of the final energy consumption in the transport sector by commodity in the TEMOA-Italy [32] Base scenario (a) and the Fit55-Net0 decarbonization one (b). The gasoline components are indicated with circle hatches, while the gas oil ones with point hatches. The category Other involves several fuels, such as aviation gasoline, jet kerosene, heavy fuel oil, natural gas, liquefied petroleum gas and synfuels consumed in pure form. The complete set of results is available at [65].

completely substituted by syndiesel in 2050, that is the only case in which a synfuel reaches 100% of blending share. However, since the agriculture sector has the lowest contribution to sectorial CO2 emissions as shown in Fig. 16, with about 4% in 2050, and since it is the only end-use sector in which the service demand corresponds to the total final energy consumption, without modeling end-use technologies, the focus here is rather on the transport sector, that contributes to about 57% of CO2 sectorial emissions in 2050. Fig. 18 compares the transport energy consumption by commodity of the Base and the Fit55-Net0 scenarios, in the period 2020–2050, in which the energy consumption increases, respectively, by 32% in the baseline scenario (Fig. 18a), and by 15% in the decarbonization one (Fig. 18b). Differences in the energy mix arise starting from 2025: besides the penetration of pure hydrogen, mainly in aviation, and the slight increase of electrification, the other changes involve the gasoline and gas oil blends, shown, respectively, with circle hatches and point hatches in Fig. 18. In particular, gasoline blend is almost completely made of fossil gasoline in the Base scenario, with a very small fraction of bioethanol, that equals the minimum shares discussed in Section 2.4: then, the consumption of gasoline blend decreases in the decarbonization scenario by almost 40% in 2050 compared to the baseline evolution, mainly due to the decrease of the fossil gasoline fraction by 41%, while also synmethanol is added to the bioethanol in the blend, with shares of 3% and 4.8%, respectively (see Table 4 for more details). Instead, gas oil blend change is more qualitative than quantitative: in 2050, its consumption is only 7% lower in the Fit55-Net0 scenario than the Base one, but fossil gas oil completely disappears in the former. Indeed, since 2030, biodiesel and syndiesel gradually substitute the corresponding fossil fuel: while the former absolute consumption is almost the same between the two scenarios, reaching about 25% in 2045, the latter is absent in the baseline, while its blending share increases up to 75% in 2045, completely decarbonizing the gas oil consumption. In the TEMOA-Italy model, the majority of the gas oil blend is consumed in road transport, which includes cars, buses, motorcycles, light commercial vehicles, and heavy and medium trucks: such a blending of LCFs allows to continue to use of conventional vehicles, even in a strong decarbonization scenario like the Fit55-Net0 one. In this perspective, Fig. 19 compares the road transport demand mix for certain years in the Base and in the decarbonization scenarios. The represented demand is the aggregation of the different service demands accounting separately for all the road transport modes included in the model instance: for each of those modes, the service demand is measured in billions of vehicle kilometers, hence the kilometers driven by the whole vehicle fleet. In 2020 the mix is the same for the two scenarios, due to the model calibration: about 75% of the demand is satisfied by gas oil vehicles, followed by gasoline vehicles, a situation in accordance with the Italian vehicle statistics [68]. Both categories refer to the traditional internal combustion engine (ICE) technology, while the *Other types* category includes vehicles consuming natural gas, liquefied petroleum gas, and hydrogen, but the latter is not consumed. Then, in 2030 gas oil and gasoline blends become the only consumed fuels: in particular, the gas oil vehicles share decreases to almost 55% in both scenarios, while the gasoline vehicles share of about 45% in the Base scenario (see Fig. 19a) is distributed among gasoline vehicles (about 23.5%) and hybrid vehicles (about 21.5%) in the Fit55-Net0 scenario (see Fig. 19b). Hybrid vehicles includes plug-in hybrid electric vehicles (PHEVs), for which an external power source can be used to recharge their electric batteries, and mild and full hybrid electric vehicles (HEVs), for which instead the recharging of the battery occurs within the vehicle operation: hence, in the model instance PHEVs consume both electricity and gas oil or gasoline, while HEVs only the latter. In particular, the possibility to use electricity in HEVs is modeled through an efficiency increase compared to the corresponding ICE-based vehicle [32,69]. In this specific case, the whole contribution comes from mild hybrid cars, that consume a gasoline blend. From these results, battery electric vehicles are completely absent: whereas they are present in the technology database of TEMOA-Italy [28], they appear to be less competitive compared to the chosen alternatives, leading to a quite unrealistic technology mix (also in 2050), as further discussed in Section 3.5. Finally, hybrid vehicles appear in 2050 also in the Base scenario, with a share of 10%, while they completely substitute gasoline vehicles in the decarbonization scenario, satisfying about 52% of the road transport demand. In particular, 75% of this contribution comes from mild hybrid cars, followed by a 21% fraction of plug-in hybrid cars, that consume gasoline and electricity. The remaining small contribution is of plug-in hybrid trucks, that instead consume gas oil and electricity.

3.5. Discussion

The dynamic CO2 emission accounting method for ESOMs described in this work is developed to allow the modeling in such tools of blending between fossil fuels and LCFs, having the latter combustion a null effect on the CO2 atmospheric concentration. Those avoided emissions would

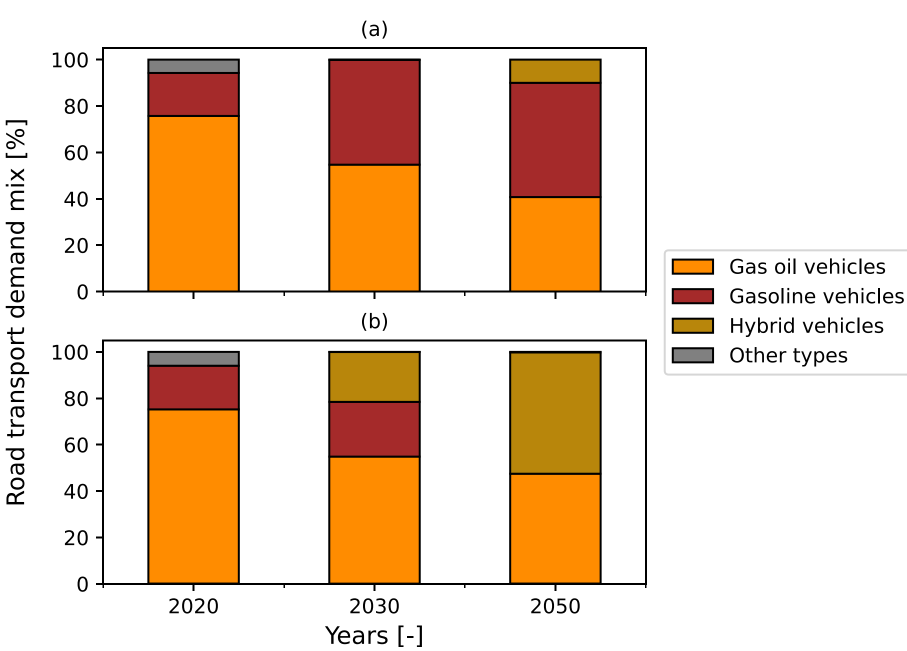

Fig. 19. Technology mix for the satisfaction of all the road transport demands modeled in the TEMOA-Italy model [32] in the Base scenario (a) and the Fit55-Net0 decarbonization one (b). Gas oil and gasoline vehicles use traditional internal combustion engines, while Hybrid vehicles include plug-in, mild and full hybrid electric vehicles. Moreover, Other types category aggregate vehicles consuming natural gas, liquefied petroleum gas and hydrogen. The complete set of results is available at [65].

not be correctly counted in the case of a static emission computation scheme, as the one traditionally characterizing ESOMs, and based on fixed and constant in-time CEFs [11,12]. Then, even if the methodology was elaborated for CO2 emissions, and applied to the TEMOA-Italy model, its flexibility allows to use this dynamic scheme in other ESOMs and to account for other GHGs, and also in case of non-null contribution to the emission commodity in question. That is the case of methane emissions from biofuel combustion, or the possible global warming potential of biogenic CO2, the latter under discussion nowadays [20,40,41]. Moreover, the flexibility of the methodology allows also to account for the avoided emissions assigning negative PEFs. Indeed, while for hydrogen and biofuels, this is done at the consumption step, for synfuels the compensation occurs at the level of CO2 sequestration, reflecting what physically happens in reality, since burning synfuels produces emissions. However, this could be a limitation in case sector-specific targets and policies has to be analyzed. That is the case, for instance, of the transport sector decarbonization, for which there is an open debate on the exclusion of synfuel-based vehicles from the ban of CO2 emitting vehicles since 2035 in the EU [70]: in this regard, the possibility to count the negative emissions at the consumption level also for synfuels could be explored, and this can be easily done in the proposed methodology, by assigning negative PEFs such as in the case of hydrogen and biofuel blending. Another example concerns the carbon pricing policies, aimed to decrease GHG emissions and support cleaner investments [71]: the pricing can be applied differently according to industries and demand sectors, such as the EU emission trading system [72], and it has been proved to directly affect the urban innovation of cities in large emitters countries like China [73]. In this context, those policies have already proven their effectiveness in reducing GHGs emissions [72,74]: however, their assessment through the dynamic methodology proposed in this work would require a careful evaluation on where to allocate the negative emissions, in case the pricing differs between different consumption sectors.

The dynamic scheme is proven to correctly function for the TEMOA-Italy model both in a base scenario and in a decarbonization one and for all the involved LCFs, namely hydrogen, biofuels, and synfuels. Being the dynamic CEFs dependent on the optimal LCF shares in the blends with fossil fuels, it is more suitable to discuss the reliability of the methodology in case of very stringent emission reduction targets, for which the mitigation potential of those blends could be fully exploited. The decarbonization scenario analyzed in this work includes the European Fit-for-55 target, and the long-term Italian one, respectively, for 2030 and 2050 [37,50]. The methodology properly works along the whole time horizon, and for very different and increasing blending shares, from a few percentage points, as in the case of bioethanol and synmethanol in transport gasoline, to >70%, as for the syndiesel in transport diesel. Indeed, the LCFs contribute to a different extent to the blending, since the technical limitations under which the current existing infrastructures and consumption technologies can handle such blends without additional costs vary between the different LCFs. In this regard, only hydrogen and synmethanol reach the maximum allowable share of 6% (in energy terms), suggesting that a less stringent constraint might favor higher blending rates: however, exceeding the maximum constraints implies higher downstream costs, to make the consumption-side technologies able to tolerate higher shares of the mixed LCFs.

In addition to the check of the methodology proper working, the decarbonization scenario results are deepened, to provide insights about the potential role of LCF blending in the Italian energy system decarbonization, rather than policy-relevant results. Indeed, the resulting role of synfuels in the decarbonization of the whole energy system, and in particular of the road transport demand, appears to be overestimated compared to the current market perspectives. In this regard, the complete absence of fully electric vehicles appears in contrast with the current transport policy framework at the national, European, and global levels [37,67,75]. All this suggests a broader robustness check on techno-economic parameters characterizing the LCF value chains, in terms of comparison to other sources, or sensitivity analysis, even if the used data sources are considered reliable, coming from well-established modeling framework and reports [14,47,76–78]– [49]. However, the penetration of LCFs qualitatively reflects the results of other policy-relevant scenarios. First, the blending of biomethane and hydrogen in natural gas (with a very similar percentage of around 10% to case-study here discussed) is foreseen in a recent analysis of TERNA and SNAM assessing the Fit-for-55 target reaching in Italy [55], while the production of synfuels in the context of power-to-gas is planned in the national long-term emission reduction strategy [37]. The latter recognizes the crucial role of CCUS to comply with the net zero emission objectives in 2050, as in the Net zero scenario of IEA [67]. Then, the high consumption of syndiesel in the transport sector fits perfectly into the most recent debate on excluding synfuels from the ban of CO2-emitting vehicles from 2035 in the EU [70]. Moreover, gas oil blends are mainly consumed in the road transport, while other transport sub-sectors are decarbonized in different ways. For instance, liquefied natural gas, hydrogen, and ammonia are used in the shipping transport starting from 2030, and this is line with the trends discussed in recent devoted studies [79].

Overall, the penetration of blended LCFs in the final energy mix generates some relevant insights. First, it suggests the possibility to reach very stringent decarbonization targets while respecting the technological neutrality principle, and without strong market and social disruptions. This can be helpful, especially in reaching the intermediate decarbonization targets, which appear to be more technically and economically challenging than the long-term ones, also considering the Sustainable Development Goal 7 of the United Nations aiming for affordable and clean energy by 2030 [80]. Indeed, LCF-fossil fuel blends can be consumed in conventional infrastructures and technologies under certain blending rates: on the one hand, this implies higher costs on the supply-side rather than in the demand-side of energy systems; on the other, this could enable investments in affordable and clean energy in countries where access to electricity and sustainable fuels is still lacking. The use of the current existing infrastructure as a ready-to-use decarbonization possibility involves also the power grids: for instance, the dynamic thermal rating has been proven to effectively increase the flexibility of those grids [81], boosting the integration of newly installed variable renewable plants [82]. Hence, an assessment of both the LCF-fossil fuel blending and strategies like the dynamic thermal rating in a unique framework would provide more insights, as other co-optimization frameworks already did [83], but on the other hand, it would require an extension of the TEMOA-Italy model scope towards unit-commitment purposes: indeed, the current version of the model is mainly used for capacity planning problems. Furthermore, such a study becomes more relevant also considering that currently, at the European level, the mixing between fossil fuels and low-carbon fuels is plausible to be less affected by supply chain risks than other technologies, considered strategic for the energy transition [84]. Lastly, other insights can arise by exploring higher blending rates, which inevitably also increase the demand-side costs. All this would be part of a more comprehensive assessment of the LCF blending role in decarbonization scenarios through ESOMs, which is also made possible by the dynamic CO2 emission accounting method described in this work.

4. Conclusions and perspectives

This work presents a methodology to correctly reckon CO2 emissions in ESOMs, particularly when considering commodities generated by a mix of fossil fuels and LCFs, such as hydrogen, biofuels, and synfuels. Indeed, ESOMs traditionally assign static emission factors to the different fuels even when taking into account variable compositions. This may lead to an overestimation of the computed emission trajectories, thus to the unreliability of the provided results. Under certain fractions, LCF blends can be handled by the current existing delivery and consumption systems without additional retrofitting costs, representing a valuable non-disruptive decarbonization alternative, possible to be studied using ESOMs. However, the emission scheme generally used in the traditional ESOM framework uses static emission factors, in the sense that it is not able to account for possible changes in the fuel composition throughout the analyzed time scale. That is a modeling limitation for LCF-fossil fuel blends since hydrogen, biofuels, and synfuels can be deemed to not affect the CO2 atmospheric concentration. Instead, the dynamic emission accounting method described here allows to consider the avoided CO2 emissions due to the blending of such LCFs. In particular, for hydrogen and biofuels avoided emissions are considered at the level of the blend consumption, implying emission reductions proportional to their blend fractions. Note that the total net contribution of synfuels is null since avoided emissions from synfuel consumption are already taken into account in sequestration processes.

The dynamic accounting method is being integrated and tested in the TEMOA-Italy model. After discussing to which extent LCFs can contribute to the reduction of CO2 emissions, according to the maximum allowable mixing share set as constraints in the model, the static and dynamic methodologies are compared in a base scenario, that has no emission reduction constraints. Looking at the blending between gas oil and biodiesel, the results show the emission overestimation in the case of static counting: as expected, the overestimation equals the fraction of biodiesel in the blend. Then, due to the absence of another blending than biodiesel and bioethanol, and due to the constrained optimization nature of the ESOM tools, the functioning of the dynamic methodology is assessed in a very stringent decarbonization scenario. The methodology is proven to correctly work for all the involved LCF blends, along the whole time horizon. In particular, some blends involve more the one LCF and to different extents, such as hydrogen, biomethane, and synmethane with fossil natural gas, biodiesel and syndiesel with fossil gas oil, and bioethanol and synmethanol with fossil gasoline. Finally, starting from the blending rates considered to check the methodology working, the results of the decarbonization scenario are deepened, to provide insights on the possible decarbonization role of blended LCFs, for future policy-relevant analyses. The results are presented in combination with the foreseen targets and evolutions included in the current energy policy framework, at the national, European, and global levels. Looking at the energy mix, blended LCFs penetrate up to about 32% of the final energy consumption in 2050, allowing to still have an energy system mainly based on gaseous and liquid fuel consumption. However, decarbonization could be ensured by the high LCF blending fractions, which constitute almost half of the gaseous fuels and two-thirds of the liquid fuels. Changes in such an energy mix are less disruptive if compared to the national and European evolutions currently foreseen since those blends can be used in the current existing delivery and consumption infrastructures. Then, this is linked to an overestimation of the emission reduction contribution of CCUS than in other decarbonization scenarios, such as the IEA Net zero scenario and the Italian long-term decarbonization strategy. However, although with even significant quantitative differences, the LCF penetration in the decarbonization scenario studied in this work qualitatively reflects the results of those policy-relevant scenarios. Indeed, hydrogen and biomethane injection into the natural gas grid in the next decade, as well as synfuel production from 2030 on, are foreseen in the Italian decarbonization strategy. Moreover, the latter and the IEA net-zero scenario consider the CCUS necessary to meet the 2050 emission reduction targets.

Future studies are going to encompass both methodological and applicative approaches. The developed methodology, tested here only for CO2 emissions, can be extended to other GHGs, such as methane and nitrous oxide, making the emission counting more comprehensive. Moreover, testing the methodology in other model instances, also developed in other ESOM frameworks, would increase its flexibility and adaptability. In this regard, two directions can be explored. The first is the modeling of the AFOLU sector, which implies a revision of the negative PEF values used for blended biofuels: this allows to assess the trade-offs behind the biofuels value chain modeling complexity. Then, avoided emissions from blended synfuels can be counted at the sectorial consumption level, comparing the related outcomes with the ones from the model instance using the methodology here described: in principle, the emission balance should be the same, but one approach could be more valuable than the other, depending on the case study objectives. Passing to the application perspectives, more policy-relevant scenarios can be studied. Firstly, a sensitivity analysis of the techno-economic parameters characterizing the LCF value chains might help to address the uncertainty behind those data, leading to more realistic analyses. Then, the scenario analysis can be enriched by studying the trade-off between higher blending rates and the eventual retrofitting costs for the consumption technologies, as well as the modeling of other LCFs, such as sustainable aviation fuels.

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CRediT authorship contribution statement

Gianvito Colucci: Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Daniele Lerede:** Writing – review & editing, Methodology. **Matteo Nicoli:** Writing – review & editing, Software, Methodology, Data curation, Conceptualization. **Laura Savoldi:** Writing – review & editing, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The source code and the description of the TEMOA modeling framework (MAHTEP version) are available at https://github.

com/MAHTEP/TEMOA/releases/tag/1.0 [29]. The specific input database related to this work is available at https://github.com/MAHTEP/TEMOA-Italy/releases/tag/2.0 [32]. The complete set of results is available at https://data.mendeley.com/datasets/69k9bwj3pw/3 [65].

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Appendix A. Techno-economic characterization of the hydrogen, synfuel, and biofuel value chains

Table A1
Techno-economic characterization of hydrogen production technologies in the TEMOA-Italy model [32,33]. Data are taken from [76], except for water electrolysis for which [77,78] are considered. INVCOST stands for investment costs, FIXOM stands for fixed operation and maintenance costs, VAROM stands for variable operation and maintenance costs, and AF stands for availability factor.

Technology	Input energy commodity	Specific consumption $\left[\frac{PJ_{in}}{PJ_{out}}\right]$		INVCOST $\left[\frac{M€}{PJ_{H2}}\right]$		FIXOM $\left[\frac{M€}{PJ_{H2}}\right]$		VAROM $\left[\frac{M€}{PJ_{H2}}\right]$		AF [−]	Lifetime [years]	
		2020	2050	2020	2050	2020	2050	2020	2050		2020	2050
Steam methane reforming*	Natural gas	1.32–1.81	1.25–1.55	6.38–58.59	5.02–36.71	0.31–1.41	0.24–1.33	0.04–0.65	0.04–0.05	0.9	20	20
Steam methane reforming w/ CCS*	Natural gas	1.52–1.65	1.40	9.03–18.72	6.07–14.29	0.45–0.94	0.36–0.76	0.20–0.53	0.07	0.9	20	20
Coal gasification*	Coal	1.75–1.77	1.25–1.75	14.67–18.18	11.13–18.18	0.45–0.87	0.45–0.71	0.16–0.22	0.12–0.22	0.8–0.9	20	20
Coal gasification w/CCS*	Coal	1.72–1.77	1.62–1.72	18.11–20.95	11.53–20.95	0.87–1.30	0.72–0.87	0.20–0.26	0.13–0.26	0.8–0.9	20	20
Heavy oil partial oxidation	Heavy fuel oil	1.30	1.30	13.69	13.69	0.68	0.68	0.14	0.14	0.9	25	25
Water electrolysis**	Electricity	1.2–1.8	1.1–1.5	15.85–177.57	6.34–31.71	0.48–5.33	0.19–0.95			0.9	3–10	8–17
Biomass steam reforming	Solid biomass	1.36	1.36	16.47	16.47	0.66	0.66	0.18	0.18	0.9	20	20
Biomass gasification*	Solid biomass	2.78–3.00	1.80–3.00	83.64–130.04	40.92–98.27	2.57–4.18	2.05–2.57	0.93–1.83	0.45–1.83	0.7–0.9	20	20
Biomass gasification w/CCS	Solid biomass	2.78	1.80	84.07	41.51	3.54	2.07	0.93	0.46	0.9	20	20
Ethanol steam reforming	Bioethanol	2.63	2.63	233.99				19.65	19.65	0.9	10	10

* These types of technologies are distinguished by size (small, medium, large) and location (centralized, decentralized), and the related parameters are represented using ranges.
** Alkaline, Polymer electrolyte membrane, Solide oxide, and anion exchange membrane electrolyzers are modeled and the related parameters are represented using ranges.

Table A2
Techno-economic characterization of hydrogen storage and delivery in the TEMOA-Italy model [32,33]. Data are taken from [76]. INVCOST stands for investment costs, FIXOM stands for fixed operation and maintenance costs, VAROM stands for variable operation and maintenance costs, and AF stands for availability factor.

Storage and delivery steps	INVCOST $\left[\frac{M€}{PJ_{H2}}\right]$		FIXOM $\left[\frac{M€}{PJ_{H2}}\right]$		VAROM $\left[\frac{M€}{PJ_{H2}}\right]$	
	2012	2025	2012	2025	2012	2025
Centralized tank	4611.11	3611.11	222.22	166.67		
Decentralized tank	2638.89	2083.33	111.11	83.33		
Underground storage	972.22	750.00	83.33	55.56		
Compression	1.37	0.86	0.20	0.12	0.03	0.02
Transmission	4.50	4.06	0.18	0.18	0.05	0.05
Liquefaction*	14.96-106.70	9.93-70.85	1.05–7.47	0.70–4.97	0.15–1.07	0.10–0.71
Road transportation	0.36	0.33	0.36	0.33		
Distribution	28.16	25.37	1.41	1.27	0.28	0.25
Refueling*	12.25-46.51	8.35-31.73	0.43–4.00	0.29–2.73	0.05–0.72	0.03–0.49
Local storage*	3.05–23.67	2.35-18.21	0.14–1.09	0.11–0.84		

* Parameter values for these steps are sectorial dependent and ranges are reported.

Table A3
Techno-economic characterization of synfuel production in the TEMOA-Italy model [32,33]. Data are taken from [76]. INVCOST stands for investment costs, FIXOM stands for fixed operation and maintenance costs, VAROM stands for variable operation and maintenance costs, and AF stands for availability factor.

Technology	CO2 specific consumption $\left[\frac{kt_{in}}{PJ_{out}}\right]$	Input energy commodity	Specific energy consumption $\left[\frac{PJ_{in}}{PJ_{out}}\right]$		INVCOST $\left[\frac{M€}{PJ_{SF}}\right]$		FIXOM $\left[\frac{M€}{PJ_{SF}}\right]$		VAROM $\left[\frac{M€}{PJ_{SF}}\right]$		AF [−]	Lifetime [years]	
			2020	2050	2020	2050	2020	2050	2020	2050		2020	2050
Methane from H2 and CO2	56.1	Hydrogen	1.27	1.22	16.65	7.93	0.83	0.40			0.95	25	25
Gas oil/Kerosene from H2 and CO2	74.07 (gas oil) 71.50 (kerosene)	Hydrogen	1.28	1.28	15.47	12.43	2.85	0.33	0.06	0.06	0.90	20	20
Gas oil /Kerosene from co-electrolysis	74.07 (gas oil) 71.50 (kerosene)	Electricity	2.33	1.83	31.57	28.22	5.70	0.66	0.12	0.12	0.90	20	20
Gas oil /Kerosene from co-electrolysis, DAC	74.07 (gas oil) 71.50 (kerosene)	Electricity	3.00	3.00	126.26	112.86	22.81	2.63	0.46	0.46	0.90	20	20
Methanol from H2 and CO2	69.30	Hydrogen	1.22	1.22	26.94	26.94	1.72	1.72	0.1	0.1	0.90	20	20
Methanol from co-electrolysis	69.30	Electricity	2.18	1.75	59.42	59.42	3.26	3.26	0.22	0.22	0.90	20	20
Methanol from co-electrolysis, DAC	69.30	Electricity	3.00	3.00	237.68	237.68	13.06	13.06	0.87	0.87	0.90	20	20

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