Dynamic Accounting for End-Use CO2 Emissions From Low-Carbon Fuels in Energy System Optimization Models

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Dynamic Accounting for End-Use CO_2 Emissions From Low-Carbon Fuels in Energy System Optimization Models

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ABSTRACT

Energy system optimization models are widely used worldwide to assess the effectiveness of decarbonization strategies. The correct accounting of greenhouse gas emissions, mainly CO2, is crucial in this field. Sectorial emissions are typically computed 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 can change throughout the model time horizon. As an alternative to static accounting, this work proposes a dynamic accounting method for the emissions avoided thanks to the contribution of hydrogen, biofuels and synfuels.

The static accounting method provides an overestimation of the emission levels compared to the proposed accounting method results, which then helps boost new low-carbon technologies in the future energy mix.

Keywords: Energy system optimization models, Hydrogen, Biofuels, Synthetic fuels, CO2 emissions, Low-carbon fuels

NOMENCLATURE

Abbreviations	
BF	Biofuel
CEF	Commodity emission factor
ESOM	Energy System Optimization Model
GHG	Greenhouse gases
H2	Hydrogen
LCF	Low-carbon fuel
PEF	Process emission factor
RES	Reference Energy System
SF	Synfuel

Symbols	
Kt	kilotons
PJ	PetaJoule
act	activity

1. INTRODUCTION

Energy System Optimization Models (ESOMs) are potent tools to analyze the effectiveness of possible energy policies in pursuing the 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 upstream sector 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.

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. Customarily, sector-specific technologies (the so-called *fuel technologies FTs*) can be accounted for to separately track fuel consumption and CO2 emissions by sector. This type of modelling allows 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 distribution network efficiency and costs, FTs are particularly useful to model the mix between two or more fuels (as shown in Fig. 1 for a FT producing sectorial

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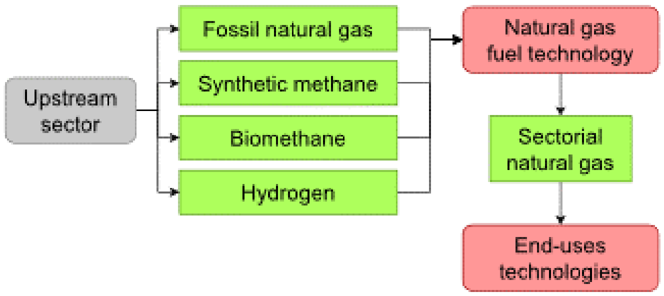

Fig. 1. Example of fuel technology for the generation of a sectorial natural gas commodity production from a mix of fossil natural gas, synthetic methane, biomethane and hydrogen in the natural gas network. Box colors: grey = supply side, red = demand side, green = energy commodity.

natural gas) occurring within the distribution infrastructure prior to 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, without deep changes in the current existing infrastructure [4], [5]. For instance, the injection of hydrogen (H2) 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]. Also, renewable transport fuels, such as biofuels and electrofuels, are considered necessary to decarbonize the transport sector in the short and medium terms. However, since dedicated transport technologies are not yet commercially available, these fuels can be used in blends with oil refined products [5].

As far as the computation of emissions is concerned, in ESOMs it is performed through commodity emission factors (CEFs) and process-specific emission factors (PEFs), as shown in Fig. 2 [7], [8]. CEFs are generally used to evaluate emissions related to combustion processes and are expressed in units of $\frac{mass_{GHG}}{energy\ cons.}$, where $mass_{GHG}$ represents the unit mass of the emitted emission of a certain GHG (typically $\mathrm{CO_2}$, $\mathrm{CH_4}$, $\mathrm{N_2O}$ or $\mathrm{SO_x}$) associated to the combustion of the quantity $energy\ cons.$ of any energy commodity. A CEF just depends on the chemical composition of the burned fuel. Differently, PEFs represent additional contributions to GHG emissions from particular technologies from different sources than fuel combustion, e.g., emissions from calcination in cement plants [9]. PEFs result then in additional contributions to total emissions from specific technologies.

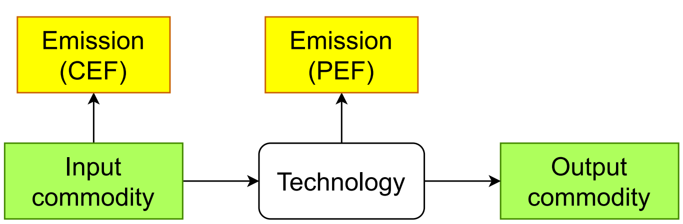

Fig. 2. Application of CEF and PEF to a generic technology and its input commodity. Box colors: white = technology, green = energy commodity, yellow = emission.

The application of CEFs to the sector-specific commodities produced by the FTs, allows to track the emissions at the level of the consumption technologies separately for each modelled sector (e.g., natural gas-based power plants or gasoline cars) [8]. However, the CEFs are fixed parameter provided a priori as input to the model, that do not consider the possible changes in the sector-specific fuel composition as in [3], [10]. 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 viable startegy of this staticity is provided by [2] in the transport sector: in case of mixing between fossil fuels and biofuels, CO2-related CEFs are applied only to the fossil commodities. While this strategy allows to count only the fossil CO2, it doesn't allow to evaluate the emissions of the end-use transport technologies (e.g., gasoline cars), since no CEFs are applied to the sectorial commodities

Instead, this work aims to provide a proper methodology to account for the emission reduction associated to the penetration of 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, here developed for, and applied to, CO2 emission evaluation in the TEMOA-Italy model [11], [12], is "dynamic", in the sense that it accounts for the fuel composition, which can vary throughout the ESOM time horizon.

2. METHODOLOGY

In a static emission counting approach CEFs and PEFs are combined to obtain the overall emission level for a technology according to Eq. (1), where: $Emission_i$ represents the global emission from technology t of the emission commodity associated to the commodity i; $Flow_{in,t,i}$ and $Flow_{out,t,i,o}$ are the consumption of the commodity i by technology t and the production of commodity o by technology t consuming commodity i, respectively.

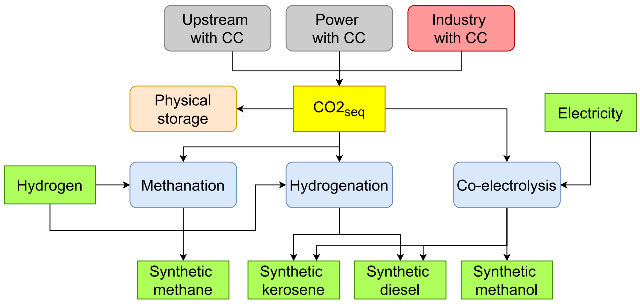

Fig. 3. CO2-based synthetic fuels production routes modelled in the present work. Box colors: grey = supply side, red = demand side, pale blue = SF production, pink = CO2 storage, green = energy commodity, yellow = Emission commodity

$$Emission_{e,t,i}[kt] = CEF_{e,i}\left[\frac{kt}{PJ}\right] * Flow_{in,t,i}[PJ] + PEF_{e,t,i,o}\left[\frac{kt}{act}\right] \cdot Flow_{out,t,i,o}[act] \quad (1)$$

The dynamic CO2 emissions accounting method is used to properly represent the effect of the mix between fossil fuels and LCFs. In general, the latter refers to those fuels the consumption of which would satisfy a GHGs emission reduction threshold (for example, at least 70 % in EU framework [13]). In this analysis, the combustion of LCFs is deemed not to affect the CO2 atmospheric concentration. That is the case of H2, biofuels (BFs) and CO2-based synthetic fuels (from now on called synfuels - SFs) and in particular:

- H2 composition does not contain any carbon atoms, independently of how it is produced. In this work, H2 can be produced from fossil fuels, using technologies with or without carbon capture (CC), and from renewable energy sources. It can also be mixed with natural gas prior to the final consumption in the demand-side sectors.

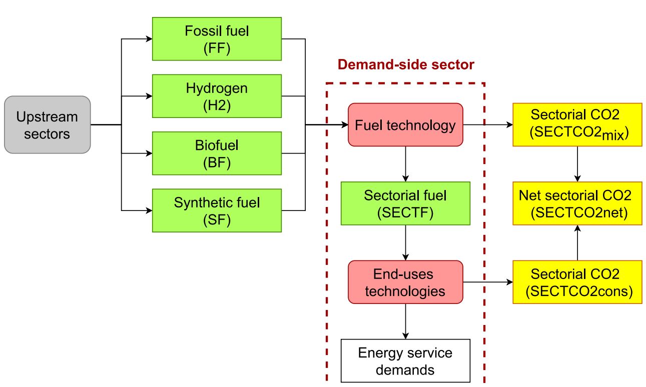

Fig. 4. Generic scheme of the dynamic accounting method for end-use CO2 emissions. Box colors: grey = supply side, red = demand side, pale blue = SF production, pink = CO2 storage, green = energy commodity, yellow = Emission commodity.

- BFs combustion emits the same amount of CO2 previously absorbed during the growth of the plants from which the biofuels are produced [14], which is not modelled. It is assumed that biomethane, bioethanol and biodiesel can be blended with natural gas, gasoline, and gas oil, respectively.
- SFs are produced starting from the CO2 previously captured in other processes (such as power plants with CC) [15], and their combustion emits the same amount of CO2 needed to produce them [2]. Fig. 3 shows the several SF production routes included in the ESOM instance considered here. Synthetic methane, synthetic diesel and synthetic kerosene can be mixed with the corresponding fossil counterparty (such as biodiesel with gas oil), while synthetic methanol can be used in blends with gasoline.

The dynamic accounting method proposed here accounts for LCFs mixing contribution to CO2 emissions reduction, envisaging the addition of PEFs assigned to sectorial FTs. In fact, one energy unit of H2 and BFs mixed with a fossil commodity through a fuel technology avoids CO2 emissions due to the consumption of one energy unit of the sector-specific commodity. On the other hand, the synfuels consumption produces an amount of CO2 already compensated at the level of CO2 sequestration processes. Hence, one energy unit of SFs mixed with a fossil commodity through a fuel technology contributes to the CO2 emissions due to the consumption of the sector-specific commodity. Fig. 4 shows the accounting of CO2 emissions in a generic demand-side sector due to consumption of a sectorial fuel, resulting from the mix between a fossil fuel and LCF(s). Note that the CO2 emissions produced in the upstream sectors are here omitted, since they are useless for the analysis. 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):

$$SECTCO2_{net}[kt] = SECTCO2_{cons}[kt] + SECTCO2_{mix}[kt] \quad (2)$$

Two terms contribute to $SECTCO2_{net}$:

1. 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.

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

2. 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 $H2$ and BFs. A PEF equal and opposite to CEF_{st} is here imputed to the FT producing $SECTF$: 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.

$$SECTCO2_{mix}[kt] = \eta_{FT}[-] \cdot (-CEF_{st}\left[\frac{kt}{PJ}\right]) \cdot (H2[PJ] + BF[PJ]) \quad (4)$$

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 ($H2, BF$ and SF).

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

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 $H2$ and BF.

$$SECTCO2_{net}[kt] = \eta_{FT}[-] \cdot CEF_{st}[\tfrac{kt}{PJ}] \cdot (FF[PJ] + SF[PJ]) \quad (6)$$

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. (7).

$$CEF_{dyn}\left[\frac{kt}{PJ}\right] = CEF_{st}\left[\frac{kt}{PJ}\right] \cdot (1 - f_{H2} - f_{BF}) \quad (7)$$

In the case of H2 and BF 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.

Note that 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 their molecules are equal to the fossil methane ones [16]. Considering the blending of gasoline with alternative fuels for car fueling, in the EU maximum of 10 $\%_{vol}$ and 3 $\%_{vol}$ of bioethanol and methanol (that can be CO_2-based synthetic), respectively, could be managed by gasoline engines [17], [18].

3. RESULTS

This section compares the dynamic CEFs for natural gas, gasoline and diesel fuel associated to different percentages of biofuels and hydrogen (the latter in the case of blending with natural gas) against the static CEFs. As explained in Section 1, the static CEFs are strictly dependent on the carbon content of fuels. The static emission factors presented in the following are taken from [19] and listed in Table 1.

Table 1. Static emission factors for natural gas, gasoline and gas oil. [19]

Commodity	$CEF_{st}\left[\frac{kt_{CO2}}{PJ}\right]$
Natural gas	56.10
Gasoline	69.30
Gas oil	74.07

It is worth to highlight that the dynamic CEFs are not know a priori, since they are not inputs to the model, but depend on the optimization process: however, according to the mixing share constraints applied to biofuels and hydrogen, it is possible to know to which extent these LCFs can contribuite to the reduction of the CO2 emissions per energy unit.

Fig. 5a shows the resulting dynamic emission factor associated to natural gas, by varying the percentage content of biomethane or hydrogen. As expected, the dynamic emission factor is linearly decreasing with increasing contents of biomethane and hydrogen. As explained in Section 2, while the maximum possible content of biomethane in the natural gas distribution network is assumed at 100%, the maximum content of hydrogen (in energy terms) is fixed at 5.4%, corresponding to 20% in volume [6] (the conversion from volume to energy units is performed according to [2]). Looking at the maximum mixing shares, 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

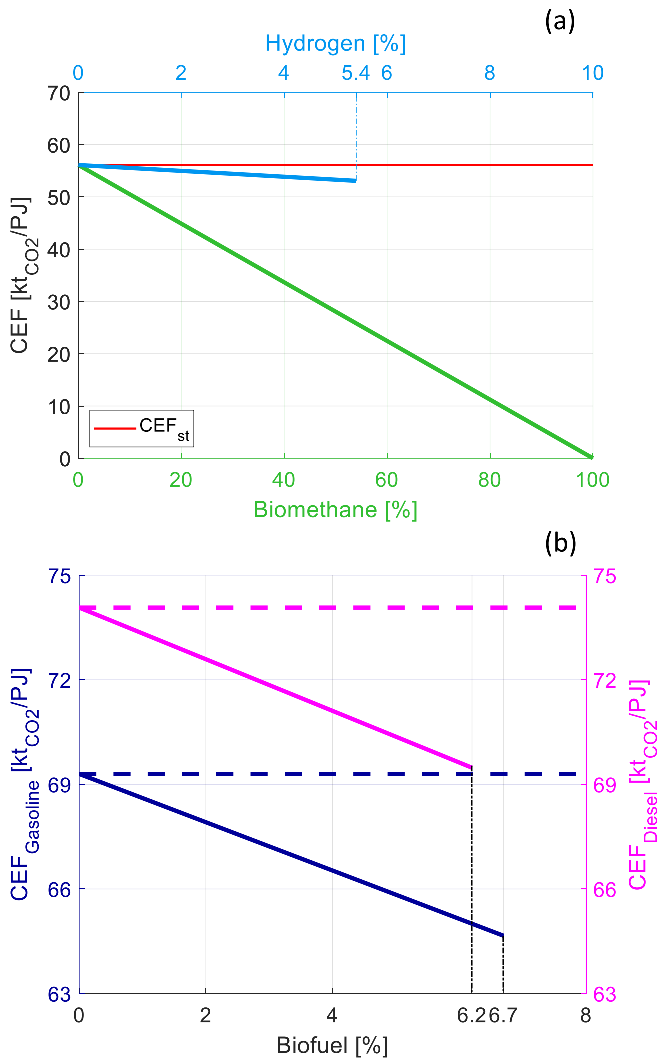

Fig. 5. (a) Dynamic emission factor for natural gas associated to different percentage contents of biomethane (green x axis) and hydrogen (blue x axis) and (b) Static (solid lines) and dynamic (dashed lines) emission factor for gasoline and gas oil associated to different percentage contents of bioethanol and biodiesel, respectively.

structure, and not only by the maximum mixing shares: hydrogen can be used to produce synthetic methane, that can be mixed to fossil methane without any limitations [20]; then, biomethane potential depends on the biomass resource availability (e.g., organic fraction of the municipal solid waste [21]) and on the biogas upgrading plants, but only a small fraction of this potential is currently exploited [22].

Fig. 5b reports the static emission factor for gasoline and the dynamic emission factor for different percentages of bioethanol in gasoline, up to 6.7% in energy and 10% in volume [23] (the conversion from volume to energy units has been performed according to [24]). It also reports the static emission factor for gas oil and the dynamic emission factor for different percentages of biodiesel in

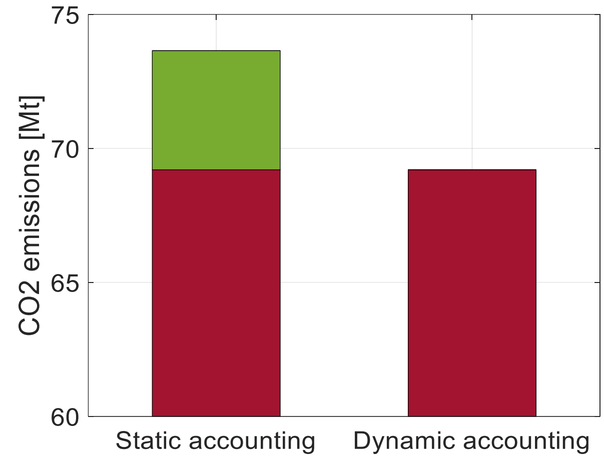

Fig. 6. Comparison between the static and dynamic accounting of the net CO2 emissions from the consumption of gas oil in the road transport in 2030: results from analysis done with [11]. Bar colors: brown = emission from fossil diesel, green = emission from biodiesel.

gas oil, up to 6.2% in energy and 7% in volume [23] (the conversion from volume to energy units is performed according to [24]): the latter share of biodiesel allows to have about the same CO2 emissions per energy unit in gas oil cars compared to cars fuelled by gasoline without bioethanol.

The static and dynamic methodologies are finally compared analyzing the net CO2 emissions resulting from the consumption of gas oil in the road transport in 2030, shown in Fig. 6 and computed using the TIMES/TEMOA-Italy model [11]. These results refer to the future evolution of the Italian energy mix according to the present situation and without any emission reduction constraint: focusing on the gas oil consumption in the road transport, the biodiesel fraction in gas oil blends is 6.0% in 2030, a value similar to the current values [25] and in accordance to the type of studied evolution. Furthermore, while the results on energy consumption are the same for both the static and dynamic accounting, since no CO2 emission constraints are applied and the optimization process is not affected by the dynamic methodology, on the other hand, the results on emissions are different. The emissions are allocated both to the fossil component (brown bars) and to the low-carbon component (green bar) when considering static CEFs. Instead, by applying the dynamic accounting, biodiesel contribution to the composition of transport gas oil reduces total CO2 emissions coming from gas oil consumption in road transport by 6.0%, a value equal to the share of biodiesel in gas oil: this result demonstrates how the static accounting methodology leads to overestimation in the calculation of CO2 emissions and that the dynamic methodology works correctly.

Due to the constrained optimization nature of the ESOM tools, the technologies resulting in lower CO2 emissions would be exploited even more if a stringent constraint on the emission level is enforced. Furthermore, under certain limitations, the current existing technologies (e.g., methane pipelines and gasoline cars) can handle FF and LCF mixes without technical modifications, hence without any further costs related to the LCFs consumpation. In fact, the possible contribution to the decarbonization from LCFs would then result in more considerable CO2 emission reduction potentials when analyzed according to the dynamic methodology.

4. CONCLUSIONS AND PERSPECTIVE

This work presents a methodology to correctly reckon GHG emissions in ESOMs, particularly when considering commodities generated by a mix of fossil fuels and low-carbon fuels, such as hydrogen, biofuels and synfuels. The dynamic accounting method described here can cope with the necessity of accounting for possibly different fuel composition throughout the analyzed time scale.

In particular, the dynamic methodology developed in this work allows to consider the avoided CO2 emissions due to the mixing of hydrogen and biofuels with fossil fuels. Moreover, the emission reduction results are proportional to their fuel composition content. On the other hand, the total net contribution of synfuels is null as avoided emissions from synfuel production are already taken into account in sequestration processes.

The dynamic accounting method is being integrated into the TIMES/TEMOA-Italy model to improve energy transition scenario analysis and the assessment of the role of low-carbon fuels in decarbonizing the energy system.

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