Analysis of standard and innovative methods for allocating upstream and refinery GHG emissions to oil products

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HIGHLIGHTS

- Traditional and innovative methods for allocating emissions at refinery level are reviewed.
- Added value has been introduced as a novel allocation method.
- Hydrogen-based consistency test has been introduced to validate the allocation methods.
- Consistent allocation methods assign negative refinery emissions to heavy products.

ARTICLE INFO

ABSTRACT

Alternative fuel policies need accurate and transparent methods to find the embedded carbon intensity of individual refinery products. This study investigates different ways of allocating greenhouse gases emissions deriving from refining and upstream crude oil supply. Allocation methods based on mass, energy content, economic value and, innovatively, added-value, are compared with the marginal refining emissions calculated by CONCAWE's linear-programming model to the average EU refinery, which has been adopted as reference in EU legislation. Beside the most important transportation fuels (gasoline, diesel, kerosene/jet fuel and heavy fuel oil), the analysis extends to petroleum coke and refinery hydrogen. Moreover, novel criteria, based on the implications due to hydrogen usage by each fuel pathway, have been introduced to test the consistency of the analyzed approaches.

It is found that only two economic-based allocation methods are consistent with the introduced criteria. These two methods also give negative refinery emissions for heavy products, which is coherent with the marginal emissions calculated through the CONCAWE refinery model. The recommended allocation methods are transparent and use only publicly available statistical data, so they may be useful not only for future EU legislation, but also in jurisdictions where a representative refinery model is not available.

1. Introduction

Current transport policies [1–5] aim to reduce greenhouse gases (GHG) emissions in transportation by replacing traditional crude oil-based fuels with alternative or renewable fuels (e.g. biofuels) [6–10]. Legislation in EU and USA incentivizes biofuels and other alternative fuels depending on their emissions savings compared with the conventional transportation fuels they replace. Therefore, the estimation of *Total Emission Intensities* (TEs) of transportation fuels, also called *Fossil Fuel Comparator* (FFC) and *Carbon Intensity Value* (CIV) respectively in

EU and USA legislations, is a current critical issue from the political and commercial viewpoints [11]. The TEs of petroleum transport fuels includes GHG emissions from upstream crude oil extraction and transport, refining, distribution, and final combustion in the vehicle. Since oil refineries produce a variety of products, a fair way must be found to allocate the refinery emissions among such products [12].

The emissions caused by refined petroleum products are correctly calculated as the difference in emissions between the global baseline refinery emissions and the same emissions when the refinery produces one marginal unit of the analyzed fuel, whilst maintaining the same

Nomenclature

Acronyms and symbols

Av, AV	added value
C	combustion emission intensity of the refinery feedstock ($gCO2eq/MJ_{crude-eq}$)
Cc	cost of crude oil input [€/MJ]
Ch	cost of refinery hydrogen [€/MJ]
CIV	Carbon Intensity Value
Cng	cost of natural gas [€/MJ]
CO2eq	Equivalent Carbon Dioxide
crude-eq	crude oil equivalent
e_{comb}	combustion factor: CO2eq emissions occurring during the combustion stage [gCO2eq/MJ]
E_{fuel}	average combustion emission intensity of refinery fuel [gCO2eq/MJ]
En	energy [MJ]
e_{ref}	CO2eq emissions allocated in the refinery stage [gCO2eq/MJ]
EU	European Union
e_{up}	upstream emissions allocated to the ith refined oil product [gCO2eq/MJ]
E_{up-C}	whole upstream emissions per MJ of crude entering into the refinery [gCO2eq/MJ]
FFC	Fossil fuel comparator
FQD	Fuel Quality Directive
GHG	greenhouse gases
H2	hydrogen
HFO	heavy fuel oil
i	ith refined oil product
ICCT	International Council on Clean Transportation
IEA	International Energy Agency
JEC	JRC-Eucar-Concawe consortium
LCA	life cycle assessment
LHV	lower heating value
LP	linear programming
m	mass of petroleum products [kg, tons]
MC	marginal carbon
NG	natural gas
np	total number of refinery products (without hydrogen)
PF	production factor
PZp	price of petroleum products [€/MJ]
RED	Renewable Energy Directive
SAV	share of added value
SEC	share of energy content
SEV	share of economic value
SMC	share of mass content
SP	share parameter
TC	annual total amount of crude oil in input [MJ]
TE	total emission intensity
TH	annual total amount of hydrogen bought on the external market [MJ]
TN	annual total amount of natural gas entering in refinery [MJ]
TP	total annual production of refined oil products [MJ]
TTW	Tank to Wheel
WTT	Well to Tank
WTW	Well to Wheel

production level of all other products [13]. These *marginal emissions* can be calculated using a detailed model of the refinery [14]: in the European context, the CONCAWE linear programming model is currently used to calculate such values for each refinery product [15]. The refining emissions from the CONCAWE marginal calculation were incorporated in the FFCs for successive JEC studies (JRC, EUCAR and CONCAWE consortium) [16], as well as for the European Union's Fuel Quality Directive.

One of the issues connected with using a refinery models is that full details of its energy, mass balances and market prices are not usually in the public domain, so that the model is not completely transparent. In order to perform a fully transparent calculation, the adopted method should rely only on public statistical data about oil refining. In particular, two different approaches can be adopted for modelling the oil refinery, in order to derive TEs of refined oil products: the *aggregate refinery-level* and the *individual refinery process-level*. The former treats the oil refinery as a black box for which overall refining emissions, production inputs and outputs of different oil products, and the related market prices, are known [17]; therefore, this approach requires emissions to be allocated among multiple products of one process, according to a certain allocation method [17–19]. On the other hand, the *individual refinery process-level* approach distinguishes detailed processes inside the oil refinery (e.g. the GREET model - http://greet.es.anl.gov/): due to this more detailed description, this approach reduces but still does not eliminate the need for emissions allocation, resulting in a more or less arbitrary choice of allocation keys. Indeed, important individual refinery processes, such as distillation and cracking, produce a number of intermediate oil products for which one emission allocation method is required.

According to ISO 14040 and 14044 [20], the preferred way of assigning emissions to multifunction processes is so-called *system expansion*: the entire process emissions are initially assigned to one product, and then a credit is given for each of the co-products, representing the emissions related to the product they substitute in the market. However, this approach can hardly be applied to oil refineries, because most of the products can only substitute other oil refinery products, leading to a circular argument. Emissions allocation to refined products is usually performed in proportion to one *allocation key*, such as mass or energy content, or economic value [21,22]. Since the same allocation key can be implemented in different ways, leading to very different results, the allocation of environmental impact among multiple products is one of the major current issues of LCA [23]. For this reason, proper criteria are needed to check the consistency of the allocation method applied. It is important to stress that policy makers are interested in the marginal *reduction* in emissions in refineries resulting from reducing the production of a particular product by replacing it with an alternative (e.g. biodiesel replacing diesel [24,25]).

This is just what the marginal approach calculates [26], so its results are suitable for deriving Fossil Fuels Comparators. Despite its limitations – especially the low transparency – the marginal method is a closest representation of the effects on the actual environmental burdens in the refinery sector. For such policy purposes, the only more transparent alternative is to find an allocation method which gives results not too far from those of the marginal model.

1.1. Objectives of the paper

In this paper, existing and innovative allocation methods are reviewed and applied to the entire EU refining sector in 2010. The specific objective of the paper is twofold:

- To account for total GHG emission intensities of conventional transportation fuels, including diesel, gasoline, jet fuel and heavy fuel oil. In addition, the analysis is applied to petroleum coke and hydrogen, which are less investigated by the literature. Refining emissions for each product are calculated based on the aggregate

refinery level, using different allocation keys: energy content, economic value and one novel method based on the added-value. The results are compared to the latest ones derived through a marginal approach calculated based on CONCAWE [27].

- To introduce and to apply *hydrogen-based consistency criteria* in order to verify whether the investigated allocation methods are able to represent the actual physical and economical relationships occurring in the refinery system. Results of the most consistent methods may serve to support policymakers in the update of Fossil Fuel Comparators for different transportation fuels.

In this paper, the entire European refinery sector is considered (EU 27, plus Norway and Switzerland) [27], with reference to year 2010. This average refinery is modeled based on the *aggregate refinery-level* approach, producing refined petroleum products by processing crude oil, natural gas and supplementary hydrogen. Notice that, in the following, *refinery hydrogen* refers to the hydrogen actually produced in the refinery. Input data used in this research are coherent with the main available data sources, such as the EUROSTAT data bank, ICCT [28], COWI [29] and IEA [6]. The coherency of several intermediate values has been also checked by comparison with relevant reports in this research field, such as COWI [29].

The rest of the paper is organized as follows: Section 2 describes the general structure of the *Well to Tank* (WTT) model, presents an overview of the analyzed allocation keys and introduces the hydrogen-based consistency criteria. Notice that this section also includes an updated and comprehensive literature review about such topics. Section 3 shows the results of allocation methods compared to the marginal reference figures, tests their validity using the aforementioned hydrogen-based consistency criteria and provides a discussion about the obtained results. Concluding remarks are finally reported in Section 4.

2. Models and methods

In this section, the Well to Tank (WTT) model is briefly introduced, allocation keys are reviewed and the hydrogen consistency test is presented.

2.1. The Well to Tank model

The Well to Wheel (WTW) methodology attempts to quantify life cycle GHG emissions and energy requirements to assess the impact of automotive fuels production and use [30,31]. A WTW chain, therefore, considers all the transformations occurring during the crude oil recovery, transport of the crude oil, refining and distribution of the finished transportation fuels (*Well-To-Tank* or WTT), and also the combustion in different powertrains, considering diverse driving-cycles (*Tank-To-Wheel* or TTW). Compared to Life Cycle Assessment (LCA), the WTW focuses on fewer stages, neglecting the energy and material consumption occurring in the construction and decommissioning of the processing plants [16,28,29,32,33].

Fig. 1 shows the system boundaries for the generic WTT model for estimating the total GHG emissions embedded in different petroleum-based fuels. The combustion emissions of fuels in their final use are added to the Well-To-Tank emissions to give the total GHG emissions associated with each fuel, in terms of grams of GHG emissions (expressed by means of the carbon dioxide equivalent emissions, in gCO_2eq) per MJ of fuel. The total GHG emissions caused by the analyzed fuels can be split into four main components:

- **Upstream emissions.** These comprise emissions from crude oil extraction and transport to the refinery. International Council on Clean Transportation (ICCT) assumes 10.0 gCO_2eq per MJ of crude oil for upstream emissions [28]. Two approaches may be used to allocate such upstream emissions on the refinery product, as described in Section 2.4.
- **Oil refinery emissions.** We calculated the total GHG emissions from European refineries in 2010 from CONCAWE [27], as the difference between the total combustion emissions of the feedstock (i.e. the sum of crude oil, natural gas and hydrogen expressed in MJ of crude oil equivalent) and the total GHG combustion emissions of all the refinery products. This results in a value of 73.36 $gCO_2eq/MJ_{crude-eq}$, which is slightly lower than that of crude oil (73.50 gCO2eq/MJ).
- **Distribution emissions**. GHG emissions from transport and distribution of diesel and gasoline have been taken from the JEC WTW model [16], while those for jet fuel, heavy fuel oil (HFO) and petroleum coke have been derived from the Ecoinvent database [34,35] (numerical values are collected in Table 1). For the EU refinery in 2010, the amount of consumed hydrogen was greater than the produced one. For this reason, emissions for hydrogen distribution from the refinery are zero.
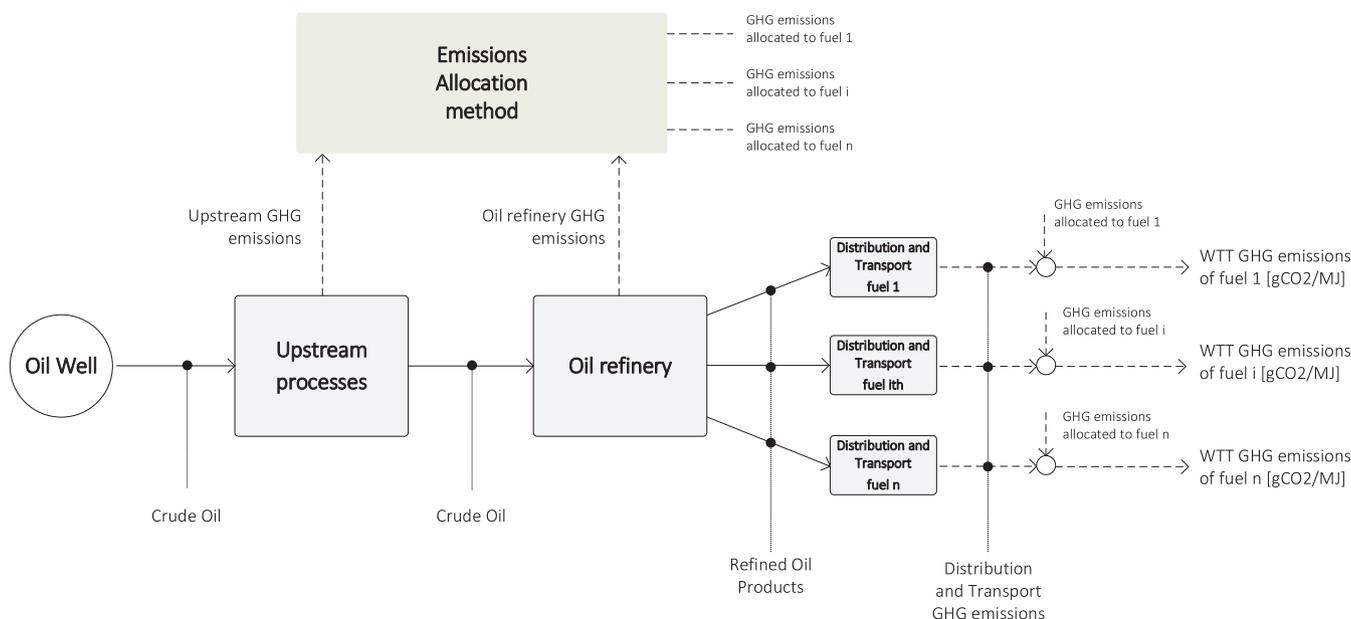

Fig. 1. Outline of the adopted Well-to-Tank model.

Table 1
Adopted values for distribution and combustion emissions of the investigated petroleum products.

Emissions [gCO$_2$eq/MJ$_{fuel}$]	Diesel	Gasoline	Jet fuel	HFO	Petroleum coke	Refinery hydrogen
Distribution	1.10	1.20	0.50	0.60	0.02	0.00
Combustion	73.00	73.30	72.20	78.10	95.60	0.00

- **Combustion emissions.** Except for hydrogen, combustion emissions represent the largest portion of the overall WTW emissions, proportional to the carbon content of each fuel. Values are taken from CONCAWE [27], and collected in Table 1. Notice that combustion emissions are not usually put into the WTT section of the WTW model. However, such emissions have been here taken into account in order to derive the total emissions intensities (TEs) for each analyzed fuel.

All the analyzed methods satisfy mass balance for the GHGs emissions in all the stages of the WTT model: in other words, the sum of the emissions allocated to the refined oil products are equal for all the proposed allocation methods (i.e. the *additivity principle* is respected [14]).

2.2. Calculating emissions of refining products based on the marginal method

As described in the introduction, the marginal method calculates the change in total refinery emissions caused by the production of one marginal unit of refined oil products, relying on a linear programming model that represents the average EU refinery sector [36–39]. Starting from a model of the whole oil refinery with baseline values for feedstock consumption, production levels and emissions, the model quantifies the change in crude oil and emissions (i.e. the marginal emissions) caused by a unit change in production of one petroleum product, whilst keeping all other products constant. This procedure for marginal emissions calculation was detailed among others by Tehrani, who proposed a numerical example of a refinery LP model and a two-stages marginal methodology for the allocation of the refinery emissions [14]. In this work, the CONCAWE model of the average EU oil refinery in year 2010 has been used [16,27]: this model works by minimizing operating costs, including the costs of oil feedstock and energy utilities, constrained by a defined level of production demand for each product, and with limited capacities of the process units. Results obtained by the marginal method will be here used as benchmark to compare results of the allocation methods described in the following.

2.3. Attributing emissions to refining products based on allocation keys

Differently with respect to the marginal method, emissions can be allocated to refined oil products based on different allocation methods, in proportion to the selected allocation key, namely: *mass, energy* or *economic value* of each oil product. In this work, allocation method based on the *added value* key is also introduced and tested. All these methods are based on different *share parameters* (SP), here defined as the *Share of Mass Content* (SMC), the *Share of Energy Content* (SEC), the *Share of Economic Value* (SEV) and the *Share of Added Value* (SAV).

2.3.1. Mass-based allocation

According to this method, emissions are allocated to multiple products based on the respective mass content of each product stream, defined by the *Share of Mass Content* (SMC) as the ratio between the total annual production of the considered ith product and the total annual refined oil products production (in tons). This approach has

been used by several researches: in particular, Wang et al. applied such allocation key to petroleum products (namely, gasoline, diesel, LPG and naphtha), comparing results obtained by different aggregation level of the analyzed oil refinery [17]. In another research, Rahman et al. performed a complete WTW analysis of transportation fuels (gasoline, diesel and jet fuel) derived from different North American conventional crudes by considering also the mass-based allocation key [33].

$$SMC_i = \frac{m_i}{\sum_{i=1}^{np} m_i} \tag{1}$$

2.3.2. Energy-based allocation

This method allocates emissions in proportion to the energy content of each stream, and it is recommended by the current *Renewable Energy Directive* (RED) to assign emissions due to biofuel production and the related by-products [2,26]. According to this method, emissions are assigned to each refined oil product based on the *Share of Energy Content* (SEC), defined for each ith product by relation (2), where m_i and LHV_i are respectively the total annual production (in tons) and the Lower Heating Value (LHV, in MJ/kg), while *np* the total number of refinery products.

$$SEC_i = \frac{m_i LHV_i}{\sum_{i=1}^{np} m_i LHV_i} \tag{2}$$

Elgowainy et al. relied on the energy-based allocation to calculate the GHG emission intensities of gasoline, diesel, jet fuel, residual fuel oil, LPG and petroleum coke by considering production data of 43 US refineries (processing the 70% of US refining capacity) [18]. A similar analysis was performed by Han et al., considering 60 large US and EU refineries [19]. Bredeson et al. found that the hydrogen content of refined oil products is one of the most important factor in increasing their energy requirements (and the related GHG emissions), but this is not always related with their energy content [21]. Therefore, they proposed a modified energy allocation method in order to produce results consistent with the refinery behavior.

2.3.3. Economic-based allocation

This method allocates GHG emissions to petroleum products based on their relative economic values, here defined as the *Share of Economic Value* (SEV) by relation (3), where m_i is the total annual production of the ith product (in tons), PZ_{pi} the price of the ith petroleum product (in €/MJ) and *np* the total number of refinery products.

$$SEV_i = \frac{m_i PZ_{pi}}{\sum_{i=1}^{np} m_{pi} PZ_i} \tag{3}$$

One criticism related to the economic-based allocation is related to the variability of its results, due to the price fluctuations of petroleum products [40]. Based on the definition of SEV, results of economic-based allocation key is affected by changes in *relative* prices of products [41], and it can be observed that the variability of such relative prices is lower compared to the variability of feedstock price. Since oil refineries production yields gradually evolve to satisfy market demand, the EU refinery set-up in 2010 reflects the relative product prices not just in 2010 but for several years before [42,43]: for such reason, the average oil products prices in the period of 2006–2010 have been here considered, estimating missing price values from the literature [27,41]. Notice that the estimated average price for hydrogen in 2010 has been here assumed as 1923 €/t$_{hydrogen}$ [44].

Wang et al. applied the economic-based allocation to oil refinery at sub-process level and compared the results with those produced through other allocation keys [17]. Pierru has also explored this method by considering the Aumann-Shapley formulation [45]. In general, literature agrees in saying that price-based methods provide results closer to the marginal method compared to other allocation keys, thus resulting in a closer representation of the actual oil refinery. This

because oil refineries increase the share of the more valuable products, at the expense of increased energy requirements: therefore, oil refineries evolve in the direction of keeping the marginal crude oil used to produce each product in proportion to the economic value of each product [17,19].

2.3.4. Added-value-based allocation

This method is here proposed as an alternative to the usual economic-based approach. Added Value (AV) is here defined as the difference between the commodity value of petroleum products and the average value of the same energy amount of refinery feedstock. According to this method, GHG emissions are allocated to refined products in proportion to their relative economic added value, here represented for each product by the *Share of Added Value* (SAV), calculated by relation (4). The numerator is the added value of the ith product (AV_i, in €/MJ) multiplied by its annual production m_i (in tons), while the denominator represents the total added value of all refined products, here defined as the difference between the value of the total production of the refinery and the cost of the oil refinery feedstock, namely crude oil, exogenous hydrogen and natural gas.

$$SAV_i = \frac{m_i AV_i}{\left(\sum_{i=1}^{np} PZ_{pi} m_i\right) - CcTC - ChTH - CngTN} \tag{4}$$

According to this method, positive values of emissions are expected to be allocated to products with higher prices compared to the feedstock, while negative values are apportioned to products with prices lower compared to the feedstock price. Despite the negative numerical values of emissions, the emissions balance of the oil refinery is respected, that is, the sum of the emissions allocated to final products will equal the total refinery emissions.

2.4. Two approaches to allocate refinery and upstream emissions

We compared two approaches for calculating how much crude oil, and hence upstream emissions from crude production and transport, to attribute to each refined oil product.

In the first method, which we call *Emissions allocation*, it was *refinery emissions* that were allocated to petroleum products simply by multiplying them by the share parameters of each product. In the second, *Feedstock allocation*, the following procedure was adopted: with reference to relations (5) and (6), the whole average combustion emissions of the crude oil feedstock ($C_{crude-eq}$, in our case equal to 73.36 $gCO_2eq/MJ_{crude-eq}$) are allocated to each refined oil products by considering the aforementioned share parameters and the production factors of each product (i.e. namely the share of each product compared to the total feedstock, PF), thus deriving the *total* emissions associated to each refined product (tc_i, $gCO_2eq/MJ_{product}$). Then the refinery emissions caused by each product ($e_{ref,i}$, $gCO_2eq/MJ_{product}$, in Table 1) are derived by subtracting the combustion emissions of each product ($e_{comb,i}$, $gCO_2eq/MJ_{product}$, in Table 1) from the obtained values. This difference must be corrected to reflect the fact that the mix of fuels burnt in refineries does not have the same chemical composition as crude oil, but they are characterized by high shares of light refinery gases with an average combustion emissions E_{fuel} of about 60 gCO_2eq/MJ [29].

$$tc_i = \frac{SP_i}{PF_i} C_{crude-eq} \tag{5}$$

$$e_{ref,i} = (tc_i - e_{comb,i}) \frac{E_{fuel}}{C_{crude-eq}} \tag{6}$$

In the case of *Emissions allocation*, similarly to refinery emissions, the *upstream emissions* E_{up-C} (here assumed as equal to 10 $gCO_2eq/MJ_{crude-eq}$) were allocated to refined products multiplying them by the share parameters of each product. In the case of *Feedstock allocation*, consistent with the method for refinery emissions, upstream emissions were allocated to each refined oil product in proportion to the ratio between refinery plus combustion emissions and total crude feedstock emissions, as represented by relation (7).

$$e_{up,i} = E_{up-C} \frac{e_{ref,i} + e_{comb,i}}{C_{crude-eq}} \tag{7}$$

2.5. The hydrogen-based consistency test

As mentioned in the introduction, the most GHG intensive production processes within oil refineries are usually characterized by large hydrogen requirements, which is highly GHG intensive in turn [18,19,21]. This is confirmed by the analysis of hydrogen production processes in the European context, resulting in an average amount of 109 $gCO_2eq/MJ_{hydrogen}$ [18,19,21]. Almost a half of the whole production of hydrogen is a fixed by-product of catalytic reforming of naphtha, which converts it into high-octane blending components for gasoline, so supplemental hydrogen comes from steam-reforming of naphtha or natural gas or by partial oxidation of heavy fuel oil fractions. Hydrogen is used in many refinery processes: it is used to convert heavy aromatic products to lighter products (e.g. gasoline, jet-fuel and diesel) by means of the hydro-cracking process. Moreover, growing amounts of hydrogen are used to reduce the Sulphur content of fuels by hydro-desulphurization, due to the increasingly strict regulations. On the other hand, heavy products (e.g. heavy fuel oil, bitumen and petroleum coke) come directly from straight-run distillation, without the need of any hydrogen-based process.

LCA standards suggest adopting the allocation method which gives results that reflect the physical and economical relationships of the system products in the most consistent way [12]: since allocation methods often underestimate the GHG emissions for hydrogen-intensive products [21], a *Hydrogen-based consistency test* is here proposed to check the consistency of the adopted allocation method. Indeed, a fair and consistent allocation of refinery emissions should allocate emissions to hydrogen-intensive products, such as gasoline, diesel and jet-fuel, rather than to heavy products from straight-run distillation.

The first proposed consistency criterion, represented by equation (8), is that the main transport fuels (gasoline, jet fuel and diesel) should be allocated more refining emissions than heavier products (e.g. HFO), and these must have, in turn, higher emissions than products obtained only by straight-run distillation (e.g. pet coke).

$$e_{ref,main\ transport\ fuels} > e_{ref,HFO} > e_{ref,pet\ coke} \tag{8}$$

The second criterion, represented by Eq. (9), establishes that allocation methods are consistent if refinery emissions allocated to hydrogen production are higher than the emissions associated to the feedstock mix required for its additional production. Since the proportions of the two fuels used for supplementary hydrogen production are unknown, the lowest emissions of the two fuels should be taken into account.

$$e_{ref,H2} \geqslant \min(e_{H2,HFO}, e_{H2,NG}) \tag{9}$$

In this paper, the following values for minimum hydrogen production emissions have been adopted: in the case of hydrogen made by steam reforming of EU-mix natural gas, emissions of 74.3 $gCO_2eq/MJ_{hydrogen}$ (with an uncertainty of ± 2%) have been considered, based on JEC-WTWv4a [16]. In the case of partial oxidation of heavy fuel oil, the refinery emissions associated to hydrogen are at least as high as the sum of the combustion and refining emissions of heavy fuel oil: the refining emissions for heavy fuel oil are one of the outputs ($e_{ref,HFO}$) of each allocation method, while the combustion emissions are reported in Table 1.

3. Applied allocation methods, results and discussion

Table 2 shows the different combinations of allocation keys and

Table 2
Combination of Upstream and Oil refinery GHG emissions allocation methods applied in this study.

Allocation method name	Allocation key	Upstream emissions allocation	Refinery emissions allocation
MC	Marginal emissions	Feedstock	CONCAWE model
En1	Energy content	Emissions	Emissions
En2	Energy content	Feedstock	Emissions
En3	Energy content	Feedstock	Feedstock
Ev1	Economic value	Emissions	Emissions
Ev2	Economic value	Feedstock	Emissions
Ev3	Economic value	Feedstock	Feedstock
Av	Added value	Feedstock	Emissions

application methods used in this study. Numerical results for the EU case study in year 2010 are reported in Table 3. Notice that numerical values of Share Parameters adopted for the analysis are reported in Table 4 (Appendix A), while, for the sake of completeness, results based on the mass allocation key are reported in Table 5 (Appendix B).

Numerical results are collected in Table 3 and graphically represented in Fig. 2. The applied methods and the results obtained through their application are commented in the following. Notice that the application of the mass allocation method gives very low emissions for hydrogen because of its high energy content (MJ/kg), and therefore this method fails in fulfilling the proposed consistency criteria. However, since mass allocation method is commonly adopted in the field of LCA, its results are reported in Appendix B.

4.1. Marginal method (MC)

Results of this method have been obtained by considering the refining emission intensities reported by CONCAWE [15,16], except for the hydrogen refining emissions (122.9 gCO$_2$eq/MJ$_{hydrogen}$), that have been calculated for the reference year 2010 through the same model. Results show that hydrogen is the product with the highest TE, despite

having zero combustion emissions, whilst HFO and petroleum coke have the lowest TE and negative refining emissions. This implies that the total refinery emissions are expected to decrease if the production of heavy oil products increases, because of the lower amount of hydrogen needed to convert the excess heavy components into lighter components. Based on MC, refining emissions of the main transportation fuels (diesel, gasoline and jet fuel) are highest for diesel, but all of them are one order of magnitude lower than the hydrogen refining emissions: this reflects the high demand for diesel in EU, prompting relatively more hydrogen to be dedicated to making extra diesel. The trend of the refining emissions is reflected also in the TEs of the main transport fuels, since their combustion emissions are very close. The results of MC satisfy the consistency criteria introduced in Section 2.5: the refinery emissions of main transport fuels (diesel, gasoline and jet fuel) are higher than those of heavy fuel oil or petroleum coke. Moreover, the total refining emissions for hydrogen (122.9 gCO$_2$eq/MJ$_{hydrogen}$) are higher than either the sum of refining and combustion emissions of heavy fuel oil according and also of emissions due to natural gas steam reforming (72.7 gCO$_2$eq/MJ$_{hydrogen}$).

4.2. Energy-based allocation 1 (En1)

According to this method, upstream and refinery emissions are allocated to each product based on their relative SEC. Results of refining and upstream emissions are the same for all petroleum products: this makes the total emission intensities (TEs) of different petroleum products different only because of their relative carbon content. Discrepancies compared to the reference emissions (MC) are small for diesel, gasoline and jet fuel, while become larger for the refining emissions of HFO, petroleum coke and hydrogen. The refining emissions for heavy fuel oil come out the same as main transport fuels, and refining emissions for hydrogen (5.8 gCO$_2$eq/MJ$_{hydrogen}$) result much lower than the combustion and refining emissions of the fuels used to produce it. Therefore, the En1 method fails both the consistency criteria presented in Section 2.5.
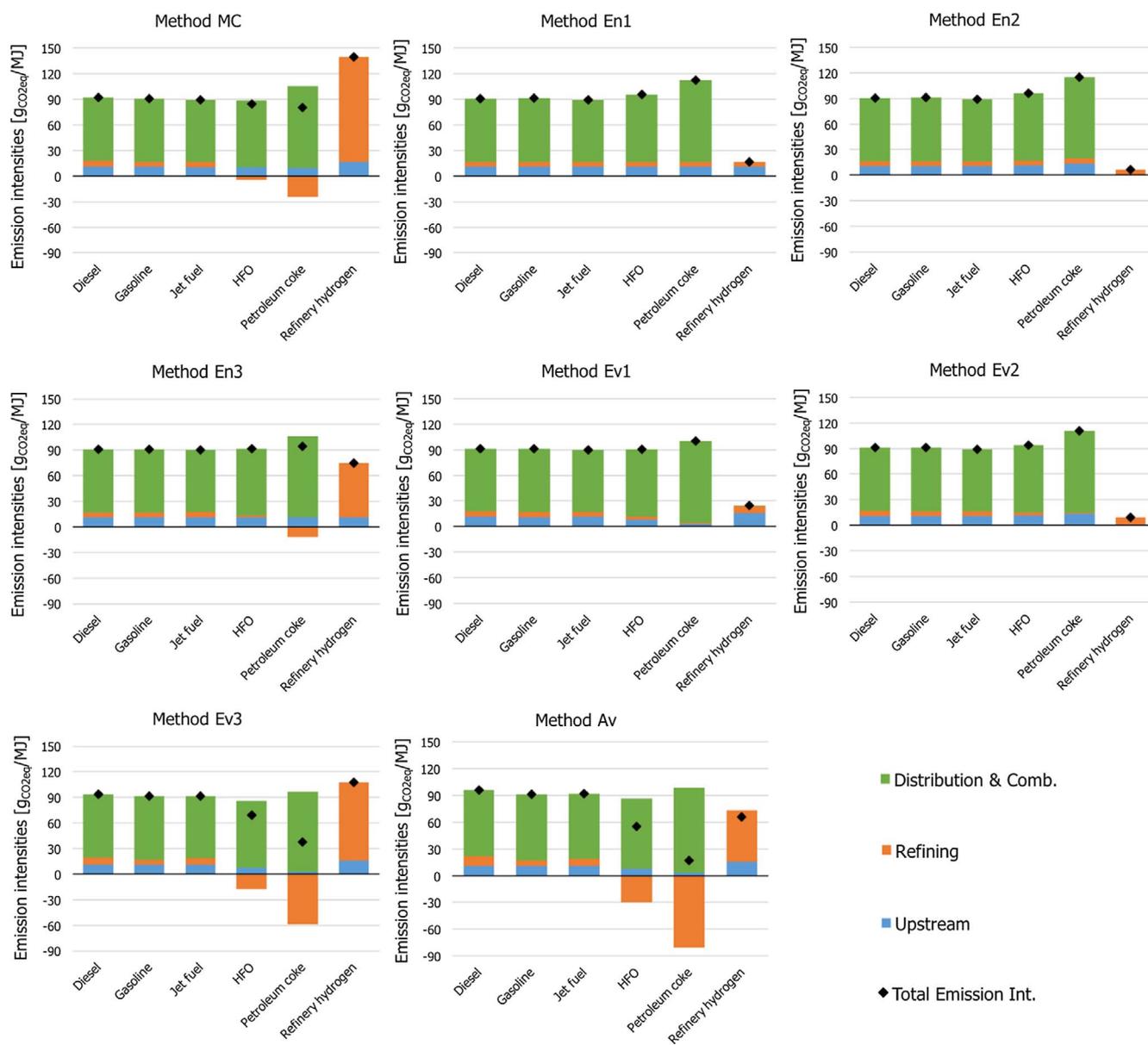
Table 3
Emission intensities assigned to each product for the considered allocation methods. All the emission intensities are expressed in gCO2eq/MJ.

Method	Well-to-Wheel phase	Diesel	Gasoline	Jet fuel	HFO	Petroleum coke	Refinery hydrogen
MC	Upstream	10.9	10.8	10.7	10.1	9.6	16.8
	Refining	7.2	5.8	6.1	−4.3	−24.8	122.9
	Total Emissions	92.2	91.1	89.5	84.5	80.4	139.7
En1	Upstream	11.0	11.0	11.0	11.0	11.0	11.0
	Refining	5.8	5.8	5.8	5.8	5.8	5.8
	Total Emissions	90.9	91.3	89.5	95.5	112.4	16.8
En2	Upstream	10.7	10.8	10.6	11.4	13.8	0.8
	Refining	5.8	5.8	5.8	5.8	5.8	5.8
	Total Emissions	90.6	91.1	89.1	95.9	115.2	6.6
En3	Upstream	11.0	11.0	11.0	11.0	11.0	11.0
	Refining	6.0	5.7	6.6	1.9	−11.9	63.9
	Total Emissions	91.1	91.2	90.3	91.6	94.5	74.9
Ev1	Upstream	11.4	11.0	11.2	7.7	2.9	15.8
	Refining	6.0	5.8	5.9	4.0	1.6	8.4
	Total Emissions	91.5	91.3	89.8	90.4	100.1	24.4
Ev2	Upstream	10.8	10.8	10.6	11.2	13.2	1.1
	Refining	6.0	5.8	5.9	4.0	1.6	8.4
	Total Emissions	90.9	91.1	89.3	93.9	110.4	9.5
Ev3	Upstream	11.4	11.0	11.2	7.7	2.9	15.8
	Refining	8.4	5.9	7.8	−17.4	−58.7	92.0
	Total Emissions	93.9	91.4	91.7	68.9	38.0	107.8
Av	Upstream	11.4	10.8	10.9	6.6	2.1	7.9
	Refining	10.3	6.0	7.9	−29.8	−80.4	57.7
	Total Emissions	95.8	91.3	91.6	55.5	17.3	65.6

Fig. 2. Comparison of emissions among the considered allocation methods.

Table 4
Product yields and allocation shares for the EU refinery sector in 2010.

PF-Production factor 2010	Diesel	Gasoline	Jet fuel	HFO	Petroleum coke	Refinery hydrogen
$[MJ_{product}/MJ_{crude-eq}]$	0.291	0.176	0.080	0.046	0.010	0.007
SP-Share Parameter [–]						
SEC	0.320	0.194	0.088	0.050	0.011	0.007
SEV (prices 2006–10)	0.332	0.194	0.089	0.035	0.003	0.011
SAV (prices 2006–10)	0.569	0.201	0.120	-0.258	-0.152	0.073

4.3. Energy-based allocation 2 (En2)

This method allocates refinery emissions based on SEC values, whilst it allocates upstream emissions based on a feedstock approach (see relation (7)). As for the En1 method, the refining emissions are the same for all petroleum products: therefore, the main parameter affecting the total emissions is the carbon content of products. Hydrogen gets very low refining emissions (5.8 $gCO_2eq/MJ_{hydrogen}$), a value lower than the combustion and refining emissions of the fuels from which it is made (83.9 gCO_2eq/MJ for HFO, 72.7 for steam-reforming of natural

gas). Therefore, method En2 fails the proposed consistency criteria.

4.4. Energy-based allocation 3 (En3)

Unlike the two previous energy-based methods, this method derives both upstream and refinery emissions from *Feedstock allocation*. This method returns similar refining emissions for diesel, gasoline and jet fuel. As for the marginal method, negative refining emission intensities are obtained for the heaviest product (petroleum coke), while for HFO the allocated emissions are slightly positive. Hydrogen refining

Table 5
Mass-based feedstock allocation method.

Well-to-Wheel step	Diesel gCO₂eq/MJ_diesel	Gasoline gCO₂eq/MJ_gasoline	Jet fuel gCO₂eq/MJ_jet fuel	HFO gCO₂eq/MJ_HFO	Petroleum coke gCO₂eq/MJ_pet-coke	Refinery hydrogen gCO₂eq/MJ_hydrogen
Upstream	10.8	10.9	10.8	11.6	15.2	3.9
Refining	5.0	5.2	5.3	5.6	12.4	22.8
Distribution	1.1	1.2	0.5	0.6	0	0
Combustion	73.2	73.3	72.2	78.1	95.6	0
Total emission intensity	**89.9**	**90.6**	**88.8**	**95.9**	**123.2**	**26.7**

emissions (63.9 gCO₂eq/MJ_hydrogen) are about half compared to those of the reference (122.9 gCO₂eq/MJ_hydrogen). The TEs for the main transport fuels and for petroleum coke are close to those of the marginal reference emissions, while the TE of hydrogen is strongly different from the reference case. The En3 method almost satisfies the first consistency criterion: the main transport fuels result in higher refinery emissions than petroleum coke, but they are slightly lower than the HFO ones. The method narrowly fails the second consistency criterion, since the refining emissions allocated to hydrogen (63.9 gCO₂eq/MJ_hydrogen) are lower than the combustion and refining emissions of HFO (80.0 gCO₂eq/MJ), and lower than emissions required to produce hydrogen from natural gas (72.7 gCO₂eq/MJ_hydrogen).

4.5. Economic-based allocation 1 (Ev1)

This method allocates refinery and upstream emissions based on values of SEV. Refining emissions for HFO (4.0 gCO₂eq/MJ) and petroleum coke (1.6 gCO₂eq/MJ) result lower than other transport fuels, but not negative as for the reference values derived from the marginal method. Total emissions for the three main transport fuels (diesel, gasoline and jet fuel) are very similar, and not far from the reference values. HFO appears to have TE similar to those of the other transport fuels even though it produces fewer emissions in the refinery stage. Hydrogen has total emissions far out of line with the reference value (139.7 gCO₂eq/MJ). Since refining emissions for main transport fuels are higher than for HFO and pet coke, this method fulfills the first consistency criterion. However, refining emissions for hydrogen (8.4 gCO₂eq/MJ) are much lower than the values adopted as testers of HFO or steam-reforming of natural gas: the second consistency criterion is therefore not respected.

4.6. Economic-based allocation 2 (Ev2)

Ev2 allocates refinery emissions based on values of SEV, while it allocates upstream emissions based on a feedstock approach (see relation (7)). Results for refinery emissions and combustion emissions are therefore the same as for method Ev1, but upstream emissions are different. These changes are small for the main transport fuels (diesel, gasoline and jet fuel), but much more significant for HFO, petroleum coke and hydrogen. More specifically, TE of heavy fuel oil (93.9 gCO₂eq/MJ) and petroleum coke (110.4 gCO₂eq/MJ) come out higher than diesel (90.9 gCO₂eq/MJ), even though they have lower emissions in the refinery stage. This method fulfils the first consistency criterion because *refining* emissions are lower for the heavy products. On the other hand, it fails the second criterion, since refining emissions of hydrogen (8.4 gCO₂eq/MJ) are much lower than the combustion and refining emissions of HFO or hydrogen production from natural gas.

4.7. Economic-based allocation 3 (Ev3)

Analogously to method En3, this method allocates both upstream and refinery emissions based on the feedstock approach, as described in Section 2.4. This method gives large differences among refining emissions of different products, and consequently strong differences in

values of TE. The heaviest oil products (HFO and pet coke) get negative refining emissions, even more negative than those calculated through the reference marginal method. Heavier products, which need less refining, have lower refinery emissions, as expected and required by the first consistency criterion. The fact that their refining emissions are negative is coherent with the reference method, which reflects the reduced emissions from the hydrocracking which is otherwise needed to convert heavy products to the main transport fuels. The total emissions for hydrogen are in the same order of magnitude than those of the reference emissions (107.8 gCO₂eq/MJ vs 139.7 gCO₂eq/MJ). Therefore, method Ev3 satisfies the two proposed consistency criteria.

4.8. Added-Value-based allocation (Av)

This method allocates refinery emissions based on values of SAV, while it allocates upstream emissions based on the feedstock approach (see relation (7)). Consistent with the marginal method, the Av method returns negative refinery emissions for heavy products (−29.8 gCO₂eq/MJ for HFO and −80.4 gCO₂eq/MJ for petroleum coke). As expected, HFO (54.6 gCO₂eq/MJ) gets lower total emissions than diesel (90.6 gCO₂eq/MJ) and gasoline (101.8 gCO₂eq/MJ), since the former needs much less refining compared to diesel and gasoline. Refining emissions for heavy products are lower than values obtained through all the other methods, including the reference results. The Av method satisfies the first consistency criterion, as the refinery emissions for the main transportation fuels are higher than the emissions of heavy products. The second criterion is also satisfied, since refining emissions for hydrogen (57.7 gCO₂eq/MJ) result as greater than the combustion plus refining emissions of HFO (48.3 gCO₂eq/MJ).

Based on the obtained results, the following comments may be highlighted:

- The considered allocation methods show large differences in the emissions allocated to hydrogen and heavy products, especially petroleum coke. This illustrates that considering also light and heavy products in testing emissions allocation methods at the aggregate refinery-level is important in comparing methods, adding relevant information.
- In general, Economic-based and Added-Value-based allocation methods give results closer to the reference method compared to the Energy-based methods. This can be explained by considering that oil refineries modify their production yields by increasing the production of valuable products (with high hydrogen content, thus highly emissions intensive) at the expense of less valuable ones, and this process continues until the extra costs involved becomes equal to the extra value generated by the products.
- With reference to Fig. 2, only two allocation methods satisfy both the proposed hydrogen-based consistency criteria: one Economic-based allocation (Ev3) and the Added-Value-based allocation (Av). Unlike to all the other allocation methods, Ev3 and Av methods allocate negative emissions to both heavy products but high positive emissions to hydrogen. Compared to the reference marginal method, such methods give lower values of TEs for hydrogen and higher ones for petroleum coke and heavy fuel oil. Considering the main

transportation fuels, both Ev3 and Av methods agree with the results of marginal method, resulting in higher refinery and total emissions for diesel than gasoline and jet-fuel. Based on the obtained results, it is possible to state that the choice among Ev3 and Av allocation methods slightly affects the GHG savings calculations from the use of alternative transportation fuels. However, on average, method Ev3 comes closer than Av to the results of the marginal method.

- Amongst the energy-based allocation methods, only results of En3 comes close to satisfying the consistency criteria, since the emissions allocated to the main transportation fuels are numerically close to the reference method. Moreover, En3 returns negative refining emissions for petroleum coke, although it differs by showing slightly positive ones for heavy fuel oil.

4. Conclusions

Current environmental policies aim to reduce GHG emissions in transportation by replacing traditional fuels obtained from crude oil with alternative fuels, such as biofuels or hydrogen. In the EU context, to assess the benefits arising from the use of alternative fuels, their total emission intensities are compared with those of the replaced conventional fossil fuels by means of the so-called Fossil Fuel Comparators (FFC). Therefore, a fair calculation of the total emission intensities (including upstream and refinery emissions) is nowadays crucial in order to inform policymakers. A methodological correct calculation of total emission intensities of petroleum products is performed by means of the *marginal method*: this method requires a detailed mathematical model of the analyzed oil refinery, including all the refinery processes and their related capacities. In the case that such models are not available, or considered not sufficiently transparent, the marginal method can be substituted by the so-called *allocation methods*, which allocate emissions based on different allocation keys, and are based on publicly available data, making them fully transparent.

In this paper, total emissions intensities have been calculated for different refined oil products (Diesel, Gasoline, Jet fuel, Heavy Fuel Oil, Petroleum Coke and Hydrogen), considering the average EU refinery in 2010. Values of Total Emissions Intensities have been calculated through the marginal method, and results compared to the ones obtained from allocation methods based on mass, energy, economic-value

keys plus the novel added-value key.

The first conclusion of this work is that when comparing the results of different allocation methods, it is important to include the results for heaviest products (e.g. petroleum coke and heavy fuel oil) and lightest ones (hydrogen). This is because different allocation methods tend to give fairly similar results for the main transport fuels (gasoline, diesel and jet-fuel/kerosene) but very different results for the heaviest and lightest products. Thus, a more sensitive, fair and comprehensive assessment can be performed if also such products are considered.

The consistency of each allocation method has been determined by comparing its results with those of the marginal method, and by fulfilling the requirements of two proposed *hydrogen-based consistency criteria*, based on specific considerations on hydrogen production processes. Only two of the investigated allocation methods satisfied the criteria: one of the Economic-value-based allocations (Ev3) and the Added-Value-based allocation (Av). Compared to method Av, results of method Ev3 are closer to results of the marginal method, thus we recommend its use. Note that Ev3 allocates the carbon intensities of the *refinery feedstock*, not only the refinery emissions, to different products. Both of the valid allocation methods En3 and Av agree with the marginal method in assigning negative refining emissions to heavy products like heavy fuel oil and petroleum coke. This implies that refineries could save overall emissions if they were able to produce more of these heavy products instead of increasing energy requirements to convert such products into lighter ones, for which there is a higher demand.

Considering only the two valid allocation methods and the reference marginal method, the range of the results is relatively small: the numerical values of European refining emissions in 2010 are: 5.8 to 6 gCO2eq/MJ for gasoline, 7.2 to 10.3 gCO2eq/MJ for diesel, 6.1 to 7.9 gCO2eq for kerosene and −29.8 to −4.3 gCO2eq for heavy fuel oil. The corresponding values for the Fossil Fuel Comparator would be 92.2–95.8 gCO2eq/MJ for diesel and 91.1–91.4 gCO2eq/MJ for gasoline.

Appendix A. Product yields and allocation shares

This appendix shows some intermediate values of the model, to allow the replication of the calculations (see Table 4).

Note that these figures are truncated versions of the ones in our spreadsheet, so using them to replicate our calculations may result in slight deviations due to round-off errors.

Appendix B. Results of the mass-based allocation method

Here are reported the results of applying allocation by mass instead of by economic value in a way similar to that used in method Ev3, which gives consistent results amongst economic-value-allocation methods. In other words, mass allocation is applied to the feedstock entering the refinery (see Table 5).

As expected, the method fails the second consistency criterion, because it gives refinery emissions for hydrogen lower than the minimum emissions from processes for producing additional hydrogen in refineries. The method also fails the first consistency criterion because the straight-run product HFO and pet coke get higher refinery emissions than the highly-refined transport fuels.

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