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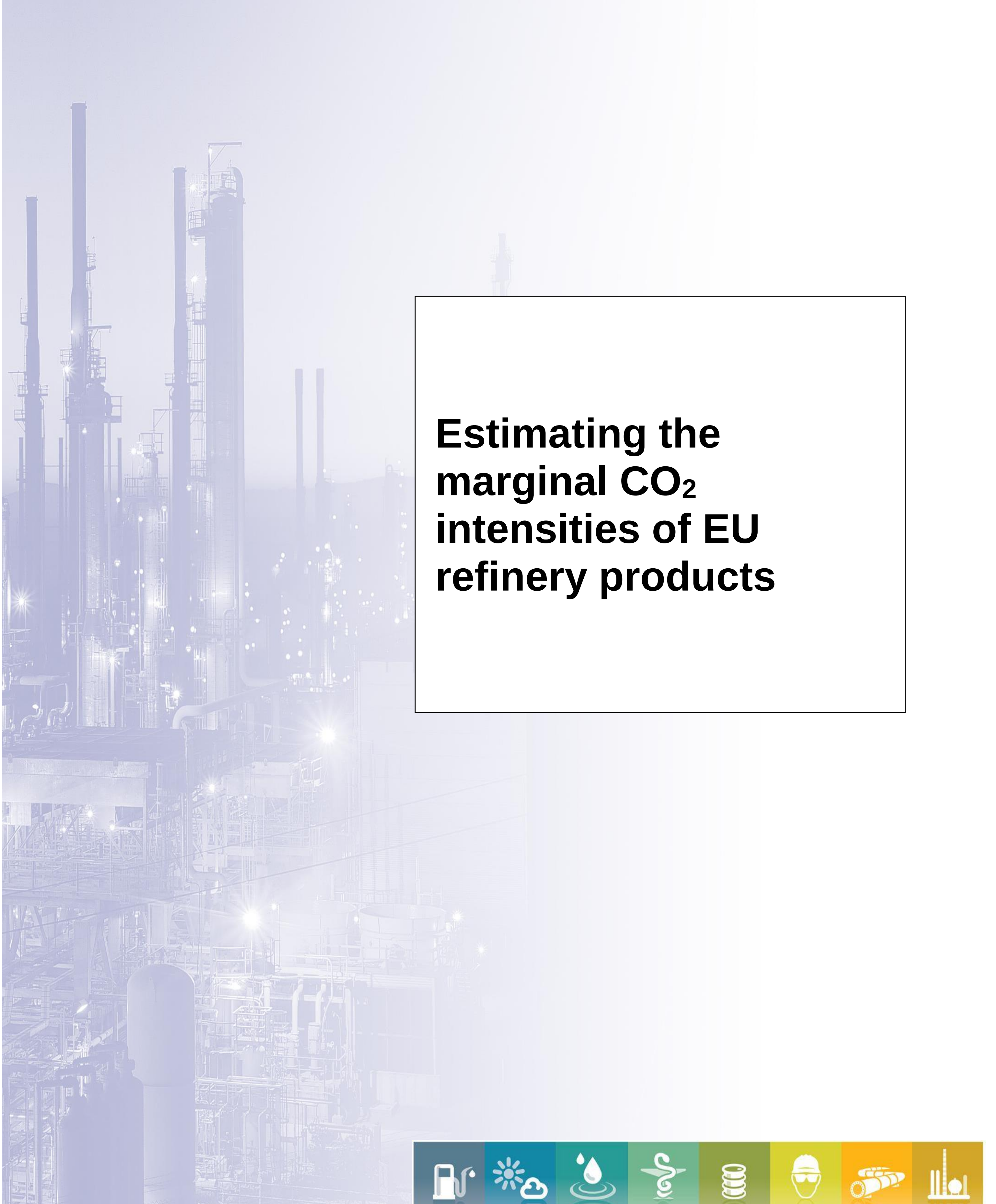

Estimating the marginal CO_2 intensities of EU refinery products

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Estimating the marginal CO_2 intensities of EU refinery products

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ABSTRACT

Estimating the CO_2 emissions associated with production of individual oil products is challenging inasmuch as they are produced simultaneously through a combination of interrelated processes. This report proposes a new methodology that utilises the specific features of the Linear Programming (LP) technique used to model refineries to produce a consistent set of CO_2 intensities for all refinery products. The methodology is described in detail and applied to a study case reflecting EU refining in 2010. Results are compared to figures obtained in previous Concawe work.

KEYWORDS

Linear Programming (LP) model, CO_2 emissions, marginal CO_2 intensity, refined product, EU refining

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SUMMARY

Estimating the CO_2 emissions associated with production of individual oil products is challenging inasmuch as they are produced simultaneously through a combination of interrelated processes. Allocation methods, although providing for a mostly straightforward set of calculations, often fail to capture crucial interactions between processes and products and can lead to unrealistic or misleading results.

In the past, Concawe proposed a methodology focused on gasoline and diesel fuel and based on marginal analysis using the in-house EU refining model. Starting from a base case a small change of demand for either fuel was introduced and the resulting change in CO_2 emissions was apportioned to that change in demand. Although it delivered figures that were considered realistic there were significant drawbacks. Firstly the approach only worked well with major products and secondly the CO_2 intensity figures were not additive (i.e. the sum of all marginal intensities would not exactly equal the total emissions of the refineries represented by the model), thereby not meeting one of the requirements of Life Cycle Assessment (LCA) studies.

The present report proposes a new methodology that utilises the specific features of the Linear Programming (LP) technique used to model refineries.

As part of the LP model solution, a marginal emission value (in tonnes of CO_2 per unit of each constraint) is generated for any constraint that is binding and has a bearing on CO_2 emissions. By design of the LP model, the sum of all marginal emission values multiplied by the value of each respective constraint is equal to the total tonnes of refinery CO_2 emissions, thereby fulfilling the additivity criterion.

The model can be adapted in such a way that the only constraining variables are final product demands and process unit capacities. Using further information available from the LP solution, an algorithm can be derived to reapportion the CO_2 emissions associated with process unit capacities to final products. In this way all CO_2 emissions can be allocated to final products.

The methodology was used to generate a full set of product CO_2 intensities for a study case representing EU refining in 2010.The results are summarised in the following table.

Products	Product demands	Product demand constraints	Reallocated process unit constraints	Total allocation to final products	Product demand constraints	Reallocated process unit constraints	Total allocation to final products	Product demand constraints	Reallocated process unit constraints	Total allocation to final products
		Emissions allocated to each product			Marginal emission intensities per tonne product			Marginal emission intensities per MJ product		
	Mt/a	Mt/a CO_2			t CO_2 / t			g CO_2 / MJ		
Chemicals	54.6	79.7	-5.4	**74.4**	1.46	-0.10	**1.36**	33.4	-2.3	**31.1**
LPG	13.0	3.6	-0.5	**3.1**	0.28	-0.04	**0.24**	6.1	-0.9	**5.2**
Gasoline	126.3	34.1	-4.2	**29.9**	0.27	-0.03	**0.24**	6.2	-0.8	**5.5**
Kerosine	56.6	17.7	-2.8	**15.0**	0.31	-0.05	**0.26**	7.2	-1.1	**6.1**
Diesel Fuel	207.1	73.4	-8.5	**64.9**	0.35	-0.04	**0.31**	8.1	-0.9	**7.2**
Heating Oil	72.5	18.9	-4.2	**14.8**	0.26	-0.06	**0.20**	6.1	-1.3	**4.7**
Marine Gasoil	7.0	1.4	-0.6	**0.9**	0.20	-0.08	**0.13**	4.8	-1.8	**2.9**
Heavy Fuel Oil	88.6	-21.6	8.2	**-13.5**	-0.24	0.09	**-0.15**	-5.9	2.2	**-3.7**
Bitumen	19.2	-8.6	0.9	**-7.7**	-0.45	0.05	**-0.40**	-11.3	1.2	**-10.1**
Petroleum coke	5.0	-4.5	0.1	**-4.4**	-0.89	0.01	**-0.88**	-25.3	0.3	**-25.0**
Lubes & Wax	5.1	2.0	1.0	**3.0**	0.39	0.21	**0.60**	9.2	4.9	**14.1**
Sulphur	3.2	-	-0.1	**-0.1**	-	-0.02	**-0.02**	-	-1.3	**-1.3**
Fuel & Losses	60.5	-	-	**-**						
Total	**718.6**	**196.2**	**-15.9**	**180.3**						

The reallocation of unit capacity constraints reduces the overall CO_2 intensity of finished products. This is because relaxation of a capacity constraint tends to give more freedom to the model to make operation more CO_2-efficient.

Heavy products (Heavy Fuel Oil, Bitumen, Petroleum coke) have negative intensities reflecting the fact that demand for heavy products reduces the need for conversion of the original crude oil barrel to lighter products.

Naphtha (chemical feed) does not feature in the table above because it is an intermediate product in the standard Concawe model, so no fixed demand is assigned. In order for a marginal value to be generated a special case needs to be established with a small naphtha (sale) demand. The CO_2 intensity figure for naphtha is in the region of 6-7 gCO_2/ MJ, i.e. higher than gasoline. Although this may be counterintuitive it can be explained by the synergy between gasoline and middle distillate production regarding redistribution of hydrogen between products.

The figures for gasoline and diesel fuel are about 20% lower than found in previous Concawe work. The approach followed in that work produced figures which were comparable to the present ones, before reallocation of capacity constraints, which accounts for about half of the difference. The other half is due to changes in base case assumptions and other changes in the model in the intervening time.

The figures generated through this method are strictly only valid for the given set of base conditions, and for specific model constraints which lead to the model adopting a marginal production strategy which may not mirror that of some refineries. A comprehensive sensitivity analysis was carried out and showed a satisfactory level of stability within a ± 2.5% range of variation of key variables around the base case. However, significantly different base cases and model constraints would correspond to different total CO_2 emissions and different distributions of marginal CO_2 intensities between products. For the same reason, the figures generated for EU as a whole cannot be applied to individual refineries that all have their specific configuration, feedstocks, product demands and operating strategies.

1. INTRODUCTION

The climate change issue has brought GHG emissions into focus, and with it, the GHG footprint of the various goods and services used in the economy. When it comes to petroleum products the main issue is their potential substitution with less GHG intensive alternatives.

The main source of GHG emissions from oil products is of course CO_2 emitted when they are combusted as fuel (which is the case for the majority of these products). There are, however, additional emissions arising from the various production and transport steps starting from crude oil and ending in a commercial product. Although there are some emissions of other GHGs on the way, the overwhelming contribution to total GHG emissions is in the form of CO_2. A significant fraction of these is incurred at the refining stage where crude oil is transformed into marketable products through a series of energy-intensive processes. In addition, refining generates so-called “process” emissions where CO_2 is produced as a result of a chemical reaction (e.g. decarbonisation of hydrocarbons to produce hydrogen).

Total CO_2 emissions from refineries are accurately monitored and measured and therefore well documented. Difficulties arise, however, when it comes to apportioning total emissions to the numerous products produced by a refinery. This is a typical example of a co-production process whereby several products are produced simultaneously through a collection of mutually dependent processes, making it impossible to isolate the production path of one particular product and therefore the CO_2 emissions attached to it. Several allocation methods to estimate average CO_2 intensities have been proposed from a simple apportionment based on mass or energy content, to more complex schemes aimed at relating each process to a number of finished products. Methods based on a static view of the refining operation ignore the complex interactions between processes and between products when the outputs change. As a result, the average CO_2 intensity values produced by static allocation methods do not reveal the interdependence of the multitude of CO_2 emission sources involved in producing each product and are unsuitable for predicting marginal intensities.

Concawe has in the past addressed the issue of apportionment of CO_2 emissions by considering marginal production i.e. what happens when, starting from a known base case, a small change to the product demand is introduced. In this way, the CO_2 footprint of the marginal production of each product could be determined. Concawe used this incremental approach in their European Refinery Linear Programming (LP) model to estimate such values for gasoline and diesel fuel and incorporated these values in the JEC Well-to-Wheels study reports [1]. However, it is not practical to do this for all refinery products. Also, even if this were done, the total of all product footprints would not exactly match the total CO_2 emissions from the base case (because each separate change represents a slightly different case), which represents a major deviation from the rules applicable to LCA studies.

In this report, we describe an innovative and scientifically rigorous method [2], exploiting the specific properties of Linear Programming models whereby the marginal CO_2 intensities of all refinery products produced in a base case can be determined simultaneously. The method is applied to a study case representative of the situation in 2010.

2. MODELLING METHODOLOGY

2.1. REFINERY MODELLING USING LINEAR PROGRAMMING (LP)

The purpose of an oil refinery is to turn crude oil into marketable products in the most efficient and economical way. A particular refinery generally serves a particular market which sets the quality of the products to be supplied and to an extent the amount of each grade. Depending on the geographical location of the refinery, there can also be opportunities to export to other markets. The refinery has access to certain crude oils and other feedstocks, the range of which is a function of its location and the way it is supplied (e.g. ships or pipelines). Finally the refinery features a certain combination of process units (generally referred to as its configuration).

Refinery operation is thus characterised by multiple real constraints arising from feedstock supply, product demand (quantity and quality) and process unit limitations. Yet there are many ways of operating within these constraints and refiners have always strived to optimise their operation in order to maximise profit or minimise costs to supply a given market demand within a given set of product prices and input costs. The tool used to that end by refiners worldwide is known as Linear Programming (LP), a mathematical technique which, given a quantity to be optimised, aims at identifying the optimum solution amongst the myriad of possible solutions to a complex problem.

In an LP model the refinery constraints are represented by a system of linear equations linking the different variables. Because there are more degrees of freedom (or variables) than there are constraints, the system has an infinite number of possible solutions. Provided that appropriate cost factors are defined as model inputs (i.e. cost of feedstocks, energy, additional plant capacity, price of products etc), a so-called “objective function” can be derived, describing the quantity to be optimised (maximum profit or minimum cost). The LP technique then provides a pathway towards the optimum solution.

For a given set of desired products, the LP solution tells the refiner how much of each available feedstock should be processed, the level at which each plant will be utilised and, more generally, which amongst all the constraints will actually be binding. Crucially it also provides information on the impact on the objective function of a marginal change in each of the binding constraints (the so-called “marginal values”). It is this last feature that can be used to assess the marginal CO_2 footprint of products.

2.2. THE CONCAWE EU REFINING LP MODEL

Since the mid-90s Concawe has operated a refinery LP model representing the combination of all refineries operating in the EU. This was originally devised to estimate the cost to EU refiners of EU legislation (mostly affecting product quality) and of expected changes in EU market demands.

Model structure

The model features a full library of refinery process units represented by a number of operating modes including feedstock type, product yield structure and all relevant quality parameters. From this a refinery can be modelled with any combination of process units.

A range of crude oils is available, representing the diversity of grades available to EU refiners.

A blending module allows finished products to be prepared according to the required quality specifications from selected intermediate streams.

In the Concawe master LP model, the EU is divided into 9 regions, each represented by a single refinery having the aggregated capacity, crude intake, process configuration and product demand of all physical refineries in that region. Due to the specific requirements of the methodology developed to generate product CO_2 intensities, a single-region model has been derived from the original 9-region model for the purpose of this study. This model then consists in a single refinery representing the aggregation of all European refineries (capacities, crude intakes, process configurations and product demands).

CO_2 emissions modelling

In response to the CO_2 emissions challenge, the model was adapted in the early years of the last decade so that it could estimate the CO_2 emissions associated with a particular operating case. This primarily requires CO_2 emission factors for combustion of refinery fuels (t of CO_2 emitted per GJ of fuel burnt), combined with fixed unit-specific energy consumption factors (GJ per t unit feed). It must also take into account structural emissions arising from specific chemical reactions (notably the production of hydrogen by reforming or partial oxidation of hydrocarbons), expressed in tonne of CO_2 per tonne of each feedstock type processed.

Because a refinery generally uses its own feeds or products for a proportion of its fuel needs the carbon contained in the input to the refinery is apportioned between products and fuels. In order to avoid any spurious carbon gain or loss as a result, it is therefore essential that the model be strictly carbon-balanced (i.e. that the amount of carbon entering the refinery in the form of feedstocks and possibly fuels equals the amount that leaves the refinery in the form of CO_2 and products). In order to achieve this, the model includes feed and product carbon contents and each operating mode of every process units must also conserve carbon.

In order for the model to generate marginal values related to CO_2 emissions, these must have an impact on the objective function. In other words CO_2 emissions must be assigned a monetary value. Although the actual number used is not crucial to the outcome, it must be sufficiently high to ensure small changes have a discernable impact on the objective function. We have used 30 €/t CO_2 (40 $/t), being the CO_2 price used in the EU Commission's Impact Assessment of the ETS directive [3].

3. METHODOLOGY FOR GENERATING MARGINAL CO_2 INTENSITIES FOR PRODUCTS

3.1. GENERATING MARGINAL EMISSION VALUES

As part of the LP solution, a marginal emission value (in tonnes of CO_2 per unit of each constraint) is generated for any constraint that is binding and has a bearing on CO_2 emissions. These emission values are "marginal" in the sense that they represent the CO_2 emissions attributable to a certain limiting constraint (for example, if the model is required to meet a certain gasoline demand, the marginal value for gasoline would represent the emissions incurred in producing the last tonne of gasoline that satisfies that demand constraint). By design of the LP technique, the sum of all marginal emission values multiplied by the value of each respective constraint is equal to the total tonnes of refinery CO_2 emissions, thereby fulfilling the additivity criterion required for Life Cycle Assessments.

The availability of the marginal emission values provides a systematic and transparent way to estimate the marginal CO_2 emissions associated with all refinery products (CO_2 intensity), taking into account all interactions within the refinery operation. Before this can be done, the modelling strategy has first to be adapted in such a way that all marginal CO_2 can be traced back to final products.

- The model constraints include product demands (tonnes), product quality specifications (e.g. sulphur content), but also feedstock availability (tonnes of crude) and process unit capacities (tonnes).
- A finished product will only generate a marginal value if its demand is seen as a constraint by the model. To this end all products must be assigned a fixed demand. These product demand constraints typically account for around 90% of all emissions.
- Because of the way product quality constraints are modelled they do not directly generate a non-zero marginal value. Instead their impact is integrated into the corresponding product demand constraints.
- Crude and feedstocks availability can be constraining, in which case they would normally generate a marginal value. This can be alleviated by specifying availability as ratios rather than fixed values.

With the adaptations described above the only marginal values that do not directly relate to products originate from process unit capacity constraints. These generate non-zero marginal values whenever the model solution fully utilises the available capacity of a certain process unit.

3.2. REALLOCATING MARGINAL EMISSIONS VALUES ASSOCIATED WITH PROCESS UNIT CAPACITY CONSTRAINTS

The LP solution provides all the elements for a structured and rigorous methodology to reapportion the capacity-related marginal emission values to final products. The calculation sequence is briefly described below. The 2010 case discussed in section 4 provides the basis for a worked example detailed in **Appendix 2**.

Step 1: Identifying constraining process unit capacities

In a given LP solution, a number of process plant capacities will be constraining (i.e. the model will have used all available capacity). Each of these will generate a non-zero marginal emission value which will need to be reallocated to final products.

Step 2: Using “Marginal Rates of Substitution” to allocate emissions to CO_2 emitting modes

The LP solution provides so-called “Marginal Rates of Substitution” (MRSs) which describe the interdependencies between all variables in the model. A subset of these variables is the streams or modes physically responsible for CO_2 emissions (essentially those variables describing fuel burning or hydrogen production). By scanning the LP solution, it is possible to identify which of these are linked to a particular process unit capacity. In other words, this means that it is possible to determine directly from the LP solution how the marginal CO_2 from step 1 is produced and how much is produced by fuel burning modes and how much by hydrogen production modes.

Each of these modes is characterised by a CO_2 “emission factor” (t CO_2 / t mode). The contribution of each CO_2-emitting mode to the total marginal emission value of a constraining process unit is given by the product of MRS and the emission factor. This provides the key for reallocating emissions from constraining process units to CO_2-emitting modes.

Step 3: Linking CO_2 emitting modes to process units

The CO_2 emitting modes can in turn be linked to those process units that produce the substance that emits the CO_2 (for instance refinery fuel gas is produced by a number of different process units). It is then logical to apportion the CO_2 burden calculated above for each mode to these process units in the proportion of their contribution to the total amount of the particular CO_2-emitting substance produced.

Step 4: Linking process units to final products

The above calculations provide a list of process units to which some marginal CO_2 has been allocated through step 2 and 3. The LP solution provides a product yield structure for each process unit. Some of these unit products are blended directly into the final product pools. Others are further processed in downstream units. Through an iterative calculation, it is then possible to arrive at a yield structure that contains only final products. The marginal CO_2 allocated to the process unit can then be further reallocated to those on a mass basis.

In this way the reallocation of the contribution of the capacity constraints to the finished product CO_2 intensities is done solely on the basis of the LP solution and is therefore entirely consistent, representing the actual interactions modelled in the LP.

The total CO_2 intensity pertaining to each finished product is the sum of the direct allocation and the amount reallocated from process unit capacities.

It is worth noting that a marginal change in the values of the product demand constraints and in the unit capacity constraints have opposite effects. Indeed an increase of product demand tends to increase CO_2 emissions (increased refinery activity) whereas an increase of unit capacity tends to de-constrain the model, leading to a more CO_2-efficient operation and therefore lower CO_2 emissions. It can thus be anticipated that the effect of the reallocation described above will be to reduce the product CO_2 intensities.

4. CASE STUDY: ESTIMATING MARGINAL CO_2 INTENSITIES OF EU REFINERY PRODUCTS IN 2010

The methodology described above was used to generate marginal CO_2 intensities for all final products within a scenario representative of the situation in 2010 in terms of refinery capacities, refinery energy intensity, feedstock availability, import/export opportunities, product demand and CO_2 emissions. An overview of the relevant input data is given in **Appendix 1**.

4.1. BASE CASE

The LP solution provides direct marginal CO_2 emission values for all refinery products (petrochemical naphtha is a special case dealt with separately below). As explained in section 3 these do not, however, account for all marginal CO_2 emissions as some is assigned to process unit capacity constraints. **Table 1** shows the unit utilisation rates pertaining to the 2010 case.

Table 1 Aggregated process unit throughputs and utilisation rates

Process unit (340 stream days/a)	**Throughput** Mt/a	**Capacity** Mt/a	**Utilisation** %
Crude distillation (CDU)	674.6	750.5	90%
Vacuum distillation (VDU)	243.7	344.0	71%
Visbreaking (VBU)	57.8	89.5	65%
Delayed Coking (DCK)	19.3	23.1	84%
Deasphalting	0.0	2.0	
Fluid Catalytic Cracking (FCC)	86.9	118.2	74%
Hydrocracking (HCK)	**74.8**	**74.8**	**100%**
Vacuum Gas Oil Hydrodesulphurisation (VGO HDS)	1.4	49.9	3%
Long Residue Hydrodesulphurisation (LR HDS)	**4.9**	**4.9**	**100%**
Short Residue Hydrodesulphurisation (SR HDS)	0.0	1.9	
Residue Hydroconversion (RHC)	0.0	9.7	
Naphtha HDT	79.1	172.3	46%
Naphtha Reformer semi-regenerative (SR Ref)	**59.7**	**59.7**	**100%**
Naphtha Reformer continuous (CCR Ref)	21.9	38.8	57%
Aromatics extraction	11.0	13.5	81%
Alkylation*	12.2	11.2	109%
Isomerisation	0.0	26.2	
Kerosine HDT	31.1	31.8	98%
Diesel HDS	**133.0**	**133.0**	**100%**
Petrochemicals	69.5	74.8	93%
Sulphur Recovery Unit* (SRU)	3.2	6.4	50%
Hydrogen production* (SMR)	0.8	1.7	48%
Hydrogen production* (POX)	**0.2**	**0.2**	**100%**
Integrated Gasification Combined Cycle (IGCC)	0.1	0.4	30%

* The figures for these units are expressed in Mt/a of product, not feed

Five of the process units show constraining capacities (i.e. 100% utilisation), with therefore a need for marginal CO_2 reallocation. The calculations are detailed in **Appendix 2**.

The complete results for the main product groups are shown in **Table 2**.

Table 2 Marginal CO_2 intensities for the main product groups

	Product demands	Product demand constraints	Reallocated process unit constraints	Total allocation to final products	Product demand constraints	Reallocated process unit constraints	Total allocation to final products	Product demand constraints	Reallocated process unit constraints	Total allocation to final products
Products	Mt/a	Emissions allocated to each product Mt/a CO_2			Marginal emission intensities per tonne product t CO_2 / t			Marginal emission intensities per MJ product g CO_2 / MJ		
Chemicals	54.6	79.7	-5.4	**74.4**	1.46	-0.10	**1.36**	33.4	-2.3	**31.1**
LPG	13.0	3.6	-0.5	**3.1**	0.28	-0.04	**0.24**	6.1	-0.9	**5.2**
Gasoline	126.3	34.1	-4.2	**29.9**	0.27	-0.03	**0.24**	6.2	-0.8	**5.5**
Kerosine	56.6	17.7	-2.8	**15.0**	0.31	-0.05	**0.26**	7.2	-1.1	**6.1**
Diesel	207.1	73.4	-8.5	**64.9**	0.35	-0.04	**0.31**	8.1	-0.9	**7.2**
Heating Oil	72.5	18.9	-4.2	**14.8**	0.26	-0.06	**0.20**	6.1	-1.3	**4.7**
Marine Gasoil	7.0	1.4	-0.6	**0.9**	0.20	-0.08	**0.13**	4.8	-1.8	**2.9**
Heavy Fuel Oil	88.6	-21.6	8.2	**-13.5**	-0.24	0.09	**-0.15**	-5.9	2.2	**-3.7**
Bitumen	19.2	-8.6	0.9	**-7.7**	-0.45	0.05	**-0.40**	-11.3	1.2	**-10.1**
Petroleum coke	5.0	-4.5	0.1	**-4.4**	-0.89	0.01	**-0.88**	-25.3	0.3	**-25.0**
Lubes & Wax	5.1	2.0	1.0	**3.0**	0.39	0.21	**0.60**	9.2	4.9	**14.1**
Sulphur	3.2	-	-0.1	**-0.1**	-	-0.02	**-0.02**	-	-1.3	**-1.3**
Fuel & Losses	60.5	-	-	**-**						
Total	**718.6**	**196.2**	**-15.9**	**180.3**						

The model was calibrated to produce CO_2 emissions close to the actual 2010 figure for the refining system that it represents (including petrochemicals). The model calculates total CO_2 emissions of 180.3 Mt/a (132.4 Mt/a from refining and 47.9 Mt/a from petrochemicals). This compares well to the actual figure of 135.4 Mt/a from refining[1] and an estimated figure of 45.1 Mt/a from the chemicals plants[2].

As mentioned in **section 3.1**, the sum total of all marginal emission values multiplied by the value of each respective constraint is equal to the total tonnes of refinery CO_2 emissions.

When considering only the subset pertaining to product demand constraints this sum total (196.2 Mt/a) is greater than the actual CO_2 emissions of the refining system. This is because these only consider the impact of product demand, all other things being equal, i.e. same refining configuration and process unit capacities.

As noted in **section 3.2**, the simultaneous relaxation of the unit maximum capacity constraints allows for a more CO_2-efficient operation and therefore leads to lower CO_2 emissions. This is the reason why the marginal CO_2 intensities of the unit maximum capacity constraints have negative values. They therefore reduce the total emissions of the refining system back to the actual value.

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[1] The European Union Transaction Log (EUTL) emissions data for "main activity type code = 2" give a total of 139.6 Mt/a CO_2 for 2010. After eliminating installations that are not refineries (e.g. chemicals plants and dedicated power plants), the corrected total for EU27 refineries is 135.4 Mt/a. The model was calibrated to this level of emissions by applying a correction factor to all the unit specific energy consumption factors.

[2] This was estimated using the 2008 average steam cracker emission factor of 0.9575 t CO_2 per t HVC (High Value Chemicals = Hydrogen+Ethylene+Propylene+Butenes+Benzene) published in a presentation to the EEPC Ethylene Seminar in 2010 [4].

The total amount of CO_2 emissions reallocated from process unit constraints to final products (15.9 Mt/a CO_2) is relatively small compared to the grand total although it can represent up to some 30% of the total for certain products.

All fuel products have relatively small refining CO_2 intensities when compared to their combustion emissions, which are in the region of 73 g CO_2/MJ. However, there are significant differences in refining CO_2 intensities between products. These differences can be related to the level of processing required for each product type. For instance diesel fuel is more CO_2 intensive than heating oil (more stringent quality specifications). Diesel fuel is also more CO_2 intensive than gasoline which is due to the specific European situation with a very large diesel vehicle market coupled with very stringent diesel fuel specifications.

The petrochemicals product group (which includes olefins and aromatics) has a much higher emission intensity than typical fuel products as the underlying processes are particularly energy-intensive. This is also the case, albeit to a lesser extent for lubes and waxes.

An apparent anomaly is the negative marginal CO_2 intensity for most heavy products (which include heavy fuel oils and bitumen). This suggests that total EU refining CO_2 emissions would increase if production of, say, bitumen, was reduced (while continuing to satisfy the total EU demand for all other refined products). Although this may appear counterintuitive, it reflects the specific operational degrees of freedom available to the LP model to achieve an increase in bitumen yield with, for example, crude runs being constrained to mirror the 2010 crude diet. Reducing the production of a heavy product implies that crude throughput must be slightly reduced while the proportion of light products in the product slate from this reduced crude input must be increased, which requires additional conversion and therefore leads to an increase in CO_2 emissions.

The figures generated through this method are strictly only valid for the given set of base conditions. The marginal intensities are not “averages” but reflect the effect of perturbations to European refinery output with the crude diet of 2010.

Different base cases would correspond to different total CO_2 emissions and different distributions of marginal CO_2 intensities between products. For the same reason, the figures generated for EU as a whole cannot be applied to individual refineries that all have their specific configuration, feedstocks and product demands. Although the same methodology could be used to generate specific CO_2 intensity figures for individual refineries, these would be of limited value and could be misleading, especially for simple refineries that specialise in the production of bitumen or lubricants. Indeed refineries are to a large extent interdependent, exchanging intermediate and finished product either directly or through the market and focussing on a particular refinery would ignore this interdependence.

4.2. SENSITIVITY CASES

The set of marginal values produced by the LP is specific to a certain case, i.e. they will change if any of the premises are changed such as product demands, product specifications, process unit capacities or feedstock availability. In a scenario where oil products would be partly and gradually replaced by alternatives, one would have to reassess the marginal values on a regular basis by adjusting the basic assumptions to reflect the current reality.

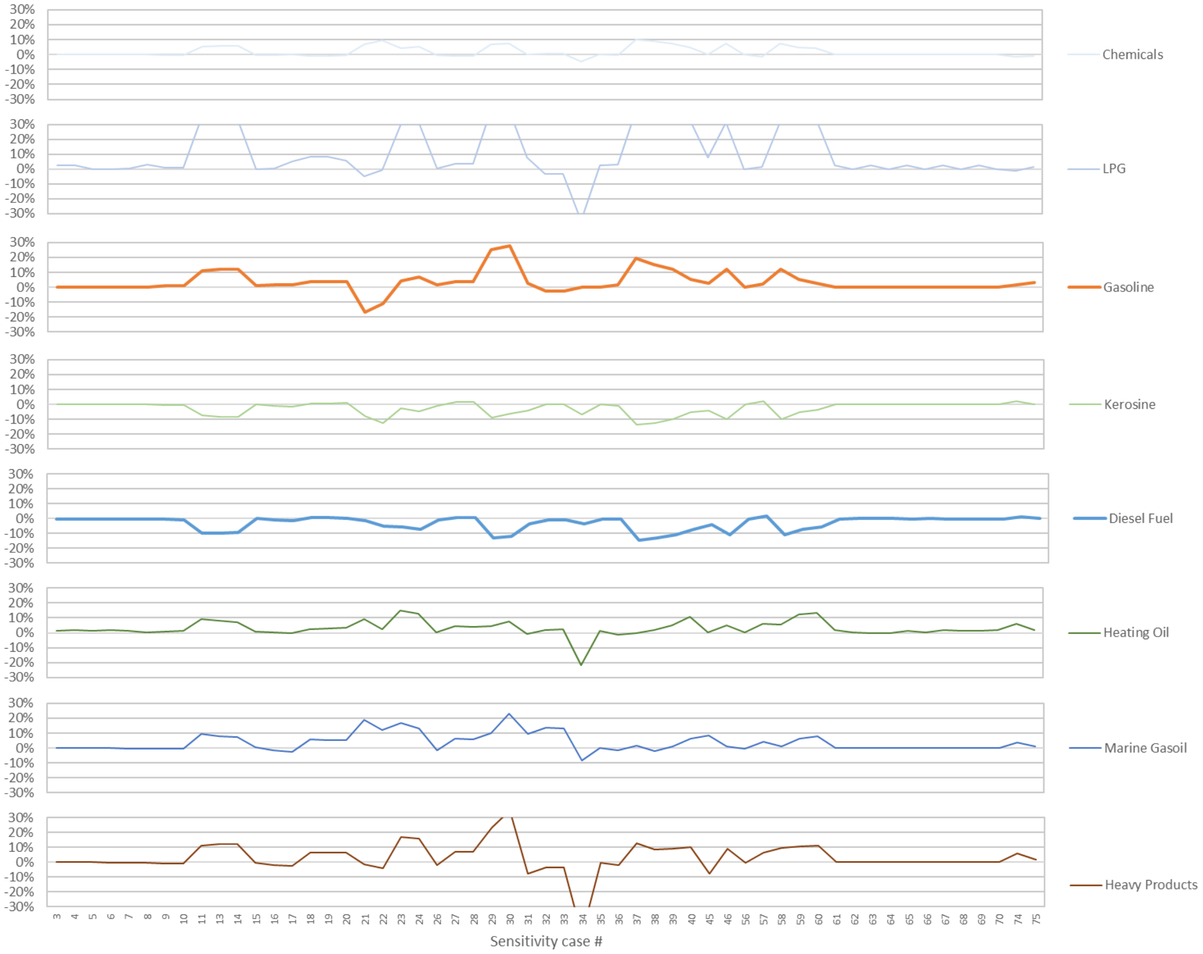
In this context, it was essential to carry out a sensitivity analysis around the given set of assumptions to ensure that the marginal emissions are stable within a reasonable range.

To this end a set of LP runs were performed where each product demand was changed in 0.5% steps between -2.5% and +2.5% around the base case value, all other parameters remaining constant. **Table 3** shows that the average of all sensitivity cases is very close to the base case value. **Figure 1** shows the range of variation of individual carbon intensities, confirming a satisfactory level of stability (for the purpose of this analysis Heavy Fuel Oil, Bitumen, Petroleum coke, Lubes and Wax and Sulphur have been combined into a single group).

Table 3 Marginal CO_2 intensities of main product groups from base case and average of sensitivity cases

CO2 intensities	**Base case** g CO_2 / MJ	**Sensitivity cases avg.** g CO_2 / MJ
Chemicals	31.1	31.7
LPG	5.2	5.7
Gasoline	5.5	5.7
Kerosine	6.1	5.9
Diesel Fuel	7.2	7.0
Heating Oil	4.7	4.9
Marine Gasoil	2.9	3.0
Heavy Products	-4.7	-4.8

Figure 1 Marginal CO_2 intensities sensitivity for the main product groups
(% of base case value)



More detailed figures for each main product group are shown in **Appendix 3**.

4.3. MARGINAL CO_2 INTENSITIES FOR NAPHTHA (PETROCHEMICAL FEED)

The Concawe model incorporates the steam crackers (olefin plants) so that, in the base case, petrochemical naphtha is an intermediate product being transferred from the refineries to the steam crackers.

In order to assess the marginal CO_2 intensity of naphtha a small naphtha demand was specified. This was done for each individual naphtha stream generated in the model and for the specific material sent to petrochemicals. The results for the main naphtha types are shown in **Table 4**.

Table 4 Marginal CO_2 intensities of naphtha streams

Stream type	**g CO_2 / MJ**
C5 - 65°C cut (various crudes)	7.1 - 7.3
C5 - 85°C cut (various crudes)	6.1 - 7.2
65°C - 155°C cut (various crudes)	4.7 - 6.4
Mixed naphtha cuts to Chemical feed (base case)	6.4

The marginal CO_2 intensities of naphtha streams are in the region of 6 to 7 g CO_2/MJ (with one exception). It is also notable that the intensities of other product groups remain stable.

The marginal CO_2 intensity of naphtha is therefore higher than that of gasoline which may appear counterintuitive inasmuch as gasoline requires more complex processing. The rationale for this is the inherent synergy between gasoline and middle distillates: in order to meet octane requirements, gasoline blending requires unsaturated components (such as aromatics and olefins) so that the production of gasoline releases hydrogen (by processing naphtha in the catalytic reformer) which is used for hydrotreating middle distillates and/or hydrocracking of heavier molecules. By contrast, (chemical feed) naphtha consists mostly of saturated components so that if more naphtha is produced for chemical feed at the expense of naphtha processed in the catalytic reformer, then more hydrogen has to be produced separately, by processes that are more CO_2-intensive than catalytic reforming. It can also be said that naphtha increases the overall hydrogen/carbon ratio of the product barrel thereby increasing the net hydrogen requirement.

5. COMPARISON WITH EARLIER CONCAWE WORK

In the context of the JEC “Well-to-Wheels” study (1), Concawe made, around 2005, an assessment of the marginal CO_2 intensity of European gasoline and diesel fuel by performing a marginal analysis of the European refining system using the CONCAWE EU refining model.

The base case was the forecasted situation in 2010 in terms of crude slate, demand and refinery configuration. Alternative cases were then built up where the demand for gasoline or diesel fuel was reduced or increased by a small amount, all other parameters remaining the same. As a result the difference in energy consumption and CO_2 emissions between the base case and an alternative case could be credibly attributed to the single change in gasoline or diesel fuel production (this is further referred to as the “incremental method”).

The figures generated in that way are shown in **Table 5** compared to the results of the current study.

Table 5 Marginal CO_2 intensities of gasoline and diesel fuel (g CO_2 / MJ)

	JEC “Well-to-Wheels”	**Current study**	
		Product sales only	After reallocation
Gasoline	7.0	6.2	5.5
Diesel Fuel	8.6	8.1	7.2

The figures derived in the current study are about 20% lower than the incremental method estimates. About half of that difference is brought about by reallocation of the unit capacity constraints emissions. The incremental method focused on a single product sales constraint at a time, allocating all of the incremental change in total CO_2 emissions to the specific change in product sales. In doing so it effectively made the assumption that all other variables (including refinery configuration and process unit capacities) remain unchanged. In that sense the figures generated by the incremental method are consistent with those obtained in the current study before reallocation of the capacity constraint emissions (see **section 4.1**). The remaining differences (about 10%) can be attributed to a combination of factors including a different base case (crude slate, product demands, quality, etc) as well as updates of the model’s refinery configuration data (capacity expansions, new units, closures, etc.) over the last decade.

The method described in the current study seeks to represent the combined and simultaneous impact of all system constraints, including both product sales and maximum unit capacities. As a result, it yields marginal CO_2-intensity values that can be expected to be lower than the incremental method.

It should be noted that, with both methodologies, gasoline displays a lower CO_2 intensity than diesel fuel (about 1.5 g CO_2/MJ less), underlining the specific European demand imbalance between the two road fuels.

6. COMPARISON WITH OTHER REFINERY CO_2 ALLOCATION METHODOLOGIES

Oil refining is a typical co-production process whereby all products are produced simultaneously and are therefore interdependent. As a result there is no straightforward manner to apportion the resources used by the refinery or its emissions between products.

Many methods have been proposed mostly based on some form of allocation. The simplest methods use an allocation key such as mass, energy content or value-added. They have the advantage of being easy to both understand and apply. They also comply with the additivity criterion for LCAs (i.e. the sum of the product allocation equals the total resources used by the refinery) and figures tend to be stable over a wide range of basic assumptions.

For all their convenience though, these methods are not founded on any physical reality as there is generally no causal link between, say, the mass or energy content of a product and its production pathway. More sophisticated methods endeavour to apportion the resources or emissions pertaining to each process unit to a particular set of products. This may be straightforward for some processes but many others have multiple functions and may also have an impact on other processes.

Generally all such methods carry the risk of ignoring complex interdependencies and synergies within the refinery, leading to conclusions that do not represent the complex reality.

The “marginal” approach is the usual method used to assess co-production cases whereby a perturbation is applied to a base case and the impact allocated to the source of the perturbation. Through a detailed analysis of the LP solution, the method proposed in this report makes it possible to ascertain the simultaneous impact of small changes in the demand of each product on the total refinery emissions while taking account of all interdependencies and interactions.

7. POTENTIAL APPLICATIONS AND LIMITATIONS

The figures generated through this method are strictly only valid for the given set of base conditions. Different base cases would correspond to different total CO_2 emissions and different distributions of marginal CO_2 intensities between products. For the same reason, the figures generated for EU as a whole cannot be applied to individual refineries that all have their specific configuration, feedstocks and product demands. Although the same methodology could be used to generate specific CO_2 intensity figures for a particular refinery, the figures thus produced would only be representative of the specific configuration and circumstances of that refinery. This is especially the case for atypical refineries that specialise in the production of bitumen or lubricants. Indeed refineries are to a large extent interdependent, exchanging intermediate and finished product either directly or through the market and focussing on a particular refinery would ignore this interdependence.

The new methodology described above provides a unique route to generate a consistent set of marginal CO_2 intensities for all major oil refinery products. Because all refinery emissions are distributed between the products this complies with one of the basic requirements of LCAs.

Since the methodology presented here is based on a marginal analysis, the resulting marginal CO_2 intensity figures for refining should only be used in consequential LCAs, for example to tackle the issue of current interest in this respect which revolves around substitution of a fraction of the existing oil products by some form of alternative product.

8. REFERENCES

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9. GLOSSARY

BTX	Benzene, toluene and xylenes
C2	A mix of FCC off-gases, ethane and lighter
C3	A mix of propane and propylene
C4	A mix of butanes and butenes
CCR Ref	Continuous Catalyst Regeneration Reforming unit
CDU	Crude Distillation Unit
CG	Cracked Gasoline (produced by the FCC unit)
CO_2	Carbon dioxide
DCK	Delayed Coking Unit
ETS	EU GHG Emissions Trading Scheme
EU	European Union
FCC	Fluid Catalytic Cracker (conversion unit processing feeds such as VGO and Coker Gas Oil, oriented towards gasoline production)
FG	Fuel Gas, mostly methane and ethane produced in various refining processes and consumed internally
GHG	Greenhouse gases
HCG	Heavy Cracked Gasoline (produced by the FCC unit)
HCK	Hydrocracker unit (conversion unit processing feeds such as VGO and Coker Gas Oil, oriented towards jet fuel and diesel fuel production)
HCO	Heavy Cycle Oil (residual product of the FCC unit)
HDS	Hydrodesulphurisation unit, for gas oils and heavier streams
HDT	Hydrotreatment unit, for kerosene and lighter streams
HFO	Heavy Fuel Oil
IGCC	Integrated Gasification Combined Cycle plant (produces electricity from residue streams such as LR, SR, VB Resid, Asphalt)
JEC	JRC-EUCAR-CONCAWE consortium
LCA	Life Cycle Assessment
LCG	Light Cracked Gasoline (produced by the FCC unit)
LCO	Light Cycle Oil (light gas oil produced by the FCC unit)
LPG	Liquefied Petroleum Gas (a market product of primarily C3 and C4 hydrocarbons)
LR	Long Residue (residual product of atmospheric distillation)

Lubes	Lubricant base oils produced from VGO and LR by dewaxing and deasphalting processes
M100	Russian high sulphur export HFO grade
MCO	Medium Cycle Oil (heavy gas oil produced by the FCC unit for HCK feed or HFO blending)
Mt/a	Million tonnes per annum
NG	Natural Gas
Pet Coke	Petroleum coke, the solid residue from the Delayed Coking Unit
POX	Partial Oxidation unit (gasification process producing syngas from residue streams such as LR, SR, VB Resid, Asphalt)
REF	Catalytic Reforming unit
RHC	Residue Hydroconversion unit
RMF	Residual Marine Fuel
RON	Research Octane Number
SMR	Steam Methane Reforming unit (produces hydrogen, usually from natural gas)
SR	Short Residue (residual product of the VDU)
SR Ref	Semi-regenerative Catalytic Reforming unit
SRU	Sulphur Recovery Unit
VB Resid	Visbroken Residue (residual product of the VBU)
VBU	Visbreaking Unit
VDU	Vacuum Distillation Unit
VGO	Vacuum Gas Oil (a VDU product in the boiling range 380-560°C)

APPENDIX 1: INPUT DATA FOR 2010 CASE STUDY

Table 1-1 Total crude oil and other feedstocks supply

Crude oil supply	**Mt/a**	**%m/m**
North Sea light sweet crude	294.0	44.6%
Middle East light sour crude	25.1	3.8%
West African light sweet crude	35.6	5.4%
Russian medium sour crude	178.0	27.0%
Condensate	9.2	1.4%
Middle East heavy sour crude	108.8	16.5%
Vacuum Residue	8.6	1.3%
Total	**659.3**	**100.0%**

Table 1-2 Total product sales (demand)

Demand	**Mt/a**	**%m/m**
Petrochemicals (1)	54.6	8.3%
LPG	13.0	2.0%
Gasoline	126.3	19.2%
Kerosine	56.6	8.6%
Diesel Fuel	207.1	31.5%
Heating Oil	72.5	11.0%
Marine Gasoil	7.0	1.1%
Heavy Fuel Oil (2)	88.6	13.5%
Bitumen	19.2	2.9%
Other (3)	13.3	2.0%
Total (4)	**658.1**	**100.0%**

(1) Olefins and Aromatics (BTX)
(2) Including residual marine fuel
(3) Lube base oil, wax, petcoke, sulphur
(4) Excluding refinery fuel and losses

Table 1-3 Imports/exports

Imports	**Mt/a**
Natural Gas	5.4
Ethane	2.5
Naphtha	6.4
Jet Fuel	14.6
Heating Oil	15.4
Russian M100 residue	15.3
Total	**59.6**

Exports	**Mt/a**
Gasoline US	13.7
Gasoline Other	22.3
HFO high sulphur	20.2
Total	**56.2**

Table 1-4 Feedstock costs and product prices
(on mass basis relative to North Sea light sweet crude)

Along with other cost information such as fixed and variable operating cost, a feedstock and product price structure is required in order to drive the model through the “margin” objective function. The absolute price level is not critical to the outcome but price ratios between crude and main products as well as between products must be realistic. Although absolute prices vary a great deal over time, these ratios are much less volatile.

Purchases	
North Sea light sweet crude	1.00
Middle East light sour crude	0.97
Middle East heavy sour crude	0.95
West African light sweet crude	0.97
Russian medium sour crude	0.94
Condensate	1.16
Vacuum Residue	0.80
Russian M100 residue	0.80
Ethane	1.57
Naphtha	1.17
Jet Fuel	1.18
Heating Oil	1.09
Ethanol	1.19
Natural Gas	1.15

Sales	
LPG	1.15
Ethylene	2.18
Propylene	1.31
Butylenes	1.23
Benzene	1.48
Toluene	1.28
Xylenes	1.41
Methanol	0.58
Gasoline EU unleaded 92RON	1.19
Gasoline EU unleaded 95RON	1.21
Gasoline EU unleaded 98RON	1.22
Gasoline US export	1.20
Gasoline Other export	1.19
Jet Fuel	1.18
Road Diesel	1.13
Non-Road Diesel	1.13
Rail Diesel	1.13
Diesel marine fuel	1.09
Inland waterways Diesel	1.09
Heating Oil	1.09
HFO very low sulphur	0.77
HFO low sulphur	0.76
HFO high sulphur	0.71
HFO high sulphur export	0.78
Residual Marine Fuel General	0.71
Residual Marine Fuel Seca	0.76
Lube base oil	1.09
Wax	1.09
Bitumen	0.63
Pet Coke	0.21
Sulphur	0.08

Table 1-5 Product quality specifications and actual model constraints

Final products specifications

			Gasoline			Jet Fuel	Road diesel	Non-road diesel*	Heating oil	Heavy fuel oils	Residual marine fuels
			92RON	95RON	98RON						
Density @ 15°C	min	kg/m3	720			775	800	806	800	900	900
	max	kg/m3	775			840	845	858	860	1000	991
Sulphur	max	ppmm	10			3000	10	570	1000		
		%m/m								0.7/1.0/1.5	1.0/1.5/3.5
Aromatics	max	%v/v	35								
Benzene	max	%v/v	1.0								
Olefins	max	%v/v	18.0								
Oxygen	max	%m/m	2.7								
Vapour pressure	max	kPa	60								
Evap 70	min	%v/v	20								
	max	%v/v	48								
Evap 100	min	%v/v	46								
	max	%v/v	71								
RON	min		92	95	98						
MON	min		82	85	88						
Cetane number	min						51				
Cetane index	min						46	44	40		
Poly aromatics	max	%m/m					8				
Viscosity @ 100^{0}C	max	cSt								35	35
Con. carbon	max	%m/m								18	18

* EU average non-road diesel quality. Some EU states had already switched from 1000ppm to 10ppm in 2010.

Model constraints (includes blending margins)

			Gasoline**			Jet Fuel	Road diesel**	Non-road diesel	Heating oil	Heavy fuel oils	Residual marine fuels
			92RON	95RON	98RON						
Density @ 15°C	min	kg/m3	725			780	815	806	800	900	900
	max	kg/m3	774			820	837	858	850	995	991
Sulphur	max	ppmm	7			700	7	570	900		
		%m/m								0.6/0.9/1.4	0.9/1.4/3.2
Aromatics	max	%v/v	34.4								
Benzene	max	%v/v	0.9								
Olefins	max	%v/v	17.7								
Oxygen	max	%m/m	1.2								
Vapour pressure	max	kPa	54								
Evap 70	min	%v/v	16.3								
	max	%v/v	41.3								
Evap 100	min	%v/v	43.5								
	max	%v/v	61.5								
RON*	min		91	94	97						
MON*	min		82	85	88						
Cetane index	min						49	44	41		
Poly aromatics	max	%m/m					7				
Viscosity @ 100^{0}C	max	cSt								35	35
Con. carbon	max	%m/m								18	18

*** Before biofuel blending*

Table 1-6 Aggregated process unit capacities[3] (total of EU-28)

Process unit	**Mt/a** (340 days)
Crude distillation (CDU)	750.5
Vacuum distillation (VDU)	344.0
Visbreaking (VBU)	89.5
Delayed Coking (DCK)	23.1
Deasphalting	2.0
Fluid Catalytic Cracking (FCC)	118.2
Hydrocracking (HCK)	74.8
Vacuum Gas Oil Hydrodesulphurisation (VGO HDS)	49.9
Long Residue Hydrodesulphurisation (LR HDS)	4.9
Short Residue Hydrodesulphurisation (SR HDS)	1.9
Residue Hydroconversion (RHC)	9.7
Naphtha HDT	172.3
Naphtha Reforming (Ref)	98.5
Aromatics extraction	13.5
Alkylation*	13.4
Isomerisation	26.2
Kerosine HDT	31.8
Diesel HDS	133.0
Petrochemicals	74.8
Sulphur Recovery Unit* (SRU)	6.4
Hydrogen production* (SMR)	1.7
Hydrogen production* (POX)	0.2
Integrated Gasification Combined Cycle (IGCC)	0.4

* The figures for these units are expressed in Mt/a of product, not feed

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[3] Based on each unit's maximum processing capacity per on-stream day, annualised by assuming 340 on-stream days per annum

APPENDIX 2: REALLOCATION OF MARGINAL CO_2 FROM CONSTRAINING PROCESS UNITS

The reallocation method briefly described in section 3.2 is illustrated here using the 2010 case study.

Step 1: Identifying constraining process unit capacities

Table 2 in the main text showed that 5 process units have constraining capacities. A non-zero marginal emission value is associated to each such unit. The CO_2 to be reallocated is the product of the marginal emission value by the throughput of the unit.

Process Unit	**Marginal emissions t CO_2 / t**	**Throughput Mt/a**	**Emissions Mt/a CO_2**
Hydrocracker (HCK)	-0.0062	74.8	-0.466
Long Residue HDS (LR HDS)	-0.0126	4.9	-0.062
Naphtha Reforming semi-regen (SR Ref.)	0.0439	59.7	2.621
Diesel HDS	-0.1301	133.0	-17.311
Hydrogen POX (H2-POX)	-0.6554	1.1	-0.698
	Total CO_2 to be reallocated		**-15.917**

Step 2: Using “Marginal Rates of Substitution” (MRSs) to allocate emissions to CO2 emitting modes

These 5 constraining units can be linked to a total of 10 CO_2 emitting modes. The corresponding MRSs, expressed in tonne mode per tonne unit throughput are shown in the table below. Combined with the CO_2 “emission factor” for each mode, they provide the emission reallocation key for each constraining process unit.

CO_2-emitting mode	H2 prod from NG	H2 prod from Asphalt*	Pet Coke gasification	NG combustion	FG combustion	C3 combustion	LR combustion	SR combustion	VB resid combustion	FCC Coke combustion	
Process Unit	**MRS (t mode / t unit throughput)**										
HCK	0.0099			-0.0199	-0.0023	0.0105	0.0292	0.0043	-0.0031	-0.0378	
LR HDS	0.0071			-0.0142	0.0137	-0.0776	0.0708	0.0010	-0.0169	0.0027	
SR Ref.	0.0026			-0.0051	0.0119	0.0194	-0.0313	-0.0001	0.0152	0.0010	
Diesel HDS	-0.0150			0.0299	-0.0203	0.0495	-0.1122	-0.0005	0.0391	0.0033	
H2 - POX	-0.2679	1.0000	0.1031	0.5340	-0.0141	-0.0530	-1.7568	0.0016	0.5431	-0.0209	
	Emissions (t CO_2 / t mode)										
	5.50	3.11	3.37	2.75	2.79	3.00	3.19	3.24	3.24	3.38	
Process Unit	**Emissions (t CO_2 / t unit throughput)**										**Total**
HCK	0.0545			-0.0547	-0.0065	0.0314	0.0929	0.0139	-0.0099	-0.1280	-0.0064
LR HDS	0.0388			-0.0391	0.0382	-0.2328	0.2256	0.0031	-0.0546	0.0091	-0.0117
SR Ref.	0.0143			-0.0140	0.0331	0.0581	-0.0998	-0.0003	0.0492	0.0034	0.0439
Diesel HDS	-0.0826			0.0821	-0.0566	0.1486	-0.3577	-0.0016	0.1265	0.0112	-0.1300
H2 - POX	-1.4735	3.1076	0.3474	1.4685	-0.0393	-0.1589	-5.6012	0.0053	1.7577	-0.0708	-0.6571
Process Unit	**Allocated emissions (Mt/a CO_2)**										**Total**
HCK	4.1	0.0	0.0	-4.1	-0.5	2.4	7.0	1.0	-0.7	-9.6	**-0.5**
LR HDS	0.2	0.0	0.0	-0.2	0.2	-1.1	1.1	0.0	-0.3	0.0	**-0.1**
SR Ref.	0.9	0.0	0.0	-0.8	2.0	3.5	-6.0	0.0	2.9	0.2	**2.6**
Diesel HDS	-11.0	0.0	0.0	10.9	-7.5	19.8	-47.6	-0.2	16.8	1.5	**-17.3**
H2 - POX	-1.6	3.3	0.4	1.6	0.0	-0.2	-6.0	0.0	1.9	-0.1	**-0.7**
Total	**-7.4**	**3.3**	**0.4**	**7.4**	**-5.9**	**24.3**	**-51.4**	**0.8**	**20.6**	**-7.9**	**-15.9**

* Hydrogen produced by Partial Oxidation of Asphalt, a residual product of Deasphalting, a process used for residue upgrading and Lubes production

Note that, for each process unit, the sum of all mode contributions equals the total marginal emissions (the small discrepancies are due to simplifications and aggregations of modes in the table as shown above).

CO_2-emitting mode	H2 prod from NG	H2 prod from Asphalt*	Pet Coke gasification	NG combustion	FG combustion	C3 combustion	LR combustion	SR combustion	VB resid combustion	FCC Coke combustion	
Process Unit	**Allocated emissions (Mt/a CO_2)**										**Total**
HCK	4.1	0.0	0.0	-4.1	-0.5	2.4	7.0	1.0	-0.7	-9.6	**-0.5**
LR HDS	0.2	0.0	0.0	-0.2	0.2	-1.1	1.1	0.0	-0.3	0.0	**-0.1**
SR Ref.	0.9	0.0	0.0	-0.8	2.0	3.5	-6.0	0.0	2.9	0.2	**2.6**
Diesel HDS	-11.0	0.0	0.0	10.9	-7.5	19.8	-47.6	-0.2	16.8	1.5	**-17.3**
H2 - POX	-1.6	3.3	0.4	1.6	0.0	-0.2	-6.0	0.0	1.9	-0.1	**-0.7**
Total	**-7.4**	**3.3**	**0.4**	**7.4**	**-5.9**	**24.3**	**-51.4**	**0.8**	**20.6**	**-7.9**	**-15.9**

Step 3: Linking CO_2 emitting modes to process units

Each mode can in turn be linked to the “source” process units that produce the CO_2 emitting substance. For instance fuel gas (FG) is produced by a number of units in the refinery. The next table shows the mass distribution of production of the particular substance relevant to each CO_2 emitting mode between the different producers.

CO_2-emitting mode	**H2 prod from NG**	**H2 prod from Asphalt***	**Pet Coke gasification**	**NG combustion**	**FG combustion**	**C3 combustion**	**LR combustion**	**SR combustion**	**VB resid combustion**	**FCC Coke combustion**
"Source" Process unit										
Chemicals	54.3%			54.3%	54.3%					
SR Ref	15.6%			15.6%	15.6%	25.8%				
VBU	2.0%			2.0%	2.0%	6.6%			100.0%	
Bitumen	1.0%			1.0%	1.0%					
CCR Ref	4.9%			4.9%	4.9%	8.2%				
CDU	1.2%			1.2%	1.2%	32.5%	100.0%			
HCG HDT	0.1%			0.1%	0.1%					
DCK	4.4%		100.0%	4.4%	4.4%	5.3%				
Diesel HDS	0.2%			0.2%	0.2%					
FCC	13.5%			13.5%	13.5%	16.3%				100.0%
VGO HDS	0.0%			0.0%	0.0%	0.0%				
HCK	1.8%			1.8%	1.8%	5.2%				
VDU								100.0%		
Kero HDT	0.1%			0.1%	0.1%					
LR HDS	0.1%			0.1%	0.1%	0.2%				
Lubes		100.0%								
Naphtha HDT	0.8%			0.8%	0.8%					

* Hydrogen produced by Partial Oxidation of Asphalt, a residual product of Deasphalting, a process used for residue upgrading and Lubes production

Natural gas (NG) is imported into refineries rather than produced internally. It is therefore not directly possible to link it to specific process units. Inasmuch as it is used in combination with fuel gas and for the same purpose, it has been postulated that the distributions are the same for both streams.

The marginal CO_2 allocated to each mode in the previous step is then further split between source process units according to their contribution to the total production.

CO_2-emitting mode	H2 prod from NG	H2 prod from Asphalt*	Pet Coke gasification	NG combustion	FG combustion	C3 combustion	LR combustion	SR combustion	VB resid combustion	FCC Coke combustion	Total
"Source" Process unit											
Chemicals	-4.04			4.00	-3.20						**-3.24**
SR Ref	-1.16			1.15	-0.92	6.27					**5.34**
VBU	-0.15			0.15	-0.12	1.59			20.63		**22.10**
Bitumen	-0.07			0.07	-0.06						**-0.06**
CCR Ref	-0.36			0.36	-0.29	1.99					**1.70**
CDU	-0.09			0.09	-0.07	7.88	-51.45				**-43.64**
HCG HDT	-0.01			0.01	-0.01						**-0.01**
DCK	-0.32		0.37	0.32	-0.26	1.28					**1.39**
Diesel HDS	-0.01			0.01	-0.01						**-0.01**
FCC	-1.00			0.99	-0.79	3.95				-7.91	**-4.77**
VGO HDS	0.00			0.00	0.00	0.01					**0.01**
HCK	-0.14			0.14	-0.11	1.26					**1.15**
VDU								0.82			**0.82**
Kero HDT	-0.01			0.01	0.00						**0.00**
LR HDS	0.00			0.00	0.00	0.04					**0.03**
Lubes		3.31									**3.31**
Naphtha HDT	-0.06			0.06	-0.05						**-0.05**
Total	**-7.44**	**3.31**	**0.37**	**7.37**	**-5.89**	**24.27**	**-51.45**	**0.82**	**20.63**	**-7.91**	**-15.92**

* Hydrogen produced by Partial Oxidation of Asphalt, a residual product of Deasphalting, a process used for residue upgrading and Lubes production

Step 4: Linking process units to final products

We have now a list of process units, each of which carries a CO_2 emissions burden. This needs in turn to be allocated to final products.

The LP solution provides a product yield structure for each process unit. As an example the FCC aggregated yields are shown below. Before they can be used, they need to be normalised to remove those streams that are used internally as fuels and therefore do not leave the refinery as final product.

Full yield structure

Product	%m/m
C2-	3.2%
C3/C4	19.8%
Light Cracked Gasoline (LCG)	29.9%
Heavy Cracked Gasoline (HCG)	14.3%
Light Cycle Oil (LCO)	16.1%
Medium Cycle Oil (MCO)	9.0%
Heavy Cycle Oil (HCO)	2.3%
Coke (on catalyst)	5.5%
Total	**100.0%**

Non-fuel products only

Product	%m/m
C2-	0.2%
C3/C4	21.2%
Light Cracked Gasoline (LCG)	32.8%
Heavy Cracked Gasoline (HCG)	15.7%
Light Cycle Oil (LCO)	17.7%
Medium Cycle Oil (MCO)	9.8%
Heavy Cycle Oil (HCO)	2.5%
Coke (on catalyst)	0.0%
Total	**100.0%**

The next table shows the mass distribution of the non-fuel FCC products between further process units feed and, in some cases final products.

FCC product	C2-	C3/C4	LCG	HCG	LCO	MCO	HCO
Process units:							
Chemical plant		4.4%					
Propylene splitter		20.3%					
Sulphur plant	100.0%						
Alkylation		53.5%					
CG splitter			60.6%				
HCG HDT				48.5%			
Diesel HDS				26.7%	52.1%		
MTBE		9.9%					
Finished products groups:							
LPG & Chemicals		10.8%					
Gasoline		1.1%	39.4%	24.8%			
Middle distillates					47.9%		
Heavy products						100.0%	100.0%

For each of the process units shown, a similar table can be generated. The procedure is then repeated until all streams have been fully allocated to final products. For the FCC the resulting mass distribution of non-fuel FCC products to final products is shown below.

	C2-	C3/C4	LCG	HCG	LCO	MCO	HCO
LPG & Chemicals		34.7%	3.5%	0.0%	0.1%		
Gasoline		65.1%	96.1%	73.5%	0.2%		
Middle distillates		0.0%	0.3%	26.3%	99.3%		
Heavy products	100.0%	0.2%	0.1%	0.2%	0.4%	100.0%	100.0%

The same calculation is made for all relevant process units. The mass distribution is then used a key to reallocate the CO_2 burden of each process unit to the final products. The results for the 2010 case study are shown below.

Final product	Distribution (%m/m)				Reallocated emissions (Mt/a CO_2)	Final allocation (Mt/a CO_2)			
	LPG & Chem.	Gasoline	Middle distillates	Heavy products		LPG & Chem.	Gasoline	Middle distillates	Heavy products
Process unit									
Chemicals	80.9%	14.3%	0.1%	4.7%	-3.2	-2.6	-0.5	0.0	-0.2
SR Ref	18.2%	80.6%	1.0%	0.2%	5.3	1.0	4.3	0.1	0.0
VBU	3.2%	5.9%	20.6%	70.3%	22.1	0.7	1.3	4.6	15.5
Bitumen	0.0%	0.0%	0.0%	100.0%	-0.1	0.0	0.0	0.0	-0.1
CCR Ref	4.7%	93.8%	1.4%	0.2%	1.7	0.1	1.6	0.0	0.0
CDU	11.1%	20.5%	48.2%	20.3%	-43.6	-4.8	-8.9	-21.0	-8.8
HCG HDT	0.0%	100.0%	0.0%	0.0%	0.0	0.0	0.0	0.0	0.0
DCK	5.4%	12.5%	27.2%	54.9%	1.4	0.1	0.2	0.4	0.8
Diesel HDS	0.1%	0.3%	98.7%	0.9%	0.0	0.0	0.0	0.0	0.0
FCC	8.5%	57.0%	21.8%	12.7%	-4.8	-0.4	-2.7	-1.0	-0.6
VGO HDS	0.2%	1.5%	94.9%	3.4%	0.0	0.0	0.0	0.0	0.0
HCK	7.8%	30.0%	56.6%	5.7%	1.2	0.1	0.3	0.7	0.1
VDU	5.7%	25.8%	31.2%	37.2%	0.8	0.0	0.2	0.3	0.3
Kero HDT	0.0%	0.1%	99.7%	0.2%	0.0	0.0	0.0	0.0	0.0
LR HDS	6.6%	44.3%	37.6%	11.5%	0.0	0.0	0.0	0.0	0.0
LCO HDT	0.1%	0.5%	98.6%	0.8%	0.0	0.0	0.0	0.0	0.0
Lubes	0.3%	1.2%	4.5%	93.9%	3.3	0.0	0.0	0.2	3.1
Naphtha HDT	14.6%	84.1%	1.1%	0.2%	0.0	0.0	0.0	0.0	0.0
				Total	**-15.9**	**-5.9**	**-4.2**	**-16.0**	**10.1**

In this way the total marginal CO_2 associated with constraining process units has been reallocated in a structured and rigorous manner to the final products.

APPENDIX 3: SENSITIVITY ANALYSIS

The results of the sensitivity analysis for each product are best illustrated by a so-called “Box and Whiskers” diagram (as proposed by Tukey).

In this case we present a diagram where data is arranged along a horizontal axis. The diagram shows the average value (Avg), the median (M) and the first and third quartile values (Q1 and Q3, i.e. the data points closest to respectively 25 and 75% of all points), which form the vertical boundaries of the box.

In addition it describes the data outside the Q1-Q3 bracket by showing end points corresponding to

- The higher of Q1 – (Q3-Q1)*1.5 or the lowest actual data point (low end point)
- The lower of Q3 + (Q3-Q1)*1.5 or the highest actual data point (high end point)

Any actual data points outside the end points bracket are also individually shown.

Example: Marine gasoil (see diagram below)

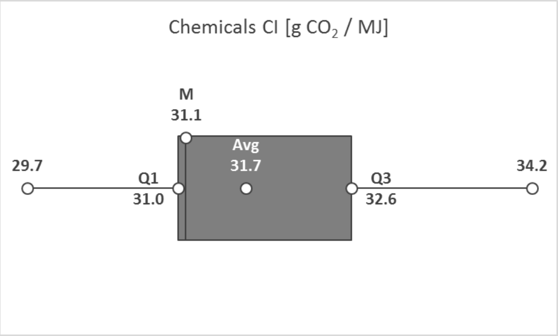
Average: 3.02 *Median: 2.93*

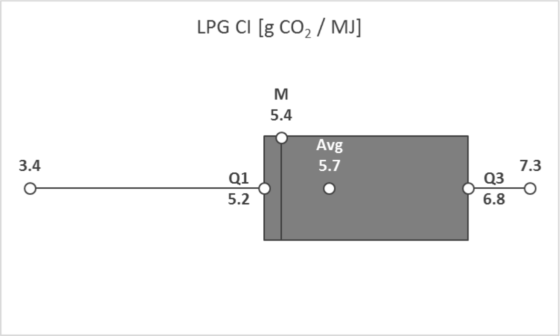
Q1: 2.92 *Q3: 3.11* *(Q1-Q3)*1.5 = 0.28*

Lowest data point: 2.68 *Highest data point: 3.59*

Low end point: higher of 2.92 – 0.28 = 2.64 or 2.68 i.e. 2.68. No data point below low end point

High end point: lower of 3.11 + 0.28 = 3.39 or 3.59 i.e. 3.39. 3 data points higher than high end point


Chemicals CI [g CO_2 / MJ]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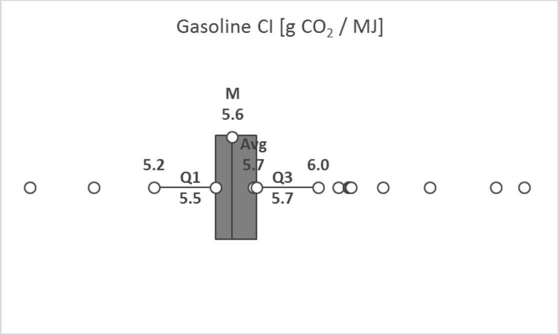
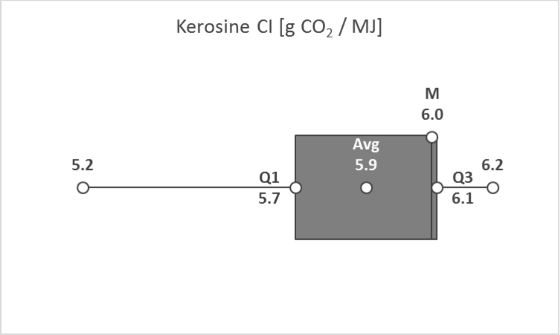
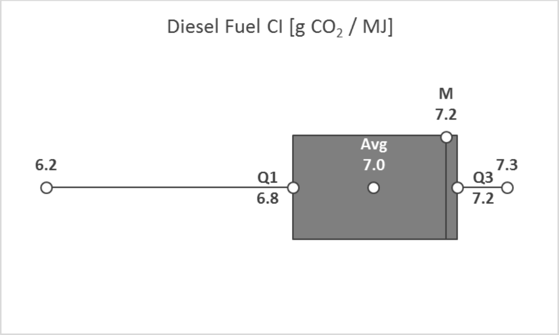
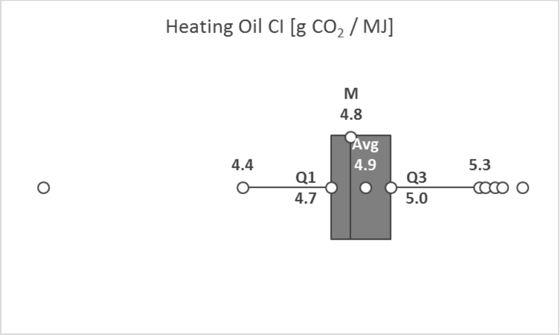
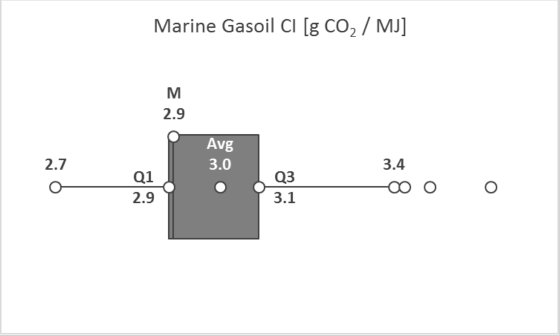
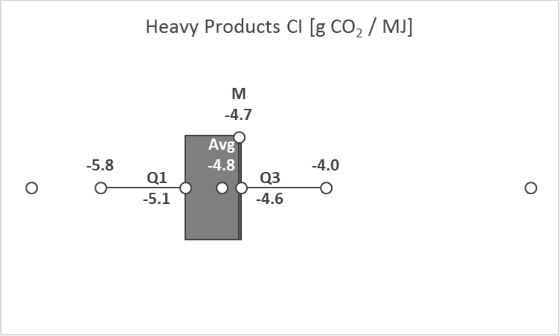

Gasoline CI [g CO_2 / MJ]


Kerosine CI [g CO_2 / MJ]


Diesel Fuel CI [g CO_2 / MJ]


Heating Oil CI [g CO_2 / MJ]


Marine Gasoil CI [g CO_2 / MJ]


Heavy Products CI [g CO_2 / MJ]

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