Allocation of CO_2 Emissions in Joint Product Industries via Linear Programming: a Refinery Example

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Résumé — **Allocation des émissions de CO_2 dans les industries à produits liés par programmation linéaire : l'exemple du raffinage** — Dans une industrie à produits liés comme celle du raffinage, la répartition des émissions de CO_2 sur les produits pétroliers n'admet pas de réponse unique. Cependant, sous certaines conditions, les modèles de programmation linéaire (PL) appliqués au raffinage fournissent une clé de répartition pertinente et unique, fondée sur la contribution marginale des produits à ces émissions. Dans ce cas, les contributions marginales en CO_2 peuvent être directement utilisées pour effectuer des études d'Analyse de Cycle de Vie (ACV). Dans cet article, nous utilisons le modèle de PL développé par l'IFP et nous appliquons la méthodologie d'allocation marginale afin d'évaluer et de comparer les contributions marginales en CO_2 de différents produits pétroliers. Nous étudions également les effets du phénomène de dégénérescence sur les résultats obtenus. Nous présentons finalement les limites de cette méthodologie pour des décisions de court terme.

Abstract — *Allocation of CO_2 Emissions in Joint Product Industries via Linear Programming: a Refinery Example* — *In joint product industries such as an oil refinery, there does not exist a unique way to fully allocate the refinery's CO_2 emissions to its oil products. Under certain conditions, however, refinery linear programming (LP) models can provide a relevant and unique allocation procedure based on the marginal contribution of each oil product to the total CO_2 emissions. In this particular case, the marginal CO_2 allocations can be directly used for Life Cycle Assessment (LCA) purposes. In this paper, we apply the marginal allocation methodology to the oil refinery LP model developed by the Institut français du pétrole (IFP) to evaluate and compare the CO_2 emissions associated with different oil products. We also study the consequences of the degeneracy phenomenon on the obtained results. Finally, the limitations of this approach for short-run decisions are discussed.*

INTRODUCTION

According to the definition of the Society of Environmental Toxicology and Chemistry (SETAC, 1993), Life Cycle Assessment (LCA) is a system analysis method which is commonly used to evaluate the environmental burdens associated with a product, process or activity throughout its life cycle from the extraction of raw materials through processing, transport, use and disposal. Any LCA analysis starts with (1) goal definition and scoping, then (2) a quantitative inventory of all inputs and outputs, followed by (3) classification and impact assessment and finally, (4) interpretation. Decision-making, identification of improvement possibilities, choice of environmental performance indicators, market claims and learning purposes are among the numerous applications of LCA studies (Tillman, 1999).

Recently, one of the interesting developments in the science of LCA methodology and procedure has been the distinction between two types of LCA: retrospective and prospective LCA (Tillman, 1999; Ekvall, 2002; Ekvall *et al.*, 2005). Retrospective LCA, or LCA with an accounting perspective, aims at describing the environmental properties of a life cycle and its subsystems. In accounting LCAs, the LCANET report (Frischknecht, 1997) recommends using average data which represent the average environmental burdens for producing a unit of the product in the system. On the other hand, prospective, consequential or change-oriented LCA is defined by its aim of modeling the environmental effects of changes within the life cycle. Its boundaries include only activities contributing to the environmental effects of the change. Marginal data are used to assess the consequence of small variations in the output of products on the environmental burdens.

Allocation in joint product systems is among the most critical issues specific to LCA. The assumptions about the allocation procedures considerably influence the results. Nevertheless, the distinction between different types of LCA has reduced the persistent methodological problems in this area (Ekvall, 2002). Allocation processes in retrospective LCA are typically solved through assigning the environmental burdens in proportion to some arbitrary physical measurements (mass, volume, energy or heat content, *etc.*) or economic property (gross sales value) of the co-products (Tillman, 1999). On the contrary, in prospective LCA allocations are avoided by enlarging the system boundaries to include all the affected processes (Ekvall *et al.*, 2005).

In general, allocation tools in LCA are based on linear homogeneous and unconstrained models to relate the environmental burdens associated with a product system to its economic outputs (Azapagic and Clift, 1995). In this regard, different methods are available (Suh and Huppes, 2005): process flow diagram, matrix representation of product system, Input-Output (IO) analysis and hybrid methods of process-based and IO-based analysis. These approaches are all based on average data and are mainly applicable in accounting LCAs. To be applicable in change-oriented LCAs, they should include data that represent marginal effects. To accurately model the marginal effects of a change, it is necessary to account for the whole economic mechanisms generated by the substitution and the opportunity cost effects of the change. A possible way to capture these latter is to use Linear Programming (LP) models. In fact, the information created through the duality in LP incorporates the complete economic effects associated with any *ad hoc* marginal variation in the system. Dual variables as well as some of their components correspond to the optimal adjustment of environmental burdens to any marginal variation in output productions and are applicable in change-oriented LCAs. In the literature, this approach has been known as the marginal allocation methodology (Azapagic and Clift, 1994, 1995, 1998, 1999a,b; Babusiaux, 2003).

This paper aims at discussing the application of LP in prospective LCAs using the allocation of the refinery's CO_2 emissions as a case study. However, we note that under certain assumptions (Azapagic and Clift, 1998, 1999a,b; Babusiaux, 2003), marginal values calculated at the solution of the LP can be used for fully assigning the refinery's CO_2 emissions to the oil products. In this particular case, the marginal allocation coefficients can be viewed as the average CO_2 contribution of oil products and be used for providing accounting LCA data. Contrary to the other distribution procedures in accounting LCA, the allocation coefficients which emerge from the LP model are based on realistic causal relations between oil products and the whole refinery system. In other words, the LP model itself detects the real type of causality between various inputs and outputs in the refinery and allocates the CO_2 emissions accordingly without having to use any arbitrary measurements. In this regard, Azapagic and Clift (1999b) show how arbitrary measurements (*e.g.*, mass or market value basis) break down in co-production industrial systems when they do not reflect the underlying physical causality and result in misleading conclusions.

The paper is organized as follows. Section 1 reviews the issue of allocating the refinery's CO_2 emissions via linear programming. Notations are introduced and the fundamental assumptions are discussed. Three major limitations of the LP approach in both retrospective and/or prospective LCA problems are introduced: multiple CO_2 coefficients in the presence of degeneracy, the additivity issue within a short-run LP framework and the erraticity phenomenon in a cost-minimization environment. In this paper, we only deal with the degeneracy and multiple optimal solutions in Section 2. The theoretical considerations are illustrated by applying them to the IFP (*Institut français du pétrole*) oil refinery model in Section 3. The last section concludes.

1 LINEAR PROGRAMMING AND THE ALLOCATION OF CO_2 EMISSIONS IN THE REFINERY

A refinery LP model contains the end-to-end configuration of the refinery with a detailed representation of processing units, blending facilities, power and utilities. Such a model describes complex interactions between different process units and is based on physical relations between crude oils, intermediate products, finished products and the pollutant emissions of the refinery. Therefore, a refinery LP model "lends itself naturally to solving allocation in multiple-function systems according to the procedure recommended by ISO 14041" (Azapagic and Clift, 1998).

1.1 Model Description

In this paper, we develop a typical European single-refinery model which operates in a cost-minimizing environment. In fact, the cost function is one of the principle tools for the analysis of production strategies made by refiners and is implied by the profit-maximization objective. The refiner's objective is to satisfy his production target (in terms of level and specification), denoted by the m-vector b, at minimum cost subject to the prevailing technology, prices and input availabilities. The oil product categories considered in this model are liquefied petroleum products (propane and butane), naphtha, gasoline, middle distillates (jet fuel, diesel and heating oils), heavy fuel oils with 1% and 3.5% mass sulfur contents and bitumen.

The term c is the given n-vector of acquisition input cost and includes all costs that are absorbed in a direct costing system. It includes the cost of crudes and feedstocks, the operating variable cost (*i.e.*, cost of catalysts, solvents and chemicals) and the exchange cost of finished products. Besides the oil product demand and capacity constraints, the most common types of other constraints are the material balance and product quality constraints. The latter guarantee the expected quality and technical requirement of finished products in blending problems such as octane number (for gasoline) or sulfur content (for diesel and heavy fuel oils), and the former represent the fact that the sum total of quantities going into some unit process or blending pool equals the sum total coming out.

Given these preliminaries, we may now state the one-period LP model of the refiner as

$$\begin{cases} \min \ c^T x \\ s.t. \\ Ax \geq b & \text{(product demand constraints)} \\ Dx = 0 & \text{(material balance constraints)} \\ E^T x - \mathcal{E} = 0 & \text{(CO}_2\text{ balance equation)} \\ Fx \leq f & \text{(capacity constraints)} \\ x \geq 0, \mathcal{E} \geq 0 \end{cases} \quad (1)$$

where $c^T x$ corresponds to the total (minimum) variable cost of the refinery. Note that in a standard form, the product

quality requirement constraints can also be formulated as $Dx = 0$. The constraints set of model (1) is a convex polyhedron and represents the refinery's technological possibility set. A detailed description of these constraints is beyond the scope of this paper and can be found in Khebri (1993) and Saint-Antonin (1998). However, one remark seems necessary about the CO_2 balance equation. The variable $\mathcal{E}$ corresponds to the total carbon dioxide emissions generated from the burning of gas fuel (ethane and propane), liquefied fuel (vacuum residue) and the coke of the catalytic cracker in the refinery, each of them being assigned a specific CO_2 emission coefficient. The choice among the refinery fuels depends on the economics and the operating state of the refinery. We assume that the refinery produces its own fuel and, for the sake of simplicity, chemical CO_2 emissions are not considered. Moreover, the utilities requirements (*i.e.*, steams and electricity) are satisfied inside the refinery from burning gas fuel and liquefied fuel.

In an environmental regulatory framework in Europe, refineries are engaged to reduce their carbon dioxide emissions. "Cap-and-trade" programs are the widely accepted approach to CO_2 reduction studies. One of the most important features of this policy is the initial allocation of emissions allowances for which several distribution methods exist in the literature (*e.g.* Kolstad, 2000). One such approach is to distribute allowances without charge to refineries based on their past emission levels. This approach is called grandfathering and gives refineries that have polluted the most in the past the most emission permits in the future. Many previous trading systems (*e.g.*, the SO_2 trading program under the 1990 Clean Air Act Amendments in the U.S.) were based on grandfathering. Another free distribution approach is to regularly update the calculation underlying the allowance allocation based on current or recent-year performance data. The nitrogen oxides regional program in the U.S. and Sweden was based on updating methods (Evans *et al.*, 2002). A third approach is the sale of allowances through an auction to the highest bidders.

In the LP framework, the CO_2 cap-and-trade policies can be formulated by introducing an upper limit, $\bar{\mathcal{E}}$, on the refinery's total emissions, $\mathcal{E}$. The dual variable associated with this constraint represents the "CO_2 value" for the refiner and should be compared with the price of CO_2 permits for any relevant decisions. This dual variable can be introduced, in a second step, into the objective function as a "CO_2 penalty" or a "Pigouvian tax"[1] on quota overruns, *i.e.*, $(\mathcal{E} - \bar{\mathcal{E}})$. Note that in a long-run equilibrium, the optimal Pigouvian tax would be equal to the CO_2 market price. This primal-dual approach provides an equivalent formulation for respecting the emission quotas initially distributed, $\bar{\mathcal{E}}$. Since the CO_2 allocation procedure does not depend upon

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[1] A Pigouvian tax is a tax levied upon each unit of pollution in an amount just equal to the marginal damage it inflicts upon society at the efficient level of output (Kolstad, 2000).

the "cap-and-trade'' policies, we have not introduced them into our basic model (1).

The following discussion shows that, in a LP formulation, some substitution coefficients derived from the final Simplex tableau correspond to the allocation coefficients and evaluate the CO_2 quantities associated with the marginal production of each oil product.

1.2 Marginal Allocation Methodology

For a general solution, let $M = \{1, 2, ..., m\}$ and $S = \{1, 2, ..., s\}$ be the sets of active demand constraints and scarce unit processes at the optimum. At this stage, we suppose that the optimal solution of the LP model (1) is not degenerate so that it has unique primal and dual optimal solutions. This strong assumption will be relaxed in Section 2.

In LP, the primal feasible basic solutions are defined as:

$$x_{\mathcal{B}} = B^{-1} \begin{bmatrix} b \\ 0 \\ 0 \\ f \end{bmatrix} \qquad (2)$$

where $x_{\mathcal{B}}$ represents the basic variables and B^{-1} corresponds to the basis inverse matrix which is pre-multiplied by the right-hand-side (RHS) vector. Any extreme point of the refinery technological possibility set, including the optimal extreme point, can be defined by relation (2). Therefore the following discussion is obviously valid for any basic feasible solution.

The dual variables y_i associated with the product demand constraints can be interpreted as their *marginal production costs*: they measure the variation of the cost function whenever the demand for one oil product is increased by one unit, while keeping demands for all other oil products constant. Similarly, the dual variables δ_j associated with the process capacity constraints can be interpreted as their *opportunity costs* at the optimum: they measure the variation of the cost function whenever the availability of one capacity constraint is increased, *ceteris paribus*.

Now let us focus on the CO_2 emission variable $\mathcal{E}$. At the optimum, $\mathcal{E}$ is a basic variable (because always positive); so an element of $x_{\mathcal{B}}$ can be expressed as:

$$\mathcal{E} = e_{\mathcal{E}}^T B^{-1} \begin{bmatrix} b \\ 0 \\ 0 \\ f \end{bmatrix} \qquad (3)$$

where $e_{\mathcal{E}}$ is the $\mathcal{E}$th unit vector ($e_{\mathcal{E}t} = 0$ for $t \neq \mathcal{E}$ and $e_{\mathcal{E}\mathcal{E}} = 1$) and $e_{\mathcal{E}}^T B^{-1}$ corresponds to the *row* of B^{-1} associated with the basic CO_2 variable $\mathcal{E}$. The row vector $e_{\mathcal{E}}^T B^{-1}$ contains several blocs which are referred to the slack variables of model (1). Simplifying (3), we get:

$$\mathcal{E} = \sum_{i \in M} \alpha_i b_i + \sum_{j \in S} \beta_j f_j \qquad (4)$$

where α_i and β_j belong to the blocs which relate $\mathcal{E}$, respectively, to the demand and capacity slack variables. The coefficient α_i corresponds to the additional emissions of CO_2 attributable to the marginal production of the ith oil product, *ceteris paribus*. Similarly, β_j refers to the additional quantities of CO_2 attributable to an extra unit of the jth scarce capacity process, *ceteris paribus*. According to the optimal technology, α_i and β_j can be positive, negative or zero (see Sect. 3.3). By using differential calculus, it can be shown that α_i and β_j capture the whole economic effects (substitution and opportunity cost effects) of a marginal variation in the ith oil product demand and jth capacity constraint at the optimum. Under the non-degeneracy assumption, these substitution coefficients are uniquely determined and directly obtainable from the optimal Simplex tableau.

One of the interesting features of LP is to transform the input activity-related emissions $\mathcal{E} = Ex$ into product- and process-related emissions *(Equation 4)*. Since the operating state of the refinery is determined by the active constraints, the CO_2 emissions are shared between both oil products and scarce unit processes at the optimum. These marginal coefficients are relevant for decision-making purposes and can be directly used for change-oriented LCAs. To be applicable in accounting LCA studies, it is necessary to reallocate the total process-related emissions (*i.e.*, $\sum_j \beta_j f_j$) over oil products (Tehrani Nejad, 2007; Babusiaux and Pierru, 2007; Pierru, 2007). In this regard, care should be taken not to fall in the realm of any arbitrary or *ad hoc* measures. In fact, this could be a valid objection to LP as a tool for accounting LCAs in the short run.

In long-run LP models, however, availability constraints are usually omitted and unit process capacities are among the endogenous variables of the problem ($f_j = 0$ for any j). Under these circumstances, the carbon dioxide emissions are fully allocated among the oil co-products and product-related parameters, α_i, can provide accounting LCA data, that is:

$$\mathcal{E} = \sum_{i \in M} \alpha_i b_i \qquad (5)$$

In the following section, we relax the non-degeneracy assumption and deal with the practical consequences of a degenerate LP on the product- and process-related CO_2 allocations.

2 MARGINAL ALLOCATION PROCEDURE UNDER DEGENERACY PHENOMENON

Using one of the Midterm Energy Market Models of the U.S. Department of Energy, Greenberg (1986) shows that most of the practical LP models are degenerate due to the model's accounting and netform structures, management practices associated with matrix generation and scenario specification. Gal (1992) also places special emphasis on weakly

redundant constraints as another major source of degeneracy in practical models.

Although weak redundant constraints have no influence on the primal admissible set, they affect the shadow prices of the remaining active constraints. Hence, their omission by pre-solving techniques can skew the oil products' marginal costs and their associated CO$_2$ allocation coefficients. As shown by the above authors, "degeneracy is a realworld phenomenon'' and should not be neglected, as is usually the case, in empirical studies. Whatever the reason, multiple optimal solutions can be the direct consequences of degeneracy in LP. Unfortunately, commercially available software does not give enough information to the user about the existence of these very common "special cases'' which could lead to wrong decisions (Roos *et al.*, 1997).

3 DEALING WITH MULTIPLE CO$_2$ ALLOCATION COEFFICIENTS

In Section 1.2 we show that, under the non-degeneracy assumption in LP, the optimal allocation coefficients (α_i and β_j) are directly derived from the optimal basis inverse B^{-1}. Whenever the optimal solution is degenerate, more than one basis B can be assigned to the optimal extreme point (*e.g.*, Gal, 1986). This phenomenon leads to multiple optimal solutions in general, and multiple CO$_2$ allocation coefficients in our context.

When the refinery LP problem possesses alternate allocation parameters, commercially available LP software, which is often based on a version of the simplex method, provides us with only with one of them. We believe that the final decision among the many possible ones should not be left to LP software, especially when the goal of the study is either an efficiency judgment or prescribing policy changes. Below, we borrow a fundamental concept from convex analysis to deal with this issue. For a complete discussion about degeneracy and multiple optimal solutions, the reader is referred to Gal (1993).

Let us denote $H(r) = \{B^1, B^2, ..., B^k\}$ the set of optimal bases, with associated CO$_2$ allocation coefficients $Z(r) = \{(\alpha_i^1, \beta_j^1), (\alpha_i^2, \beta_j^2), ..., (\alpha_i^k, \beta_j^k)\}$. By analogy to the shadow prices in LP under degeneracy (see *e.g.*, Roos et al., 1998 for details), there exist only two allocation parameters for each oil product (or combination of oil products) and scarce input (or combination of scarce inputs). These two-sided allocation coefficients correspond to the right- and left-partial derivatives of the CO$_2$ response function (*Equation 4*). Hence, care must be taken to distinguish between "the CO$_2$ contribution of one more unit of the ith oil product (α_i^+) or jth scarce input (β_j^+)'' and "the CO$_2$ contribution of one less unit of the same oil product (α_i^-) or scarce input

(β_j^-)'':

$$\begin{cases} \alpha_i^+ = \frac{\partial \mathcal{E}}{\partial b_i^+} \neq \frac{\partial \mathcal{E}}{\partial b_i^-} = \alpha_i^- & i \in M \\ \beta_j^+ = \frac{\partial \mathcal{E}}{\partial f_j^+} \neq \frac{\partial \mathcal{E}}{\partial f_j^-} = \beta_j^- & j \in S \end{cases} \tag{6}$$

Note that in a non-degenerate LP, $\alpha_i^+ = \alpha_i^- = \alpha_i$ and $\beta_j^+ = \beta_j^- = \beta_j$ for any i and j.

In the RHS perturbation analysis, the *directional derivative theorem* says that each optimal basis B^r has a set of *compatible or admissible directions* (Greenberg, 1986), and associated values provide the rate of change of the minimum total cost of the refinery. An interesting result of the theory of compatibility (Greenberg, 1986) is that the optimal basis that yields the marginal cost of the ith oil product is the one which contains its associated CO$_2$ allocation coefficient. Contrary to the marginal cost analysis, however, the two-sided product- and process-related allocation coefficients do not necessarily correspond to the extremal marginal allocations.

Identifying the compatible bases associated with the demand and capacity constraints variation requires traversing the optimal bases set $H(r)$. An interesting way to reach the compatible bases more easily is to perform a parametric analysis on the RHS of the desired constraints (see Gal, 1986 for further details).

In conclusion, $\alpha_i^+(i \in M)$ and $\beta_j^+(j \in S)$ are the relevant CO$_2$ allocation coefficients for any change-oriented LCA study and represent, respectively, the additional carbon dioxide emissions attributable to the marginal production of the ith oil product and the extra availability of the jth unit process.

Note that in general, $\alpha_i^+(i \in M)$ and $\beta_j^+(j \in S)$ do not belong in general to the same optimal basis, and as a consequence

$$\mathcal{E} \neq \sum_{i \in M} \alpha_i^+ b_i + \sum_{j \in S} \beta_j^+ f_j \tag{7}$$

In other words, when the LP model is degenerate, the relevant marginal coefficient-based allocations overestimate or underestimate the total CO$_2$ emissions of the refinery. As a consequence, even for long-run situations, LP models do not provide exact accounting LCA data (see Sect. 3.3). Therefore, the degeneracy issue is another valid objection to the LP as a tool for retrospective LCA studies for users of one or more of the oil co-products.

4 CASE STUDY

The goal of this case study is to evaluate and to compare the carbon dioxide contents associated with the marginal production of joint oil products, produced in a European refinery structure. To this end, we have used the IFP model (described in Sect. 1.1, with 485 constraints and 1035 variables) and extracted the CO$_2$ allocation coefficients from the optimal simplex matrix.

4.1 General Framework of the Model

4.1.1 Refinery Scheme

The LP refinery model retained here corresponds to a typical European fluid catalytic cracking (FCC) refinery of 10 million metric tonnes per year of crude oil processing capacity. The processing units are atmospheric and vacuum distillations, a catalytic reformer, an isomerization unit, a catalytic cracker combined with an alkylation unit, a Mild HCK unit, a MTBE unit, a gas oil hydrodesulfurization unit, a visbreaker to process residues and finally, a Claus unit process. Since the refinery is supposed to operate at the short run, all the units are limited by their installed capacity.

The standard refining process described by the model can be summarized as follows: three typical crude oils; namely, Brent, Arabian Light and Arabian Heavy crudes [2] and some imported feedstocks of atmospheric residue type [3] are separately distilled in the distillation column at atmospheric pressure. Depending upon requirements, two sets of oil cuts (the temperature at which a product is cut) are considered in the model. In the atmospheric distillation unit, various fractions are separated according to their boiling points. Light fractions are used to make gasoline and naphtha whilst middle fractions are used to produce gas oil and kerosene. The heaviest fractions are distilled again under vacuum to produce vacuum distillate and vacuum residue. The major part of the vacuum residue is fed to a visbreaker, to reduce the viscosity of the fuel oil products that enables the minimization of the contribution of light distillate products, the excess vacuum residue being used as refinery fuel. The vacuum distillate is converted by a fluid catalytic cracker into a gasoline blending component and light cycle oil for blending into the diesel pool. The fluid catalytic cracking is combined with an alkylation unit and operates following two severities. The sulfur specifications for gasoline, middle and heavy oil products require the use of various hydrodesulfurization units. A Claus sulfur recovery processing is also modeled to convert the H_2S into liquid sulfur.

On the other side, a catalytic reforming unit converts low-octane naphthas into high-octane gasoline blending components called reformates where hydrogen is a by-product. An isomerization unit is also modeled to convert n-paraffins into isoparaffins of substantially higher octane number.

4.1.2 Oil Product Demand

Though oil products' demand has continued to increase, expansion of existing capacity has still not taken place in European refineries. High capacity utilization, some investments and increased imports of middle distillates (diesel, jet

fuel and heating oil) are required in order to meet demand. Imports from Russia and Central Europe are helping to fill the Western European diesel gap. At this time, the primary focus for the European refineries is to boost the production of middle distillates (especially diesel) while reducing gasoline output or keeping it stable.

This tight supply-and-demand market is worsened by the tightening of product specifications: gasoline and "on-road'' diesel sulfur content was reduced to 50 ppm in 2005 and will be reduced to 10 ppm by January 2009. In addition, the total aromatics content was reduced from 42 vol% to 35 vol% in 2005. Since 2000, the olefins and benzene contents have been limited to 18 vol% and 1 vol%, respectively. A review of European Union diesel specifications is scheduled for 2006 (Houdek, 2005).

In this paper, we consider the specifications of the year 2000 *(Table 1)* to evaluate the CO_2 contents associated with the marginal production of oil products. Further studies are being investigated based on oil product specifications of 2005 and 2009.

TABLE 1

Specifications of gasoline and diesel (year 2000)
Source: Panorama IFP 2005

Quality	Gasoline	Diesel
Sulfur max. (% m)	0.015	0.0 35
Cetane (point)	–	51
Poly-aromatics max. (% m)	–	11
RON min. (point)	95	–
MON min. (point)	85	–
Aromatic max. (% vol.)	42	–
Olefin max. (% vol.)	18	–
Oxygen max. (% m)	2.7	–
Benzene max. (% vol.)	1.0	–

4.2 Model Calibration for 2000

In the process of abstracting and simplifying a real system the model loses information and needs to be verified against actual behavior. The evaluation of carbon dioxide contents based on a LP model that shows a wide divergence between its optimal solutions and the actual production and cost patterns of a typical refinery is unacceptable. Here, we have adopted the following criteria to validate the model. Firstly, the oil production level of the refinery should correspond to the European market structure of the year 2000. Secondly, marginal costs of oil products are examined to ensure that they are between their respective Custom-Insurance-Fret (CIF) and Free-On-Board (FOB) prices. The third criterion is based on a utilization rate test for the unit processes. The fourth is a utility production test that considers any excess production of utilities is unreasonable at the optimum. Finally, the active quality constraints and their

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(2) These are considered to be typical of the quality of crudes currently available in European refineries.

(3) The imports of feedstocks are limited to 0.43 million tonnes.

associated dual values are verified to ensure that they do not diverge from the European refinery constraints and performances.

Based on the above validation criteria, the calibrated level of oil products is summarized in Table 2.

TABLE 2

Calibrated production level for oil products
Units: million tonnes

Oil products	Production level	% total production
Propane	0.20	2.0
Butane	0.10	1.0
Naphtha	0.70	7.0
Gasoline	2.27	22.7
Jet fuel	0.50	5.0
Diesel	2.90	29.
Heating oil	1.15	11.5
Heavy fuel oil 1%S	0.60	6.
Heavy fuel oil 3.5%S	0.50	5.0
Bitumen	0.40	4.0
Fuel refinery	0.68	6.8
TOTAL	10.0	100

Note that the oil product demand is equal to the refinery production plus the net exchange (imports - exports) for each finished product. For some technical reasons, discussed in the next section, we do not allow the possibility of exchange for gasoline and middle distillates (*i.e.*, jet fuel, diesel and heating oil). In the optimal production plan, only butane and heavy fuel oil 1%S are exported.

Although the refinery structure is gasoline-oriented (because of the FCC unit whose major function is to produce gasoline), nearly half of its production is middle distillates. This is consistent with the European refineries' production structure which tries to increase their middle distillate products while reducing or keeping stable their gasoline output.

The results of the verification/calibration experiments are extensive. Here, we only overview the most significant ones. First, the refinery fuel mixes results felt within the range of the observed actual refinery fuel: 70% gas fuel and 30% liquefied fuel. Second, as shown in Table 1, the amounts of gasoline and heavy fuels were overestimated by 3% and 0.95% and the middle distillates production was underestimated by 2%. This occurred because of the gasoline configuration of the refinery and the lack of various technical flexibilities which were not considered in the model. Third, the alternation in the production of middle distillates and gasoline as diesel production increased was replicated. The parametric results confirmed the capability of the IFP model to correctly reproduce the logical evolution of the product mix.
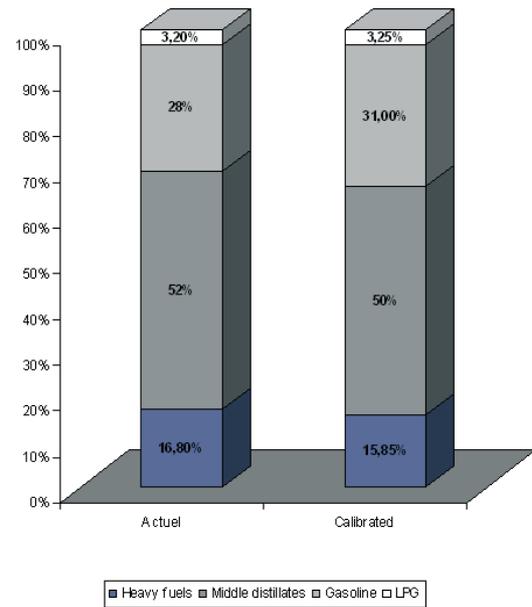

Figure 1

Oil product outputs: calibrated results against the base year 2000.

4.3 Allocation of carbon dioxide emissions

The typical refinery discharges 1.974 million tonnes of CO$_2$ emissions at the optimum, *i.e.*, 20% of the crude oil processed [4]. Due to the optimal active constraints of our model, the total CO$_2$ emissions are shared between both oil products and unit processes (see *Tables 3, 4*). The calculated marginal contents (*i.e.*, α_i and β_j) are therefore relevant for decision-making purposes in prospective LCA studies where the implications of both final products and unit process expansion are of interest (Azapagic and Clift, 2000).

Several remarks are in order. First, note that, as far as the LP model is degenerate, one should distinguish between the substitution coefficients (*i.e.*, α_i and β_j) and the relevant product- and process-related emissions (*i.e.*, α_i^+ and β_j^+). In this regard, we performed further parametric analysis to derive the relevant CO$_2$ allocation for each active constraint. For instance, Table 3 shows that producing one additional tonne of diesel would cause a total increase in CO$_2$ emissions of 1.112 tonnes (α_{diesel}^+) and not 0.851 tonnes as indicated by its corresponding substitution coefficient (α_i). Similarly, the relevant marginal CO$_2$ allocation of gasoline (β_j^+) is nearly 10% higher than its substitution coefficient (β_j). As a consequence, the relevant total allocated CO$_2$ to gasoline and middle distillates (jet fuel, diesel and heating oil) are

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(4) This amount corresponds to the actual CO$_2$ emissions of the French refineries in 2005.

0.20 and 1.18 million tonnes, more than what is calculated by the substitution coefficients at the optimum.

TABLE 3

CO_2 emissions allocated to oil products

Oil products	Substitution coefficients α_i (tCO$_2$/t)	Allocation parameters α_i^+ (tCO$_2$/t)	Total allocated CO$_2$ (million t)
Butane	0.000	0.000	0.000
Naphtha	0.677	0.778	0.544
Gasoline	0.761	0.850	1.929
Jet fuel	0.836	1.096	0.548
Diesel	0.851	1.112	3.225
Heating oil	0.808	1.067	1.227
Heavy fuel oil 1%S	0.000	0.000	0.000
Heavy fuel oil 3.5%S	-0.171	-0.171	-0.085
Bitumen	-0.307	-0.405	-0.162
TOTAL			*7.114*

The same interpretation applies to the process-related CO_2 emissions (β_j and β_j^+ in *Table 4*). These results illustrate the importance of degeneracy analysis in empirical LP studies.

TABLE 4

CO_2 emissions allocated to scarce unit process and feedstocks

Oil products	Substitution coefficients β_i (tCO$_2$/t)	Allocation parameters β_i^+ (tCO$_2$/t)	Total allocated CO$_2$ (million t)
Atmospheric distillation	-0.351	-0.478	-4.780
Vacuum distillation	-0.060	-0.087	-0.409
Mild HCK	-0.129	-0.177	-0.018
Isomerization	-0.352	-0.349	-0.087
Feedstocks	-0.023	-0.023	-0.010
TOTAL			*-5.304*

As shown in Table 3, the marginal CO_2 emissions α^+ associated with butane and heavy fuel oil 1%S are zero at the equilibrium solution. These values result from the fact that the additional demand of butane and heavy fuel oil 1%S is met by decreasing their exportation level without any extra production activity and, therefore, any extra CO_2 emissions. The same conclusion is true when a given oil product is imported at the optimum. Since our objective is to evaluate the marginal CO_2 contributions of gasoline and middle distillates (specially diesel), we do not allow the model the possibility of exchanging these products.

Besides, marginal allocated CO_2 emissions to heavy fuel oil 3.5%S and bitumen are negative, which means that their marginal production decreases the total CO_2 of the refinery

by 0.171 and 0.405 tonnes, respectively. Not intuitive a priori, these results can be perfectly calculated by analyzing the substitution coefficients associated with the refinery fuels. Producing one additional tonne of heavy fuel oil 3.5%S increases the internal consumption of the gas fuel (ethane and propane) and FCC coke by 0.06 and 0.03 tonnes, respectively, which generates 0.288 additional tonnes of CO_2 emissions. On the other hand, the consumption of the liquefied fuel (vacuum residue) decreases by 0.143 tonnes which induces a reduction of 0.459 tonnes of carbon dioxide emissions. This cost-efficient arbitrage (0.288 - 0.459 = - 0.171) results in a negative marginal contribution of CO_2 for heavy fuel oil 3.5%S. Thus, from an environmental point of view, it would be cleaner to increase the production of the heavy fuel oils in the refinery (because of their lesser energy consumption), a result which is in sharp contrast with the actual evolution of the oil products' demand in Europe.

Finally, comparing the marginal CO_2 coefficients in Table 3 leads to the following conclusion: forcing a FCC refinery to boost its production of middle distillates while reducing its gasoline output leads to a higher marginal CO_2 content associated with middle distillate products (especially diesel) as compared with gasoline. This conclusion could even worsen with the tightening of the "on-road" diesel specifications. Note that, however, since the CO_2 emissions are not fully allocated to the oil products, the marginal CO_2 contributions (*i.e.,* α_i^+) should not be directly compared with the other accounting allocation methods used by LCA practitioners [5]. As shown in Table 3, the total allocated CO_2 to oil products based on their marginal contents (7.114 million tonnes) is nearly 3.5 times more than the total unallocated CO_2 emissions of the refinery (1.947 million tonnes). This is especially due to the fact that all the process-related emissions (*i.e.,* β_j^+) are all negative at the optimum (*cf. Table 4*). Moreover, under degeneracy the relevant allocation coefficients (α_i^+ and β_j^+) underestimate the total CO_2 emissions by nearly 7% (*cf. Equation 7*).

5 FURTHER REMARKS

The results shown in Tables 3 and 4 depend naturally on the optimal solution and change with the operating state of the refinery. In other words, the allocated CO_2 emissions are not fixed but change to reflect changes in the system parameters such as the evolution of oil products' demand.

Since the allocation values (*i.e.,* α_i and β_j) are derived from the optimal basis inverse matrix B^{-1}, their response to the rim (RHS and cost vectors) parametric changes are erratic and unpredictable. Unlike the predictable behavior

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(5) Most accounting LCA studies come to the opposite conclusion: due to a higher number of gasoline processing units in FCC refineries, the average CO_2 content of gasoline is higher than that of diesel.

of marginal production costs, $y^{(6)}$, which increase gradually in function of output productions, the marginal CO_2 contents change abruptly as solutions move from one extreme point on the convex set to another. This erratic behavior in the system arises mainly from active capacity constraints whose CO_2 allocation coefficients (*i.e.*, β_j) are spread over the product-related CO_2 emissions (*i.e.*, α_i) at the optimum. This unpredictable response of the LP-based CO_2 allocations is the third valid objection to LP for accounting LCA perspectives. Due to this erratic behavior, the comparison of the products' marginal CO_2 contents requires special precautions. In particular, it is recommended to perform a parametric analysis to fully compare the evolution of the CO_2 allocations of various oil products.

Besides, a number of developments could also enable the reduction of the sensitivity of the LP-based CO_2 allocations. Moving averages may seem to be an appealing suggestion for this issue by smoothing out the curving lines and making it easier to identify the direction of the trend. They will not predict any change in trend, but can be rather used for trend-following purposes. However, it should be noted that when the marginal CO_2 allocations' curve is not trending, moving averages can give misleading signals.

An environmentally-effective way to obtain non-erratic CO_2 allocation coefficients is to minimize the total carbon dioxide emissions of the refinery, rather than its variable costs, subject to the same set of constraints as in model 1. In this case, the CO_2 allocation coefficients correspond to the dual variables associated with demand constraints and are piecewise linear, non-decreasing, convex and continuous on its domain in b. In the European refinery context, where the production of middle distillates are boosted, we implemented this approach and observed that the optimal components of diesel and gasoline remained almost the same in both cost-minimization and emissions-minimization frameworks. This result is of importance because the environmentally-effective CO_2 -based coefficients for automotive fuels which follow a more predictable trend could replace their respective cost-effective CO_2 contributions (α) in prospective LCA studies (Tehrani Nejad and Saint-Antonin, 2007).

CONCLUSION

In this paper we distinguished between the allocation procedures in retrospective (accounting) and prospective (change-oriented) LCAs. Allocations in prospective LCA are relevant for economic decisions and require marginal data reflecting the whole economic mechanism (substitution and opportunity cost effects) of a change. These data can be successfully provided by non-degenerate LP models. Under degeneracy in LP, dual variables and marginal CO_2 allocations should be interpreted with precaution. We brought a theoretical and practical answer to this issue.

Under particular conditions, the marginal allocation data generated by LP can also be applicable in retrospective LCA studies. Contrary to the arbitrary physical measurements (mass, volume, energy, *etc*.), the allocation coefficients which emerge from the LP model are based on realistic causal relations between oil products and the whole refinery system. In other words, the LP model itself detects the real type of causality between various inputs and outputs in the refinery and allocates the CO_2 emissions accordingly without having to use any arbitrary measurements.

Besides the degeneracy issue in LP which is common to both types of LCAs, we raised two other valid objections to LP as a tool for retrospective LCA studies. First, the non-additivity character of the product-related CO_2 emissions whenever capacity constraints are active at the optimum. In this case, the CO_2 allocations associated with oil products are perfectly relevant for prospective LCA but inapplicable directly in accounting LCAs. Second, we discussed that unlike the marginal production costs, the LP-based CO_2 allocations change abruptly as the demand of one product increases gradually. Due to this unpredictable behavior, it is highly recommended to perform a parametric analysis to fully compare the evolution of the CO_2 allocations of various oil products. In this regard, different suggestions to reduce the sensitivity of the LP-based CO_2 allocations were also introduced.

For the case study considered here, we focused on a prospective LCA approach to evaluate and to compare the carbon dioxide emissions associated with the marginal production of joint oil products in a typical refinery.

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(6) It is well known that in model 1, the objective value is piecewise linear, non-decreasing, convex and continuous on its domain in b for fixed input variable cost c.

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