Oil & Gas Science and Technology – *Rev. IFP*, Vol. 58 (2003), No. 6, pp. 685-692

Allocation of the CO_2 and Pollutant Emissions of a Refinery to Petroleum Finished Products

D. Babusiaux[1]

1 Institut français du pétrole, 1 et 4, avenue de Bois-Préau, 92852 Rueil-Malmaison Cedex - France
e-mail: denis.babusiaux@ifp.fr

Résumé — Affectation des émissions de CO_2 et de polluants d'une raffinerie aux produits finis pétroliers — Les risques de changement climatique vont conduire l'industrie du raffinage à réduire autant que possible ses émissions de gaz à effet de serre et principalement de CO_2. Afin de mieux apprécier ces émissions, *Total* et l'*IFP* se sont associés pour développer une modélisation appropriée par programmation linéaire, testée sur une raffinerie française.

Dans le cadre de cette étude s'est posé le problème de l'affectation des émissions de CO_2 aux différents produits du raffinage. Il existe une infinité de clés de répartition possibles. Celle que nous proposons, et dont nous montrons la pertinence, s'appuie sur la détermination d'un « contenu marginal » en émissions de chaque produit. Celui-ci peut être déterminé par les modèles de programmation linéaire. Nous précisons (à l'aide d'un « théorème » très simple) dans quelles conditions les contenus marginaux ont une structure de contenus moyens. Nous donnons enfin quelques indications sur les résultats obtenus.

Abstract* — *Allocation of the CO_2 and Pollutant Emissions of a Refinery to Petroleum Finished Products — *The risks of climate change are pressing the refining industry to minimize its greenhouse gas emissions, and chiefly CO_2. To gain a closer understanding of these emissions,* Total *and* IFP *have joined hands to develop an appropriate linear programming model, tested on a French refinery.*

One element of the study addressed the problem of allocating CO_2 emissions to the different refinery products. An infinite number of allocation methods are available. The one proposed by the authors, who demonstrate its relevance, is based on the calculation of a "marginal emissions content" of each product, which can be determined by linear programming models. The authors (using a very simple "theorem") identify the conditions in which marginal contents have an average content structure, and go on to provide details about the results obtained.

INTRODUCTION

A comparison of the environmental impacts of energy systems demands the analysis of greenhouse gas and pollutant emissions associated with each of the different operations, from production to the end use of the energy. The life cycle analysis methodology was developed to facilitate the corresponding calculations. In automotive transport, this means accounting for the different links of the "well to wheel" chain, by allocating the impacts associated with the production and transport of oil and gas, with refining in the case of conventional petroleum fuels, and with conversion to mechanical energy by engines.

Refining raises a specific problem insofar as it leads to the manufacture of joint products. There are innumerable ways to allocate the pollutant and greenhouse gas emissions of a plant among the different finished products. Most analyses use an accounting that relies on pro rata calculations by weight or energy content. Nonetheless, while the issue of the average contribution of a product's manufacture to emissions eludes any single answer, the marginal contribution can be calculated, particularly using the linear programming models routinely used in the refining industry. The marginal contribution must clearly serve as a reference in examining decisions on manufacturing, import or product exchanges between refineries or between refining zones. And this contribution should serve as a basis to determine any applicable Pigou tax. This article attempts to clarify the conditions in which a marginal emissions content has the properties of an average content, *i.e.* that represents a means of allocation of emissions between the finished products. We have accordingly demonstrated a "theorem" that is very simple but appears to be novel. The method was developed as part of a joint study by *IFP* and *Total*. The aim was to achieve a better grasp of the CO_2 emissions of a refinery in connection with modeling by linear programming.

The presentation here puts emphasis on CO_2 emissions, not only because they are the subject of the study mentioned, but also for the sake of simplification. The following arguments and formulations are nonetheless easily adaptable to other greenhouse gases and pollutants. It is also clear that the methodology proposed can be generalized to any industrial process with joint products.

1 LINEAR PROGRAMMING IN REFINING

Linear programming is routinely used in the refining industry to draw up annual, quarterly and monthly[1] programs involving crude oils (distillation cut points, unit operating severities), procurements and finished product sales. Certain modeling options may vary from one company to another, such as planning frequency, procedures for incorporating nonlinearities, the integration or not of several refineries and of the distribution, the use of seasonal models involving several periods, etc. All linear programming methods in refining are nonetheless constructed on the same general principles that we briefly recall in this section, before tackling the problem of CO_2 emissions.

The **aim** is to maximize a profit or to meet a given demand for finished products at minimum cost. Both formulations are naturally equivalent if the second option is associated with finished product buying and selling possibilities (import and export). To facilitate certain presentations, we shall adopt the second option below, considering a problem of cost minimization, with sales of production surpluses in excess of fixed demand appearing with a negative cost.

The **main variables** are the flows of crude oil and products to be processed, intermediate products and finished products corresponding to each of the possible allocations of these products within the refinery.

Among the main equations, **material balance equations** are the most numerous. They express the equality between an available quantity of a given intermediate product (product yield at the exit of a unit multiplied by the quantity of feedstock processed) and the quantities used corresponding to the different possible destinations of this product.

In actual fact, unit yields are not constant. They depend on operating conditions and the relations are no longer linear. This difficulty is often circumvented by considering two or more "severities" (operation conditions), and the problem is formulated as if several distinct units exist, their characteristics corresponding to the different possible operating conditions of the same unit.

Moreover, product yields and grades usually depend on the type of feedstock and the crude oil employed. In this case, there must be a set of equations for each type of feedstock and each crude. The nonlinearity of certain relations is sometimes accounted for by means of iterative processes.

Demand equations reflect the fact that the sum of the quantities of intermediate products used in blends to produce a finished product, possibly as indicated above, less export sales and plus import purchases, should serve to meet the demand for this product.

Quality equations express the obligation, for each finished product, to meet the legal specifications as well as a number of technical requirements. For automotive fuels, these are density, vapor pressure, octane numbers (of total fraction and light fractions), distillation points, sensitivity, aromatics and olefins content; and for medium distillates and heavy fuel oils, density, sulfur content, viscosity, pour point, cetane number (for engine diesel).

When these grades fail to meet a weight or volumetric linear blending law, the corresponding constraints are written using blending index tables.

(1) Here, we shall ignore day-to-day manufacturing programs which raise combinatory problems of a different order.

Capacity and availability equations reflect the capacity limitations of existing units, crude oil availability limitations, etc.

To obtain an accurate representation of the relations analyzed, a large number of constraints and variables is often necessary, and the models employed in the industry generally contain several hundred, indeed thousands, of constraints and variables.

Note also that the use of this type of model is not restricted to the analysis of short-term manufacturing plans. Linear programming models are also used to analyze investment decisions. In this case, added to the above variables are variables representing the unit capacities to be built. The incorporation of nonlinearities (economies of scale) and possibly a combination of alternative choices, can give rise to mixed integer programming models (with continuous and integer variables).

2 MODELING CO_2 EMISSIONS

Refinery operations release pollutants and greenhouse gases, some of which have regulatory limits. In the United States, sulfur and nitrogen oxides are the subject of markets for tradable emission rights, encouraging the quest for the cheapest reductions. To grapple with the problem of climate change, carbon dioxide emissions must also be reduced. *BP* and *Shell* have pledged commitments accordingly, and each has introduced an in-house market for CO_2 emission rights. *Total* is committed to limit its emissions. In France, the *AERES (Association des entreprises pour la réduction de l'effet de serre)* includes most of the big energy consuming industries that have pledged voluntary commitments to limit their emissions. They include refiners operating in continental France. Finally, despite the United States refusal to ratify the Kyoto Protocol, the draft European directive calls for the establishment of a market for tradable rights. Most refiners are therefore prepared to include a "CO_2 constraint" in drawing up production programs and examining investment projects.

The linear programming models mentioned above incorporate a representation of the production and use of utilities (fuels, steam, electricity) from which CO_2 emissions can be calculated. Until recently, however, the reduction of these emissions was not a priority. Hence the degree of detail of the data used and the modeling formulations employed preclude a precise knowledge of the emissions, and a 20% margin of error was commonly announced.

The need to upgrade linear programming methods has led *IFP*, *Elf* and *Total* (before their merger) to join in developing an appropriate model. The aim is to quantify the consequences of production or investment decisions on the energy balance and CO_2 emissions of a typical refinery or a set of refineries. Modeling must also serve to analyze the impact, in terms of emissions, of changes in various parameters, like those pertaining to the demand and supply structure, finished product quality specifications, pollutant release limits, developments in plant technical characteristics, etc.

The corresponding study was carried out with aid from the *Fonds de soutien aux hydrocarbures*. The modeling principles were tested on the case of a *Total* group refinery. This is not the place to go into the details of this study, and we shall merely address two specific points in the rest of this article.

The first corresponds to a commonplace remark. The model includes a variable corresponding to CO_2 emissions. It is calculated very simply from the consumptions of the different fuels used in the refinery, each of them being assigned a specific CO_2 emission coefficient.

The second point relates to the modeling option selected. It consists in integrating, in the objective function, a cost associated with CO_2 emissions. No doubt this cost is known today only in a small number of specific cases where a market for emission rights already exists (in-house markets of *BP* and *Shell* previously mentioned). The coefficient allocated to a ton of carbon dioxide is hence considered as a parameter, and the sensitivity of the results to the value of this parameter must naturally be analyzed. This approach was preferred to others, like those involving more sophisticated multi-criteria analyses, because of its simplicity and because the price per ton of carbon or CO_2 is an increasingly popular reference.

Note also that if quota overruns are taxed, the total quantity of emissions should be considered as the sum of an untaxed quantity and a quantity subject to penalty, with only the latter appearing in the objective function.

3 THE ALLOCATION OF EMISSIONS TO PETROLEUM FINISHED PRODUCTS

The risk of climate change, and the looming rarefaction of fossil energy resources, have spawned studies of different alternative methods of production of motor fuels, biomass and the production of liquid hydrocarbons from natural gas (Fischer-Tropsch process), and possibly from coal. Different propulsion systems are also being developed, electric motors powered by fuel cells and hybrid vehicles. A comparison of the environmental impacts and the analysis of the consequences on greenhouse gas emissions must account for all the necessary operations, from production and distribution to the end use of the energy, including all the links of the "well to wheel" chain. Life cycle analysis (LCA)[2] methodology was developed to facilitate and standardize the calculations. A system is thereby broken down into steps, each corresponding to a module accurately describing an elementary production, conversion, transport or distribution operation,

(2) Cf for example Consoli (1993).

and allowing identification of the inputs, the conversion yield, output flows and pollutant and greenhouse gas releases.

The production of conventional petroleum fuels raises a special problem. The products of the refining industry are linked, implying an infinite number of means of allocation of the emissions of a plant to the different finished products. Existing studies rely on different methods. In the most common[3] for each refining unit, emissions are allocated to the products (intermediate or finished) in proportion to the quantities manufactured, by mass or by volume, and possibly according to their energy content or economic value.

When a "well to wheel" system is analyzed, the CO_2 emissions are essentially generated during fuel combustion. Yet, refining emissions are not negligible, and justify the application of less arbitrary methods. We propose to adopt a marginal approach.

4 THE MARGINAL APPROACH

Note first that this method is not a novel one. It was suggested by *IFP* in the late 1970s (Leprince *et al.*, 1981). It was the subject of the thesis of Azapagic (1996)[4] who analyzed its potential contributions and computation methods by linear programming. Yet, surprisingly, she does not seem to ask the question as to the extent to which the marginal contents of emissions concerned could constitute a means of allocation of all the emissions. We shall deal with this question after introducing the concept of marginal content. We begin with an ordinary observation: the problem of allocating a refinery's pollutant and greenhouse gas emissions is similar to that of allocating its processing costs to the different finished products.

Allocating Costs

This is a now classic question. A number of general principles can be set forth. When a manufacturing or marketing decision for a product is being examined, the marginal production cost must be compared with the selling price (or the marginal revenue if price is not independent of marketed quantities). When manufacturing programs are drawn up using linear programming, the marginal costs of the different products are obtained from the optimization results. For a cost minimization model under the constraints to satisfy a production demand, the marginal costs are equal to the dual variables associated with the demand equations. The question also arises whether the sale or production at a given price is or is not profitable. For a company manufacturing a single product, the answer is given by comparing the selling price with the average production cost. But for a company with joint products, no single definition of the average cost of a product applies, and any means of allocation of the total processing cost over the finished products is arbitrary. Solutions that rely on marginal costs nonetheless have a special relevance.

The Duality Property of Linear Programs

At the optimum, the sum of the products of the dual variables by the right hand side (RHS) coefficients of the constraints associated with these variables is equal to the value of the economic function. Thus when a refining model only has nonnull right hand side coefficients that are associated with demand equations, the sum of the products of the marginal costs by the quantities demanded is equal to the processing costs, or at least to total costs taken into account in the economic function. Marginal costs accordingly constitute a means of allocation of the operating costs, in other words, they have an average cost structure.

Marginal Emissions Content

In order to minimize the greenhouse gas emissions of a refinery, the ideal solution is obviously to shut it down, and to import the petroleum product. However, the greenhouse effect is global, regardless of the place where the releases occur. By contrast, let us consider a less naive alternative. To meet additional gasoline demand, an oil company can boost its production or resort to imports. If the only criterion is the impact of the decision on the greenhouse effect, the emissions that would be generated by the production at one refinery or the other, importer or exporter, would have to be compared. In other words, the marginal contribution of the gasoline to the CO_2 emissions at each of the manufacturing points should be compared. Similarly, at a macroeconomic level, in order to define a gasoline or diesel tax as a function of the emissions associated with their production, the marginal emissions content of these products should clearly serve as a basis for calculating the tax. In short, as a rule, the relevant analysis is often the one that relies on marginal values.

Remark: Here the **marginal content** of a product refers to the additional quantities of emissions generated by its manufacture in a refinery, and not the emissions that occur at the time of its combustion, which are normally easier to calculate.

When refining programs are drawn up using a linear programming model like the one described in Section 2, the marginal emissions contents of the different products are directly obtained from the optimization results. In fact, the table of results at the optimum gives the relations between the basic variables (which are generally a nonnull value) and the off-base variables, which are null at the optimum. The

(3) Among recent studies: Weiss *et al.* (2000), Argonne National Laboratory (2001), GM *et al.* (2002).

(4) Reference unknown to us at the time when we developed this approach.

variable representing the CO_2 emissions is a basic variable. Let us consider the relation linking it to the non basic variables. These include the slack variables associated with binding constraints. The coefficient of the slack variable associated with a non binding demand constraint for a product measures the marginal contribution of this product to the CO_2 releases. The marginal contribution of a product for which demand is not binding is zero because the marketing of an additional ton of this product is achieved from a production surplus, hence without additional production activity.

5 COST FUNCTION ASSOCIATED WITH EMISSIONS AND ALLOCATION TO PRODUCTS

The introduction of a "CO_2 penalty" into the objective function is unnecessary to analyze the extent to which marginal contents offer a key to the allocation of emissions. It nonetheless facilitates the presentation. We shall therefore first consider a linear programming model like the one mentioned in Section 2.

The objective function is composed of two terms. The first corresponds to the operating cost which traditionally appears in refining models. For the long-term models used to analyze investment decisions, this first term, in addition to the actual operating costs, includes the investment costs of the units to be built. The second term is associated with CO_2 emissions. In this section, we shall assume it to be proportional to the quantities released and term as "penalty" the correspondent coefficient, whether a Pigou tax or a price for tradable emission rights.

Generalization of the Duality Property of Linear Programs

The property that we demonstrate in the Annexe is a generalization of the classic duality property reviewed in Section 4: at the optimum, the sum of the products of the dual variables by the RHS coefficients of the constraints associated with these variables is equal to the value of the economic function. When the economic function is composed of two elementary economic functions, the proposed approach requires breaking down each dual variable into two elementary dual variables. By considering a cost function to be minimized, as we do here, the dual variables are interpreted as marginal costs. The first elementary dual variable is accordingly interpreted as an operating marginal cost while the second corresponds to a CO_2 marginal emission cost. The property is stated as follows: at the optimum, the sum of the products of the "operating" dual variables by the RHS of the constraints associated with these variables is equal to the value of the operating cost. **The sum of the products of the "emission" dual variables by the RHS of the constraints associated with these variables is equal to the CO_2 emission cost.**

Linear programming models used to define refinery operating programs reveal several types of non-zero data as RHS of the constraints. Consumptions requirements appear as RHS of equations associated with finished product production, import and export balances. Also observable are non-zero values as RHS of constraints on unit capacity limitation and on crude availability.

When a model is used to analyze investment decisions, in order to determine optimal unit capacities, these capacities are variables of the problem and the corresponding equations have no RHS. Moreover, for long-term studies, crude availability constraints are seldom introduced.

Hence it often happens that the only non-zero RHS of an investment model are those of demand equations. Let us consider this special case. As recalled earlier, dual variables (marginal costs) supply a key to allocating all operating and emission costs to finished products. In view of the generalized duality property, marginal operating costs ("operating" dual variables) supply a means of allocating a operating costs to finished products, and "emission" dual variables a key to allocating emission costs.

To go from a (marginal) emission to a marginal CO_2 content cost, it suffices to divide it by the "penalty" coefficient. **The CO_2 marginal contents provide a means of allocating CO_2 emissions.**

Note also that marginal CO_2 contents can be calculated in cases where the cost associated with emissions is nil. The structural property of average content remains valid in this case.

6 LESSONS AND DEVELOPMENTS

The first results obtained on the models described here are rich in lessons. They may be rather different from those obtained with conventional LCA. The main differences concern the marginal contents of gasolines and diesels. Classic analyses indicate a gasoline emission content that is generally higher than that of diesels, reflecting the fact that refineries have more gasoline processing units than diesel processing units. The marginal contents calculated with the approach proposed here naturally depend on the structure of the refinery concerned, the assumptions concerning demand and its evolution, product specifications, crude oil procurement, etc. They are sometimes in line with the results of previous studies. But for a fairly large number of scenarios, they reveal higher emission contents for diesels than for gasolines. In certain cases, negative gasoline marginal contents are even obtained. These results, which are not intuitive a priori, are perfectly explained *a posteriori* and reflect the difficulties that could be encountered in certain cases by refiners wishing to boost their diesel production.

While the proposed method already yields interesting results, a number of developments are still required. The principles of the modeling and allocating of emissions to finished products are very simple. Yet applications raise various problems. Thus the transition from a margin maximization model to a cost minimization model may lead to cases of degeneration. The analysis of the dual variables accordingly demands special precautions. Moreover, the method should be extended to cases in which the model employed contains equations other than the demand equations, possessing nonnull second members. These questions are under examination at present. When the answers are obtained, they should help to broaden the fields of application.

REFERENCES

Azapagic, A. (1996) Environmental System Analysis: the Application of Linear Programming to Life Cycle Assessment. *PhD Thesis*, University of Surrey.

Babusiaux, D. (2000) Les émissions de CO_2 en raffinerie et leur affectation aux différents produits finis. *Cahiers de l'économie*, **41** (working paper), Institut français du pétrole.

Consoli F. (ed.) (1993) *Guidelines for Life-Cycle Assessment: A "Code of Practise"*, SETAC (Society for Environmental Toxicology and Chemistry), Bruxelles.

Evans, J.R. and Baker, N.R. (1982) Degeneracy and the (mis)interpretation of sensitivity analysis in linear programming. *Decision Sciences*, **13**, 2, April.

Huppes, G. and Schneider F. (eds.) (1994) *Allocation in LCA*, SETAC Europe, Bruxelles.

Leprince, P., Arlie, J.P. and Raimbault, C. (1981) Comment calculer le coût énergétique des produits d'origine pétrolière et de leurs substituts d'origine charbonnière ou végétale. *Revue de l'Institut français du pétrole*, **36**, 1.

Palmer, K. (1984) *A Model Management Framework for Mathematical Programming*, Wiley, New York.

Pierru, A (2002) Extension d'un théorème de dualité en programmation linéaire - Application à la décomposition de coûts marginaux de long terme. *Cahiers de l'économie*, **50** (working paper), Institut français du pétrole.

Weiss, M.A., Heywood, J.B., Drake, E.M., Schafer, A. and Auyeung, F.F. (2000) A life-cycle analysis of new automobile technologies. *Energy Laboratory Report* MIT EL 00-003.

AFNOR (1997) NORME ISO 14040: *Environmental Management - Life Cycle Assessment - Principles and Framework*, Paris.

Argonne National Laboratory (2001) *Well-to-Wheel Energy Use and Greenhouse Gas Emissions of Advanced Fuel/Vehicle Systems - North American Analysis*. http://www.transportation.anl.gov/ttrdc/assessments/ta_papers.html#total

GM (2002) *Well-to-Wheel Analysis of Energy Use and Greenhouse Gas Emissions of Advanced Fuel/Vehicle Systems. A European Study*, September 2002, http://www.lbst.de/gm-wtw.

Final manuscript received in November 2003

ANNEXE

GENERALIZATION OF THE DUALITY PROPERTY

Notations

Let us consider a linear program written in standard form (after any introduction of slack variables designed to go from inequations to equations):

$$\text{Min} \quad \begin{aligned} &F = CX \\ &AX = b \\ &X \geq 0 \end{aligned} \qquad \text{(P1)}$$

We consider an objective function defined as the sum of two economic functions that we call elementary economic functions F' and F''. The generalization to any number of elementary functions is immediate.

$$\text{Min} \quad \begin{aligned} &F = F' + F'' \\ &F' = C'X \\ &F'' = C''X \\ &AX = b \\ &X \geq 0 \end{aligned} \qquad \text{(P2)}$$

where:
X is the vector whereof the n components are the n variables of the model;
C, C' and C'' are row vectors (with n components);
A is a matrix with dimensions $m \times n$, of rank m.

Characterization of an Optimal Solution

The marginal analysis will be conducted from an optimal solution. Note however that the theorem that we shall demonstrate has been generalized by Pierru (2002) and remains valid for a nonoptimal base solution. We assume that the optimal solution is a nondegenerate base solution.

We make a partition of the vector X and denote:
Y, the subvector of the basic variables; $\overline{Y}$, the subvector of the nonbasic variables:

$$X = [Y\overline{Y}]$$

B and $\overline{B}$, the matrices associated respectively with all the subscripts of the basic and nonbasic variables and component A:

$$A = [B\overline{B}]$$

We similarly consider the vectors D' and $\overline{D}'$, making up C', associated with the set of subscripts of the basic and nonbasic variables:

$$C' = [D' \ \overline{D}']$$

$$C'' = [D'' \ \overline{D}'']$$

The equations of the initial problem are written accordingly:

$$F' = [D' \ \overline{D}'] \begin{bmatrix} Y \\ \overline{Y} \end{bmatrix}$$

$$F'' = [D'' \ \overline{D}''] \begin{bmatrix} Y \\ \overline{Y} \end{bmatrix}$$

$$BY + \overline{BY} = b$$

We consider a nondegenerate base solution, with inversible B. At the optimum, the value of Y is given by:

$$Y = B^{-1}b$$

Duality, Review and Notations

Let Π denote the vector of the dual variables. This vector can be defined by the equation:

$$\Pi = DB^{-1}$$

The duality property is written:

$$\Pi b = CX$$

At the optimum, the values of the dual variables correspond to the marginal costs (variations of the economic function) associated with the different constraints of the problem, which can be formulated as follows:

$$\Pi b = F$$

$$\Pi_j = \frac{\partial F}{\partial b_j} \qquad (j = 1, 2, ..., m)$$

Elementary Dual Variables

Let us return to the initial problem, where the objective function F is composed of two elementary economic functions F' and F''. The question is now to break down the marginal costs into two terms, each representing the variations of an elementary economic function. To do this, it suffices to define:

$$\Pi' = D'B^{-1}$$

$$\Pi'' = D''B^{-1}$$

It is clear that:

$$\Pi' + \Pi'' = \Pi$$

Moreover, Π' and Π'' clearly have the classic properties of a dual vector. In fact:

$$\Pi' b = D'B^{-1}b = D'Y = F'$$

$$\frac{\partial F'}{\partial b_j} = \Pi'_j \qquad (j = 1, 2, ..., m)$$

$$\Pi'' b = D''B^{-1}b = D''Y = F''$$

$$\frac{\partial F''}{\partial b_j} = \Pi''_j \qquad (j = 1, 2, ..., m)$$

Note that the numerical values of the variables Π'_j and Π''_j are directly given by the linear programming codes which supply the simplex tableau at the optimum. In fact, if we refer to the above formulation (P2) of the problem analyzed, it suffices to observe that the variables F' and F'' are necessarily basic at the optimum. They can therefore be expressed as a function of the nonbasic variables, and particularly as a function of the slack variables associated with the binding constraints. The marginal costs Π'_j and Π''_j are the coefficients of the slack variable associated with the constraint of subscript j appearing in the equations giving F' and F''.