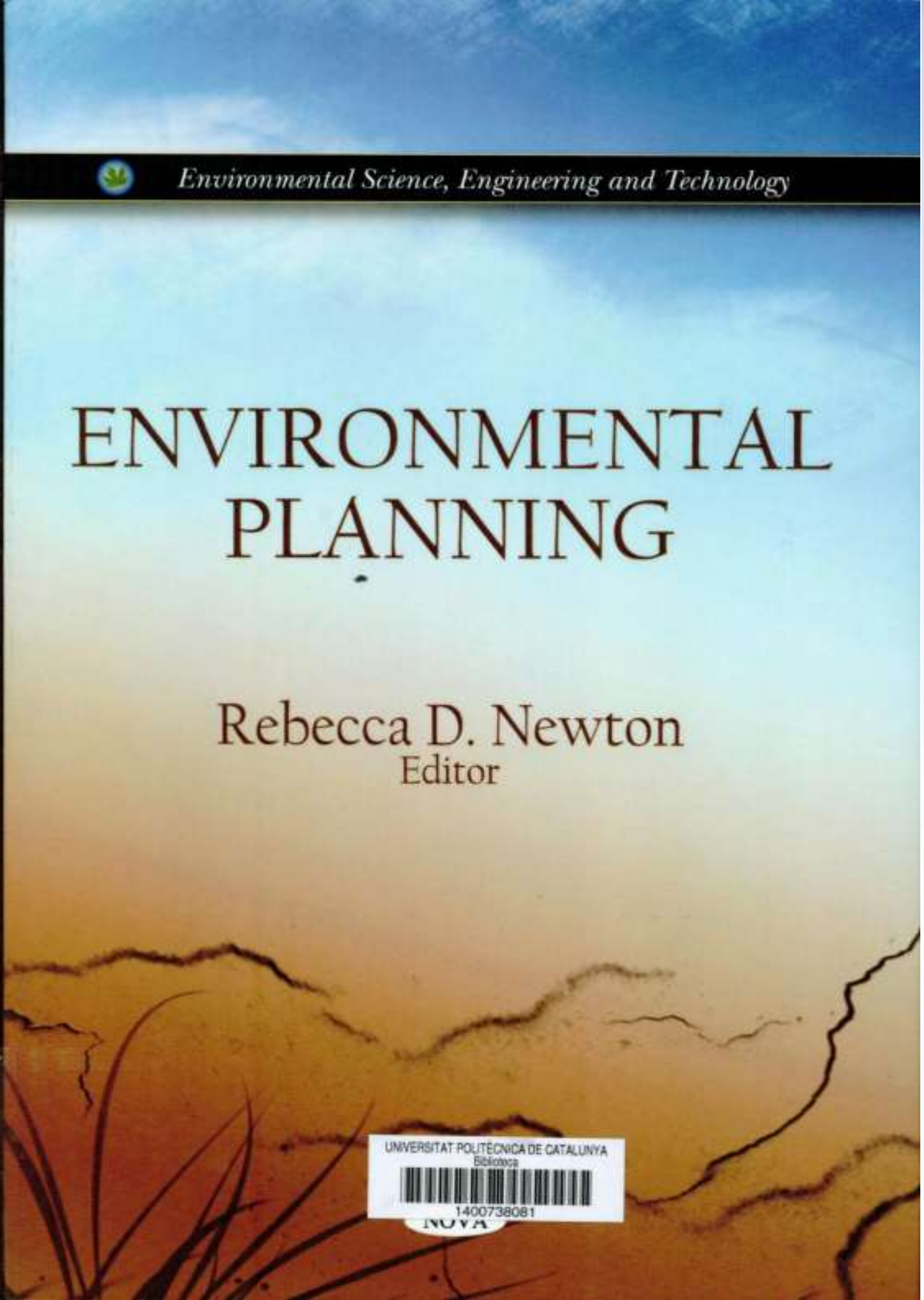

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Chapter 1

ENVIRONMENTAL CONSIDERATIONS IN STRATEGIC AND TACTICAL PLANNING OF SUPPLY CHAINS

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ABSTRACT

Corporate approaches towards reducing its environmental footprint cannot be undertaken in isolation. Nowadays, it is recognized that a concerted effort is required, embracing the different supply chain entities, in order to correctly estimate environmental burdens and to propose effective environmental strategies. Such an effort poses an important and complex challenge to managers. On the one hand, the economic and environmental trade-offs existing within a supply chain network must be pondered so as to make proper decisions. This is not a straightforward task;, thus, analytical tools are desirable to support environmental decision-making. On the other hand, environmental performance is seldom quantified appropriately. Traditional current accounting practices which do not clearly consider environmental issues and the availability of diverse environmental metrics make it arduous to assess firms' environmental performance.

This chapter proposes the use of analytical tools to tackle environmental planning. The proposed approach addresses the optimization of the supply chain planning and design by considering economic and environmental issues. The strategic decisions contemplated in the mathematical model are facility location, processing technology selection and the production–distribution planning. The Life Cycle Assessment (LCA) approach is envisaged to incorporate the environmental aspects of the model. The IMPACT 2002+ methodology is selected to perform the impact assessment within the SC since it provides a feasible implementation of a combined midpoint–endpoint evaluation.

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Moreover, traditional accounting practices have been extended to include different costs associated with environmental issues. The environmental costs estimation has been carried out using a Total Cost Assessment (TCA) approach and taking into consideration a CO_2 trading scheme as well.

Additionally, the model performs an impact/cost mapping along the nodes and activities that comprise the supply chain. Such mapping allows focusing financial efforts to reduce environmental burdens to the most promising subjects. The mathematical formulation of this problem becomes a multi-objective MILP (moMILP). Criteria selected for the objective function are damage categories impacts, overall impact factor and net present value (NPV) considering different environmental costs. The main advantages of this model are highlighted through a realistic case study of a maleic anhydride SC production and distribution network in Europe.

1. Introduction

Supply Chain Management (SCM) can be defined as the handling of material, information and financial flows through a network of organizations interconnected with the aim of producing and delivering goods or services to consumers. SCM has been a major source of competitive advantage in the global economy. Moreover, it is well recognized that an optimum management of the Supply Chain (SC) offers a key opportunity for preserving a firm's value. The proper handling of a SC should be concerned with the sharing of responsibility from various aspects of performance which include environmental matters. It has been realized that significant improvements in terms of environmental performance and market competitiveness may be achieved by concentrating efforts from all SC partners. Actually, managerial practice related to environmental issues has expanded from a narrow focus on pollution control within a single firm to include a larger set of inter-organizational management decisions, programs, tools, and technologies that prevent pollution before its generation (Klassen and Johnson, 2004). Consequently, these issues are being considered in recent works and call for further research in the integration of environmental management with SC operations.

The aforementioned integration may be achieved through the emerging concept regarded as "Green Supply Chain Management" (GrSCM), which is defined as the integration of environmental thinking into SCM, including product design, raw materials sourcing and selection, manufacturing process selection, delivery of final product to the consumers as well as end of life management of the product after its useful life (Srivastava, 2007). Traditionally, the methodologies devised to assist SC operation and design have focused on finding a solution that maximizes a given economic performance indicator while satisfying a set of operational constraints imposed by the manufacturing/processing technology and the topology of the network. In recent years, however, there has been a growing awareness of the importance of including environmental and financial aspects associated with the business decision support levels (Puigjaner and Guillén, 2007). In fact, there are some documented success stories of enterprises that have integrated environmental and SCM issues. For instance, Hart (1997) has presented the Xerox's Asset Recycle Program which redirects 90% of all materials and components for its photocopiers through reuse, remanufacturing, and recycle; in this case, annual savings are estimated in US$300 million. Also, Hoeffer (1999) has reported a scrap management system deployed by Daimler-Chrysler which allows for

annual savings of US$4.7 million. These examples illustrate the potential benefits that can be achieved by integrating environmental aspects along the SC.

The environmental science and engineering community have developed several systematic methodologies for the detailed characterization of the environmental impacts of chemicals, products, and processes. All of these methodologies have embodied the concepts of life cycle, i.e., they are based on a Life Cycle Assessment (LCA) which is described in a series of ISO documents (ISO14040, 1997). The LCA framework includes the entire life cycle of the product, process or activity, encompassing extraction and processing of raw materials; manufacturing, transport and distribution; re-use, maintenance recycling and final disposal. Most importantly, it takes a holistic approach, bringing the environmental impacts into one consistent framework, wherever and whenever these impacts have occurred or will occur (Guinee et al., 2001).

Examples of these methodologies in the field of process systems engineering are the Minimum Environmental Impact (MEI) methodology (Stefanis et al., 1995), the Waste Reduction (WAR) algorithm (Young and Cabezas, 1999), the Optimum LCA Performance (OLCAP) framework (Azapagic, 1999; Azapagic and Clift, 1999), the Environmental Fate and Risk Assessment tool (EFRAT) (Chen and Shonnard, 2004) and the methodologies proposed by Alexander et al. (2000) and by Guillén-Gosálbez et al. (2008). All these methodologies are based on the incorporation of an optimization step into the four classical phases that comprise an LCA study, namely, goal definition, life cycle inventory-LCI, life cycle impact assessment-LCIA and interpretation (see Figure 1). All of the former methodologies optimize process conditions or topology just considering a single SC echelon. Also common to all of them is the implementation of multi-criteria optimization strategies in order to evaluate the trade-off between economic and environmental issues.

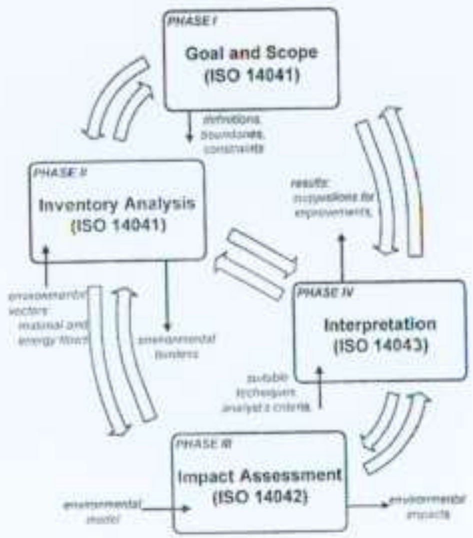

Figure 1. Life cycle assessment steps (Puigjaner & Guillén-Gozalbez, 2008)

The concept of SC refers to the network of interdependent entities (i.e., retailers, distributors, transporters, warehouses and suppliers) that constitute the processing and distribution channels of a product from the supply of its raw materials to its delivery to the final consumer. Because an LCA study ideally covers a cradle-to-grave approach, it can be clearly seen that LCA fits as a suitable tool for quantitatively assessing the environmental burdens associated with designing and operating a SC. Two possible LCA approaches can be distinguished, namely, comparison/selection and improvement (Klassen and Greis, 1993). The former approach focuses on identifying environmentally preferable products or processes alternatives as an attempt to leverage marketplace and financial forces in order to displace environmentally harmful activities (Klöpffer and Rippen, 1992). The latter one uses LCA as a tool to identify the SC stages that have a particularly strong negative impact on the environment, and thus, where improvements would be most beneficial. This last alternative allows improving the allocation of limited management time and financial resources within the SC (Freeman et al., 1992). Both types of analysis are performed in this chapter by means of an SC design-planning optimization model.

Some works have already addressed the integration of LCA and SC models. Recently, Mele et al. (2008) have shown a quantitative tool for decision making support in the design of sugar cane to ethanol SCs. Also, Hugo and Pistikopoulos (2005) have shown how a set of SC network designs can form an environmentally conscious basis for the investment decisions associated with strategic SC level. Similarly, Chakraborty et al. (2003, 2004), propose a methodology for long term operation and planning. Their proposed framework uses as an MILP formulation with a planning horizon of typically five years. In their approach the estimation of wastes are inputs and the decisions to be made include choosing the plant-wide waste treatment facility. The planning also incorporates a forecast on environmental regulation and a CO_2 emission cap is enforced as a constraint into the model.

One topic that deserves further attention is the accounting of environmental costs. It is generally recognized that environmental accounting words such as "full", "total" and "life-cycle" are used to indicate that not all costs are captured in traditional accounting and capital budgeting practices (Rosselot & Allen, 2002). The principle followed is that if costs are properly accounted for, business management practices that foster economic performance will also foster superior environmental performance. However, the major proportion of costs arising from environmental damage is borne by the natural environment and the wider community. Since these costs fall outside the conventional accounting framework of the polluter, they are called external costs or externalities. Several techniques below the environmental cost assessment (ECA) umbrella have been developed to assess such costs and to further include them into traditional accounting practices. In this regards, Hertwig et al. (2002) and Xu et al. (2005) propose a methodology which incorporates economic, environmental and sustainability costs combined in the objective function to be optimized. The economic function includes a simplified version of the Ache's Total Cost Assessment (TCA) metrics while the environmental impact is assessed using the WAR methodology. The environmental impact is included in the optimization function as a given percentage of the raw material costs (Xu et al., 2005). The plants modeled include an agro-chemical complex plant which also incorporates several CO_2 processing facilities. In Singh et al. (2007) the same problem is studied using the Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI) metrics but without considering the environmental impact as a cost. The authors show that improving the environmental performance for some impact potentials worsens others. Thus, attempts to optimize global warming ends-up increasing fossil fuel usage, human health and photochemical smog.

It has been pointed out that tools, specifically LCA models, should be useful in pursuing more effective climate change policies and international trade should be included within this type of analysis. With regard to this, it is noteworthy that climate change policies are applied based on the temporal distribution of emissions. Usually SC environmental impacts are evaluated at the end of the planning horizon, and the temporal distribution is disregarded at all in the case of LCA. Consequently, the incorporation of constraints associated to the temporal emission distributions is necessary when studying climate change policies in a SC planning model.

This chapter describes an analytical approach for SC design and planning focusing on environmental impact and its sources. The approach applies mixed integer modeling techniques. The model is optimized so as to select the most appropriate technology, the appropriate raw material/service supplier and the most convenient production and distribution profiles. The mathematical model encompasses direct emissions, purchased energy emissions, raw materials production emissions and transport distribution emissions. LCA concepts are embedded in the approach, and going further in order to attain a comprehensive LCA application, not merely an overall environmental impact indicator is calculated but also partial environmental impact categories are studied. Furthermore, the impact associated to every SC echelon is mapped aiming at discovering possible opportunities to focus management efforts and resources for environmental impact reduction. The temporal emission distribution is considered for the calculation of environmental and financial metrics, accounting for possible emissions trading. In this way the traditional LCA scheme is extended by including the emissions temporal distribution.

2. Environmental and Operations Planning

This chapter deals with the strategic-tactical problem associated to the optimal design and operation of a SC network taking into account environmental considerations.

The SC network consists of a number of existing multi-product manufacturing sites and distribution centers at given locations, a number of potential locations where either a manufacturing site or distribution center or both of them can be installed, and finally a number of sales regions and suppliers at fixed locations. In general, each product can be produced at several plants located at different locations using different technology equipment. The production capacity of each manufacturing/processing site is modeled by relating the nominal production rate per activity to the availability of the equipment technology at each plant. Distribution centers are described by upper and lower bounds on their material handling capacity and they can be supplied from more than one manufacturing plants and can supply more than one market place. Given the manner the problem is modeled, materials flows between any facilities may appear if selecting such flow allows improving the performance of the SC. Each market demands one or more products. A market may be served by more than one distribution center, or even directly from any manufacturing site. The mathematical model is an analytical tool intended to support managers on planning decisions such as:

Damage oriented or end-point methods such as Eco-indicator 99 (Goedkoop & Spriensma, 2001) or EPS (Steen, 1999), try to model the environmental mechanism up to the damage to a given area of protection.

Most methods differ on the way mid- or end-point impacts are measured and in the way that weights are assessed for each impact. Moreover not all methods consider the same environmental areas of protection, or how each mid-point indicator affects the end-point. However there is a tendency to define indicators at common mid-points to ensure simplicity in their definitions and to minimize perceived uncertainty (Finnveden et al., 2009). While reliable end-point modeling seems within reach for some categories such as acidification, cancer effects and photochemical ozone formation, it is still under development for climate change (a mid-point indicator is still used early along the environmental mechanism, i.e. increase in radiative force), and the end-point modeling is encumbered with large uncertainties due to many unknowns of the global climate system and due to the long time horizon of some of the involved balances (Finnveden et al., 2009).The selection between one of the impact assessment methods or the usage of different mid-point models from different methods is a matter of the decision maker and the goal that the study follows.

Here, the environmental metrics used are the ones devised in the work of Humbert et al. (2005), which presents an implementation working at both mid-point and end point (damage) levels. For each environmental intervention two characterization factors are proposed, which eases model implementation. Their methodology, IMPACT 2002+, is mainly a combination between IMPACT 2002 (Pennington et al., 2005), Eco-indicator 99 (Goedkoop and Spriensma, 2001) using egalitarian factors, CML (Guinee et al., 2001) and the Intergovernmental Panel on Climate Change (IPCC) considerations for CO_2 emissions. IMPACT 2002+ has grouped similar category end-points into a structured set of damage categories by combining two main schools of impact model methods: classical impact assessment methods (CML/IPCC) and damage oriented methods (Eco-indicator 99). This methodology proposes a feasible implementation of a combined mid-point/damage-oriented approach. It links all types of LCI results via 15 mid-point impacts (human toxicity, respiratory effects, ionizing radiation, ozone layer depletion, photochemical oxidation, aquatic ecotoxicity, terrestrial ecotoxicity, terrestrial acidification/nitrification, aquatic acidification, aquatic eutrophication, land occupation, global warming, non-renewable energy and mineral extraction) to four areas of protection end-point categories (human health, ecosystem quality, climate change-global warming potential and resources).

Table 1. Pollution control expenditures, for selected industrial sectors in the US (Rosselot & Allen, 2002)

Industry sector capital expenditures	As a % of sales	As a % of value added	As a % of total
Petroleum	2.25	15.42	25.7
Primary metals	1.68	4.79	11.6
Chemical manufacturing	1.88	3.54	13.4

This approach contains the advantages of being able to calculate both mid- and end-point indicators.

Within the presented model, and in order to avoid emission double counting, raw material emissions are not aggregated to product manufacturing, similarly transport and energy consumption are considered separately.

2.2. Legislation Constraints and CO_2 Trading

From another standpoint, as the planet warms up, so does legislation to reduce greenhouse gas (GHG) emissions worldwide. Within this scenario much of the opportunity to manage carbon (CO_2) emissions effectively relies on the capacity of the organization to have an overall view of its specific responsibility and associated cost, from a life-cycle point of view. With estimated economic damage of about US$85 for each ton of CO_2, capping GHG emissions and establishing a price tag on them became inevitable (Stern, 2006). Regarding to eco-taxes, Brennan, (2007), emphasizes that several different economic instruments are available for the government to encourage greater environmental responsibility, such as: (i) emission charges related to quantity and quality of pollutant and damage done; (ii) user charges for treatment of discharges, related to cost of collection, disposal and treatment; (iii) tradable/marketable permits, which enables pollution control to be concentrated amongst those who can do it economically without increasing total emissions, and (iv) deposit refund systems involving refundable deposit paid on potentially polluting products.

Due to the former considerations environmentally benign process designs are bound to be more profitable, given that they will incur in lower waste treatment and environmental compliance costs while converting a higher percentage or raw materials into saleable products (Khor et. al., 2007). This is also true for the case of recycle options where the benefits from avoiding manufacturing impacts tend to dwarf energy/materials used for recycling the materials (Constable et al, 2009), which makes design of environmentally benign supply chains worth of consideration.

In the case of tradable permits there exists SO_2 (acid rain program) and NO_x air emission markets for some zones in the USA[1], and there is a European Union Emission Trading System (EU-ETS) market[2] for CO_2 emissions. The idea behind these schemes is to make firms pay for their emissions so that a financial incentive to decrease them is provided. A cap is set on emissions, businesses are allowed to buy or sell from each other the right to emit emissions. Firms exceeding their emissions cap have to buy extra credits to cover the excess, providing an incentive for them to operate under the capped level, while those that do not use up all their allowances can sell them, providing the least-polluting firms with extra revenue and an incentive to further reduce emissions (Young, 2008). In this sense, organizations should expect to be charged for their CO_2 emissions and consequently much of the opportunity to address CO_2 emissions rests on SCM, compelling companies to look for new approaches to manage CO_2 emissions effectively. Most certainly, this CO_2 related charge will force a change in the way organizations run their SCs (Butner et al., 2008).

Several institutions (e.g. the California Climate Action Registry (CCAR), The Climate Registry (TCR), the World Resources Institute (WRI), World Business Council for

[1] http://www.epa.gov/airmarkets/index.html
[2] http://ec.europa.eu/environment/climat/emission/index/_en.htm

Sustainable Development (WBCSD) have determined protocol definitions for carbon registries in order to help organizations analyze their CO_2-footprints. Nevertheless, according to Matthews et al. (2008) the scope of these protocols varies with regards to emission sources, generally suggests estimating only direct emissions (Tier 1) and emissions from purchased energy (Tier 2), with less focus on the SC context which will lead to large underestimates of the overall CO_2 emissions. The authors propose a footprint estimation that includes the total SC up to the production gate, also known as cradle-to-gate approach (Tier 3). Furthermore, the authors refer to Tier 4 emission estimations when the whole product life-cycle is taken into account by considering emissions occurring during distribution and product end of life. This extended scope is expected to better aid effective environmental strategies since both firms and consumers have an important influence over the carbon footprints through their "purchase" decisions.

3. The Mathematical Model

This chapter describes a comprehensive tool that can be used to assist in the planning and design of a SC under economical and environmental impacts considerations. The resulting model is solved by using a multi objective MILP (moMILP) algorithm, which allows observing possible environmental tradeoffs between damage categories and the economic indicator. This approach reduces the value-subjectivity inherent to the assignment of weights in the calculation of an overall SC environmental impact, which is also calculated. The analysis of partial environmental impacts for every echelon is performed with the aim of discovering improvement opportunities; this analysis also provides information about where to focus emission control activity and hints on possible strategies for emission reduction at source. The temporal emissions distribution and trading schemes considerations contributes to understand how regulatory schemes may induce environmental impact reductions.

The mathematical formulation of the LCA-SC problem is briefly described next. The variables and constraints of the model can be roughly classified into three groups. The first one concerns process operations constraints given by the SC topology. The second one deals with the environmental model used while the third refers to the economic metric applied.

3.1. Supply Chain Design - Planning Model

The design-planning approach presented is a translation of the State Task Network (STN) formulation (Kondili et al., 1993) to SC modeling, which has been presented in the work of Laínez et al. (2009). Such a formulation is suitable to collect all SC node information through a single variable, which eases the environmental and economic metrics formulation. This way SC node characteristics are modeled with a single equation set, since manufacturing nodes and distribution centers are treated in the same way as well as production and distribution activities. Subsequently, it turns out that the model most important variable is $P_{ijff't}$; which represents the specific activity of task i performed using technology j receiving input materials from site f and "delivering" output materials to site f' during period t. Indeed, to

model a production activity it must receive and deliver material within the same site (P_{ijfft}). In case of a distribution activity, facilities f and f' must be different. The model's equations are briefly described in the next paragraphs. The separation between tasks and technologies allows for a flexible formulation of different scenarios.

Materials mass balance must be satisfied in each of the nodes. Eq. (1) represents the mass balance for each material (state in the STN formulation) s consumed at each potential facility f in every time period t. Parameter α_{sij} is defined as the mass fraction of material s that is produced by task i performed using technology j; T_s set refers to those tasks that have material s as output, while $\bar{\alpha}_{sij}$ and $\bar{T}_s$ set, refer to tasks that consume material s.

$$S_{sft} - S_{sft-1} = \sum_{f'}\sum_{i \in T_s}\sum_{j \in (J_i \cap J_{f'})} \alpha_{sij} P_{ijf'ft} - \sum_{f'}\sum_{i \in \bar{T}_s}\sum_{j \in (J_i \cap J_f)} \bar{\alpha}_{sij} P_{ijff't} \qquad (1)$$

$$\forall s, f, t$$

The model assumes that process parameters are fixed (such as reaction conversion, separation factors, temperatures, etc.), this is one of the reasons for the model to be linear. In this sense α_{sij} and $\bar{\alpha}_{sij}$ are fixed and constant due to the replacement of all the potentially non-linear relationships by fixed specified parameters. This assumption is acceptable since the model deals with strategic and tactical decisions. Such decision levels require the usage of aggregated figures in which some details (e.g. process operating parameters, scheduling decisions) are disregarded, making the decision making process manageable. Equation (2) models the temporal changes in facility capacities, in this sense the model allows for the simultaneous consideration of design and retrofit of SCs. Equation (3) serves for total capacity (F_{jft}) bookkeeping taking into account the amount increased during planning period t (FE_{jft}).

$$V_{jft} FE^L_{jf} \le FE_{jft} \le V_{jft} FE^U_{jf} \qquad \forall f, j \in \tilde{J}_f, t \qquad (2)$$

$$F_{jft} = F_{jft-1} + FE_{jft} \qquad \forall f, j \in \tilde{J}_f, t \qquad (3)$$

Equation (4) ensures the total production rate in each plant to be greater than a minimum desired production rate and lower than the available capacity. Furthermore, parameter β_{jf} defines a minimum utilization rate of technology j in site f, while $\theta_{ijff'}$ determines the resource utilization factor.

$$\beta_{jf} F_{jft-1} \le \sum_{f'}\sum_{i \in I_j} \theta_{ijff'} P_{ijff't} \le F_{jft-1} \qquad \forall f, j \in \tilde{J}_f, t \qquad (4)$$

$\theta_{ijff'}$, is the capacity utilization rate of technology j by task i whose origin is location f and destination location f'. This parameter is one of the key factors to be determined when addressing aggregated planning problems, considering strategic and tactical decisions. This operational model may be applied in continuous as well as in semi-continuous processes. Firstly let us consider the continuous processes. For these cases, the capacity utilization factor is a conversion factor, which allows taking into account the equipment j capacity in site f in terms of task i kg of produced material per time unit. In this way the $\theta_{ijff'}$ factor is the maximum throughput per planning period. On the other hand, this parameter is closely related to tasks operation time in the case of semi-continuous (batch) processes. Notice that in this kind of production processes the time period scale utilized in aggregated planning is usually larger than the time a task (production/distribution activity) requires to be performed. Therefore, the sequencing-timing problem of short term scheduling is transformed into a rough capacity problem where aggregated figures are used. It is important to have in mind that capacity is expressed as equipment j available time during one planning period, then $\theta_{ijff'}$ represents the time required to perform task i in equipment j per unit of produced material. Thus, once operation times are determined this parameter can be easily estimated. Eq. (5) forces the amount of raw material s purchased from site f at each time period t to be lower than an upper bound given by physical limitations (A_{sft}). Also, the model assumes that part of the demand can actually be left unsatisfied because of limited production or supplier capacity. Thus, Eq. (6) forces the sales of product s carried out in market f during time period t to be less than or equal to demand.

$$\sum_{f'}\sum_{i \in T_s}\sum_{j \in J_i} P_{ijff't} \leq A_{sft} \qquad \forall s \in RM, f \in Sup, t \tag{5}$$

$$\sum_{f'}\sum_{i \in T_s}\sum_{j \in J_i} P_{ijf'ft} \leq Dem_{sft} \qquad \forall s \in FP, f \in Mkt, t \tag{6}$$

For further model details the reader should refer to Laínez et al. (2009).

3.2. Supply Chain - Environmental Model

The application of the LCA methodology to a SC requires of four steps, namely (i) goal setting, (ii) life-cycle inventory (LCI), (iii) life-cycle impact assessment (LCIA), and (iv) results interpretation towards improvement.

Regarding goal setting, it is important to define the boundaries of the system under study, and which is the functional unit (FU) or service that the SC will provide. Boundaries in the case of the chemical industry are usually drawn from cradle to gate, this is due to the fact that most chemicals are used in different ways and the use phase of products made of these chemicals is too difficult to model appropriately. Consequently raw material extraction, its processing and shipment to a market are considered as part of the chemical SC system. Regarding the FU, commonly a certain amount of product produced is considered.

The LCI step requires the estimation of SC environmental interventions (emissions or natural raw material consumptions) which requires assessment of raw material producers,

transportation and product manufacturingimpacts. This step is the most time consuming within a LCA due to the large amount of information that is required to be gathered, however the usage of LCI databases eases this issue.

The results of the LCI step of the LCA can be interpreted by means of different environmental metrics. Environmental interventions are translated into metrics related to environmental impact as end-points or mid-points metrics by the usage of characterization factors (CFs), this translation is the LCIA. These metrics differ in their position along the environmental damage chain (environmental mechanism).

The equations of the environmental model are briefly described next. Equation (7) models IC_{aft} which represents the mid-point a environmental impact associated to site f which rises from activities in period t; $\psi_{ijff'a}$ is the a environmental category impact CF for task i performed using technology j, receiving materials from node f and delivering them at node f'.

$$IC_{aft} = \sum_{j \in J_f}\sum_{i \in I_j}\sum_{f'} \psi_{ijff'a} P_{ijff't} \qquad \forall a, f, t \tag{7}$$

Similarly to the case of α_{sij} and $\bar{\alpha}_{sij}$, the value of $\psi_{ijff'a}$ is fixed and constant, provided that all environmental impacts are directly proportional to the activity performed in that node (P_{ijfft}). This issue is common practice in LCA, where all direct environmental impacts are considered linear with respect to the FU (Heijungs and Suh, 2002). In the case of transportation the FU commonly considered is the ammount of kg of material transported a given distance [kg·km]. Consequently the value of $\psi_{ijff'a}$ can be calculated by Eq. (8) in the case of transportation, which considers the distance between sites ($distance_{ff'}$) and where ψ^{T}_{ija} represents the a environmental category impact CF for the transportation of a mass unit of material over a length unit. The study of environmental impacts associated to transport or production can be performed by setting the indices summation over the corresponding tasks (i.e $i \in Tr$ or $i \in NTr$).It should be noted that environmental impacts associated to materials transport are assigned to their origin node.

$$\psi_{ijff'a} = \psi^{T}_{ija} distance_{ff'} \qquad \forall i \in Tr, j \in J_i, a, f, f' \tag{8}$$

Equation (9) introduces $DamC_{gft}$ which are a weighted sum of all mid-point environmental interventions combined using g end-point damage factors ζ_{ag} and then further normalized with $NormF_g$ factors. Equation (10) is used to compute the g normalized end-point damage along the whole SC ($DamC^{SC}_{g}$).

$$DamC_{gft} = \sum_{a \in A_g} NormF_g \zeta_{ag} IC_{aft} \qquad \forall g, f, t \tag{9}$$

$$DamC_g^{SC} = \sum_f \sum_t DamC_{gft} \qquad \forall g \tag{10}$$

CO_2 emissions trading is modeled by introducing Eq. (11). The climate change damage category accounts for all the equivalent-CO_2 kg. Eq. (11) states that the total equivalent CO_2 emission occurring in the SC (Tier 4 emissions do not considering for product use and end of life emissions, given that fall outside system boundaries) in period t to be equal to the free allowance emissions cap ($MaxCO_{2t}$) plus the extra rights bought to emit ($Buy_t^{CO_2}$) minus the sold rights ($Sales_t^{CO_2}$) in period t. T_L is the subset of those periods when the emission trading is executed, usually every year. In this model it is assumed that any amount of rights can be sold or obtained at the emissions market. L is the number of periods that accounts for the emission trading interval (e.g., in case that emissions trading occurs yearly and each period t represents one month, L is equal to 12).

$$\sum_f \sum_{a \in A_g} \sum_{t'=t-L+1}^{t} \zeta_{ag} IC_{aft'} = MaxCO_{2t} + Buy_t^{CO_2} - Sales_t^{CO_2} \tag{11}$$
$$\forall g = ClimateChange, t \in T_L$$

Equations (12) and (13) sum up the environmental damage category results for each site f and for the whole SC, respectively.

$$Impact_f^{2002} = \sum_g \sum_t DamC_{gft} \qquad \forall f \tag{12}$$

$$Impact_{overall}^{2002} = \sum_f \sum_g \sum_t DamC_{gft} \tag{13}$$

$DamC_g^{SC}$ or $Impact_{overall}^{2002}$ are both used as objective functions in the moMILP formulation. In this sense the use of damage categories is sometimes preferred given that they are easier to comprehend compared to mid-point values.

3.3. Supply Chain - Economic Model

Many economic performance indicators have been proposed to assess the economic performance of a SC network design. The most traditional indicators are profit, NPV, and total cost. Other more holistic measures have been recently proposed. Laínez et al. (2007) proposed a model that pursues the maximization of a financial key performance indicator, the corporate value of the firm at the end of the time horizon. The corporate value is computed by a discounted-free-cash-flow (DFCF) method which can be introduced as part of the mathematical formulation. Most SC modeling approaches usually ignore net working capital (NWC), which represents the variable assets associated with the daily SC operations (e.g., material inventories, accounts receivable, accounts payable). By using the DFCF method to compute the corporate value, the actual capital cost, the changes in NWC, the liabilities and other financing funds required to support SC operations and thus liquidity are explicitly considered when appraising SC performance. Next, expressions to calculate (i) operating revenue, (ii) operating cost, and (iii) capital investment are presented which would eventually permit integration with detailed financial models. Here, NPV will be used for the sake of simplicity and comprehensiveness. The application of other kind of metrics is out of the scope of this chapter, given the specific characteristics of the problem addressed in this work.

Operating revenue is calculated by means of net sales which are the income source related to the normal SC activities. Thus, the total revenue incurred in any period t can be easily computed from products sales executed in period t as stated in Eq. (14).

$$ESales_t = \sum_{s \in FP} \sum_{f \in Mkt} \sum_{f' \notin (Mkt \cup Sup)} Sales_{sff't} Price_{sft} \qquad \forall t \tag{14}$$

In order to calculate overall operating cost an estimation of indirect costs and direct costs are required. The total fixed cost of operating a given SC structure can be computed using Eq. (15). Where $FCFJ_{jft}$ is the fixed unitary capacity cost of using technology j at site f.

$$FCost_t = \sum_{f \notin (Mkt \cup Sup)} \sum_{j \in J_f} FCFJ_{jft} F_{jft} \qquad \forall t \tag{15}$$

The cost of purchases from supplier e, which is computed through Eq. (16), includes raw materials purchases, transport and production resources.

$$EPurch_{et} = Purch_{et}^{rm} + Purch_{et}^{tr} + Purch_{et}^{prod} \qquad \forall e, t \tag{16}$$

The purchases ($Purch_{et}^{rm}$) associated to raw materials made to supplier e can be computed through Eq. (17). It should be noted that in this formulation and for the case of raw material suppliers and transport providers each one of them uses a different technology. Variable χ_{est} represents the cost associated to raw material s purchased from supplier e.

$$Purch_{et}^{rm} = \sum_{s \in RM} \sum_{f \in F_e} \sum_{i \in T_s} \sum_{j \in J_i} P_{ijft} \chi_{est} \qquad \forall e \in E_{rm}, t \tag{17}$$

The costs of production and transportation are determined by Eqs. (18) and (19), respectively. Here, $\rho_{eff't}^{tr}$ denotes the e provider unitary transportation cost associated to material movement from location f to location f' during period t. τ_{ijft}^{ut1} represents the unitary production cost associated to perform task i using technology j, whereas τ_{ijft}^{ut2} represents the unitary inventory costs of material s storage at site f, both of them using provider e during period t.

$$Purch_{et}^{tr} = \sum_{i \in Tr} \sum_{j \in J_i \cap J_e} \sum_{f} \sum_{f'} P_{ijff't} \rho_{eff't}^{tr} \qquad \forall e \in \bar{E}_{tr}, t \tag{18}$$

$$Purch_{et}^{prod} = \sum_{f} \sum_{i \in Tr} \sum_{j \in (J_i \cap J_f)} P_{ijfft} \tau_{ijfet}^{ut1} + \sum_{s} \sum_{f \in (Sup \cup Mkt)} S_{sft} \tau_{sfet}^{ut2} \qquad \forall e \in \bar{E}_{prod}, t \tag{19}$$

In the case of τ_{ijfet}^{ut1}, this parameter entails restrictions associated with α_{sij} and $\bar{\alpha}_{sij}$, which forces the plant to operate at the same fixed conditions, meaning that the amount of utilities and labor spent is proportional to the amount of raw material processed. However the utilities and labor unitary cost may change in time. Moreover, possible cost decrease associated to economies of scale are disregarded by using the former assumption, higher production rates are associated linearly to higher production costs. Finally, the total investment on fixed assets is computed through Eq. (20). This equation includes the investment made to expand the technology's capacity j in facility site f in period t ($Price_{jft}^{FJ} FE_{jft}$).

$$FAsset_t = \sum_{f} \sum_{j} Price_{jft}^{J} FE_{jft} + I_{ft}^{J} JB_{ft} \qquad \forall t \tag{20}$$

In order to take into consideration the compliance with environmental regulations the environmental cost (Net_t^{env}) is considered as in the TCA methodology. These costs include type 2 costs related to waste treatment costs, and environmental reporting, and type 3 costs related to environmental liabilities.

$$Net_t^{env} = Cost_t^{WT} + Cost_t^{Compliance} + Cost_t^{EnvLiabilities} \qquad \forall t \tag{21}$$

Waste treatment (WT) costs ($Cost_t^{WT}$) are usually pooled for the whole site, and consequently are very hard to quantify, however there exists order of magnitude prices ($Price_w^{WT}$) that can be used for the calculation of the waste treatment cost depending on the WT facility to different w sinks (e.g. air, water, landfill or incineration, see Sinclair-Rosselot and Allen, 2002), and the waste flow ($Flow_{wt}^{WT}$).

$$Cost_t^{WT} = \sum_{w} Price_w^{WT} Flow_{wt}^{WT} \qquad \forall t \tag{22}$$

In the case of regulatory costs, these are also "hidden" when a project is evaluated; given that these costs are usually personnel costs associated to staff that might divide their time between many different tasks. In the case of the US, the Resource Conservation and Recovery Act (RCRA) requires to maintain records, to notify, and to report for relevant legislations while in the case of the EU similar legislation is found (e.g., REACH, EMAS). These activities entail several costs, which can be roughly estimated considering: a frequency of occurrence ($FreqOcc_{rt}$), and an associated cost for the generation of the required documents ($CostDoc_r$). In the case of the RCRA, some guidelines are available, see appendix E Sinclair-Rosselot and Allen, 2002.

$$Cost_t^{Compliance} = \sum_{r}^{reports} FreqOcc_{rt} CostDoc_r \qquad \forall t \in T_L \tag{23}$$

Similarly to compliance costs, environmental liabilities can be estimated by assuming a frequency of environmental ($FreqLiability_{lt}$) events that might end in: administrative or civil fines ($CostFine_l$).

$$Cost_t^{EnvLiabilities} = \sum_{l}^{possibleliabilities} FreqLiability_{lt} CostFine_l \qquad \forall t \in T_L \tag{24}$$

The net income due to emissions trading ($Net_t^{CO_2}$) is calculated by Eq. (25). Here, $Cost^{CO_2}$ and $Price^{CO_2}$ represent the emission right cost and price respectively.

$$Net_t^{CO_2} = Price_t^{CO_2} Sales_t^{CO_2} - Cost_t^{CO_2} Buy_t^{CO_2} \qquad \forall t \in T_L \tag{25}$$

Equation (26) represents the calculation of profit at period t. To conclude, NPV is computed by means of Eq. (27).

$$Profit_t = ESales_t + Net_t^{CO_2} - Net_t^{env} - (FCost_t + \sum_{e} EPurch_{et}) \quad \forall t \tag{26}$$

$$NPV = \sum_{t} \left(\frac{Profit_t - FAsset_t}{(1+rate)^t} \right) \tag{27}$$

The selection of the discount rate (*rate*) for any time discounted metric is subject to controversy, given that it represents the trade-off between the enjoyment of present and future benefits and affects directly intergenerational aspects of sustainability. Higher values of *rate* devaluate future impacts and consequently they count little on long time horizon projects, which could be perceived as contrary to the interest of future generations[3]. In some cases it has been suggested to adopt very low discount rates (even zero), in cases where mortality or extinction of species is possible. As pointed out by Gasparatos et al. (2008), most CBAs have used the Kaldor-Hicks criterion[4] allowing for some social actors to lose and not be compensated provided that society gains as a whole. Identically to the case of a weighting set for a composite environmental index, the selection of a given discount rate is highly subjective and should represent the decision maker beliefs in terms of intergenerational aspects.

Finally, the SC network design-planning problem whose objective is to optimize a given set of objective functions can be mathematically posed as follows:

$$\underset{\mathcal{X},\mathcal{Y}}{Min}\left\{-NPV, DamC_g^{SC}, Impact_{overall}^{2002}\right\}$$

subject to

$$\text{Eqns. (1) to (27)}$$

$$\mathcal{X}\in\{0,1\};\mathcal{Y}\in\mathbb{R}^{+}$$

Here X denotes the binary variables set, while Y corresponds to the continuous variable set.

4. Case Study: A Supply Chain for Maleic Anhydride

The case study used to illustrate the concepts behind the presented strategy addresses a SC design problem comparing different technologies for maleic anhydride (MA) production. MA is an important raw material used in the manufacture of phthalic-type and unsaturated polyester resins, co-polymers, surface coatings, plasticizers and lubricant additives (USEPA, October 1980). Two main technologies are available for its manufacture by catalytic oxidation of different hydrocarbons, benzene or butane (Chen and Shonnard, 2004). Main process reactions are as follows:

$$Butane\ Route: C_4H_8+3O_2\rightarrow C_4H_2O_3+3H_2O \tag{28}$$

$$Benzene\ Route: C_6H_6+4.5O_2\rightarrow C_4H_2O_3+2CO_2+2H_2O \tag{29}$$

[3] This could lead to a non-equitable distribution of costs and benefit through time by forcing future generations to bear a disproportionate cost.

[4] A project should be undertaken if the size of benefits is such the gainers could compensate the losers in theory though compensation would not have to be actually carried out.

From an atom economy point of view (Domenech et al., 2002), the procedure considering the conversion of butane/butene is more environmentally friendly (see Eq. (28)), because all butene C atoms end up as MA, while for benzene reaction (see Eq. (29)), only 67% of C atoms are converted into MA. Also for the butane reaction, the oxygen efficiency is greater than in the benzene reaction (50% vs. 33%); just in terms of hydrogen consumption benzene reaction renders a higher atom efficiency than butane reaction (33% vs. 25%). Several factors such as advances in catalyst technology, increased regulatory pressures, and continuing cost advantages of butane over benzene have led to a rapid conversion of benzene- to butane-based plants, consequently to the conversion of the whole MA SC (Felthouse et al., April 26, 2001).

The SC under study comprises raw material extraction facilities, processing sites, distribution centers and marketplaces, fitting a cradle to distribution center approach. Different raw material suppliers are modeled considering that each of them provides the same commodities quality, but the production is performed using different technologies. Two technologies can be implemented: (i) based on benzene (MA Technology 1) and (ii) based on butane (MA Technology 2) feedstock. Table 2 shows raw materials requirements for each of these technologies.

Table 2. Different raw material consumption (α_{sij}) per kg of MA, based on literature data. (EcoinventV1.3, 2006)

Technology	MA Technology 1 Benzene based	MA Technology 2 n-Butane based
Electricity consumption [kWh]	0.540	1.08
Propane-butane [kg]	0.000	0.99
Benzene [kg]	1.026	0.00
CO_2 direct emissions [kg]	1.800	3.87

Figure 2. SC node location in the proposed case study. Bt1 and Bt2 show n-butane suppliers, Bz1 and Bz2 show benzene suppliers; Site1-3 show possible MA production sites and M1-5 are possible markets for MA sale. Number in parenthesis below node name shows general node numbering *fc*1-14

Table 3. Environmental impact for 1 kg of MA production (not considering raw materials nor transport) and raw materials production ($\psi_{iff'a}$) (EcoinventV1.3, 2006)

Impact category	Unit	MA Tech 1 (Benzene)	MA Tech 2 (Butane)	Benzene, Supplier 1 (coke plant-Bilbao-*fc*3)	Benzene, Supplier 2 (pyrolisis-gasoline-Rotterdam-*fc*4)	n-Butane Supplier 1 (refinery-Rotterdam-*fc*6)	n-Butane Supplier 2 (proxy mix-Le Havre-*fc*5)
Carcinogens	kg C_2H_3Cl	1.4E-09	0.0E+00	3.9E-01	2.0E-01	6.3E-03	9.1E-02
Non-Carcinogens	kg C_2H_3Cl	2.7E-04	0.0E+00	1.4E-02	8.9E-04	7.6E-03	7.5E-03
Respiratory inorganics	kg PM2.5	0.0E+00	0.0E+00	4.3E-03	1.3E-03	8.1E-04	1.5E-03
Ionizing radiation	Bq C-14	0.0E+00	0.0E+00	1.3E+01	5.9E-03	9.3E+00	2.2E+01
Ozone layer depletion	kg CFC-11	0.0E+00	0.0E+00	2.4E-07	2.9E-11	4.7E-07	1.4E-07
Respiratory organics	kg ethylene	7.9E-06	1.3E-05	9.2E-03	9.2E-04	8.5E-04	1.4E-03
Aquatic ecotoxicity	kg TEG water	8.8E-07	2.3E-07	1.5E+02	6.0E+01	1.5E+02	1.0E+02
Terrestrial ecotoxicity	kg TEG soil	1.7E-07	3.2E-07	3.4E+01	2.4E-02	3.1E+01	1.7E+01
Terrestrial acid/nutri	kg SO_2	0.0E+00	0.0E+00	2.5E-02	3.8E-02	1.5E-02	3.9E-02
Land occupation	m^2org.arable	0.0E+00	0.0E+00	2.0E-02	1.4E-05	3.4E-03	4.8E-03
Aquatic acidification	kg SO_2	0.0E+00	0.0E+00	6.6E-03	8.3E-03	6.3E-03	9.4E-03
Aquatic eutrophication	kg PO_4 P-lim	5.4E-04	5.4E-04	1.6E-05	4.4E-06	3.5E-04	4.4E-04
Global warming	kg CO_2eq.	1.8E+00	3.9E+00	6.4E-01	1.4E+00	5.6E-01	1.6E+00
Non-renewable energy	MJ primary energy	0.0E+00	0.0E+00	5.4E+01	7.1E+01	5.6E+01	6.7E+01
Mineral extraction	MJ surplus energy	0.0E+00	0.0E+00	3.4E-03	2.5E-04	2.6E-03	1.5E-02

A simplified potential network is proposed and restricted to Europe (see Figure 2). Tarragona (*Site*1-*fc*7), Estarreja (*Site*2-*fc*8) and Drusenheim (*Site*3-*fc*9) are considered to be possible facilities location nodes. Benzene is supposed to be available at Bilbao (*Bz*1-*fc*3) and Rotterdam (*Bz*2-*fc*4), while n-butane can be supplied from again Rotterdam (*Bt*1-*fc*6) and Le Havre (*Bt*2-*fc*5). MA is supposed to be sold at four markets located at Madrid (*M*1-*fc*10), Paris (*M*2-*fc*11), Munich (*M*3-*fc*12), Lisbon (*M*4-*fc*13) and Barcelona (*M*5-*fc*14).

The environmental impacts associated to MA production without consideration of raw material production, transportation and electricity consumption are found in Table 3. Two potential benzene suppliers are considered, benzene can be obtained from a coke plant (Benzene Supplier-Tech 1-*Bz*1), or from a 50% mixture of ethylene reforming and pyrolysis gasoline (Benzene Supplier-Tech 2-*Bz*2). For the case of butane production, two suppliers are considered, one that is a proxy model obtained from a European typical refinery (Butane Supplier-Tech 1-*Bt*1-*fc*6), and another one from a mixture of the top 20 most important organic chemicals (Butane Supplier-Tech 2-*Bt*2-*fc*5). The LCI values were retrieved from the LCI database EcoinventV1.3 (2006) and using SimaPro 7.1.6 (PRe-Consultants-bv, 2008), were converted directly to the IMPACT 2002+ mid-point indicators. The environmental impact for raw material production can be also found in Table 3 which does not consider impacts associated to transportation.

Two different types of transportation services are assumed to be available: Lorries in two different sizes (16 and 32 ton). Benzene is a chemical that is liquid at standard conditions and therefore stored and transported as a liquid. Butane, on the other hand, is a gas at standard conditions and therefore needs to be liquefied in order to be transported and stored. In this case butane liquefaction has been considered during its production, and consequently both products are transported in liquid state, with similar environmental impacts by the same kg·km. Regarding electricity consumption, medium voltage electricity production from different countries grid is considered. Environmental impacts associated to transport services and electricity consumption are found in Table 4. Raw material, electricity, product and transportation prices were estimated from current economical trends, see Table 5 and 6. For the case of NPV optimization return rate is assumed to be 25%.

Capital investment associated to equipment and its operating costs are based on previously published results which were obtained using process simulation of different MA production flow sheets (Chen and Shonnard, 2004). These figures are from a design basis of 2.27×10^7 kg of MA/year (see Table 7).

Thirty-seven monthly planning periods are considered. The model has been implemented in GAMS which is algebraic modeling software (Brooke et al., 1998). The formulation of the SC-LCA model leads to a MILP with 15440 equations, 137652 continuous variables, and 1093 discrete variables. It takes 13.2 CPU s to reach a solution with a 0% integrality gap on a 2.0 GHz Intel Core 2 Duo computer using the MIP solver of CPLEX (ILOG-Optimization, 2008).

Table 4. Environmental impact associated to transport services (ψ^{T}_{0e}) and electricity production (ψ_{iifr}), for typical European countries. (EcoinventV1.3, 2006)

Impact category	Unit	Transport lorry 32ton [tn·km]	Transport lorry 16ton [tn·km]	Electricity supplier 1 [kWh]	Electricity supplier 2 [kWh]
Carcinogens	kg	1.2E-03	2.0E-03	1.6E-04	1.4E-04
Non-Carcinogens	kg	2.4E-03	3.9E-03	1.4E-04	1.4E-04
Respiratory inorganics	kg PM2.5	2.8E-04	6.5E-04	3.7E-05	2.8E-05
Ionizing radiation	Bq C-14	1.4E+00	3.8E+00	1.1E-01	3.8E+00
Ozone layer depletion	kg CFC-11	2.3E-08	4.9E-08	5.1E-09	1.7E-09
Respiratory organics	kg C_2H_2	1.7E-04	6.7E-04	1.1E-05	4.1E-06
Aquatic ecotoxicity	kg TEG water	1.8E+01	3.2E+01	1.9E+00	1.9E+00
Terrestrial ecotoxicity	kg TEG soil	1.1E+01	1.8E+01	5.2E-01	3.4E-01
Terrestrial acid/nutri	kg SO_2	7.6E-03	1.5E-02	8.7E-04	5.0E-04
Land occupation	m^2org-arable	1.3E-03	4.7E-03	5.8E-05	7.3E-05
Aquatic acidification	kg SO_2	1.2E-03	2.4E-03	3.0E-04	1.9E-04
Aquatic eutrophication	kg P-lim	1.6E-05	3.4E-05	2.0E-06	5.3E-07
Global warming	kg CO_2	1.6E-01	3.6E-01	5.2E-02	3.6E-02
Non-renewable energy	MJ primary	2.8E+00	6.0E+00	7.4E-01	8.2E-01
Mineral extraction	MJ surplus	1.3E-03	1.9E-03	6.8E-05	9.0E-05

Table 5. Raw material prices available at different suppliers (χ_{est}), and MA mean prices available at different markets ($Price_{sft}$)

Commodities		Price/cost [$]
Electricity [kWh]	Supplier-Tech 1	0.057
	Supplier-Tech 2	0.038
Benzene [kg]	Supplier-Tech 1 (Coke plant – Bilbao – *fc*3)	0.171
	Supplier-Tech 2 (Pyrolisis gasoline – Rotterdam – *fc*4)	0.214
Butane [kg]	Supplier-Tech 1(Refinery – Rotterdam – *fc*6)	0.224
	Supplier-Tech 2 (Proxy – Le Havre – *fc*5)	0.280
Maleic anhydride [kg]		1.672

Table 6. Raw materials and product transportation cost ($ $10^{-4}/(km{\cdot}kg)$, ρ^{tr}_{eff})

Raw Material (RM)	Transport Cost (32 ton)	Transport Cost (16 ton)
Benzene	2.99	2.69
MA	2.75	2.48
Butane	4.25	3.83

Table 7. Facilities capital investment ($Price^{FJ}_{jft}$) and operating cost (τ^{ut1}_{ijfe}), $1·$10^7$

	MA Technology 1 Benzene based	MA Technology 2 n-Butane based
Capital investment	1.61	1.95
Operating cost	1.42	1.30

In order to evaluate comparable alternatives, the first step has consisted on determining a SC which maximizes NPV, which is used to fix a total production rate. From the supplied data, it is found that the production rate should be of 813x10^3 ton of MA for a 3 years planning horizon. Then, since two objective functions are to be optimized, namely NPV and IMPACT 2002+, the multi-objective optimization procedure known as the weighted sum is followed (Statnikov and Matusov, 1995). In order to be able to make comparisons not only the production rate is the same for both solutions, but the amount of sales has been set to the same Figure The selected figure is the resulting from NPV optimization.

Following this procedure, Figure 3 shows the obtained dominant SC that maximizes NPV. It is found that its production is based on benzene feedstock, which is bought from both available suppliers; moreover production of MA is located in Estarreja (*fc*8) and Drussenheim (*fc*9). Alternatively, by the minimization of the environmental impact indicator, subject to the same production/sales rate, the resulting SC (Figure 4) uses butane as feedstock and buys raw materials from a single supplier. In this sense n-butane is selectively bought from one single supplier (*fc*6, refinery in Rotterdam) and is processed at all three possible manufacturing sites (*fc*7-*fc*9). Arrows width in figures 3 and 4 shows activity level.

Tables 8 and 9 summarize the most significant values corresponding to both solutions regarding environmental and economic aspects.

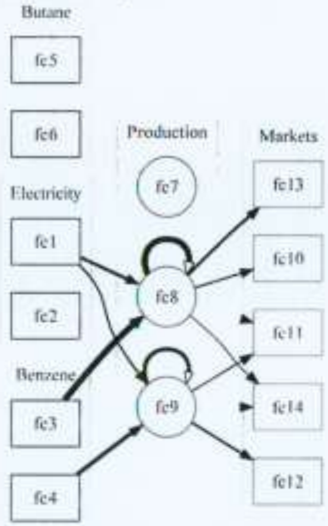

Figure 3. SC configuration for the most profitable SC option (NPV optimization). Arrows width shows activity level. It shows a benzene based SC with production of MA located in Estarreja (*fc*8) and Drussenheim (*fc*9)

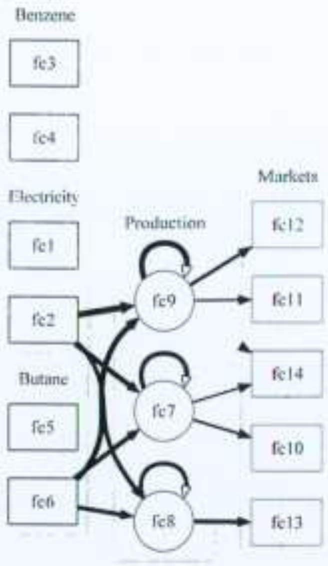

Figure 4. SC configuration for the most environmental friendly option (overall impact 2002+ optimization). Arrows width shows activity level. It shows that n-butane is selectively bought from one single supplier (*fc6*, refinery in Rotterdam) and is processed in all three possible manufacturing sites (*fc7*-*fc9*)

Table 8. Environmental impacts arising from single economic and overall environmental objective function optimization results [Impact 2002+ pts]

End-point impact category	Impact 2002+ Optimization		NPV Optimization	
	Direct value	Normalized value	Direct value	Normalized value
Human Health	7.87E+02	1.11E+05	3.03E+03	4.27E+05
Ecosystem Quality	3.55E+08	2.59E+04	3.35E+08	2.45E+04
Climate Change	3.85E+09	3.89E+05	2.62E+09	2.65E+05
Resources	4.94E+10	3.26E+05	5.69E+10	3.76E+05
Impact 2002+	8.52E+05		1.09E+06	
SC-structure	Figure 4		Figure 3	

Table 9. Economic aspects arising from single objective optimization (NPV and Impact 2002+). [m.u.]

Economic aspect	Impact2002+ Optimization		NPV Optimization	
	Non discounted	Discounted	Non discounted	Discounted
Investment	1.61E+08	1.61E+08	1.09E+08	1.09E+08
Raw Material Cost	2.28E+08	1.59E+08	2.31E+08	1.61E+08
RM Transport Cost	4.52E+08	3.15E+08	1.37E+08	9.36E+07
Product Transport Cost	7.92E+07	5.53E+07	1.08E+08	7.52E+07
Production cost	4.69E+08	3.27E+08	5.10E+08	3.56E+08
Fixed cost	3.62E+07	2.53E+07	2.91E+07	2.03E+07
Sales	1.36E+09	9.50E+08	1.36E+09	9.50E+08
Profit	-6.56E+07		2.37E+08	
NPV		-9.44E+07		1.32E+08
IRR		-31.06%		99.10%

Figure 5 shows the distribution of the environmental impacts along SC echelons for these two cases, this kind of analysis are the ones that entail the fourth step of the LCA methodology. According to Bauman and Tillman (2004), most LCA studies show that the production of materials often causes a dominant proportion of the environmental impact of a product, whereas assembly often causes a very minor proportion. However, if the product requires energy during its use phase, this phase often dominates the environmental profile, whereas if the product is used in a more passive way, the production phase dominates; notably the production of materials. In spite of transport being a major source of pollution in society, transportation and distribution often contribute less to the environmental impact than expected. In the presented case study raw material production is the most important factor contributing to the overall environmental impact in both single objective optimization cases; while electricity consumption and transportation are the least impacting aspects. This clearly shows that activities to reduce environmental impact should be focused on raw material production echelon. Moreover, from Figure 5, it can also be concluded that if raw material production would be disregarded then different solutions would be obtained, thus showing the influence of "purchase" decisions on the environmental impact of a SC.

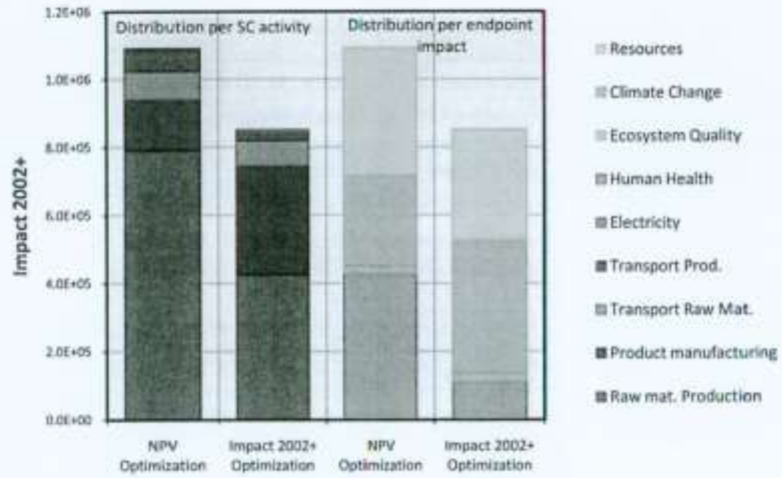

Figure 5. Distribution of environmental impacts for single objective optimization solutions, according to different SC activities and end-points

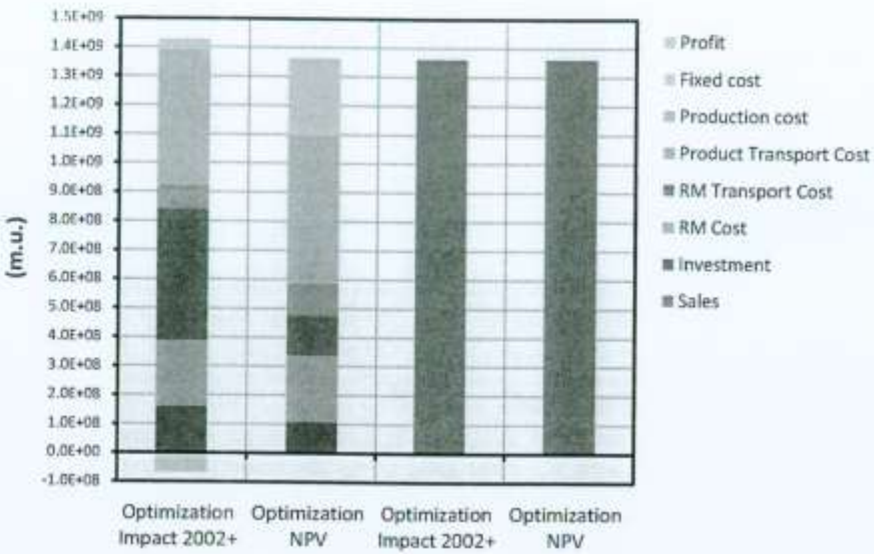

Figure 6. Distribution of costs for single objective optimization solutions, distributed in different SC activities

In the case of minimization of environmental impact, a negative NPV and Internal rate of return (IRR) are found. If the costs are analyzed it can be seen (Figure 6 clarifies this situation), that raw material transportation cost associated to environmental impact minimization is significantly higher and is the most significant difference between economic and environmental optimizations. This difference is due to the following reasons: butane suppliers locations are far from production facility locations, butane transport cost is 42% higher than benzene cost, and the environmental impact optimization selects lorries of 32tons which are less polluting, but more expensive (see table 5). The second and third biggest differences between the obtained solutions are regarding investment and fixed operating costs which also penalize butane based production. A comparison of the distribution of environmental impacts can be seen in Figure 7.

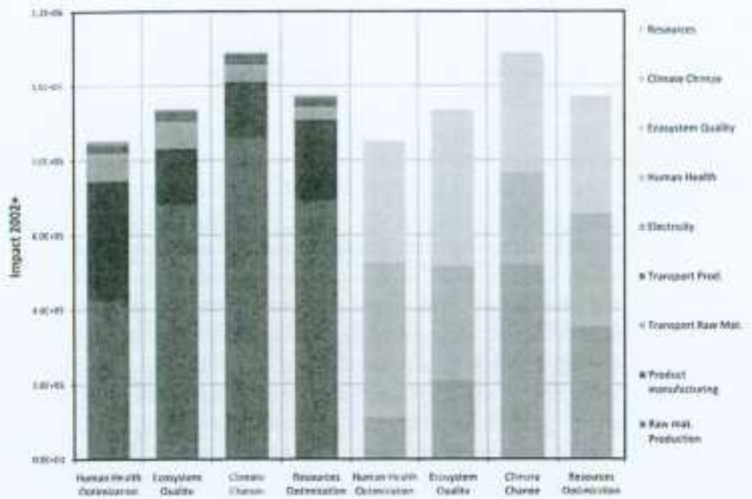

Figure 7. Distribution of environmental impacts along SC activities and end-point categories for single end-point environmental optimization

Table 10. Single end-point optimization results distributed along different environmental end-point metrics. Last row presents the resulting overall Impact 2002+ [Impact 2002+ pts].

End-point indicator	Human Health Optimization	Ecosystem Quality Optimization	Climate Change Optimization	Resources Optimization
Human Health	110953	210863	520133	353555
Ecosystem Quality	25946	12633	27337	24271
Climate Change	388736	293764	219817	279434
Resources	326140	418723	320895	315826
Impact 2002+	851776	935983	1088183	973085
SC configuration	Figure 7 (a)	Figure 7 (b)	Figure 7 (c)	Figure 7 (d)
SC raw materials	n-Butane	Benzene	Benzene	n-But+Ben

Table 11. Environmental impact associated to different SC activities for single end-point optimization [Impact 2002+ pts].

SC activity	Human Health Optimization	Ecosystem Quality Optimization	Climate Change Optimization	Resources Optimization
Raw mat. Production	427169	684044	862463	695986
Product manufacturing	318002	147994	147994	213013
Transport Raw Mat.	75313	73128	46546	34968
Transport Prod.	20470	25406	25770	20401
Electricity	10822	5411	5411	8717

Tables 10 and 11 show the solutions associated to the cases in which each end-point indicator is optimized.

Table 10 rows show, as expected, that the minimum value for each of the partial environmental impacts is obtained by the optimization of such objective function. The solution obtained by optimization of the human health end-point is the same as the one obtained when optimizing the overall Impact 2002+, a SC based on butane as in Figure 4 and Figure 8 (a). One of the reasons for this is due to the fact that the weighting and normalization coefficients for that end-point value are the largest in the methodology. Interestingly, each one of the other end-point optimizations provides with a different SC structure, see Figures 8 (b,c,d). In the case of ecosystem quality and climate change optimization (Figures 7 b and c), the production is based on benzene and the SC structures are similar to the one depicted in Figure 3. The difference between solutions is the MA production load on each different site and the benzene supplier which in the case of ecosystem quality is the provider that uses pyrolisis gasoline (*fc*4 located in Rotterdam) and the case of minimisation of climate change is a coke plant (*fc*3 located in Bilbao). Please note that arrows widths are wider in the case of nodes close to the supplier, to minimise environmental impact from transportation. In the case of resources impact optimization it is based on a combined use of benzene and butane technologies (see Figure 8(d)). Regarding the optimization of ecosystem quality and climate change, they both show minimum amount environmental impact due to electricity.

One alternative to reduce SC environmental impacts may be to look for new feedstock providers whose production processes are more environmental friendly. It is also important to notice that Human Health impacts are considerable high in both solutions. In the case of NPV optimization this fact is due to benzene toxic properties. It is expected that CO_2 emissions trading considerations will make the butane based production more economically attractive. This aspect is analyzed in the next section.

There is SC-structure dependence against its total production. Other works related to SC design and environmental issues consider that demand must be completely fulfilled. This assumption leads to an invariable total production rate and suboptimal solutions. In Figure 9 iso-production/sales curves correspond to solutions following this assumption. For these cases minimum overall impact always leads to negative NPVs. These solutions are obviously dominated by the zero-production/sale solution (origin). This trade-off is absolutely necessary. Regardless of emissions, every productive sector has a "break-even" point below which "profit" becomes negative. It establishes the minimum production capacity required to make a profitable business. Further analysis on this issue is presented later. The actual Pareto curve is shown in Figure 9 as a continuous black line which is obtained by allowing unfulfilled demand (i.e. not considering a fixed required amount). It can be seen that positive NPVs can be achieved by reducing the MA production.

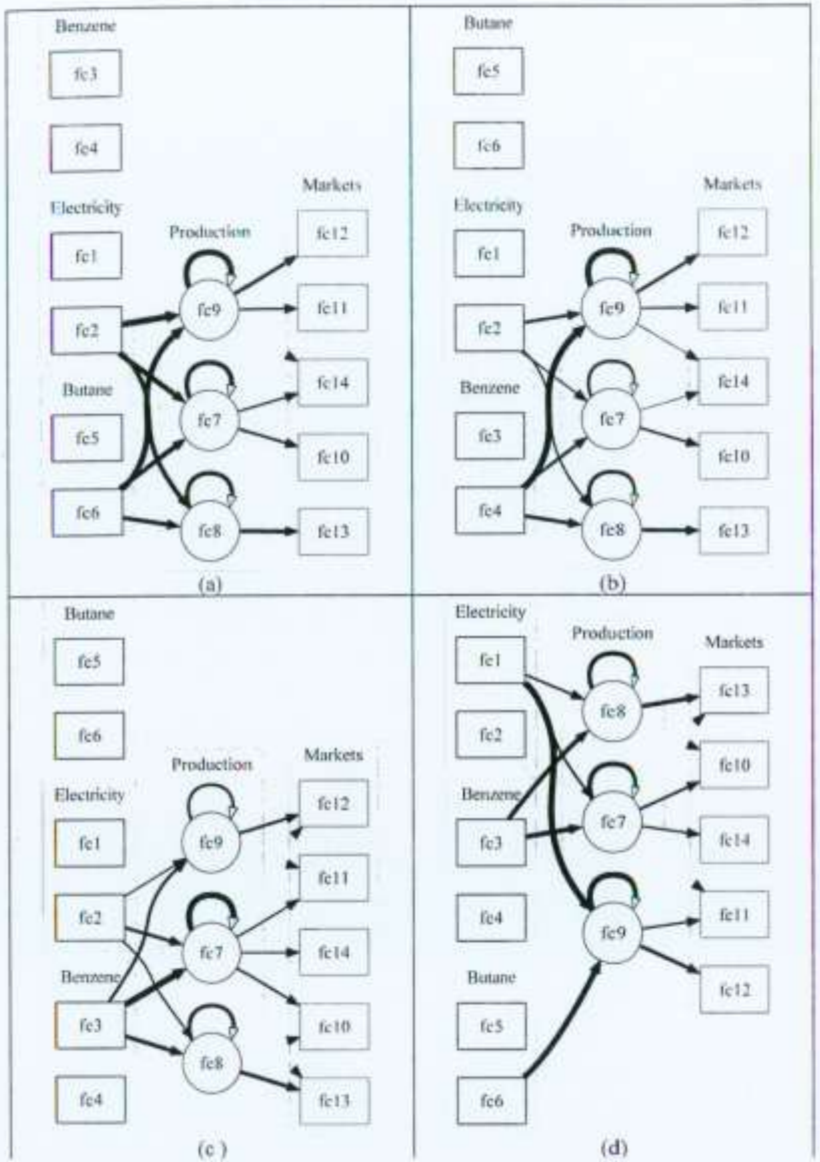

Figure 8. a,b,c,d. Different SC configurations obtained from the optimization of each end-point indicator, (a) Human Health, (b) Ecosystem quality, (c) Climate change and (d) resources

In order to explicitly consider the conflict between environmental and economic issues, here the overall impact indicator has been optimized against NPV for different production amounts. Results obtained in this way draw a clear picture of the problem, which is basic for a more objective selection among the different alternatives. As it can be observed (see Figure 8 and 9), the multi-objective optimization results in a set of Pareto solutions, connecting lines do not represent solutions, and only the vertices of the curve are feasible SC alternatives. Within this set of non-dominated solutions the decision maker must select one. The stake holder's selected solution will depend on the weights that he/she subjectively assigns to each of the objectives (i.e., NPV and Impact2002+). Several multi-attribute decision analysis (MADA) techniques are available for this purpose, for a review of these techniques the reader is referred to the work of Seppälä et al. (2002).

With regards to the effect of interest rate on the optimal SC configuration, an analysis was performed by increasing gradually the annual interest rate from 0% to 40%, while optimizing the NPV. The obtained results are shown in Figure 10.

Figure 10 shows that for interest rates lower than 7.5% one SC structure is found. This SC is based on the installation of benzene and butane based production technologies and is similar to the one shown in Figure 8d. For values of interest rate greater than 7.5% the optimal NPV SC is based on the production of MA from benzene only and has the same structure as the one shown in Figure 3. It is worth emphasizing that in this case increases in the interest rate will render solutions that prioritize early cash flows rather than end of project ones.

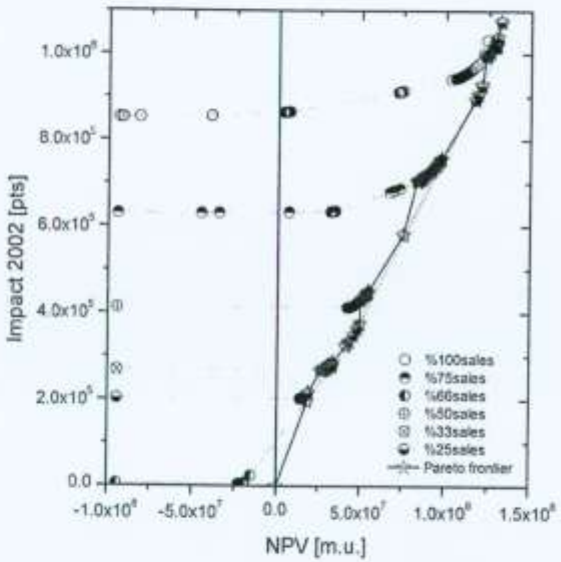

Figure 9. Iso-production/sales curves for different production amounts based a per-centage of best NPV sales value. Continuous line shows Pareto frontier for overall envi-ronmental impact vs. NPV

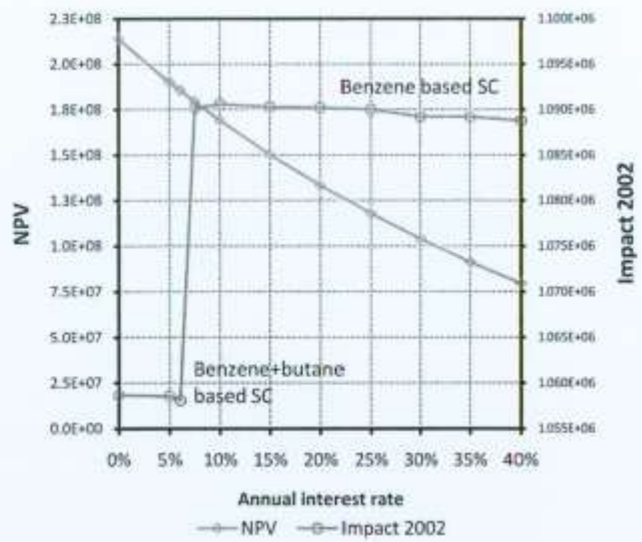

Figure 10. Net present value optimization results for different values of interest rate

4.1.1. CO_2 emission trading considerations

In order to take into account CO_2 emissions, values for maximum free emissions caps must be available. One possible way of assessing such value is to take the best available technology (BAT) in terms of CO_2 emissions. Chen and Shonnard (2004) have studied both MA production schemes finding through simulation optimum flow sheets (see Table 12). Given that their data does not consider steam co-production, the BAT value has been increased accordingly (32%), in order to be comparable to the one reported by EcoinventV1.3 (2006). It has been found that producing MA from butane has the lowest CO_2 emissions and will be used to set the free emission quota available. Tier 1, Tier 2 and Tier 3 CO_2 emissions were retrieved from EcoinventV1.3 (2006).

In the economic formulation it is considered that CO_2 emissions credits are bought at the end of each year in order to cope with CO_2 emissions that exceed the maximum allowed considered using the BAT. The trading cost and price of emission rights is considered as US$23 which is a proxy of the values currently found in the trading market.

Table 12. CO_2 emissions associated to the production of 1 kg of MA (EcoinventV1.3, 2006), and BAT data ($MaxCO_2t$) adopted from Chen and Shonnard (2004).

	MA Technology 1 Benzene based	MA Technology 2 n-Butane based
BAT Tier 2 CO_2 emissions [kg]	3.41	3.02
Tier 1 CO_2 emissions [kg]	1.80	3.87
Tier 2 CO_2 emissions [kg]	2.05	4.38
Tier 3 CO_2 emissions [kg]	3.53	4.93

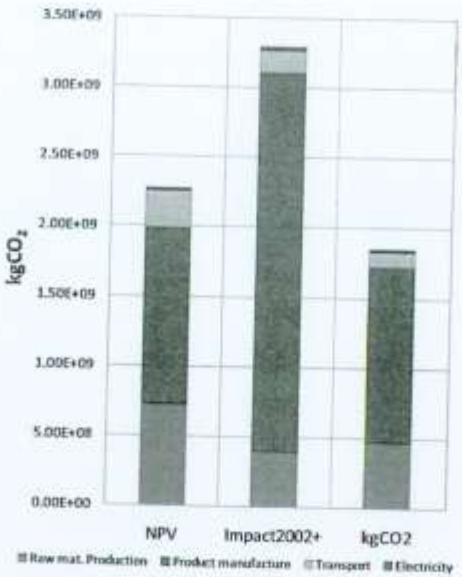

Figure 11. Emissions allocation along the SC for the maximum NPV configuration, the minimum overall impact configuration, and minimum emissions

It is noteworthy that the optimal SC configuration considering the emissions trading scheme remains equal to the one obtained when optimizing NPV without this consideration (Figure 3) independently of the free emissions cap and the emission right price. Let us recall that the minimum overall environmental impact is achieved by installing butane based technologies, while the most profitable is based on benzene as feedstock. The CO_2 emission allocation along the SC is depicted in Figure 11 for the maximum NPV, minimum overall impact, and minimum CO_2 emissions network configurations, optimized taking into account the CO_2 trading scheme. The least CO_2 pollutant configuration is based on benzene technology. It can be observed from this figure that the optimal overall impact configuration (butane based) is the one that emits more CO_2, most of it coming from the MA production. Under the trading scheme this configuration would be strongly penalized. As aforementioned, it was expected that regulatory pressures would lead to a conversion of benzene- to butane-based plants since benzene is considered to be more environmental harmful. Actually, benzene based SCs show greater overall impact (see Table 8 and 10), being human health their more impacting damage category due to benzene's carcinogenicity. However, a CO_2 trading emission scheme as the one modeled in the case study will not cause benzene based production to move towards butane; on the contrary, it can be a factor leading to change butane based into benzene based MA production.

4.1.2. Product and raw material subsidies

From the results found from single objective optimization of NPV and Impact 2002+, it was found that an IRR of nearly 100% is associated to a MA production SC based on

benzene, while production based on butane is the most environmentally friendly but is not profitable (see Table 8). Another possible way of solving this issue, instead of taxes on CO_2, is to have a government subsidy on the production of MA based on butane. This subsidy could be of different forms which can be grasped from the distribution of cost in Figure 6. In this sense the possible options are (i) increase of MA selling price, (ii) a decrease in the cost of production of MA and (iii) decrease of butane and MA related transportation costs. Points (i) and (ii) are similar, in the sense that both are based on the kg of MA produced. Figure 12 shows the change in the IRR value for the SC based on butane when increasing the subsidy per kg of MA produced. Table 13 shows the MA government subsidies results for different IRR values.

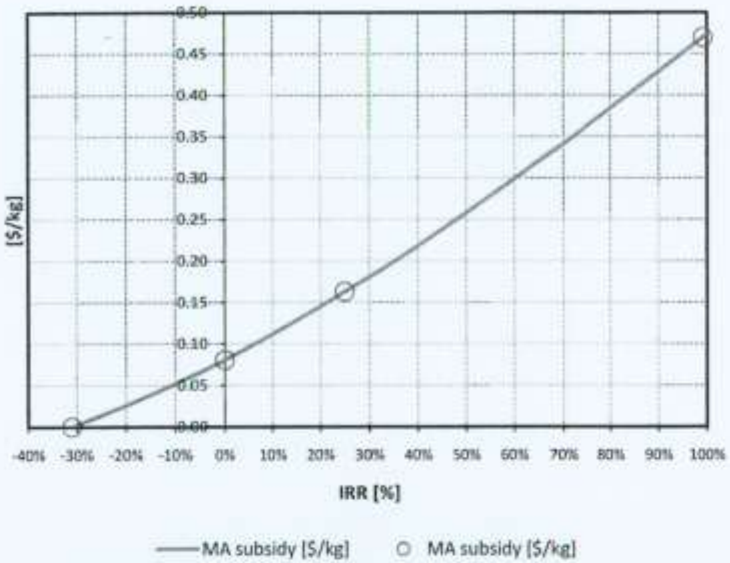

Figure 12. IRR values for different amount of government subsidy based on MA production

Table 13. Current and possible MA prices and production government subsidies

IRR [%]	MA subsidized price [$/kg]	Operating cost subsidy [$/kg]
-31.1%	1.672	0.000
0.0%	1.753	0.081
25.0%	1.835	0.163
99.1%	2.142	0.470

Table 14. MA and n-butane transportation cost with and without government subsidies

IRR [%]	Butane subsidy [\$/kg·km]	Butane Transport Cost [\$/kg·km]	MA subsidy [\$/kg·km]	MA Transport Cost [\$/kg·km]
-31.1%	0	4.25E-04	0	2.75E-04
0.0%	6.17E-05	3.63E-04	2.28E-04	4.73E-05
25.0%	1.27E-04	2.98E-04	4.69E-04	-1.94E-04
99.1%	3.89E-04	3.56E-05	1.43E-03	-1.16E-03

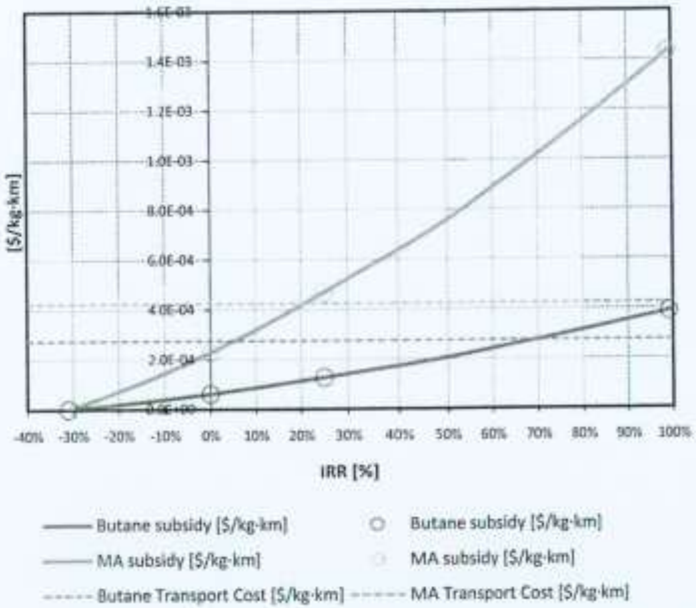

Figure 13. IRR values for different amount of government subsidy based on transports of MA and butane

In the case of transportation costs associated to MA and n-butane, Table 14 and Figure 13 show the obtained results. The analysis was performed considering one single transport being subsidized, and it is found that a subsidy on butane transportation is more efficient than one on MA. However in both cases in order to make the butane based SC equally profitable than the benzene one, government subsidies are bigger than the actual transportation cost (negative values in Table 14 indicate a higher subsidy than the cost). On the contrary in the case of a subsidy on MA production or sale price, a subsidy of 0.538 €/kg of butane (being it as sales price or operating cost reduction) will make the butane based SC as profitable as the one based on benzene.

5. Conclusion

This chapter presents an approach for designing and planning environmentally friendly and profitable SC. The model consists of a multi-period MILP that accounts for the multi-objective optimization of economic and environmental interventions. The model considered the long-term strategic decisions (e.g., installation of plants, selection of suppliers, manufacturing sites, and distribution centers) with the mid-term planning for SCs. Each end-point damage categories was considered as an objective function in order to avoid the subjectivity associated with their aggregation into an overall environmental impact indicator, showing the various SC possibilities obtained for each indicator. The Impact2002+ metric was adopted as a measure of overall environmental impact. Moreover, joint consideration of end point damages and trading schemes enables the proposed approach to support (i) assessment of current regulatory policies and (ii) definition of more adequate policy parameters (e.g., free emissions allowance cap for each industry, emissions trading price, subsidies).

A maleic anhydride SC case study is presented where two potential technologies are available. Two problems were solved, a first approach that did not consider CO_2 trading scheme and a second one (see subsection 2.2) that took it into account. We have shown the possibility of tackling such problems with ease. A SC for MA production based on butane was found to be more environmentally friendly than one based on benzene. In this sense the current model allowed for possible selection between obtained optimal solutions. Most of the works related to SC and environmental issues consider a fixed production/demand; it was demonstrated that such constraint leads to dominated solutions. By allowing unsatisfied demand, the actual Pareto curve was obtained.

Raw material production was found to be the most important contributor to overall environmental impact, while transportation and electricity consumption were the least important. This clearly shows that the current model allows for selection of improvement actions and the necessity for an approach with visibility of the whole SC. Recall the environmental impact potential significant dependence on "purchase decisions which cannot be assessed without a SC approach. Additionally, it was determined by using the optimization model that the production process was the activity that emits the most CO_2.

Additionally, the model may help to discover interesting facts. For example, it turns out that the CO_2 trading scheme will favor benzene-based over butane-based production. The results obtained for this specific case study question the suitability of a single CO_2 trading scheme applicability to every industry sector: different regulatory schemes may be required in different industrial scenarios. Current regulations merely consider climate change damage which certainly is a very important factor but other aspects such as human health, ecosystem quality and abiotic resources usage should be also considered so that effective industrial changes regarding the environment are induced. In this sense the utilization of a multiobjective optimization for each damage category has shown to be helpful at discovering insights regarding how different policies will affect SC strategic and tactical decisions. We believe that one of the main achievements of this work is not building and solving a complex SC-environmental model, instead it is to emphasize the dangers related to deploying CO_2 emission related policies in isolation from other pollution related issues. Also, it has been shown how this type of model can be used to determine subsidies policies in order to actually drive industry towards more environmental practices. On the other hand, it is important to point out that environmental metrics for the interpretation of life cycle inventories involve determining aggregated measures. Usually, normalizing factors are used to determine the weight of each damage factor (climate change, human health, resources depletion, ecosystem quality) in the overall measure which may favor different solutions. When this type of analysis is performed for the selection among different design alternatives, which will be active during a long time horizon, a careful sensitivity/uncertainty analysis related to the application of these normalizing factors is required. Such analysis can be done by using a multi-criteria optimization that accounts for end-point damage categories as presented in this chapter.

Obviously, nowadays the environmental impact associated with SC decisions at all levels is of high significance. However, approaches that address the environmental impact evaluation at the operational level (scheduling and distribution) are scarce. On the other hand, as stated by Papageorgiou (2009), there is an increasing interest in reverse logistics and closed loop SCs mainly because they are expected to diminish firms' environmental burden. Notwithstanding, most of the approaches developed so far do not assess the environmental reward or impact of such kind of operations (Fleischmann et al., 2001; Schultmann et al., 2003; Amaro & Barbosa-Póvoa, 2008).

Further work should be focused on the consideration of uncertainty, which is an important factor that may influence the decisions regarding trading schemes. Another potential extension is to analyze how decisions related to the short-term may contribute to reduce environmental burdens.

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NOTATION

Indices	
e	suppliers
f, f'	facility locations
i	tasks
j	equipment technology
s	materials (states)
t, t'	planning periods

(Continued)

a	mid point environmental impact categories
g	end point environmental impact categories
w	possible waste treatment sinks
r	considered reports for environmental compliance
l	considered environmental liabilities

Sets	
A_g	set of midpoint environmental interventions that are combined into endpoint damage factors g
E_{rm}	set of suppliers e that provide raw materials
$\hat{E}_{prod}$	set of suppliers e that provide production services
$\overline{E}_{tr}$	set of suppliers e that provide transportation services
F_e	set of locations f where supplier e is placed
FP	set of materials s that are final products
I_j	set of tasks i that can be performed in technology j
$\overline{J}_e$	technology j that is available at supplier e
$\tilde{J}_f$	technology j that can be installed at location f
J_i	technologies that can perform task i
Mkt	set of market locations
RM	set of materials s that are raw materials
Sup	set of supplier locations
T_L	set of periods when the emissions trading is executed
T_s	set of tasks producing material s
$\overline{T}_s$	set of tasks consuming material s
Tr	set of distribution tasks

Parameters	
A_{sft}	maximum availability of raw material s in period t in location f
Dem_{sft}	demand of product s at market f in period t
$Cost_t^{co_2}$	emissions right cost in period t
$distance_{ff'}$	distance from location f to location f'

(Continued)

$FCFJ_{jft}$	fixed cost per unit of technology j capacity at location f in period t
I^J_{ft}	investment required to establish a processing facility in location f in period t
$MaxCO_{2t}$	free allowance emissions cap at period t
$NormF_g$	normalizing factor of damage category g
$Price_{sft}$	price of product s at market f in period t
$Price_t^{co_2}$	emissions right price in period t
$Price_w^{WT}$	price for residues treatment to sink w
$Flow_{wt}^{WT}$	Mass flow of residues to treatment sink w at period t
$FreqOcc_{rt}$	frequency of occurrence of report r during period t
$CostDoc_r$	cost for the generation of the required documents r
$FreqLiability_{lt}$	frequency of occurrence of liability l during period t
$CostFine_l$	cost associated to the expected liability l
$Price^J_{jft}$	investment required per unit of technology j capacity increased at facility f in period t
$rate$	discount rate
α_{sij}	mass fraction of task i for production of material s in equipment j
$\bar{\alpha}_{sij}$	mass fraction of task i for consumption of material s in equipment j
β_{jf}	minimum utilization rate of technology j capacity that is allowed at location f
ζ_{ag}	g end-point damage characterization factor for environmental intervention a
$\theta_{ijff'}$	capacity utilization rate of technology j by task i whose origin is location f and destination location f'
$\rho^{tr}_{ff't}$	unitary transportation costs from location f to location f' during period t
τ^{ut1}_{ijfet}	unitary cost associated with task i performed in equipment j from location f and payable to external supplier e during period t
τ^{ut2}_{sfet}	unitary cost associated with handling the inventory of material s in location f and payable to external supplier e during period t

(Continued)

χ_{est}	unitary cost of raw material s offered by external supplier e in period t
$\psi_{aijff'}$	a environmental category impact CF for task i performed using technology j receiving materials from node f and delivering it at node f'
ψ^T_{a}	a environmental category impact CF for the transportation of a mass unit of material over a length unit

Binary Variables	
V_{jft}	1 if technology j is installed at location f in period t, 0 otherwise
Continuous Variables	
$Buy_t^{co_2}$	amount of emissions extra rights bought in period t
$DamC_{gft}$	normalized endpoint damage g for location f in period t
$DamC_g^{SC}$	normalized endpoint damage g along the whole SC
$EPurch_{et}$	economic value of purchases executed in period t to supplier e
$ESales_t$	economic value of sales executed in period t
$FAsset_t$	investment on fixed assets in period t
$FCost_t$	fixed cost in period t
$Fjft$	total capacity of technology j during period t at location f
FE_{jft}	capacity increment of technology j at location f during period t
IC_{aft}	midpoint a environmental impact associated to site f which rises from activities in period t
$Impact_f^{2002}$	total environmental impact for site f
$Impact_{overall}^{2002}$	total environmental impact for the whole SC
$Net_t^{co_2}$	Net income due to emissions trading in period t

(Continued)

Net_t^{env}	Net cost associated to type 2 and 3 environmental costs in trading period t
$Cost_t^{WT}$	Environmental type 2 cost related to waste treatment for period t
$Cost_t^{Compliance}$	Environmental type 2 cost related to environmental compliance for period t
$Cost_t^{EnvLiabilities}$	Environmental type 3 cost related to possible environmental liabilities for period t
NPV	net present value
$P_{ijff't}$	activity magnitude of task i in equipment j in period t whose origin is location f and destination location f'
$Profit_t$	profit achieved in period t
$Purch_{et}^{pr}$	amount of money payable to supplier e in period t associated with production activities
$Purch_{et}^{rm}$	amount of money payable to supplier e in period t associated with consumption of raw materials
$Purch_{et}^{tr}$	amount of money payable to supplier e in period t associated with consumption of transport services
$Sales_t^{co_2}$	amount of emissions rights sold in period t
$Sales_{sff't}$	amount of product s sold from location f in market f' in period t
S_{sft}	amount of stock of material s at location f in period t
Superscripts	
L	lower bound
U	upper bound

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