

Multi-objective optimization of environmentally conscious chemical supply chains under demand uncertainty

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Abstract

In this work, we analyse the effect of demand uncertainty on the multi-objective optimization of chemical supply chains (SC) considering simultaneously their economic and environmental performance. To this end, we present a stochastic multi-scenario mixed-integer linear program (MILP) with the unique feature of incorporating explicitly the demand uncertainty using scenarios with given probability of occurrence. The environmental performance is quantified following life cycle assessment (LCA) principles, which are represented in the model formulation through standard algebraic equations. The capabilities of our approach are illustrated through a case study. We show that the stochastic solution improves the economic performance of the SC in comparison with the deterministic one at any level of the environmental impact.

Keywords: supply chain management; mixed-integer linear programming; risk management; multi-objective optimization; life cycle assessment; optimization under uncertainty.

1. Introduction

Supply chain management (SCM) aims at the efficient integration of suppliers, manufacturers, warehouses and stores, in order to ensure that products are manufactured and distributed in the right quantities, to the right locations, and at the right time thereby maximizing the system's performance (Simchi-Levi et al., 2000). Traditional SCM performance indicators focused on quantifying the economic outcome (Beamon, 1999). In the last decade, the incorporation of environmental concerns along with economic criteria in the decision-making process has gained wider interest (Grossmann and Guillén-Gosálbez, 2010). This trend has motivated the development of systematic methods for reducing the environmental impact in SCM. Among the tools that are available, those based on multi-objective optimization (MOO) have been increasingly used for this purpose, mainly because they treat environmental aspects as additional objectives rather than as constraint imposed on the system. This approach therefore allows identifying solutions where significant environmental savings are obtained at a marginal increase in cost.

The scientific community has not yet reached an agreement on the use of a universal indicator for objective environmental impact assessment. It has become clear, however, that the environmental performance should be assessed over the entire life cycle of a process in order to avoid local solutions that shift environmental burdens from one echelon of the supply chain to another. Life cycle assessment (LCA) is a methodology that arose in response to this situation. LCA is a quantitative performance tool for evaluating the environmental loads associated with a product, process, or activity over its entire life cycle ('from the cradle to the grave') (Guinée et al., 2001). LCA adopts a holistic view that considers all material and energy flows that

enter or exit the system. These flows include material and energy resources, as well as emissions to air, water and land, which are referred to as environmental burdens. These burdens are generated by activities encompassing extraction and refining of raw materials, transportation, production, use and waste disposal of final products. The combined use of LCA and MOO was formally defined by Azapagic and Clift (1999), and since then has found many applications in a wide variety of environmental problems (for a review see Grossmann and Guillén-Gosálbez, 2010). Among these applications, the environmentally conscious design of chemical SCs has been the focus of an increasing interest in the last years. In a seminar paper, Mele et al. (2005) addressed the optimization of SCs with economic and LCA-based environmental concerns through a combined simulation-optimization approach. Hugo and Pistikopoulos (2005) proposed a MILP formulation for the long-range planning and design of SCs, in which the environmental performance was measured via the Eco-indicator 99 (Goedkoop and Spriensma, 2001). Bojarski et al. (2009) introduced an MILP formulation for the design and planning of SCs considering economic and environmental issues, which incorporated the CML 2001 methodology to assess their environmental performance. Guillén-Gosálbez and Grossmann (2009) (see also Grossmann and Guillén-Gosálbez, 2010) proposed two MINLP formulations for the design of chemical SCs under uncertainty that explicitly consider the variability of the life cycle inventory of emissions and damage assessment model, respectively.

Most of the works that combine MOO and LCA rely on deterministic approaches (Applequist et al., 2000; Simchi-Levi et al., 2000; Talluri and Baker, 2002; Guillén et al., 2006a) that assume that all model parameters are nominal and show no

variability. In practice, however, it might be difficult to perfectly know in advance several key parameters, such as product demand, prices and availabilities. These parameters should be thus regarded as uncertain. Chemical process industries, in particular, are affected by many uncertainty sources that influence their economic and environmental performance (Sahinidis, 2004). In this context, deterministic models that neglect these uncertainties may lead to solutions that perform well in the most likely scenario but show poor performance under other plausible circumstances (Guillén-Gosálbez and Grossmann, 2009).

The most important and extensively studied source of uncertainty in SCM has been the demand (Gupta and Maranas, 2000; Gupta et al., 2000; Tsiakis et al., 2001; Gupta and Maranas, 2003; Balasubramanian and Grossmann, 2004; Sahinidis, 2004; Guillén et al., 2005; Guillén et al., 2006b; Guillén et al., 2006d; Guillén et al., 2006c; You and Grossmann, 2008; Ejikeme-Ugwu et al., 2011). This is due to the fact that meeting customer demand is what mainly drives most SC planning initiatives. Product demand fluctuations over medium-term (1-2 years) to long-term (5-10 years) planning horizons may be significant (Gupta and Maranas, 2000). Deterministic SC models fail to capture the effect of demand variability on the trade-off between lost sales and inventory costs.

To the best of our knowledge, the works by Guillén- Gosálbez and Grossmann were the only ones that studied the effect of uncertainties in the environmentally conscious design and planning of chemical SCs. Particularly, the authors developed mathematical programming tools that accounted for the variability of the life cycle inventory of emissions and characterization factors involved in the evaluation of the

environmental performance of SCs (Guillén-Gosálbez and Grossmann, 2009; Guillén-Gosálbez and Grossmann, 2010).

In this work, and as a step forward in our previous research, we study the effect of another uncertainty source (i.e., demand uncertainty) on the economic and environmental performance of SCs. Several previous works have studied this source of uncertainty in SCM, but to the best of our knowledge, there is no single contribution that has addressed its impact on both, the economic and environmental performance of SCs. We formulate the SC design problem under uncertainty as a multi-objective stochastic MILP that seeks to maximize the expected profit and minimize the probability of exceeding a given environmental limit. The capabilities of our approach are illustrated in the discussion of a case study that addresses the design of a petrochemical supply chain.

The remainder of this article is organized as follows. The problem of interest is first formally stated, and the assumptions made are briefly described. The problem data, decision variables and objectives are also introduced at this point. The stochastic mathematical model that considers explicitly the demand uncertainty is then presented. The solution procedure is described in the following section. The capabilities of the approach proposed are then illustrated through a case study based on a European petrochemical SC. The conclusions of the work are finally drawn in the last section of the paper.

2. Problem statement

In this work we consider a generic three-echelon SC (production-storage-market) as the one depicted in Figure 1. This network includes: a set of plants with a set of

available technologies, where products are manufactured; a set of warehouses where products are stored before being shipped to final markets; and a set of markets where products become available to customers.

The problem addressed in this article can be formally stated as follows. Given are a fixed time horizon divided into a set of time periods, a set of potential locations for the SC facilities, the capacity limitations associated with these technologies, the prices of final products and raw materials, the investment and operating cost of the SC and environmental data (emissions associated with the network operation and damage assessment model). The demand, which is assumed to be uncertain, is described through a set of scenarios with given probability of occurrence.

The goal of the study is to determine the configuration of the SC along with the associated planning decision that simultaneously maximize the expected total net present value (NPV) and minimize the environmental impact under demand uncertainty. Decisions to be made are of two types: structural and operational. The former include the number, location and capacity of the plants (including the technologies selected in each of them) and warehouses to be set up, their capacity expansion policy and the transportation links between the SC entities. The operational decisions are the production rate at the plants in each time period, the flows of materials between plants, warehouses and markets, and the sales of final products.

3. Stochastic mathematical model

Several methods have been proposed to deal with uncertainty in SCM. The most widely used approaches are control theory, fuzzy programming, robust optimization,

and stochastic programming (Guillén et al., 2006c). The approach proposed in this work relies on a two-stage stochastic MILP that pertains to the last group of methods. In our case, stage-1 decisions, which are taken before the uncertainty is resolved, are given by the design variables, like establishing a new plant or warehouse. In contrast, stage-2 decisions, which are made after the uncertainty is revealed, model operational variables (mainly production levels and transportation flows) that can be adjusted according to the uncertainty resolution. We assume that the uncertain parameters are described by a set of explicit scenarios with given probability of occurrence. Such scenarios together with their associated probabilities must be provided as input data to the model. In our case, these scenarios are generated from probability distributions using sampling methods.

We describe next a stochastic programming MILP model based on the one introduced by Guillén-Gosálbez and Grossmann to tackle uncertainties in the life cycle inventory of emissions and damage assessment model (Guillén-Gosálbez and Grossmann, 2009). The model equations are classified into three main blocks: mass balance equations, capacity constraints and objective function equations. These sets of equations together with the model variables are described in detail next.

3.1 Mass balance constraints

The mass balance must be satisfied for each node embedded in the network. Thus, for each plant j and chemical p the purchases (PU_{jpts}) made during period t plus the amount produced must equal the amount transported from the plant to the warehouses (Q_{jkpts}^{PL}) plus the amount consumed in every scenario s :

$$PU_{jpts} + \sum_{i \in \text{OUT}(p)} W_{ijpts} = \sum_k Q_{jkpts}^{PL} + \sum_{i \in \text{IN}(p)} W_{ijpts} \quad \forall j, p, t, s \quad (1)$$

In Eq. (1), W_{ijpts} denotes the input/output flow of p associated with technology i at plant j in time period t and scenario s .

For each product, the total purchases are constrained within lower (\underline{PU}_{jpt}) and upper limits (\overline{PU}_{jpt}) in every scenario s . These bounds are given by the product availability in the current market place:

$$\underline{PU}_{jpt} \leq PU_{jpts} \leq \overline{PU}_{jpt} \quad \forall j, p, t, s \quad (2)$$

Equation (3) represents the material balance for each technology i installed at plant j in every scenario s .

$$W_{ijpts} = \mu_{ip} W_{ijp'ts} \quad \forall i, j, p, t, s \quad \forall p' \in MP(i) \quad (3)$$

In this equation, μ_{ip} denotes the material balance coefficient for technology i and chemical p , whereas $MP(i)$ is the set of main products corresponding to each technology.

Equation (4) represents the mass balance for the warehouses. Here, for each scenario s , the inventory of the previous time period ($INV_{kpt-1,s}$) plus the amount transported from plant j to warehouse k must equal the material flow from the warehouse to the markets (Q_{klpts}^{WH}) plus the final inventory at time period t .

$$INV_{kpt-1,s} + \sum_j Q_{jkpts}^{PL} = INV_{kpts} + \sum_l Q_{klpts}^{WH} \quad \forall k, p, t > 1, s \quad (4)$$

Products sales at the markets (SA_{lpts}) are determined from the amount of materials sent by the warehouses, as it is stated in Eq. (5):

$$SA_{lpts} = \sum_k Q_{klpts}^{WH} \quad \forall p, l, t, s \quad (5)$$

Finally, Eq. (6) forces the total sales of product p at market l in period t and scenario s to be greater than the minimum demand target level (\underline{D}_{lpts}) and lower than the maximum demand (\overline{D}_{lpts}).

$$\underline{D}_{lpts} \leq SA_{lpts} \leq \overline{D}_{lpts} \quad \forall p, l, t, s \quad (6)$$

3.2 Capacity constraints

The production rate of each technology i in plant j , for each time period t and scenario s , must be lower than the existing capacity, C_{ijt}^{PL} , and higher than a minimum desired percentage, τ , of this existing capacity.

$$\tau C_{ijt}^{PL} \leq W_{ijpts} \leq C_{ijt}^{PL}, \quad \forall i, j, t, s \quad \forall p \in MP_i \quad (7)$$

The capacity of plant j in time period t is calculated from the existing capacity at the end of the previous period plus the expansion in capacity carried out in t , CE_{ijt}^{PL} :

$$C_{ijt}^{PL} = C_{ijt-1}^{PL} + CE_{ijt}^{PL} \quad \forall i, j, t \quad (8)$$

The capacity expansions are constrained within lower and upper limits, which are denoted by $\underline{CE}_{ijt}^{PL}$ and \overline{CE}_{ijt}^{PL} , respectively.

$$\underline{CE}_{ijt}^{PL} X_{ijt}^{PL} \leq CE_{ijt}^{PL} \leq \overline{CE}_{ijt}^{PL} X_{ijt}^{PL} \quad \forall i, j, t \quad (9)$$

In Eq. (9), binary variable X_{ijt}^{PL} indicates the occurrence of the capacity expansion. This variable takes the value of 1 if technology i at plant j is expanded in capacity in time period t , and 0 otherwise.

Similarly, as with the plants, we define a continuous variable to represent the capacity of the warehouses, C_{kt}^{WH} . Equation (10) forces the total inventory kept at warehouse k at the end of time period t in each scenario s (INV_{kpts}) to be less than or equal to the available capacity:

$$\sum_p INV_{kpts} \leq C_{kt}^{WH} \quad \forall k, t, s \quad (10)$$

In order to cope with fluctuations in demand, the storage capacity (C_{kt}^{WH}) must be twice the summation of the average storage inventory level kept at the warehouse in each scenario s (IL_{kts}):

$$2IL_{kts} \leq C_{kt}^{WH} \quad \forall k, t, s \quad (11)$$

The value of IL_{kts} is calculated from the output flow of materials and the turnover ratio of the warehouse (tor_k), which represents the number of times that the stock is completely replaced per time period:

$$IL_{kts} = \frac{\sum_l \sum_p Q_{lkpst}^{WH}}{tor_k} \quad \forall k, t, s \quad (12)$$

The capacity of the warehouse at any time period is determined from the previous one and the expansion in capacity executed in the same period:

$$C_{kt}^{WH} = C_{kt-1}^{WH} + CE_{kt}^{WH} \quad \forall k, t \quad (13)$$

The capacity expansion is also bounded within lower and upper limits.

$$\underline{CE_{kt}^{WH}} X_{kt}^{WH} \leq CE_{kt}^{WH} \leq \overline{CE_{kt}^{WH}} X_{kt}^{WH} \quad \forall k, t \quad (14)$$

This constraint makes use of the binary variable X_{kt}^{WH} , which equals 1 if an expansion in the capacity of warehouse k takes place in time period t and 0 otherwise.

The existence of a transportation link between plant j and warehouse k in period t and scenario s is represented by the binary variable Y_{jkt}^{PL} . A zero value of this variable prevents the flow of materials from taking place, whereas a value of 1 allows it within some lower and upper limits:

$$\underline{Q}_{jkt}^{PL} Y_{jkt}^{PL} \leq \sum_p Q_{jkpts}^{PL} \leq \overline{Q}_{jkt}^{PL} Y_{jkt}^{PL} \quad \forall j, k, t, s \quad (15)$$

3.3 Objective functions

The SC design model previously described must attain two different targets. The economic objective is represented by the NPV, whereas environmental concerns are quantified by the global warming potential (GWP), as described by the IPCC 2007 (Intergovernmental Panel on Climate Change) (Hischier R., 2010). Our model shows a different economic and environmental performance in each scenario. One objective of the mathematical formulation is to maximize the expected value of the resulting NPV distribution, $E[NPV]$. To control the probability of meeting unfavourable scenarios with high GWP values, we minimize as well the GWP in the worst (i.e., most unfavourable) scenario. The calculation of these two objectives is described next.

3.3.1 Expected NPV

At the end of the time horizon, different NPV values are obtained for each scenario, NPV_s , once the demand uncertainty is resolved. The expected value of the resulting distribution is determined from these values as follows:

$$E[NPV] = \sum_s prob_s NPV_s \quad (16)$$

where $prob_s$ is the probability of scenario s .

The NPV_s is calculated as the summation of the discounted cash flows (CF_{ts}) generated in each of the time periods t in which the time horizon is divided:

$$NPV_s = \sum_t \frac{CF_{ts}}{(1 + ir)^{t-1}} \quad \forall s \quad (17)$$

In this equation, ir represents the interest rate. The cash flow in each time period is determined from the net earnings (i.e., profit after taxes), and the fraction of the total depreciable capital ($FTDC_t$) that corresponds to the period:

$$CF_{ts} = NE_{ts} - FTDC_t \quad t = 1, \dots, NT - 1, \forall s \quad (18)$$

In Eq. (19), we consider that in the cash flow of the last time period ($t = NT$), part of the total fixed capital investment (FCI) will be recovered. This amount, which represents the salvage value of the network, may vary from one type of industry to another.

$$CF_{ts} = NE_{ts} - FTDC_t + svFCI \quad t = NT, \forall s \quad (19)$$

where sv is the salvage value fraction of the network.

The net earnings are obtained by subtracting costs and taxes from total incomes. Taxes accrued in period t are determined from the tax rate (φ) and gross profit (i.e., difference between incomes, total cost and depreciation, DEP_t):

$$NE_{ts} = incomes - costs - \varphi(incomes - (costs + DEP_t)) \quad \forall t, s \quad (20)$$

The total cost accounts for purchases of raw materials, operating cost, inventory costs, and transportation cost, as shown in Eq. (21):

$$\begin{aligned}
NE_{ts} = & (1 - \varphi) \left[\sum_l \sum_p \gamma_{lpt}^{FP} SA_{lpts} - \sum_j \sum_p \gamma_{jpt}^{RM} PU_{jpts} \right. \\
& \sum_i \sum_j \sum_{p \in MP(i)} v_{ijpt} W_{ijpts} - \sum_k \pi_{kt} IL_{kts} + \sum_j \sum_k \sum_p \psi_{jkpt} \lambda_{jk}^{PL} Q_{jkpts}^{PL} \\
& \left. - \sum_k \sum_l \sum_p \psi_{klpt} \lambda_{kl}^{WH} Q_{klpts}^{WH} \right] + \varphi DEP_t \quad \forall t, s
\end{aligned} \tag{21}$$

In this equation, γ_{lpt}^{FP} and γ_{jpt}^{RM} denote the prices of final products and raw materials, respectively. Furthermore, v_{ijpt} denotes the production cost per unit of main product p manufactured with technology i at plant j in period t , π_{kt} represents the inventory cost per unit of product stored in warehouse k during period t , and ψ_{jkpt}^{PL} and ψ_{klpt}^{WH} are the unitary transports cost. The depreciation term is calculated with the straight-line method:

$$DEP_t = \frac{(1-sv)FCI}{NT} \quad \forall t \tag{22}$$

where the total fixed cost investment (FCI) is determined from the capacity expansions made in plants and warehouses as well as the establishment of transportation links during the entire time horizon as follows:

$$\begin{aligned}
FCI = & \sum_i \sum_j \sum_t \left(\alpha_{ijt}^{PL} CE_{ijt}^{PL} + \beta_{ijt}^{PL} X_{ijt}^{PL} \right) + \sum_k \sum_t \left(\alpha_{kt}^{WH} CE_{kt}^{WH} + \beta_{kt}^{WH} X_{kt}^{WH} \right) + \\
& + \sum_j \sum_k \sum_t \beta_{jkt}^{TR} Y_{jkt}^{PL} \\
FCI = & \sum_i \sum_j \sum_t \left(\alpha_{ijt}^{PL} CE_{ijt}^{PL} + \beta_{ijt}^{PL} X_{ijt}^{PL} \right) + \sum_k \sum_t \left(\alpha_{kt}^{WH} CE_{kt}^{WH} + \beta_{kt}^{WH} X_{kt}^{WH} \right) + \\
& + \sum_j \sum_k \sum_t \beta_{jkt}^{TR} Y_{jkt}^{PL}
\end{aligned} \tag{23}$$

Here, parameters α_{ijt}^{PL} , β_{ijt}^{PL} and α_{kt}^{WH} , β_{kt}^{WH} are the variable and fixed investment terms corresponding to plants and warehouses, respectively. β_{jkt}^{TR} is the fixed investment term associated with the establishment of transportation links between plants and warehouses.

The total capital investment is constrained to be lower than an upper limit, as stated in Eq. (24):

$$FCI \leq \overline{FCI} \quad (24)$$

Finally, the model assumes that the payments of the fixed capital investment are divided into equal amounts distributed over the entire planning horizon. Hence, variable $FTDC_t$ is calculated as follows:

$$FTDC_t = \frac{FCI}{NT} \quad \forall t \quad (25)$$

3.3.2 Environmental Impact Assessment

In this work, we follow a combined approach that integrates LCA with optimization tools. This framework was first proposed by Stefanis and Pistikopoulos (Stefanis et al., 1995, 1997) and formally defined by (Azapagic and Clift, 1999).

Following this general approach, the environmental impact is quantified by the global warming potential (GWP) indicator, as described by the IPCC 2007 (Intergovernmental Panel on Climate Change) (Hischer R., 2010). Direct global warming potentials (GWPs) are expressed taking as reference the impact of carbon dioxide. GWPs estimate the relative global warming contribution of one kg of a particular greenhouse gas compared to the emission of one kg of carbon dioxide.

We perform a cradle-to-gate analysis to determine the total amount of global warming emissions released to the environment during the entire life cycle of the SC. GWPs are published for time horizons of twenty, one hundred and five hundred years (Pennington et al., 2000). Here, we use GWPs for one hundred years. We consider three main sources of emissions that contribute to the GWP damage: the consumption of raw materials (GWP_s^{RM}), the energy requirements (GWP_s^{EN}) and

the transportation tasks (GWP_s^{TR}). Hence, the total GWP for each scenario

(GWP_s^{total}) is determined as follows:

$$GWP_s^{total} = GWP_s^{RM} + GWP_s^{EN} + GWP_s^{TR} \quad \forall s \quad (26)$$

Mathematically, the impact is determined from the purchases of raw materials

(PU_{jpts}), production rates at the manufacturing plants (W_{ijpts}) and transport flows

(Q_{jkpts}^{PL} and Q_{klpts}^{WH}), as stated in Eq. (27):

$$\begin{aligned} GWP_s^{total} = & \sum_j \sum_p \sum_t IMP_p^{RM} PU_{jpts} + \sum_i \sum_j \sum_{p \in MP(i)} \sum_t IMP^{EN} \eta_{ijp}^{EN} W_{ijpts} \\ & + \sum_j \sum_k \sum_p \sum_t IMP^{TR} \lambda_{jk}^{PL} Q_{jkpts}^{PL} + \sum_k \sum_l \sum_p \sum_t IMP^{TR} \lambda_{kl}^{WH} Q_{klpts}^{WH} \quad \forall s \end{aligned} \quad (27)$$

In this equation, IMP_p^{RM} , IMP^{EN} , IMP^{TR} denote the cumulative life cycle impact assessment (LCIA) results associated with the consumption of 1 kg of raw material p , 1 MJ of energy, and transportation of 1 tonne 1 km of distance, respectively. These LCIA values are available in environmental database such as Ecoinvent (Frischknecht et al., 2005). In Eq. (27), λ_{jk}^{PL} and λ_{kl}^{WH} denote the distance between plants and warehouses and warehouses and markets, respectively. Finally, η_{ip}^{EN} represents the consumption of energy per unit of product p manufactured with technology i at plant j . This includes utilities such as electricity, steam, fuel, and cooling water.

3.3.3 Risk management metric for the environmental impact

Stochastic programming models typically optimize the expected value of the objective function distribution. As will be discussed later in the section 5.2, this strategy provides no control on the variability of the objective function in the

uncertain parameters space. Furthermore, the minimization of the expected environmental impact can lead to unrealistic solutions that do not represent any operational policy. For these reasons, in this work the variability of the GWP is controlled by appending to the objective function the worst case scenario (WC) risk metric (Birge and Louveaux, 1997). This stochastic metric is easy to implement and leads to good numerical performance in stochastic models (Bonfill et al., 2004). The worst case is determined from the maximum GWP attained over all the scenarios as follows:

$$GWP_s \leq WC \quad \forall s \quad (28)$$

4. Solution procedure

The overall bi-MILP formulation can be finally expressed in compact form as follows:

$$(M) \quad \begin{array}{l} \max_{x, x_s, y} \{ E[NPV](x, x_s, y); -WC(x, x_s, y) \} \\ s.t. \quad \text{Eqs. 1-28} \end{array} \quad (29)$$

Here, x generically denotes first stage continuous variables associated with structural decisions, while x_s denote second-stage decisions that depend on the scenario that finally materializes. In Eq. (29) y represents binary variables that model the existence of SC facilities and transportation links. The solution to this problem is given by a set of Pareto alternatives representing the optimal trade-off between the two objectives. In this work, these Pareto solutions are determined via the ε -constraint method (Ehrgott, 2005) which entails solving a set of instances of the following single-objective problem M1 for different values of the auxiliary parameter ε :

$$\begin{aligned}
(M1) \quad & \max_{x, x_s, y} \{E[NPV]\} \\
& s.t. \quad \text{Eqs. 1-28} \\
& \quad \quad WC \leq \varepsilon \\
& \quad \quad \underline{\varepsilon} \leq \varepsilon \leq \bar{\varepsilon}
\end{aligned} \tag{30}$$

where the lower and upper limits within which the epsilon parameter must fall are obtained from the optimization of each separate scalar objective. As the environmental impact increases as the economic performance of the SC also augments, we obtain the highest value for the WC of the GWP (that is $\bar{\varepsilon}$) by solving the following problem (M1a), where only the expected NPV objective is maximized:

$$\begin{aligned}
(M1a) \quad & (\bar{x}, \bar{x}_s, \bar{y}) = \arg \max_{x, x_s, y} \{E[NPV]\} \\
& s.t. \quad \text{Eqs. 1-28}
\end{aligned} \tag{31}$$

From the solution of problem (M1a), we calculate $\bar{\varepsilon} = WC(\bar{x}, \bar{x}_s, \bar{y})$. The best environmental performance of the SC is obtained regardless of the economic aspect. Hence we obtain the lowest value for the WC of the GWP (that is $\underline{\varepsilon}$) as the optimum value of the objective function for the next mono-objective problem:

$$\begin{aligned}
(M1b) \quad & \underline{\varepsilon} = \min_{x, x_s, y} \{WC\} \\
& s.t. \quad \text{Eqs. 1-28}
\end{aligned} \tag{32}$$

5. Case study

We revisit herein the first example introduced by Guillén-Gosálbez and Grossmann (Guillén-Gosálbez and Grossmann, 2009) that addresses the optimal retrofit of an existing SC established in Europe. The superstructure of this case study is shown in

Figure 2. The SC under study comprises 1 plant and 1 warehouse that are both located in Tarragona (Spain), and 4 final markets that are located in the following European cities: Leuna (Germany), Neratovice (Czech Republic), Sines (Portugal) and Tarragona. There are 6 different technologies available to manufacture 6 main products: acetaldehyde, acetone, acrylonitrile, cumene, isopropanol and phenol (

Figure 3). The demand is expected to increase in Leuna and Neratovice, so the problem consists of determining whether it is better to expand the capacity of the existing plant or open a new one in Neratovice, which would be closer to the growing markets. The existing plant has an installed capacity of 100 kton/year of each available technology, whereas the capacity of the existing warehouse equals 100 kton. No limits are imposed on the total number of expansions of plants and warehouses. The lower and upper limits for the capacity expansions are 10 and 400 kton/year for plants, and 5 and 400 ktons for warehouses, respectively. Furthermore, no upper limits on the purchases of raw materials are fixed. We set zero upper limits on purchases of intermediate and final products, as outsourcing is not allowed. The lower and upper bounds on the flows of materials between plants and warehouses and warehouses and markets are 5 and 500 kton/ year in both cases, respectively. The turnover ratio is equal to 10, while the initial inventories at the warehouses are assumed to be zero. No minimum production levels are defined for the plants. The interest rate, the salvage value and the tax rate are equal to 10%, 20% and 30%, respectively. In this example, we assume low transportation costs equal to 1.7 ¢/ton km. All the problem data can be found in Tables 1-7 of the original paper (Guillén-Gosálbez and Grossmann, 2009). Demand uncertainty is represented by 100 scenarios generated from a normal distribution with given mean value and standard deviation using the sampling algorithm MT19937 implemented in Matlab, which is based on the Mersenne Twister generator (Matsumoto and Nishimura, 1998). The mean value of each distribution is defined according to the deterministic (nominal) demand upper bound, $\overline{D_{lpt}^{MK}}$. The standard deviation of each distribution was set to

10 %. The demand lower bound for each scenario, $\underline{D}_{lpts}^{MK}$, is calculated as the demand upper bound for each scenario, \overline{D}_{lpts}^{MK} , times the demand satisfaction parameter, D_{sat} . A minimum demand satisfaction target level of 55 % of the maximum demand must be attained for each scenario in each of the years of a 3-year time horizon.

The model was implemented in GAMS ([Rosenthal, 2012](#)) and solved to global optimality (i.e., optimality gap of 0%) with CPLEX 12.1. The LCIA data were retrieved from the Ecoinvent database ([Hischier R., 2010](#)).

Figure 4 shows the Pareto curve obtained by following the proposed procedure. As seen, there is a clear trade-off between the economic indicator, $E[NPV]$, and the WC since reductions in environmental impact can only be achieved by compromising the economic benefit. Note that each point of the Pareto set in

Figure 4 entails a specific SC structure and set of planning decisions.

Figure 5 and

Figure 6 show the SC configurations of the extreme solutions (minimum WC and maximum expected NPV, respectively) for the first year. The capacities of the technologies (denoted by the letter Q) are expressed in tons and represented by numbers inside the black rectangles. Note that these capacities (variable C_{ijt}^{PL}) correspond to structural decisions that do not depend on the scenarios. Inside the same rectangles, we show the six production rates for the corresponding main products of each technology (letter F). As these variables (W_{ijpts}) are scenario-dependent, we provide only their expected values. The numbers inside each green rectangle represent the expected values of the upper bound level (denoted by SUB), total sales (denoted by SA) and lower demand (denoted by SLB). The numbers next to the arrows represent expected materials flows (denoted by TRA and TRB). As seen, the extreme solutions differ in the transportation flows between warehouses and markets and total network capacity. In the maximum $E[NPV]$ solution, part of the total production (85%) is made at the new plant that will be opened in Neratovice (Czech Republic), and then shipped to the warehouse located in the same city and distributed from there to the final markets, including the one located in Tarragona (Spain). In this case, the model takes advantage of the lower investment and production costs in Czech Republic compared to those in Spain. In contrast, in the minimum WC, the probability of sending products from Neratovice to the market located in Tarragona is very low, 0.3 % (this probability is 12 times higher in the maximum $E[NPV]$ solution). The second difference concerns the SC capacity, which is lower in the minimum environmental impact design (83 % of the SC capacity in the maximum expected NPV solution). In the minimum WC solution, the

production rates are reduced and the demand satisfaction level drops to values close to its lower limit, whereas in the maximum NPV solution, the level of sales is close to its upper limit.

Figure 7 depicts the probability distribution of the NPV associated with the extreme Pareto solutions. As observed, as the WC decreases from the maximum value

3.17×10^9 kg CO₂-Eq (

Figure 7b) to its minimum value, 2.40×10^9 kg CO₂-Eq (

Figure 7a), the probability distributions of the NPV are shifted to the left. For instance, the probability of surpassing a NPV value of US\$ 1.32×10^8 (dashed line in

Figure 7a and 7b) is 0.66 in the maximum economic performance solution, and only 0.13 in the minimum worst case one.

Figure 8 shows for the extreme solutions the contribution of the 3 main sources of environmental impact (raw materials production, utilities generation and transportation tasks) in all of the scenarios. Note that the extraction of raw materials represents the most significant contribution to the total impact.

5.1 Comparison between stochastic and deterministic solution

To further highlight the importance of using a stochastic model, we compared the solutions produced by the deterministic and stochastic approaches. Note that the deterministic model can be easily obtained from the stochastic one (eqs. (1)-(27)) by defining only one single scenario which corresponds to the mean demand. Hence, we first solved the deterministic MILP maximizing the NPV and minimizing the GWP, thereby generating a set of SC designs and associated planning decisions. These SC configurations were next fixed in the stochastic model in which we maximized the expected NPV and minimized the WC fixing the structural continuous and binary variables $(x^{\text{det},\text{struct}}, y^{\text{det},\text{struc}})$ to the values provided by the deterministic model:

$$\begin{aligned} \max_{x, x_s} \{ & E[NPV](x^{\text{det},\text{struct}}, x, x_s, y^{\text{det},\text{struc}}); -WC(x^{\text{det},\text{struct}}, x, x_s, y^{\text{det},\text{struc}}) \} \\ & s.t. \quad \text{Eqs. 1-28} \end{aligned} \quad (33)$$

Figure 9 shows the expected NPV and WC of the solutions generated with the stochastic and deterministic models. As seen, the stochastic solution dominates the deterministic design when we consider the two dimensional space given by the expected NPV and worst case. The difference between both solutions along the Pareto front varies between US\$ 1.9×10^6 and US\$ 1.0×10^6 depending on the worst case value, but it is always above 1 % of the economic performance shown by the stochastic solution. This is a clear proof that the use of a stochastic formulation is highly recommendable in this context.

5.2 Disadvantages of the expected impact for the environmental objective

Finally, to illustrate the disadvantages of minimizing the expected impact instead of the worst case, we solved the stochastic model maximizing the expected NPV and imposing a bound on the expected impact of 2.55×10^9 kg CO₂-Eq. We then fixed the SC configuration computed by this model, and solved the stochastic model again maximizing the expected NPV and removing any bound on the expected impact.

Figure 10 depicts the largest demand and the sales of products attained by the fixed configuration in both cases (i.e., in the models with and without the constraint on the expected environmental impact) and in every scenario, which inform about the demand satisfaction level reached in every scenario. The latter values (demand satisfaction levels in the stochastic model without any environmental constraint) represent the most profitable operating mode, that is, the operating mode that would lead to the largest benefits. Indeed, for the model without any environmental constraint (

Figure 10b), the product sales match the product demand. In contrast, the demand satisfaction levels obtained when the environmental constraint is added reflect a policy consisting of making as much profit as possible while still fulfilling the environmental legislation. As observed in

Figure 10a, there are cases (for example, in scenarios 26 and 29, or in scenarios 76 and 96) in which the demand is very similar, but the product sales greatly differ. In practice, the stochastic model behaves in a rather conservative manner in some scenarios (29 and 76), and more aggressively in others (scenarios 26 and 96). This solution follows this strategy in order to satisfy the expected environmental performance sought while maximizing at the same time the expected benefit. Hence, this solution does not reflect any realistic policy, since the way to operate the SC in one scenario depends on the performance attained in others, which makes no sense in a real industrial environment. In contrast, the WC reflects a clear strategy: to make as much profit as possible while ensuring at the same time a minimum environmental performance.

6. Conclusions

This article has addressed the optimal design and planning of chemical SC under demand uncertainty. The problem was mathematically formulated as a bi-criterion stochastic MILP that accounts for the maximization of the expected NPV and minimization of the environmental impact performance (GWP). The variability of the latter criterion, quantified according to LCA principles, was controlled using the worst case metric. The capabilities of the model were highlighted through its application to a case study. The solutions obtained by the proposed approach, which provide valuable insights into the design problem, are intended to guide decision-makers towards the adoption of more sustainable process alternatives. Our stochastic approach maximizes the expected profit while satisfying at the same time a maximum allowable environmental impact. Numerical results show that the stochastic design improves the deterministic one and should be therefore the

preferred choice in practice. Finally, we showed that the minimization of the expected environmental impact leads to unrealistic results, and should be therefore avoided.

Acknowledgements

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Nomenclature

Sets/Indices

I/i set of manufacturing technologies indexed by i

J/j set of plants indexed by j

K/k set of warehouses indexed by k

L/l set of markets indexed by l

P/p set of products indexed by p

S/s set of scenarios indexed by s

T/t set of time periods indexed by t

Subsets

$MP(i)$ set of main products p of technology i

$IN(p)$ set of manufacturing technologies that consume p

$OUT(p)$ set of manufacturing technologies that produce p

Parameters

D_{sat} demand satisfaction factor [dimensionless]

$\overline{D_{lpt}^{MK}}$ deterministic value of the maximum demand of product p sold at market l in period t [tons]

$\overline{D_{lpts}^{MK}}$ maximum demand of product p sold at market l in period t in scenario s [tons]

$\underline{D_{lpts}^{MK}}$ minimum demand of product p to be satisfied at market l in period t in scenario s [tons]

ir interest rate [dimensionless]

$\overline{PU_{jpt}}$ upper bound on the purchases of product p at plant j in period t [tons]

$\underline{PU_{jpt}}$ lower bound on the purchases of product p at plant j in period t [tons]

$\overline{SA_{lpts}}$ upper bound on the sales of product p at market l in time period t in scenario s [tons]

$\underline{SA}_{lp ts}$	lower bound on the sales of product p at market l in time period t in scenario s [tons]
sv	salvage value fraction of the network [dimensionless]
tor_k	turnover ratio of warehouse k [dimensionless]
α_{ijt}^{PL}	variable investment coefficient associated with technology i at plant j in time period t [$\$ \cdot \text{ton}^{-1}$]
α_{kt}^{WH}	variable investment term associated with warehouse k in time period t [$\$ \cdot \text{ton}^{-1}$]
β_{ijt}^{PL}	fixed investment term associated with technology i at plant j in time period t [$\$$]
β_{kt}^{WH}	fixed investment term associated with warehouse k in time period t [$\$$]
β_{jkt}^{TR}	fixed investment term associated with the establishment of a transport link between plant j and warehouse k in time period t [$\$$]
$\gamma_{lp t}^{FP}$	price of final product p sold at market l in time period t [$\$ \cdot \text{ton}^{-1}$]
γ_{jpt}^{RM}	price of raw material p purchased at plant j in time period t [$\$ \cdot \text{ton}^{-1}$]
η_{ijp}^{EN}	energy consumed per unit of chemical p produced with manufacturing technology i at plant j [TFOE/ t p], (Tons of Fuel Oil Equivalent = 41.868 GJ)
λ_{jk}^{PL}	distance between plant j and warehouse k [km]
λ_{jk}^{WH}	distance between warehouse k and market l [km]
ξ_d	weighting factor for damage category d
μ_{ip}	mass balance coefficient associated with product p and manufacturing technology i [dimensionless]
π_{pkt}	inventory cost per unit of product stored p in warehouse k during period t [$\$ \cdot \text{ton}^{-1}$]

φ	tax rate [dimensionless]
v_{ijpt}	production cost per unit of main product p manufactured with technology i at plant j in period t [$\$/\text{ton}^{-1}$]
ψ_{pjkt}^{PL}	unitary transport cost of product p sent from plant j to warehouse k in time period t [$\$/\text{ton}^{-1}\cdot\text{km}^{-1}$]
ψ_{klpt}^{WH}	unitary transport cost of product p sent from warehouse k to market l in time period t [$\$/\text{ton}^{-1}\cdot\text{km}^{-1}$]
τ	minimum desired percentage of the installed capacity that must be utilized [dimensionless]

Variables

C_{ijt}^{PL}	capacity of manufacturing technology i at plant j in time period t [tons]
C_{kt}^{WH}	capacity of warehouse k in time period t [tons]
CE_{ijt}^{PL}	capacity expansion of manufacturing technology i at plant j in time period t [tons]
CE_{kt}^{WH}	capacity expansion of warehouse k in time period t [tons]
CF_{ts}	cash flow in period t in scenario s [\\$]
DEP_t	depreciation term in period t [\\$]
FCI	Total fixed capital investment [\\$]
$FTDC_t$	fraction of the total depreciable capital that must be paid in period t [\\$]
GWP_s^{EN}	contribution to the total GWP due to the energy consumed by the utilities in scenario s [kg CO ₂ -Eq]
GWP_s^{RM}	contribution to the total GWP due to consumption of raw materials in scenario s [kg CO ₂ -Eq]
GWP_s^{TR}	contribution to the total GWP due to the transportation of the materials between the nodes of the SC in scenario s [kg CO ₂ -Eq]
GWP_s^{total}	total Global Warming Potential in scenario s [kg CO ₂ -Eq]

IL_{kts}	average inventory level at warehouse k in time period t in scenario s [tons]
INV_{kpts}	inventory of product p kept at warehouse k in period t in scenario s [tons]
NE_{ts}	net earnings in period t (profit after taxes) [\$]
NPV	net present value [\$]
NT	number of time periods [dimensionless]
PU_{jpts}	purchases of product p made by plant j in period t in scenario s [tons]
Q_{jkpts}^{PL}	flow of product p sent from plant j to warehouse k in period t in scenario s [tons]
Q_{klpts}^{WH}	flow of product p sent from warehouse k to market l in period t in scenario s [tons]
SA_{lpts}	sales of product p at market l in time period t in scenario s [tons]
W_{ijpts}	input/output flow of product p associated with technology i at plant j in period t in scenario s [tons]
X_{ijt}^{PL}	binary variable (1 if the capacity of manufacturing technology i at plant j is expanded in time period t , 0 otherwise) [dimensionless]
X_{kt}^{WH}	binary variable (1 if the capacity of warehouse k is expanded in time period t , 0 otherwise) [dimensionless]
Y_{jkt}^{PL}	binary variable (1 if a transportation link between plant j and warehouse k is established in time period t , 0 otherwise) [dimensionless]

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Figure Captions

Figure 1. Superstructure of the three-echelon SC taken as reference.

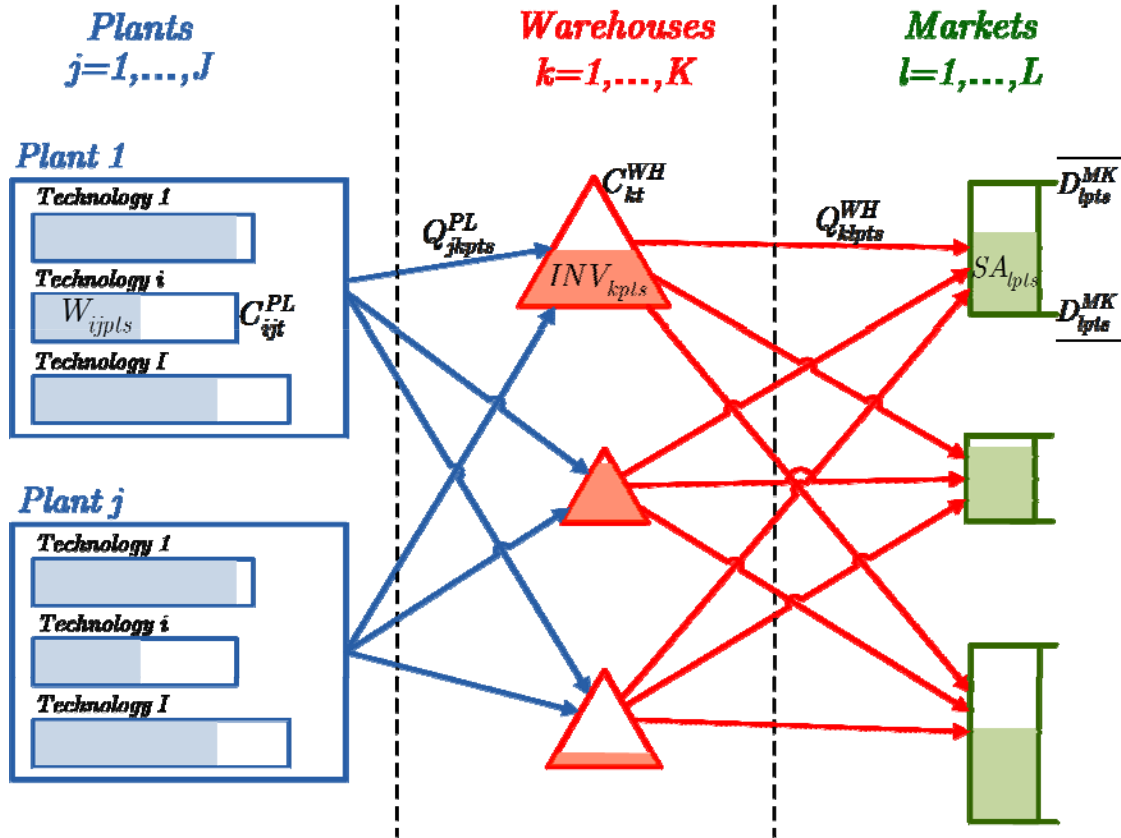


Figure 2. Superstructure of the case study.

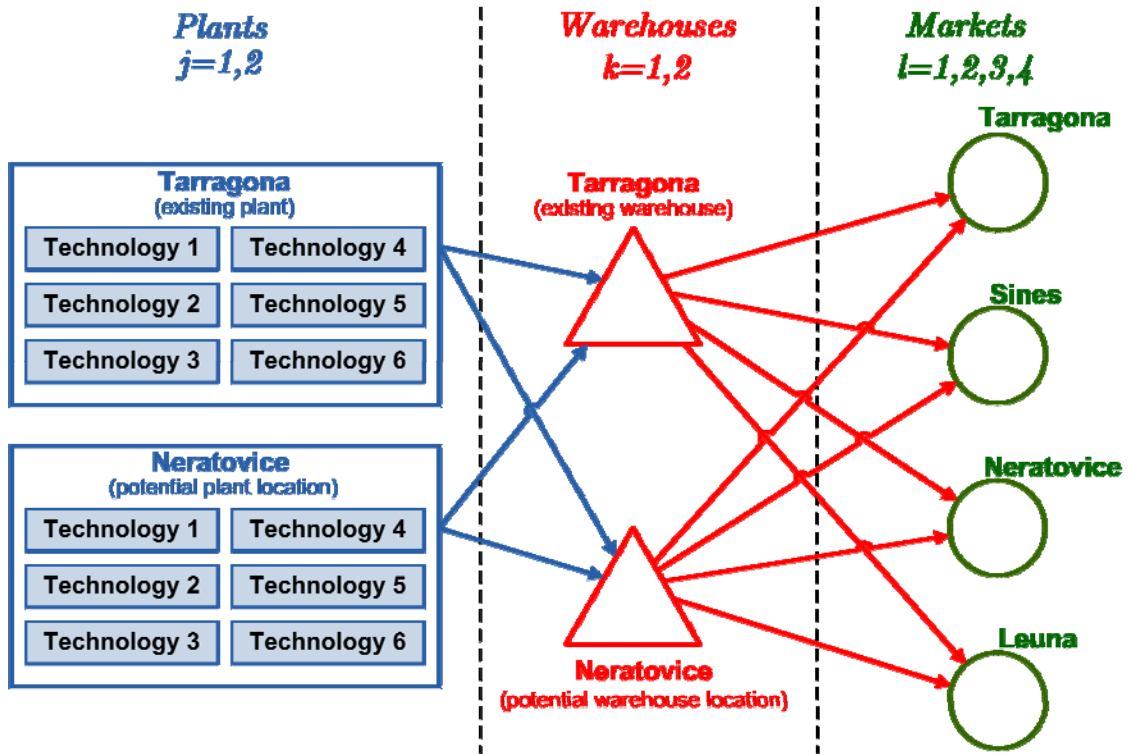


Figure 3. Available technologies at each plant.

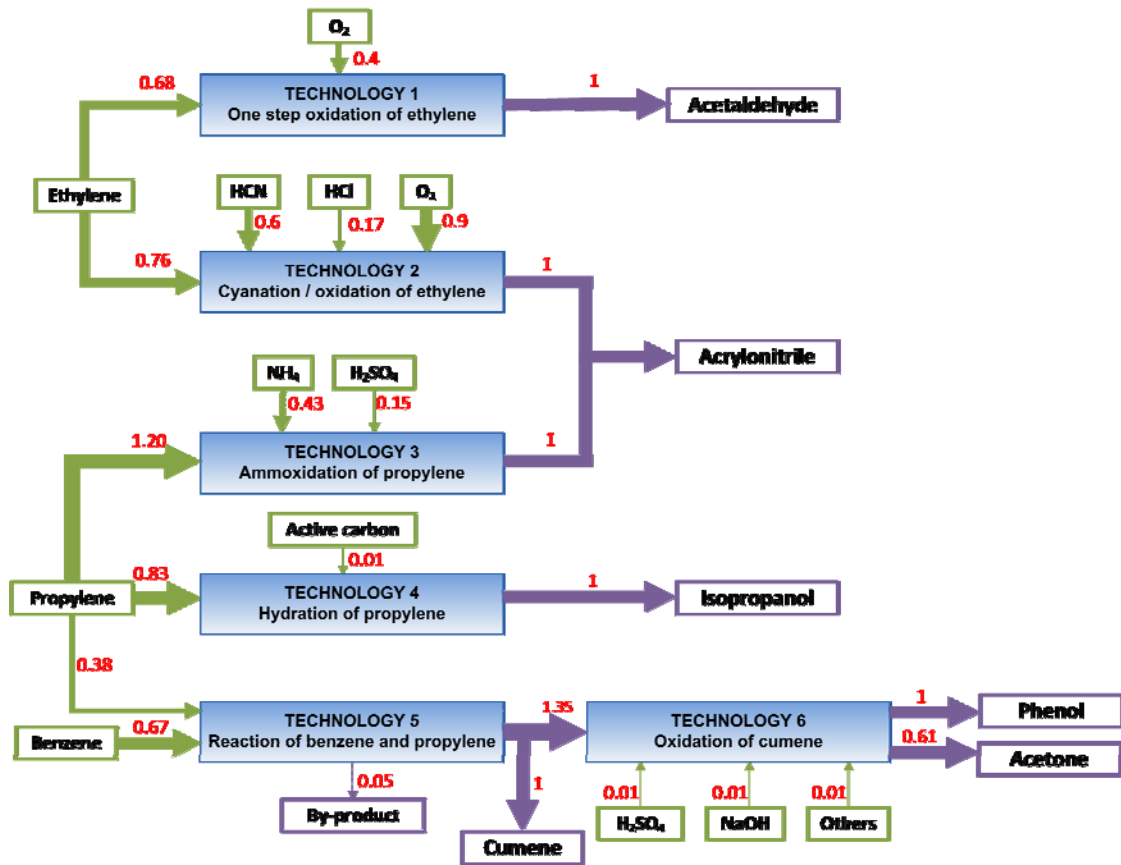


Figure 4. Pareto set of solutions for the environmental impact and economic performance.

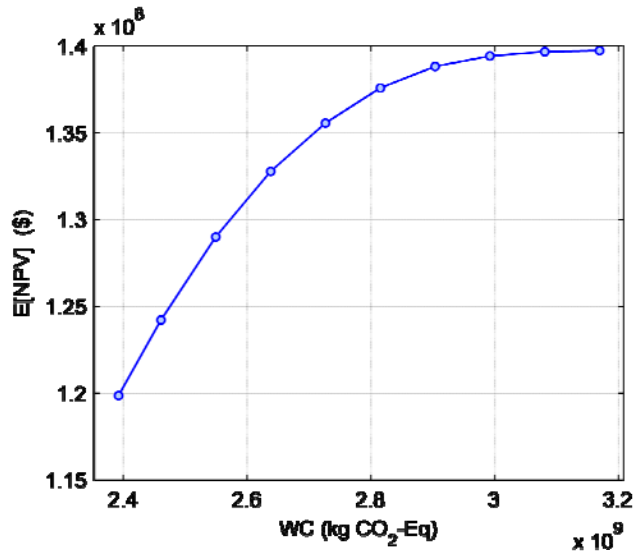


Figure 5. SC Topology for the extreme solution corresponding to the minimum WC.

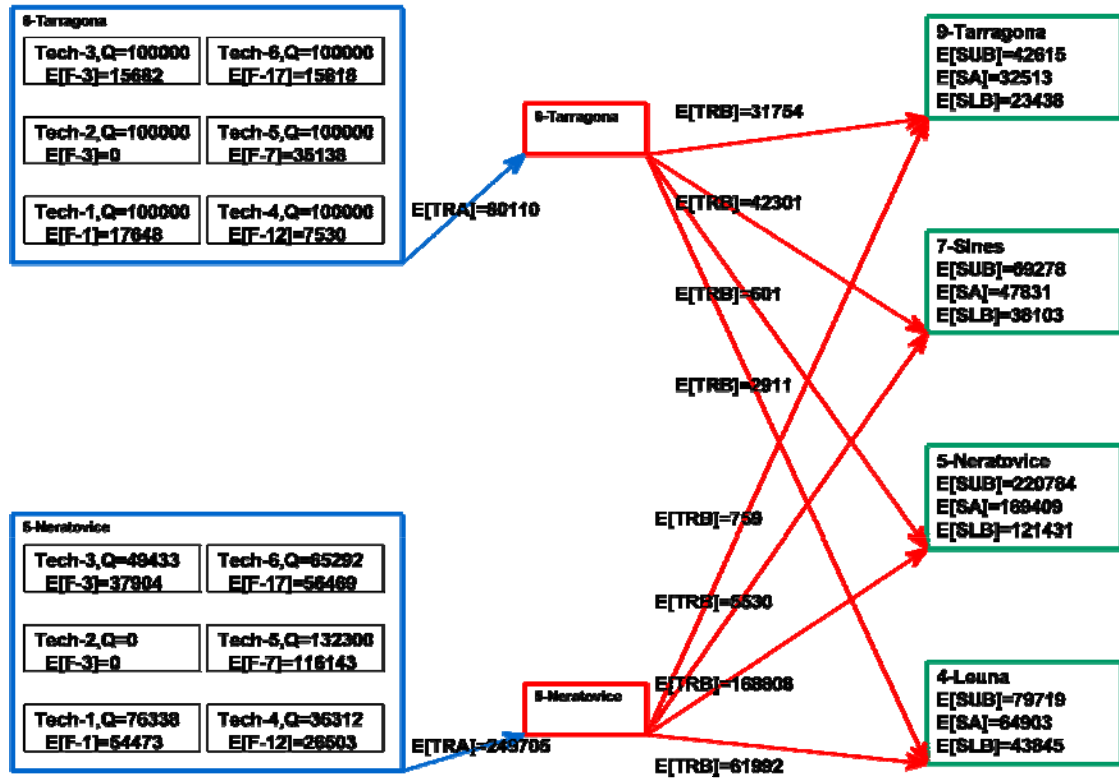


Figure 6. SC topology for the extreme solution corresponding to the maximum

$$E[NPV]$$

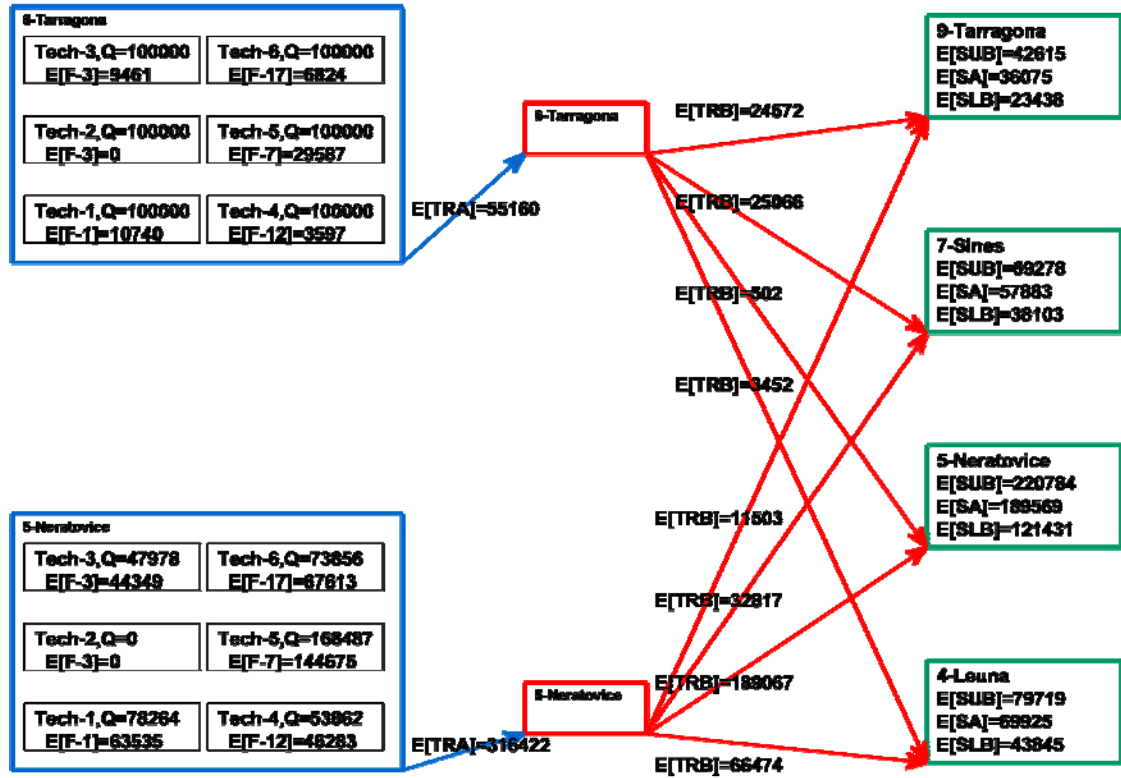


Figure 7. NPV distribution for the extreme Pareto solutions: a) minimum WC; b)

maximum expected NPV

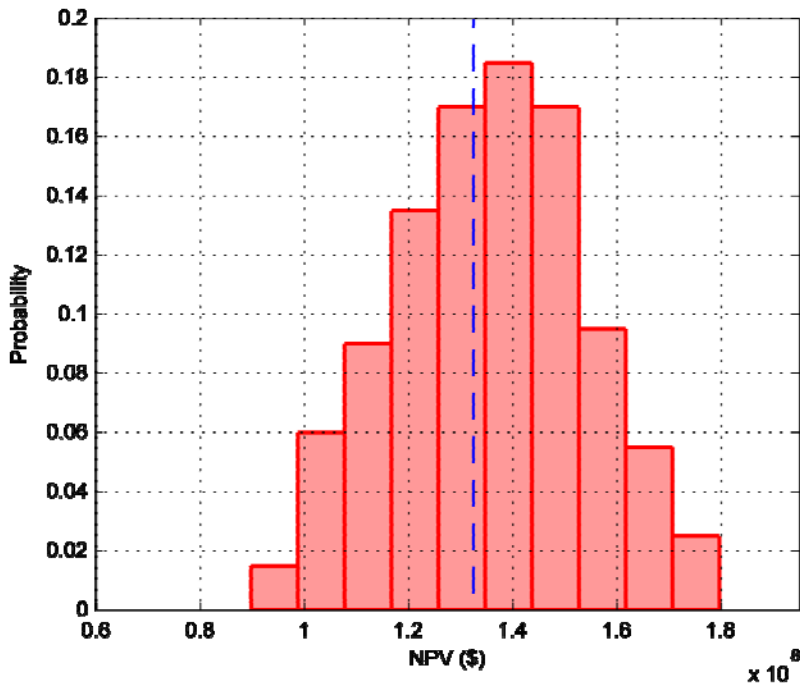
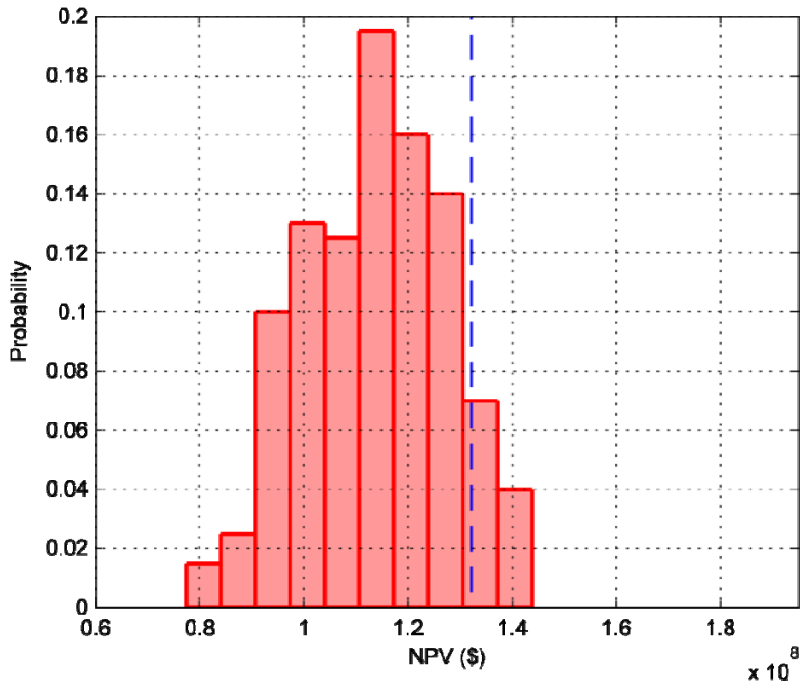


Figure 8. Contribution of the 3 main sources of environmental impact in each scenario for the extreme solutions: a) minimum WC; b) maximum expected NPV.

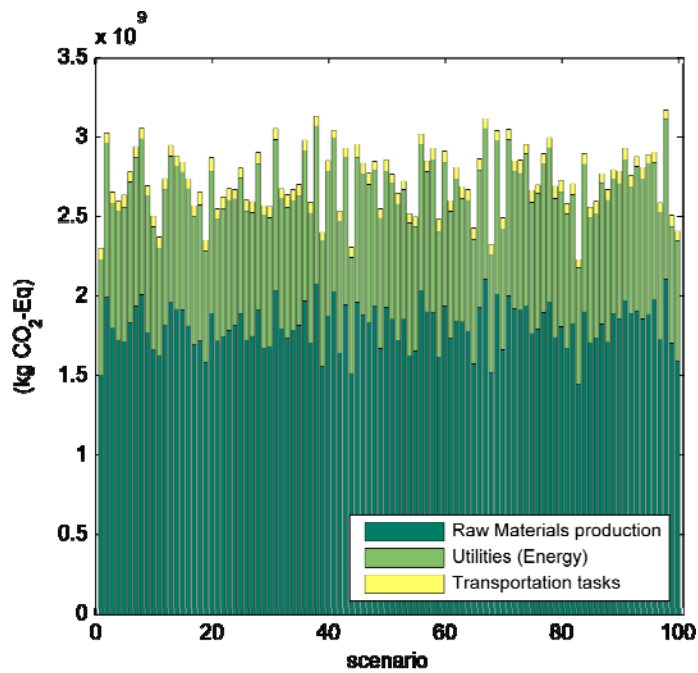
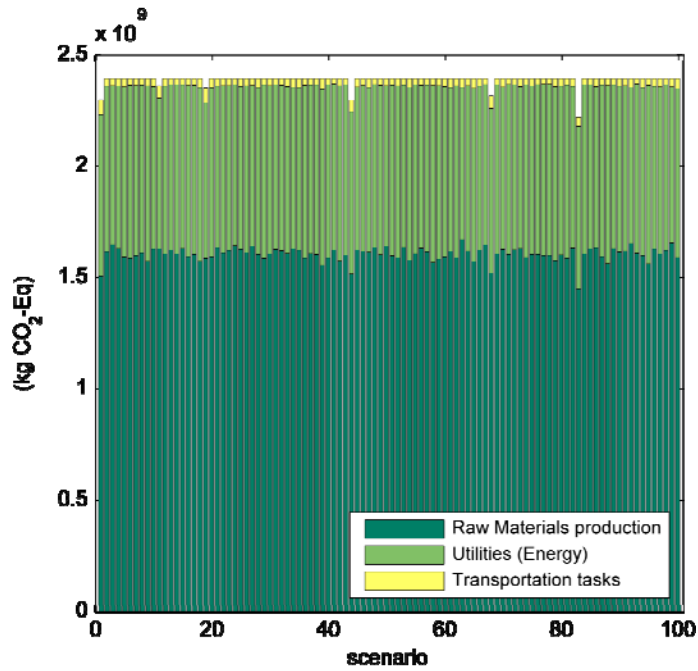


Figure 9. Comparison for the two Pareto set of solutions obtained by the stochastic design and by the deterministic design evaluated with the stochastic model.

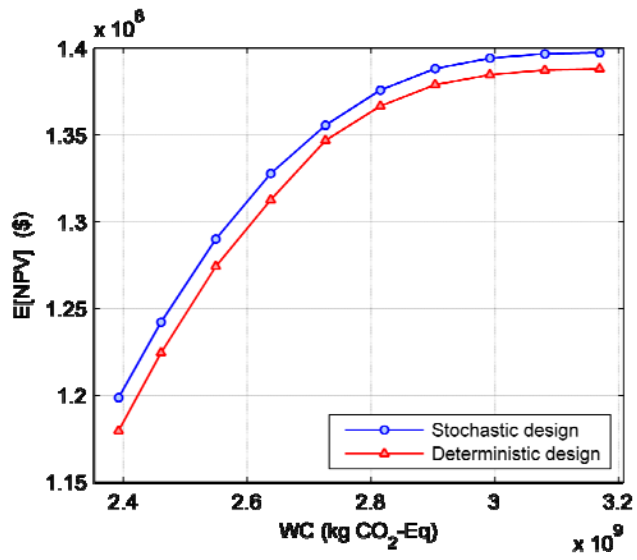


Figure 10. Demand upper limit and sales for all the scenarios for the product cumene in the market Neratovice during the first year: a) model with a bound on the expected environmental impact; b) model without any constraint on the expected environmental impact.

