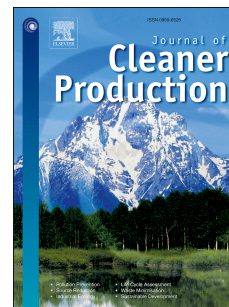


Journal Pre-proof

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A cooperative game strategy for designing sustainable supply chains under the emissions trading system

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Highlights

- Optimum supply chain management under the carbon-trade policy is addressed.
- Cooperation among different companies leads to economic and environmental benefits.
- Cooperative game theory ensures the stability of cooperation (grand coalition).
- CO₂ price evolution, predicted by ARIMA models, affects the supply chain behavior.

Abstract

The growing environmental concerns, as well as governments policies regarding greenhouse gas (GHG) emissions, promote Supply Chain (SC) design and management strategies that simultaneously benefit companies in economic terms and the society by reducing the total CO₂ emissions. Some game theoretic approaches have been applied to SC design and management, most of them in competitive game schemes. However, there is a lack of studies within the cooperative game framework. To fill this gap, in this paper cooperative games theory has been applied to motivate cooperation among companies for the optimum management of a SC for the chemical industry in Europe under the existing Emissions Trading System (ETS), which represents a financial incentive to cut off GHG emissions. We present a novel methodology that integrates the SC economic and environmental assessment, including carbon trading policy, within the cooperative game framework. The companies involved in the SC are considered as players participating in a cooperative game. The results highlight that when the companies cooperate in a grand coalition, that is, all the companies work in a cooperating SC, the NPV is higher and the environmental impact, assessed as the Global Warming Potential (GWP), is lower than the overall NPV and GWP achieved by the companies acting individually. The stability of the grand coalition is assured by finding a profit share drawn from the core of the game. Additionally, a sensibility analysis has been carried out with the aim of appraising the effect of the key parameters of the carbon trading policy (i.e. CO₂ price and emissions cap) on the game, showing that the more restrictive the conditions are, the more advantageous the cooperation is.

Keywords: CO₂ cap-and-trade, cooperative games, optimum supply chain management, ARIMA price prediction.

1 Introduction

The objective of supply chain (SC) management is to be efficient and cost-effective across the entire system, which involves integration of suppliers, manufacturers, warehouses and stores (Simchi-Levi et al., 2000). However, as well as other topics related to industrial development, SC networks demand the application of the sustainability principles during their process design. One major motivation for this trend is the growing environmental concerns regarding climate change, which has led governments to adopt specific policies to reduce greenhouse gas (GHG) emissions. One of these policies are market-based instruments to reduce emissions, which can also represent a financial incentive for companies. In this sense, in 2005 it was launched the European Union Emissions Trading System (EU ETS), which aims to reduce GHG emissions by at least 40 % from 1990 levels by 2030 (European Commission, 2014). Although the EU ETS was the world's first international emissions trading system, there are other national systems already operating, which the EU cooperate with through the International Carbon Action Partnership (ICAP). The ETS is based on the cap-and-trade principle, which consists on setting a cap on the total amount of GHG that can be emitted by installations covered by the system. Within the cap, the companies receive emission allowances each year which they can trade with as needed. Each allowance provides companies the right to emit one ton of CO₂. If a company's emissions are higher than the number of allowances free allocated by the government, it can buy more from another company with allowances surplus. The cap is reduced annually by a linear reduction factor, so total emissions fall over time. The current method of allocating allowances is auctioning. According to the EU ETS Directive, at least 50 % of the revenues generated from the auctioning of allowances should be used for climate and energy purposes (European Commission, 2017).

1.1 Supply Chains under the ETS

Within this framework, industries involved in the ETS must reconsider their SC network strategies to reduce their GHG emissions as much as possible, so they do not have to buy extra rights, that would reduce their net income. The cap-and-trade regulation policy is one of the most effective emission reduction mechanisms and has been widely implemented (Xu et al., 2016). Comparing with the other globally used carbon regulatory practice (carbon tax), carbon trading mechanism results in better supply chain performance in terms of emissions generation and cost (Zakeri et al., 2015). Ramudhin et al. (2010) were the firsts to propose a carbon market sensitive

planning for sustainable supply chain network design (Chaabane et al., 2012). They apply the methodology to an example derived from the steel industry. Chaabane et al. (2012) presented a mathematical model for the design of sustainable supply chains over their life cycle. Ruiz-Femenia et al. (2012) analyzed the effect of incorporating the carbon emissions trading to the optimal design of a SC in the chemical industry taking into account the uncertainty in the CO₂ emission allowances price. They apply their model to a petrochemical SC previously studied by Guillén-Gosálbez and Grossmann (2009). Fareeduddin et al. (2015) presented optimization models based on carbon regulatory policies for a closed-loop supply chain considering strict carbon caps, carbon tax, and carbon cap-and-trade. Xu et al. (2016) analyzed the behavior of a two-echelon SC under the cap-and-trade regulation using different mechanisms of cooperation, such as revenue sharing and two-part tariff contracts. The authors also carried out a sensitivity analysis to determine the effect of the emissions cap and market price.

As pointed out by many authors (Chen et al., 2016; Hua et al., 2011; Ruiz-Femenia et al., 2012; Xu et al., 2016; Zakeri et al., 2015), one key point for the SC planning and management under the carbon trade scheme is the CO₂ allowances price, which in turn represents a great uncertainty source due to market dependency. In fact, since the implementation of the EU ETS, CO₂ price has undergone a constant variation along the entire period (historic CO₂ allowances price data are available on Market Insider website). After the low levels (around 5 €) achieved during the period 2012-2017, the CO₂ allowances price rose dramatically (more than 25 €/ton CO₂), and this trend is expected to be maintained during the next years due to the planned reduction in the carbon cap.

Therefore, an accurate method for the prediction of the allowances price is decisive for the design of a cost and environmental-effective SC. Different models, such as statistical and econometric models, artificial intelligence models, and ensemble (hybrid) models have been proposed in the literature to forecast the carbon price (Zhu et al., 2018) as well as other commodity prices (Contreras et al., 2003). One of the most popular models used for this purpose is the autoregressive integrated moving average (ARIMA) models (Box et al., 1994), as they can characterize nonlinear data (Zhou et al., 2014) and exhibit the advantage of its ease of use, accuracy and mathematical soundness (Contreras et al., 2003; Zhu and Wei, 2013).

1.2 Game theory strategies in supply chain

Due to the globalization of markets, business decisions on SC management are influenced not only by a single decision-maker but by several. Within this framework of multi-decision maker, game theory, which predicts the rational strategic behavior of individuals in conflicting or cooperating situations, seems to provide an adequate modeling basis for problems in SC management (Drechsel, 2010; Leng and Parlar, 2005). The field of game theory may be divided roughly in two parts, namely non-cooperative game theory (each player optimizes its own objective and does not care for the effect of its decisions on others) and cooperative game theory (all players share the same objective). In turn, non-cooperative games are divided in sequential and simultaneous games (Cachon and Netessine, 2004) depending on the decision making sequence. In sequential games, players acting later have knowledge about decisions of early players (e.g. Stackelberg game), while in simultaneous games all players make decisions simultaneously (Gao, Jiyao and You, Fengqi, 2017). Game theory, specially non-cooperative sequential games, has been successfully applied to many fields, some of them of great importance in the chemical industry such as the facilities safety (Chen et al., 2020; Wu et al., 2020; Zhang and Reniers, 2018).

The main concern regarding non-cooperative game theory applied to industrial SCs is whether this approach provides a solution that maximizes the total profit under Nash equilibrium (Zamarripa et al., 2012). On the other hand, one of the main questions when applying cooperative game theory to SC networks is whether cooperation is stable, that is, whether there exists an allocation of the joint profit among all parties (companies involved in the SC) so that there is no company or group of them that can obtain a greater benefit from that assigned within the coalition. Both competitive and cooperative game theories have been used by many authors to design effective SC managing strategies. Nagarajan and Sošić (2008) published a review where different models based on game theory are analyzed and Fiestras-Janeiro et al. (2011) provided a review of the applications of cooperative game theory in the management of centralized inventory systems. Yue and You (2014) presented a mathematical model for the optimal design of non-cooperative three-echelon biorefineries SC using the leader-follower approach (Stackelberg game). This same approach was later used to optimize the design of shale gas supply chains under economic and life cycle criteria (Gao, J. and You, F., 2017a, b). Zamarripa et al. (2013) addressed the SC planning problem through a multi-objective optimization of two SCs acting in both competing and cooperating scenarios to lead the decision-making process. This work was an extension of a previous one (Zamarripa et al., 2012) in which the SC planning is performed under competition

environment. Madani and Rasti-Barzoki (2017) developed a competitive mathematical model of government as the leader and two competitive green and non-green supply chains as the followers. More recently, Zheng et al. (2019) have employed cooperative and non-cooperative game theoretic analyses to characterize interactions among different parties of a three-echelon closed-loop supply chain (which involves remanufacturing and recycling used products); Jamali and Rasti-Barzoki (2019) examined different variables in a SC considering different game scenario; Li (2020) considered the social responsibility of a SC considering four non-cooperative game situations and Carrero-Parreño et al. (2019) have studied the economic and environmental benefits of cooperation in water management in the shale gas industry.

Although some of the aforementioned literature presented SC design models including environmental concerns, none of them accounted for specific carbon emission policies. In this sense, and Xia et al. (2020) analyzed the impact of carbon trading on low-carbon supply chain under different production modes. They apply a non-cooperative game model between low-carbon and ordinary products, based on which they analyzed the impact of carbon trading on unit retail price, sales volume, sales profit and consumer surplus. Xing et al. (2020) used Stackelberg games to study the changes in expected utility of supply chain and its members brought by changes in carbon emission trading price, consumers' low-carbon awareness, carbon emission and competition of third-party recyclers. Halat and Hafezalkotob (2019) presented a study aiming to optimize the inventory cost of a three stage SC applying a Stackelberg game between the government and the SC, where the government is the leader and the SC is the follower in decision making, under four different carbon emission regulations (i.e. carbon cap, carbon tax, carbon trade, and carbon offset). Using a similar game approach, Du et al. (2015) analyzed the impact of emission cap-and-trade mechanism in an emission-dependent supply chain. Other authors (Tong et al., 2019) also used this game structure but with different players. In their study the SC is led by the retailer and manufacturers act upon the retailer's action. Within this framework, they developed an evolutionary game to analyze the SC behavior under a cap-and-trade system. Yang et al. (2017) considered vertical (among different levels of the SC) and horizontal (among entities of the same level of different SCs) cooperation for two competitive supply chains consisting of one manufacturer and one retailer, under the cap-and-trade scheme. In the vertical direction, the manufacturer is the leader and the retailer the follower and in the horizontal direction, there is a Nash game about the emission reduction decisions between manufacturers.

Table 1 presents a summary of the reviewed literature presenting game theoretic approaches to the SC management including the main features of their models in comparison with the model described in the present study.

Table 1. Comparison between this paper and related studies reviewed.

Authors	Environmental impact	Carbon trading	Carbon price forecast	Game theory	
				Non-cooperative	Cooperative
Zamarripa et al. (2013)				√	√
Yue and You (2014)				√	
Du et al. (2015)		√		√	
Gao and You (2017a, b)				√	
Yang et al. (2017)	√			√	
Madani and Rasti-Barzoki (2017)	√			√	
Zheng et al. (2019)				√	√
Jamali and Rasti-Barzoki (2019)	√			√	
Halat and Hafezalkotob (2019)		√		√	
Tong et al. (2019)		√		√	
Xia et al. (2020)		√		√	
Xing et al. (2020)		√		√	
Li (2020)				√	
This study	√	√	√		√

As shown in Table 1, most of the literature reviewed regarding game theoretic approach to the design and performance of SC under the carbon trade system apply competitive (or non-cooperative) game strategies, specially the Stackelberg game (leader-follower). However, to the best of our knowledge, there is a lack of literature regarding cooperative game strategies applied to SC management, especially in the context of carbon cap-and-trade. Indeed, (Agi and Hazir, 2019) in a recent review pointed out the scarcity of studies applying cooperative game concepts to green supply chain management. Although economic advantages in horizontal cooperation (i.e. companies belonging to the same SC stage) have been proven (Drechsel, 2010), there is also a research gap regarding the environmental interest of this type of cooperation in SC. To fill this gap, in this work we explore not only the economic but also the possible environmental benefit of cooperation among different companies that manufacture same chemical products within the EU ETS scheme. Thus, the main novelties of our study

are: 1) the application of cooperative games theory to the optimal design of sustainable Supply Chains for petrochemical industries; 2) exploring, besides the economic advantage, the possible environmental benefit of horizontal cooperation among companies; 3) incorporating the carbon trading policy to a multi-period optimization SC model; and 4) the use of ARIMA methodology for the prediction of CO₂ allowances price in the time horizon considered. As far as we know, this is the first time that these four features are integrated in a modeling framework that can be used to lead decision and policy makers.

The remainder of the paper is organized as follows: section 2 describes the problem statement, in section 3 the methodology and mathematical formulation is detailed, sections 4 and 5 present the case study selected and main results obtained and, finally, in section 6 the conclusions drawn from the results are exposed.

2 Problem statement

We consider a three-echelon SC for the chemical industry consisting of production, storage and market stages. The general network includes a set of plants, placed in different locations in Europe, with their respective associated warehouses and a set of markets, where the products manufactured at plants are sold under certain demand limits. The sets of plants, warehouses and markets are indexed by j , k and l , respectively. Every plant has 6 available technologies (indexed by i), which are used to obtain 6 different chemical products (indexed by p). Assuming a possible horizontal cooperation among firms (i.e. plants), the respective warehouses can be shared among all plants, so the minimum product total demands imposed by the markets can be satisfied at the maximum profit. Therefore, all possible connections among plants, warehouses and markets are considered for the cooperating SC planning (Figure 1). This SC superstructure is based on that originally presented by Guillén-Gosálbez and Grossmann (2009), which study was later extended by other authors (Ruiz-Femenia et al., 2013; Ruiz-Femenia et al., 2012). The main difference between our proposed SC and that previously analyzed is that we consider that each plant (and respective warehouse) belongs to a different firm, while in the mentioned studies all possible plants and warehouses belong to the same company. Those authors studied whether to expand the capacity of an existing plant or build a new one in another location in respond to a demand increase. Conversely, in this study we assume that all plants exist and can satisfy markets demand by their own. The key question here is whether the overall and individual performance can be improved if all companies work together in a

cooperative SC. In that way, the overall and individual profit increase, as well as the total GHG emissions decrease, since chemical plants are considered emission-dependent industries (Du et al., 2015). Remark that, despite cooperation, all companies preserve their own identity and facilities, as well as their capacity to fulfill their customers demand.

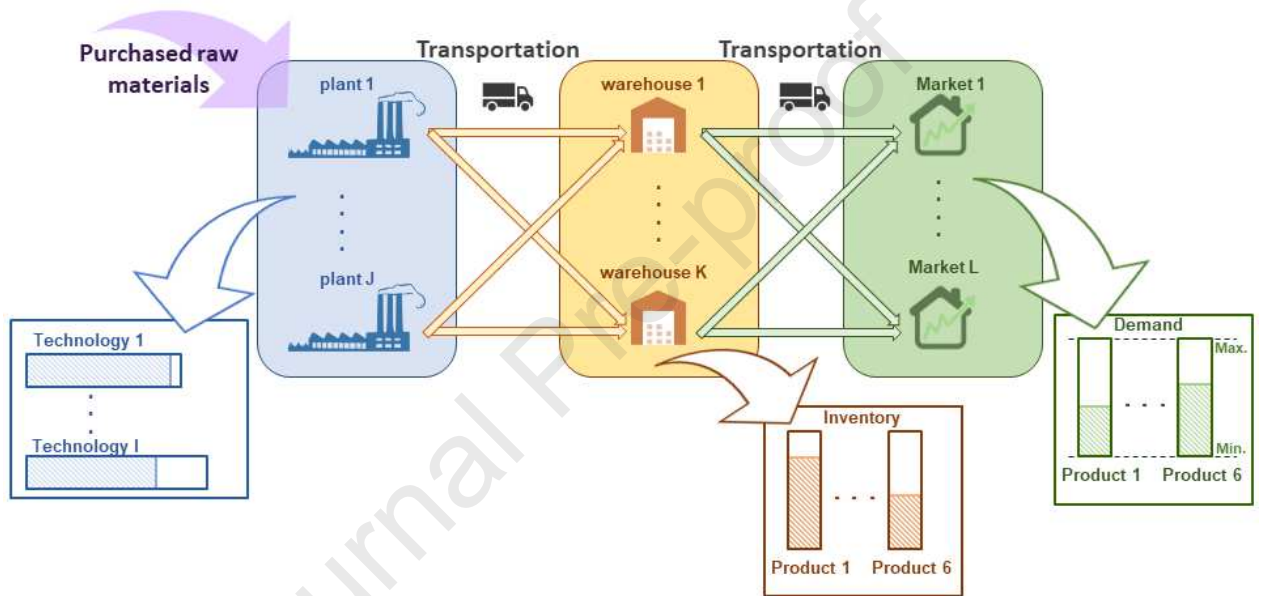


Figure 1. Superstructure of the SC network with horizontal cooperation.

The problem is formally stated as follows. Given are: a time horizon divided into a set of time periods (indexed by t), the specific locations for the SC facilities (plants, warehouses and markets), capacity expansion limitations for the technologies available in plants, prices of final products and raw materials, investment and operating costs, maximum and minimum product demands in markets, CO₂ allowances price forecast, environmental data (emissions associated with the network operation) and emissions cap imposed to each plant. First, it must be checked that the optimal structure and planning decisions of a cooperating SC is economical and environmentally more efficient than SCs individually managed. Then, the goal is to determine how to share that global benefit among all firms comprising the coalition formed, so that none of them wants to abandon it and work alone or in smaller coalitions. To this aim, the cooperative game theory is applied using the core concept, originally introduced by

Gillies (1953), as allocation method to ensure the stability of the so-called grand coalition

3 Methodology and mathematical formulation

The methodology applied in this work is illustrated in Figure 2, where its three main components (supply chain model, its economic and environmental assessment and the cooperative game theory) and the connections among them (i.e., information flows) are showed. The input data required are divided into 3 groups: supply chain data; LCIA results for the GWP indicator; and historic CO₂ allowances price, which in turns feed the ARIMA model to compute the price forecast (see section 3.2). The SC model (see section 3.1.1 for a detailed description), where different companies cooperate, sends the SC assessment part the values of the decision variables required to compute the NPV and GWP (see section 3.1.2 and 3.1.3, respectively), which are linked by the carbon cap-and-trade model. The economic performance (i.e., NPV value) of a particular SC design is sent back to the SC model part. The companies that form a specific coalition in the SC model are fixed by the information flow received from the cooperative game theory unit (specifically from the solution of the MILP subproblem), which in turn receives the NPV that assess that coalition forwarded by the SC model part. These four information flows progress iteratively until the stopping criterion of the row generation algorithm (see section 3.3.2) is satisfied, and the main outcome of our approach, a profit allocation in the core (defined in section 3.3.1) that guarantees the stability of the grand coalition, is achieved.

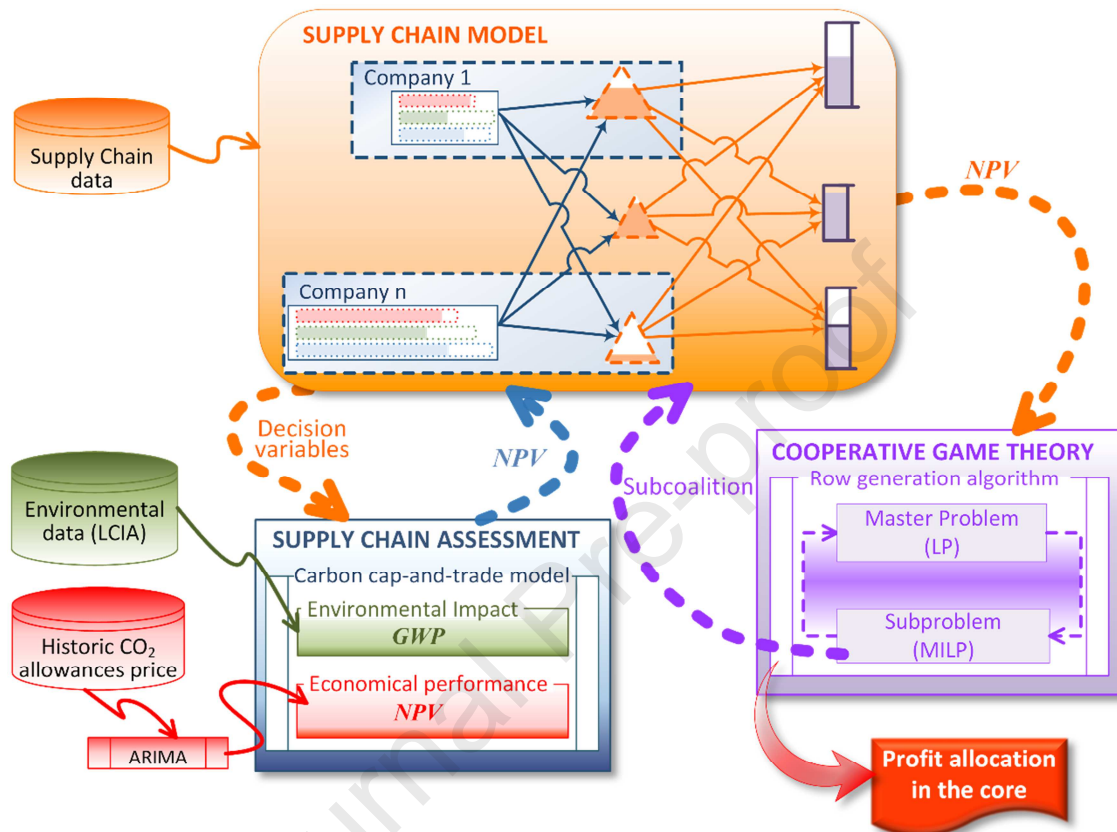


Figure 2. General scheme of the methodology to determine a profit allocation that promotes cooperation among all companies, by integrating the supply chain model, its environmental and economical assessment and the cooperative game theory, given the supply chain data, the LCIA data and the historic CO₂ allowances price.

3.1 Supply Chain Model

The design problem is formulated as a multi-period mixed integer linear programming problem seeking to maximize the NPV of the cooperating SC. The main blocks of equations are mass balances and capacity constraints at plants and warehouses, environmental assessment equations, which includes the carbon trading model, and the economic objective function. In this paper, we show only the main equations of the model, the interested reader can find the detailed model in Guillén-Gosálbez and Grossmann (2009) and Ruiz-Femenia et al. (2013).

3.1.1 Mass balances and capacity constraints

At each node of the SC network (i.e. plants, warehouses and markets) the mass balance must be satisfied. Figure 3 shows a scheme of the main flows among nodes of the SC, where PU_{jpt} denotes the purchases made during period t for each plant j and chemical product p ; W_{ijpt} is the input/output flow of chemical p associated with technology i at plant j in time period t ; INV_{kpt} the inventory of warehouse k during t for product p ; SA_{lpt} represents the sales of p during t in market l . This value must lie between a minimum and a maximum demand $(\underline{D}_{lpt}, \overline{D}_{lpt})$. Q_{jkpt}^{PL} and Q_{klpt}^{WH} are the amount of p transported in time period t from plant j to warehouse k and from warehouse k to market l , respectively. The mass balance for each plant reads (Eq. (1))

$$PU_{jpt} + \sum_{i \in OUT(p)} W_{ijpt} = \sum_k Q_{jkpt}^{PL} + \sum_{i \in IN(p)} W_{ijpt} \quad "j, p, t \quad (1)$$

In Eq. (1) $IN(p)$ and $OUT(p)$ are subsets of technologies that produce and consume p , respectively.

Similarly, the mass balance for each warehouse reads (Eq. (2))

$$INV_{kpt-1} + \sum_j Q_{jkpt}^{PL} = \sum_l Q_{klpt}^{WH} + INV_{kpt} \quad "k, p, t \quad (2)$$

Where INV_{kpt-1} represents the initial inventory, that is, the inventory in the previous time period $(t-1)$.

Finally, product sales in markets are defined by the material flows from the warehouses, as Eq. (3) states

$$SA_{lpt} = \sum_k Q_{klpt}^{WH} \quad "p, l, t \quad (3)$$

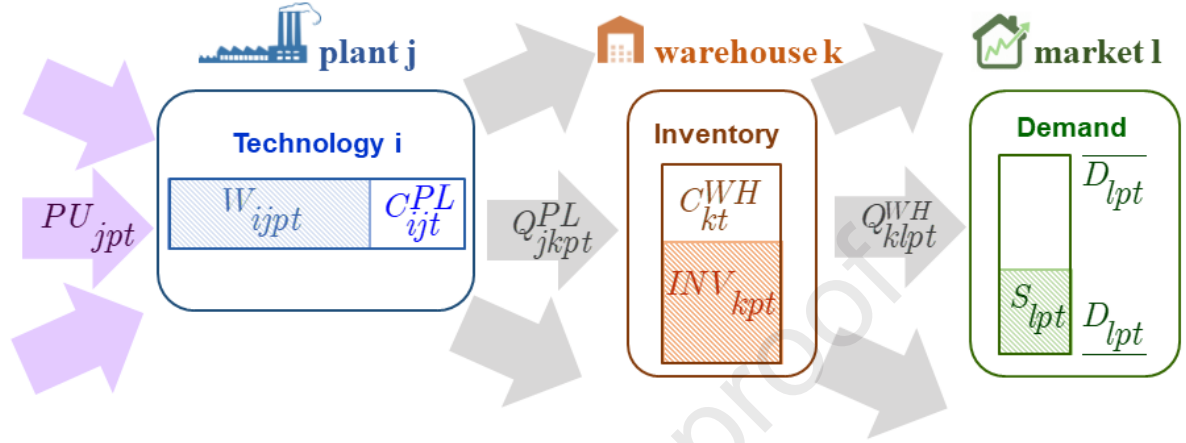


Figure 3. Scheme of the mass flows through the SC network.

In Figure 3, C_{ijt}^{PL} and C_{kt}^{WH} are the capacity of technology i at plant j and the capacity of warehouse k in time period t , respectively. These capacities are calculated as follows (Eqs. (4) and (5))

$$C_{ijt}^{PL} = C_{ijt-1}^{PL} + CExp_{ijt}^{PL} \quad \forall i, j, t \quad (4)$$

$$C_{kt}^{WH} = C_{kt-1}^{WH} + CExp_{kt}^{WH} \quad \forall k, t \quad (5)$$

In Eqs. (4) and (5), C_{ijt-1}^{PL} and C_{kt-1}^{WH} are the existing capacities at the end of the previous time period ($t - 1$), and $CExp_{ijt}^{PL}$ and $CExp_{kt}^{WH}$ are the capacity expansions that can occur during t , which are bounded within lower and upper limits, as stated in Eqs. (6) and (7), respectively

$$\underline{CExp_{ijt}^{PL}} y_{ijt}^{PL} \leq CExp_{ijt}^{PL} \leq \overline{CExp_{ijt}^{PL}} y_{ijt}^{PL} \quad \forall i, j, t \quad (6)$$

$$\underline{CExp_{kt}^{WH}} y_{kt}^{WH} \leq CExp_{kt}^{WH} \leq \overline{CExp_{kt}^{WH}} y_{kt}^{WH} \quad \forall k, t \quad (7)$$

y_{ijt}^{PL} and y_{kt}^{WH} are binary variables whose values are 1 if the mentioned capacity expansions occur in time period t .

Additionally, the production rate of the main product p in technology i in plant j , must be lower than the existing technology capacity and higher than a desired minimum which is calculated as a percentage, τ , of this capacity (Eq. (8))

$$\sum_{i \in MP(i)} C_{ijt} \leq W_{ijpt} + C_{ijt} \quad \forall i, j, t \quad \forall p \in \hat{MP}(i) \quad (8)$$

where the subset $MP(i)$ defines the main product p associated with technology i .

Similarly, the total inventory of warehouse k in time period t must not exceed the available warehouse capacity, as shown in Eq. (9)

$$\sum_p \hat{a}_p \text{INV}_{kpt} \leq C_{kt}^{WH} \quad \forall k, t \quad (9)$$

Finally, the existence of transportation links between plants and warehouses as well as from warehouses to markets is defined by the binary variables x_{jkt}^{PL} and x_{klt}^{WH} , respectively. When these variables take the value of 1, the corresponding flow is allowed within certain bounds, as stated in Eqs. (10) and (11)

$$\underline{Q}_{jkpt}^{PL} x_{jkt}^{PL} \leq \hat{a}_p \underline{Q}_{jkpt}^{PL} \leq \overline{Q}_{jkpt}^{PL} x_{jkt}^{PL} \quad \forall j, k, t \quad (10)$$

$$\underline{Q}_{klpt}^{WH} x_{klt}^{WH} \leq \hat{a}_p \underline{Q}_{klpt}^{WH} \leq \overline{Q}_{klpt}^{WH} x_{klt}^{WH} \quad \forall k, l, t \quad (11)$$

3.1.2 Environmental impact assessment

The environmental impact is quantified using the Life Cycle Assessment (LCA) principles. Specifically, we make use of the global warming potential (GWP) indicator, as described by the intergovernmental panel on climate change 2007 (IPCC) (Hischer R., 2010), which estimates the relative contribution to the global warming of one kg of a GHG compared to the emission of one kg of CO₂. We consider three main sources of emissions- transportation (GWP^{TR}), energy requirements (GWP^{EN}) and raw materials consumption (GWP^{RM})- that contribute to the total GWP (Eq. (12)).

$$GWP_t^{total} = GWP_t^{TR} + GWP_t^{EN} + GWP_t^{RM} \quad \forall t \quad (12)$$

To compute the three contributions to the total GWP in Eq. (12), the environmental data and the values of the decision variables that directly influence each environmental impact source for GWP are required. For this environmental metric, we use a time horizon of 100 years. LCA databases offer data for three different time horizons, 20, 100 and 500 years (Pennington et al., 2000). As regards the decision variables, GWP^{TR}

is calculated from the transport flows ($Q_{jkpt}^{PL}; Q_{klpt}^{WH}$), GWP^{EN} from the production rates (W_{ijpt}) and GWP^{RM} from the raw materials purchases (PU_{jpt}), as follows

$$GWP_t^{TR} = \mathring{a}_j \mathring{a}_k \mathring{a}_p \text{Imp}^{TR} l_{jk}^{PL} Q_{jkpt}^{PL} + \mathring{a}_k \mathring{a}_l \mathring{a}_p \text{Imp}^{TR} l_{kl}^{WH} Q_{klpt}^{WH} \quad " t \quad (13)$$

$$GWP_t^{EN} = \mathring{a}_i \mathring{a}_j \mathring{a}_p \text{Imp}^{EN} h_{ijp}^{EN} W_{ijpt} \quad " t \quad (14)$$

$$GWP_t^{EN} = \mathring{a}_i \mathring{a}_j \mathring{a}_{p \dot{M}P(i)} \text{Imp}^{EN} h_{ijp}^{EN} W_{ijpt} \quad " t \quad (15)$$

$$GWP_t^{RM} = \mathring{a}_j \mathring{a}_p \text{Imp}_p^{RM} PU_{jpt} \quad " t \quad (16)$$

In Eqs. (13), (14) and (16), Imp^{TR} , Imp^{EN} and Imp_p^{RM} represent the life cycle impact assessment (LCIA) result for the GWP indicator due to the transportation of 1 ton of mass 1 km of distance, the usage of 1 MJ of energy and the consumption of 1 kg of raw material p , respectively. These values are taken from Ecoinvent database (Frischknecht et al., 2005b).

In Eq. (13), l_{jk}^{PL} is the distance from plant j to warehouse k , while l_{kl}^{WH} is the distance from warehouse k to market l , and in Eq. (14), h_{ijp}^{EN} denotes the energy consumed per unit product of the main product p produced by technology i in plant j , which includes electricity, steam and cooling water.

The overall GWP during the entire time horizon of the SC is calculated as

$$GWP^{total} = \mathring{a}_t GWP_t^{total} \quad (17)$$

3.1.3 Objective function

The objective of the SC design is to maximize the Net Present Value (NPV), calculated by Eq. (18)

$$NPV = \sum_t \frac{CF_t}{(1+ir)^{t-1}} \quad (18)$$

Where CF_t is the summation of the discounted cash flows in each period of time t and ir is the interest rate. The cash flow is defined as the net earnings (NE_t) (i.e. profit after taxes) minus the fraction of the total depreciable capital ($FTDC_t$), at each time period except the last one (Eq. 19) for which we consider that a fraction of the total fixed capital investment (FCI) will be recovered (salvage value ratio, sv) (Eq. (20)).

$$CF_t = NE_t - FTDC_t \quad t = 1, \dots, NT - 1 \quad (19)$$

$$CF_t = NE_t - FTDC_t + sv FCI \quad t = NT \quad (20)$$

The net earnings are obtained by subtracting costs and taxes from total incomes. The revenues are determined from sales of final products, whereas the total cost includes the purchases of raw materials, the operating and inventory costs associated with plants and warehouses, the transportation cost and the depreciation, which is considered to vary linearly with time. Regarding FCI , it is determined from the capacity expansions of plants and warehouses as well as the establishment of transportation links. For further description of the calculation of NE_t and FCI see Guillén-Gosálbez and Grossmann (2009).

The environmental performance of the SC is incorporated to the objective function by monetizing the GWP_t through the emissions trading model, presented in Eq. (21), which states that the total equivalent CO_2 (CO_2 -eq) emitted equals the maximum emissions corresponding to the free allowances given by the government ($Cap_t^{CO_2}$) plus the extra rights to emit bought ($Buy_t^{CO_2}$) minus the rights sold ($Sales_t^{CO_2}$).

$$GWP_t^{total} = Cap_t^{CO_2} + Buy_t^{CO_2} - Sales_t^{CO_2} \quad \forall t \quad (21)$$

The net income ($Net_t^{CO_2}$) due to emissions trading is calculated by Eq. (22)

$$Net_t^{CO_2} = Price_t^{CO_2} Sales_t^{CO_2} - Cost_t^{CO_2} Buy_t^{CO_2} \quad \forall t \quad (22)$$

Where ($Price_t^{CO_2}$) and ($Cost_t^{CO_2}$) are the emission allowances price and cost, respectively, which can be equal or different (Letmathe and Balakrishnan, 2005). In this study we assume the same value for both parameters.

The value of $Net_t^{CO_2}$ is included as another income of the SC in the NE_t calculation.

3.2 CO₂ allowances price forecast

As aforementioned, the prediction of the emissions allowances price is a key factor for the optimal design of the SC under the carbon trading scheme through a time horizon. To this purpose, we apply the ARIMA model using the historical CO₂ emissions price data.

ARIMA models are generally denoted as ARIMA(p, d, q), where the autoregressive order, p, the order of differencing, d, and the moving average order, q, must be identified. In this model, carbon price is a linear function of past values and error terms and can be mathematically expressed as in Eq. (23) (Zhu and Wei, 2013)

$$Y_t = u + a_1 Y_{t-1} + a_2 Y_{t-2} + \dots + a_p Y_{t-p} - e_t - b_1 e_{t-1} - b_2 e_{t-2} - \dots - b_q e_{t-q} \quad (23)$$

where Y_t is the carbon price obtained by differencing d times; u is the average value of the data set; e_t is the error at period t (hypothetical white noise) and $e_{t-1}, e_{t-2}, \dots, e_{t-q}$ are the errors of past forecasted values, assumed to be independent and identically distributed with a mean of zero and a constant variance of σ^2 (i.e., $\{e_t\} \sim i.i.d.(0, \sigma^2)$); and $\alpha_1, \alpha_2, \dots, \alpha_p$ and $\beta_1, \beta_2, \dots, \beta_q$ are the parameters to be estimated.

To determine the order of the AR (autoregressive) and MA (moving average) components, it is usual to build a time series basic diagnostics chart with the autocorrelation (ACF) and partial autocorrelation functions (PACF) (Shumway, 2017), or use criteria based on penalty factors such as Akaike information criteria (AIC) and Bayesian information criteria (BIC) (Brockwell, 2016).

3.3 Cooperative games model

The main objective of cooperative game theory is to establish a contract between all players (in this case, each company is considered to be a player) to divide the total wealth generated collectively (Gilles, 2010). This contract can be based on power or fairness exclusively or on a mixture of both. The preferred game form to describe cooperative games is the characteristic function form, which represents the negotiation process to allocate the profit generated by the interactive decision process. This negotiation process leads to a balance in which none of the players or group of them (i.e., coalition) have incentives to oppose the proposed agreement. The resulting set of

allocations form the so-called core of the game. The main properties of the core are detailed below.

3.3.1 Core definition and properties

Given a set of players, $N = \{1, 2, \dots, N\}$, any subset of them is called a coalition ($S \subseteq N$), being the grand coalition that formed by all players, $S = N = \{1, 2, \dots, N\}$. Thus, the total number of possible coalitions is $2^{|N|}$. Any player and coalition among them are considered as decision makers. The characteristic function, $v : 2^{|N|} \rightarrow \mathbb{R}$, is a vector function that assigns a profit value to each coalition (S), which is the best outcome that players forming coalition S can attain without cooperating with the players not belonging to S . The profit share allocated to player n is denoted by p_n , so the vector composed by all these shares, $p = (p_1, p_2, \dots, p_{|N|})$, gives an allocation of the total profit for the grand coalition. Since there must be an incentive to cooperate, otherwise, cooperation will not occur and the outcome will be inefficient, the profit allocations should fulfill some properties (Drechsel, 2010). One of these properties is *efficiency*, which states that the profit of the grand coalition must be equal to the summation of the profit shares (Eq. (24))

$$v(N) = \sum_{n \in N} p_n \quad (24)$$

Another desirable property, called *individual rationality*, specifies that the profit attained by a player cooperating is at least as high than the profit while acting alone (Eq.(25))

$$p_n \geq v(\{n\}) \quad \forall n \in N \quad (25)$$

Individual rationality can be extended to *coalitional rationality* as described in Eq. (26)

$$\sum_{n \in S} p_n \geq v(S) \quad \forall S \subseteq N \quad (26)$$

If Eqs. (25) and (26) are met, we can assure that the grand coalition is stable since no player has any motivation to form a smaller coalition S . Any profit allocation that guarantees efficiency and rationality properties is called an imputation. By merging

efficiency and rationality properties, given a set of players N and a characteristic function ν , a core C is defined as the following set:

$$C(N, \nu) := \left\{ p \in \mathbb{R}^{|N|} \mid \sum_{i \in N} p_i = \nu(N) \text{ and } \sum_{i \in S} p_i \leq \nu(S) \quad \forall S \subseteq N, S \neq \emptyset \right\} \quad (27)$$

Therefore, any profit share, π , drawn from the core (i.e. is a non-dominated imputation) ensures the stability of the grand coalition.

In terms of mathematical programming, the core specifies a constraint satisfaction problem of the form:

$$\begin{aligned} \min \quad & z = 1 \\ \text{s.t.}, \quad & \sum_{i \in N} p_i = \nu(N) \\ & \sum_{i \in S} p_i \leq \nu(S) \quad \forall S \subseteq N, S \neq \emptyset \\ & p_i \geq 0 \quad \forall i \in N \end{aligned} \quad (28)$$

Note that the only reason to introduce a dummy objective function in problem (28) is for the purpose of using an optimization solver to obtain a point of the core, but the whole core results by solving the constraint satisfaction problem.

The core can be easily illustrated in a triangular diagram for a three-player game (Maschler et al., 1979). In Figure 4, each point of the triangle represents a profit allocation $p = (p_1, p_2, p_3)$ in which the efficiency constraint (Eq. (24)) holds. The vertices of the triangle display the maximum profit attainable for each player, that is, if the total benefit of the grand coalition is assigned to one of the players. Figure 4 a) and b) show the feasible region defined by individual and coalitional rationality constraints, respectively. The intersection area of both regions satisfies all the constraints and hence, constitutes the core of the game (Figure 4 c). For a numerical illustration see Carrero-Parreño et al. (2019).

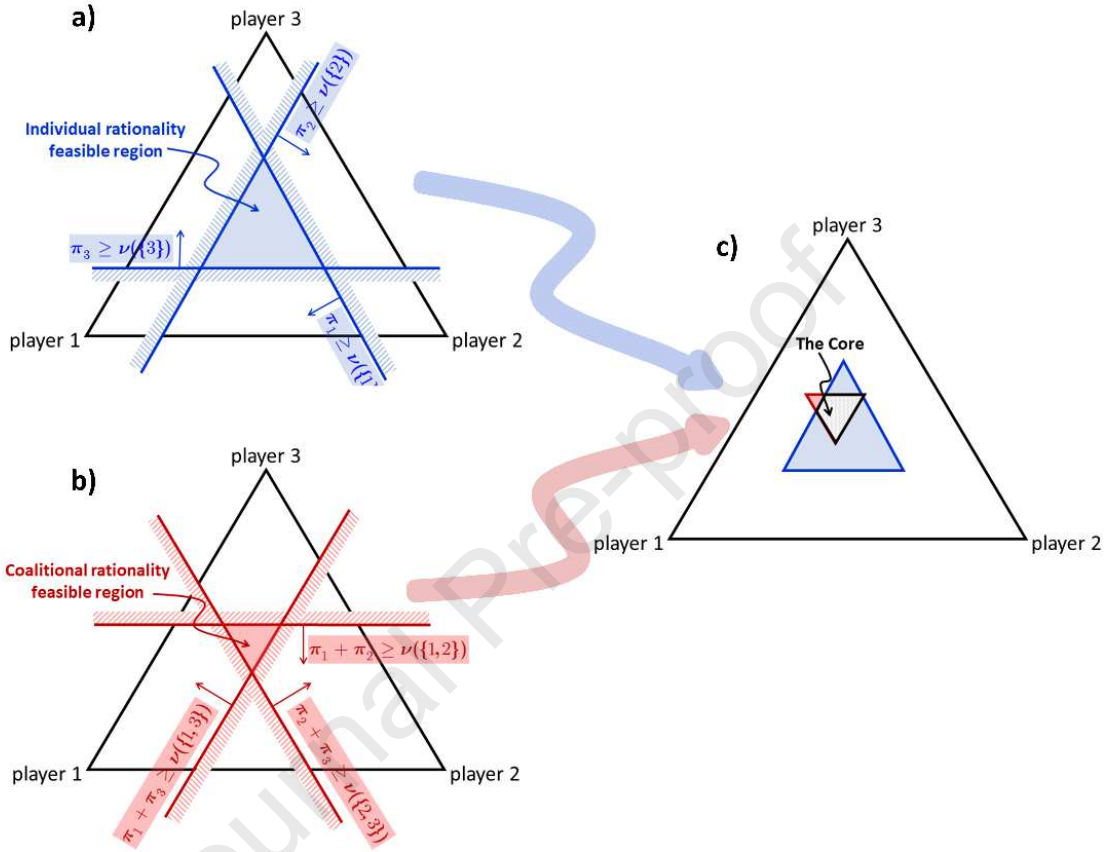


Figure 4. Geometric interpretation of a three-player game using a triangular diagram: a) region (blue shaded) defined by the individual rationality constraints; b) region (red shaded) defined by the coalitional rationality constraints; and c) the intersection of the two previous regions defined the core of the game.

3.3.2 Row Generation Algorithm

As mentioned before, the number of possible coalitions is $2^{|N|}$, therefore this number rises exponentially with an increasing number of players and so does the number of constraints specified for the core definition (Eq. (27)). To address this problem, Drechsel and Kimms (2010) introduced a row generation procedure in order to avoid computing the constraints for all possible coalitions to find a core element. To address this problem, Drechsel and Kimms (2010) introduced a row generation procedure in order to avoid computing the constraints for all possible coalitions to find a core element. Using this procedure, with the necessary modifications on the algorithm to compute the maximum profit of the SC instead of the minimum cost, it is possible to

apply the core solution concept for the planning and management of a SC composed of many collaborating companies.

First, an initial set of coalitions Σ is defined. The algorithm starts with a relaxed version of the whole problem (28), denoted as the master problem $MP(\Sigma)$, and adds missing relaxed constraints over several iterations aiming to obtain an element of the core without adding all the constraints. The master problem is a linear programming problem (LP) of the form

$$\begin{aligned}
 \min \quad & w \\
 \text{s.t.}, \quad & \sum_{n \in N} p_n = n(N) \\
 & \sum_{n \in S} p_n + w \geq n(S) \quad \forall S \in \Sigma \\
 & p_n \geq 0 \quad \forall n \in N \\
 & w \geq 0
 \end{aligned} \tag{29}$$

If the optimal solution, $\{w^{\hat{a}}, p_n^{\hat{a}}\}$, of the $MP(\Sigma)$ gives a result of $w^{\hat{a}} = 0$, the core exists, otherwise the game has an empty core, that is, the grand coalition would not be possible and effective sub-coalitions should be found. In this case, the algorithm stops. In the case that the core is non-empty, we continue with the procedure by seeking a new coalition $S' \in \Sigma$ ($S' \neq N$) for which profit allocation is not in the core, that is, it does not meet the rationality constraint (Eq. (26)), so $\sum_{n \in S'} p_n^{\hat{a}} < n(S')$. If such coalition S' cannot be found, then the algorithm stops because the allocation yielded by the $MP(\Sigma)$ solution, $p_n^{\hat{a}}$, is in the core. To find out whether a coalition S' exists, we fix the profit allocation to the values provided by the $MP(\Sigma)$ solution, $p_n^{\hat{a}}$, and solve the following Mixed Integer Linear Programming (MILP) subproblem

$$\begin{aligned}
 \max \quad & m \\
 \text{s.t.}, \quad & \text{SC model constraints}(x) \\
 & \sum_{n \in S'} p_n^* u_n + m = n(S') \\
 & m \in \mathbf{R} \\
 & u_n \in \{0, 1\}
 \end{aligned} \tag{30}$$

where u_n is a binary variable that takes the value 1 when player n is in coalition S' and 0 otherwise. The value of these binary variables at the optimal solution provides the coalition that violates most the core constraint. In case this coalition is found, the algorithm continues by computing the total profit for this coalition, adding the relaxed constraint (31) to a new instance of the $MP(\Sigma)$, where $S = S \cup \{S'\}$, and repeating the process through successive iterations until no coalition that violates the core constraint is found. In this case, the optimal values of p_n obtained in the previous master problem define a core allocation.

$$\sum_{n \in S'} p_n + w^3 n(S') \quad (31)$$

4 Case study

The mathematical model described in section 3 is applied to a case study consisting of a cooperative SC composed by seven companies (considered as players participating in a cooperative game), each of which manages a plant and a warehouse located in different parts of Europe, namely: 1-Frankfurt (Germany), 2-Kazincbarcika (Hungary), 3-Leuna (Germany), 4-Mantova (Italy), 5-Neratovice (Czech Republic), 6-Tarragona (Spain) and 7-Wloclaweck (Poland). All plants have 6 technologies installed, which are used to manufacture 6 main products (particularly, acetaldehyde, acetone, acrylonitrile, cumene, isopropanol and phenol) as described in case study 1 presented by Guillén-Gosálbez and Grossmann (2009). The total number of chemicals involved in this SC is 18. The 6 main products are sold in 4 final markets placed in Leuna, Neratovice, Sines (Portugal) and Tarragona. Figure 5 presents the approximate geographical distribution of the mentioned SC entities. In Table A.1 and Table A.2 of Appendix A the distances between plants and warehouses and between warehouses and markets, respectively, are shown.

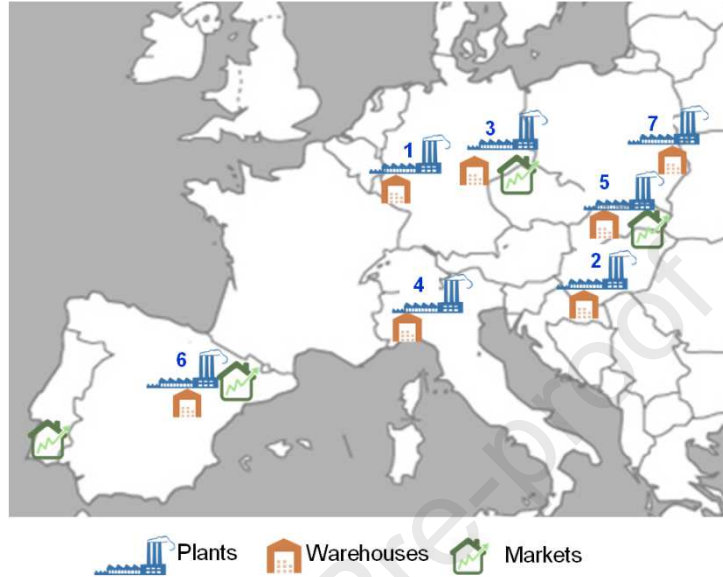


Figure 5. Geographical distribution of plants, warehouses and markets: 1-Frankfurt, 2-Kazincbarcika, 3-Leuna, 4-Mantova, 5-Neratovice, 6-Tarragona and 7-Wloclaweck.

We fix the time horizon to 10 periods, being each period one year long. We consider that all technologies available in all plants have the same initial capacity ($C_{ijt=1}^{PL}$), 20 ktons/year, while all warehouses have an initial capacity ($C_{kt=1}^{WH}$) of 20 ktons and the initial inventory for all of them ($INV_{kpt=1}$) is 0. The lower and upper limits for the capacity expansions are 10 and 400 ktons/year for plants, and 5 and 400 ktons for warehouses, respectively. The purchases of raw materials are limited to 32 ktons/year and purchases of intermediate and final products are not allowed to prevent outsourcing.

The total demand in markets is divided among all companies, so all of them must satisfy their corresponding demand portion. The maximum demand of chemicals (\overline{D}_{lpt}) for the first time period is shown in Table A.3, assuming an increase of 5 % per time period. In this study we consider that at least 90 % of this demand must be satisfied (\underline{D}_{lpt}). The prices of the chemical products as well as other SC design parameters can be found in Appendix A.

The lower and upper bounds on the flows of materials between plants and warehouses $(\underline{Q}_{jkpt}^{PL}; \overline{Q}_{jkpt}^{PL})$ and warehouses and markets $(\underline{Q}_{klpt}^{WH}; \overline{Q}_{klpt}^{WH})$ are 5 and 500 ktons/year in both cases.

The initial GHG emissions cap $(Cap_{t=1}^{CO_2})$ for each plant is set to 2×10^8 kg CO₂-eq, which is estimated from data of emission rights assignment published by Spanish government. In addition, we establish an annual reduction rate of 2.2 % according to the phase 4 (2021-2030) of the EU ETS (European Commission, 2015).

5 Results

In this section we present, firstly, the most suitable ARIMA(p, d, q) model for our case study and its resulting predictions for the CO₂ prices. Then, we describe the structure and performance of the optimum SC described in section 4 when the companies take part in a 7-player cooperative game. Finally, a sensitivity analysis has been carried out in order to assess the effect of the key parameters of the carbon trading model (i.e. CO₂ price and cap) on the game.

5.1 CO₂ allowances price forecast

To apply the ARIMA model for the prediction the CO₂ allowances price through the time horizon considered, firstly, the most suitable parameters p, d and q must be determined. To this aim, the first step is differencing de non-stationary time series data set (raw data retrieved from Market Insider website (2020)) in order to get a stationary one. Normally, the correct order of differencing is the lowest that yields a time series which fluctuates around a well-defined mean value. In our case, applying a difference of order d equal to 1, the data set becomes stationary as shown in Figure 6.

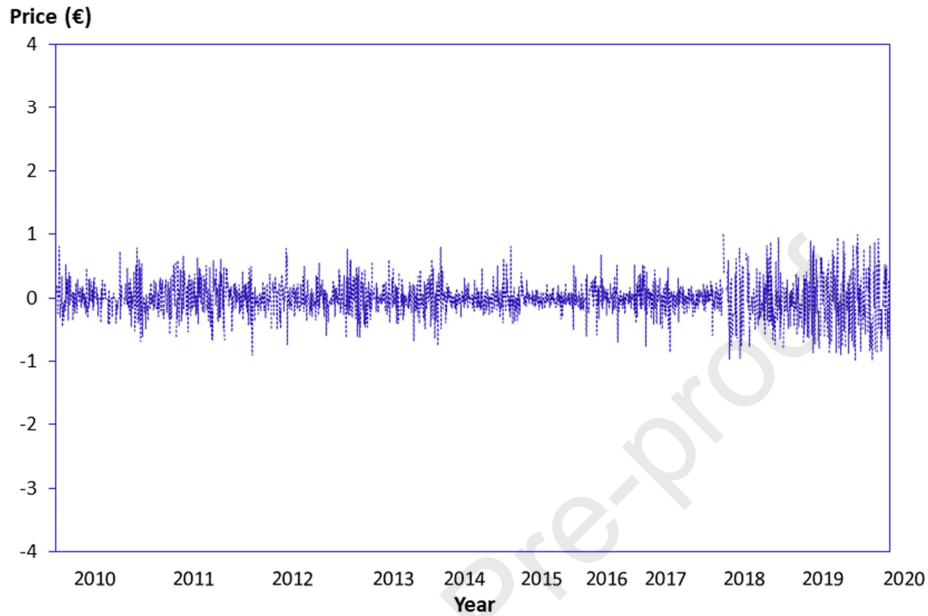


Figure 6. Result of the first order differentiation of the raw data set.

Then, the parameters p and q have been identified by calculating AIC and BIC for different ARIMA($p, 1, q$) models. The lowest values of AIC and SBC define the best model, which turned out to be 4 for both p and q . Using this ARIMA(4,1,4) model together with a Monte Carlo simulation, the CO₂ allowances price has been predicted for different scenarios from 2020 to 2030. The simulation has been carried out using the Econometrics Matlab Toolbox. Figure 7 presents the results of the CO₂ allowances price prediction. The grey line shows the CO₂ allowances price historical data since 2010 (data retrieved from Market Insider website (2020)). The solid black line represents the mean value for the price predicted by the model for the period 2020-2030 while the dotted lines are the highest and lowest values predicted within a 95% confidence interval.

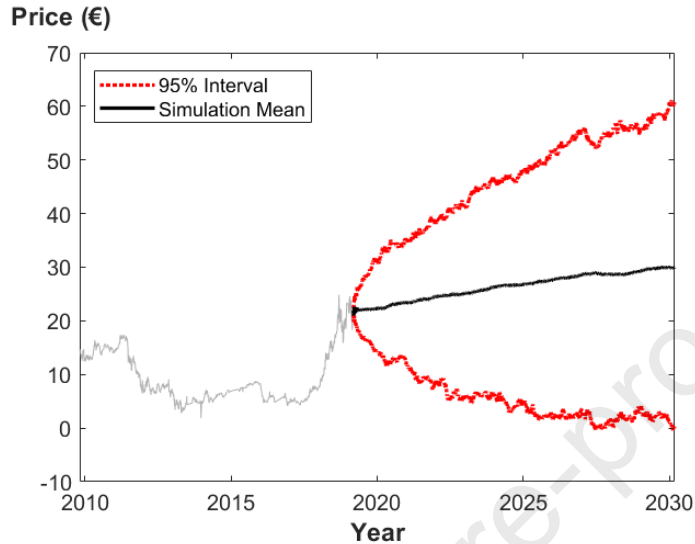


Figure 7. CO₂ allowances price forecasting.

5.2 Cooperative 7- player game

Given the mean value of the CO₂ allowances price predicted by the ARIMA(4,1,4) model as the base case, we have analyzed the performance of the cooperative SC described in section 4. In the first place it must be determined whether the cooperation among all players (i.e., grand coalition) is advantageous in comparison with the overall performance of all companies working separately. To this aim, we optimize the SC model for each sub-coalition formed by a unique company and for all the players working together. Table 2 shows the maximum NPV attained as well as the GWP generated by each company working individually and cooperating in the grand coalition to satisfy the markets demand of products for the considered time horizon. As can be observed, the NPV achieved by the grand coalition (308.59 M€) is higher and the GWP (14.092 Mton CO₂-eq) of the grand coalition lower than the summation of the NPVs (240.73 M€) and GWPs (14.391 Mton CO₂-eq) corresponding to each company working separately. Specifically, the grand coalition improves the economic and environmental performance of the SC in approximately 28 % and 2 %, respectively. Although a decrease of 2 % may seem unimportant, it represents nearly 300 ktons less CO₂-eq emitted into the atmosphere, which would have a positive impact on reducing climate change.

Table 2. NPV and GWP for each company acting separately and for the grand coalition.

Player n (company)	NPV_n (M€)	GWP_n^{total} (Mtons CO ₂ -eq)
1	23.17	2.032
2	42.87	2.087
3	12.27	2.024
4	33.24	2.053
5	52.41	2.046
6	30.67	2.086
7	46.10	2.063
$\sum_n NPV_n$ $\sum_n GWP_n^{total}$	240.73	14.391
Grand coalition	308.59	14.092

Once proven that forming the grand coalition is both economically and environmentally beneficial, the NPV obtained for the grand coalition must be shared among companies in a proper way, so that all of them are willing to cooperate and none have incentive to deviate from the grand coalition. Since the number of possible sub-coalitions in a 7-players game is very high ($2^7 = 128$), the core allocation was found by means of the row generation algorithm described in section 3.3.2, which is a relaxed version of the whole problem that would require an individual rationality constraint (Eq. (25)) for each one of the 128 sub-coalitions. This algorithm starts with an initial set Σ of 8 coalitions, which includes the 7 seven sub-coalitions formed by a unique player and the grand coalition. To build the constraints that define the first Master problem (Eq. (29)), we need to write the individual rationality constraint (Eq. (25)) for each company. The RHS of these inequalities are the values of the characteristic function for each sub-coalition formed by a unique company, computed previously by optimizing the SC model (Table 2, NPV_n column). The other constraint required to formulate the first master problem is the efficiency constraint (Eq. (24)), whose LHS has already been computed (the NPV of the grand coalition). The solution of this first master problem offers a profit share among companies ($\pi_1^a=91.03$, $\pi_2^a=42.87$, $\pi_3^a=12.27$, $\pi_4^a=33.24$, $\pi_5^a=52.41$, $\pi_6^a=30.67$, $\pi_7^a=46.10$) that belongs to the core of the game. Next, after fixing this profit allocation we formulate the first MILP subproblem (Eq. (30)) and solve it to find the sub-coalition that violates most the rationality constraint. For instance, for the first subproblem, the sub-coalition found is $S'=\{2,3,4,5,6,7\}$. From that sub-coalition, a coalitional rationality constraint (Eq. (26)) can be added to the first master problem to build the

second one, whose solution provides a new profit allocation for the second subproblem, which in turn is solved to complete the second iteration. From here, the algorithm performs successive iterations until the stopping criterion is satisfied, no sub-coalition is found by the subproblem at iteration 14 (Table 3 shows the iteration progress). Comparing the values of NPV_n in Table 2 with the last iteration provided in Table 3, corresponding to the ultimate core imputation, it is clear that the payoff assigned to each company forming the grand coalition is higher than the maximum NPV that they could achieve working individually or forming any other smaller coalition (i.e. individual and coalitional rationalities, Eqs. (25) and (26), are fulfilled).

Table 3. Iteration progress of the row generation algorithm with the optimal profit allocation from the master problem solution and the coalition found by the subproblem.

	MP(Σ) solution (M€)							Subproblem solution
	p_1^*	p_2^*	p_3^*	p_4^*	p_5^*	p_6^*	p_7^*	Coalition S'
Iteration 1	91.03	42.87	12.27	33.24	52.41	30.67	46.10	$S' = \{2,3,4,5,6,7\}$
Iteration 2	23.17	42.87	12.27	33.24	120.27	30.67	46.10	$S' = \{1,2,3,4,6,7\}$
Iteration 3	23.17	97.29	12.27	33.24	65.84	30.67	46.10	$S' = \{1,3,4,5,6,7\}$
Iteration 4	23.17	42.87	12.27	33.24	52.41	98.53	46.10	$S' = \{1,2,3,4,5,7\}$
Iteration 5	33.83	50.98	28.07	33.24	65.84	50.53	46.10	$S' = \{3,4,7\}$
Iteration 6	33.83	50.98	35.81	33.24	58.10	50.53	46.10	$S' = \{1,4,5,7\}$
Iteration 7	33.83	50.98	25.40	43.65	58.10	50.53	46.10	$S' = \{1,3,5,6,7\}$
Iteration 8	33.83	43.23	23.47	45.59	65.84	50.53	46.10	$S' = \{2,3,6,7\}$
Iteration 9	33.83	50.98	33.15	35.91	65.84	42.79	46.10	$S' = \{2,3,4,6,7\}$
Iteration 10	23.17	50.98	12.27	33.24	65.84	30.67	92.41	$S' = \{1,2,3,4,5,6\}$
Iteration 11	33.83	47.54	27.77	41.28	61.54	50.53	46.10	$S' = \{4,7\}$
Iteration 12	33.83	47.54	26.87	41.28	61.54	50.53	47.00	$S' = \{2,3,4,7\}$
Iteration 13	33.83	47.54	26.87	41.28	61.54	50.53	47.00	$S' = \{1,2,3,5,6,7\}$
Iteration 14	33.83	49.04	26.87	39.78	62.91	47.66	48.49	$S' = \{\emptyset\}$

Both the LP master problem and the MILP subproblem have been modeled using GAMS (General Algebraic Modeling System) and solved with CPLEX 12.7.0.0. Table

4 indicates the problem size for both models corresponding to the worst case, which is the last iteration for the master problem as it includes the highest number of coalitional rationality constraints, and the subproblem with highest CPU time. In terms of CPU time, the subproblem uses 3.5 times more resources than the Master Problem, being 10 s, approximately, the total time used by the row generation algorithm to produce the outcome.

Table 4. Model statistics for the two types of models solved in the row generation algorithm.

	Master Problem (LP)	Subproblem (MILP)
Number of equations	22	5666
Number of variables	9	8056
Number of binary variables	-	301
CPU time (s)	0.157	0.547

As commented before, the formation of the grand coalition is not only advantageous in terms of economic benefit but also in terms of environmental performance. On the one hand, the introduction of the cap-and-trade policy induces the companies to minimize their CO₂ emissions since they must buy additional rights to emit if they exceed the free allowances granted by the governments. Besides, they have the possibility of obtaining extra incomes by selling the surplus of allowances, which also impacts their economic performance. Figure 8 depicts the contribution of the net income due to the emissions trading ($Net_t^{CO_2}$) to the net earnings (NE_t) of the SC network developed by the grand coalition. During the first time periods, the total emissions remain below the carbon cap, thus a percentage of the net earnings correspond to the sales of emissions rights. From time period 5, the free emission allowances allocated are not enough to cover the total emissions of the SC, therefore part of the incomes must be employed to buy extra rights to emit. This is due to the joint effect of the carbon cap reduction and products demand growth in markets with time.

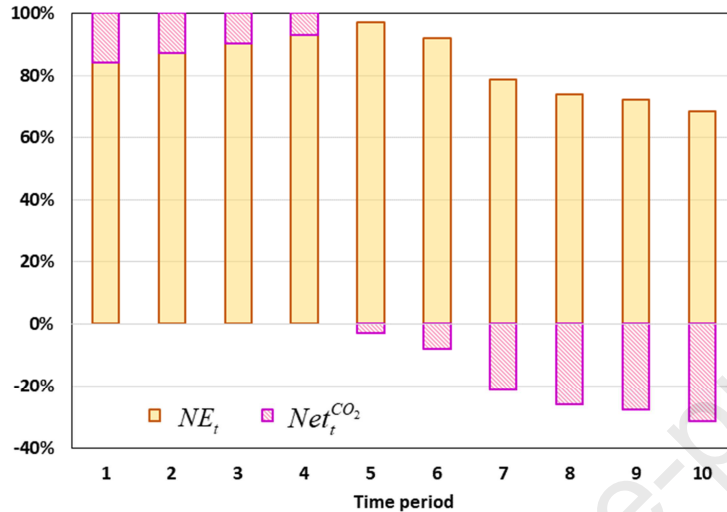


Figure 8. Contribution of the net income due to carbon trading to the net earnings of the SC.

On the other hand, the possibility of sharing facilities among the companies cooperating in the SC allows to optimize the resources involved in the environmental impact assessment as well as the transportation links between the SC entities. As can be observed in Figure 9, except for time periods 5 and 7, the CO₂ equivalent emitted by the grand coalition is lower than that emitted by the plants working without cooperation. This difference is especially noticeable for the last time periods, where the demands of the different chemicals in markets are the largest.

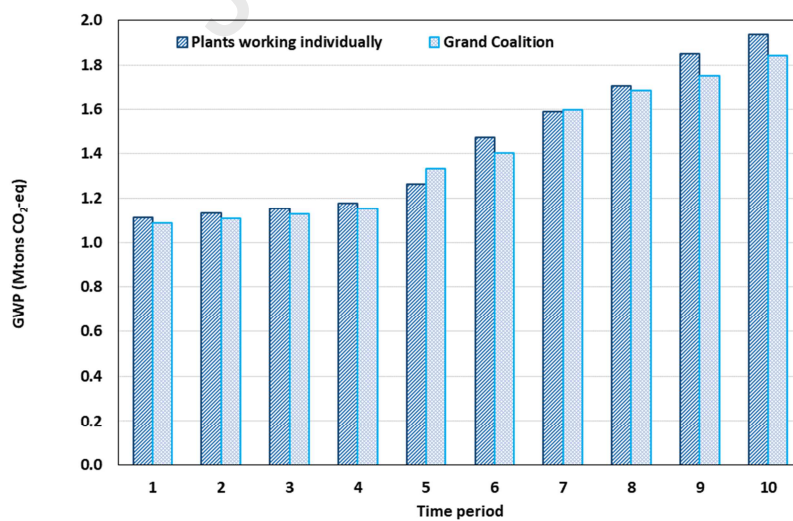


Figure 9. GWP (Mtons CO₂-eq) generated by all companies working individually and by the grand coalition.

Analyzing the total production in plants, depicted in Figure 10, there is a great difference among the production of plants depending on their respective investment and operating costs (see Appendix A, Table A. 5, Table A. 6 and Table A. 7). The plant with the lowest costs (that located in Neratovice) is the one that contributes most to markets supplies. In addition, there is a market placed in the same location, which in turn accounts for the highest demand (Table A. 3) and lowest price (Table A. 4) of all chemicals. This circumstance further favors the productivity of this plant. On the other hand, the plants with lower productions are those with the higher costs (namely Frankfurt and Leuna). Specifically, Leuna, despite being situated in the same city as the market with the second highest demand, has a very low production due to its high investment and operating costs.

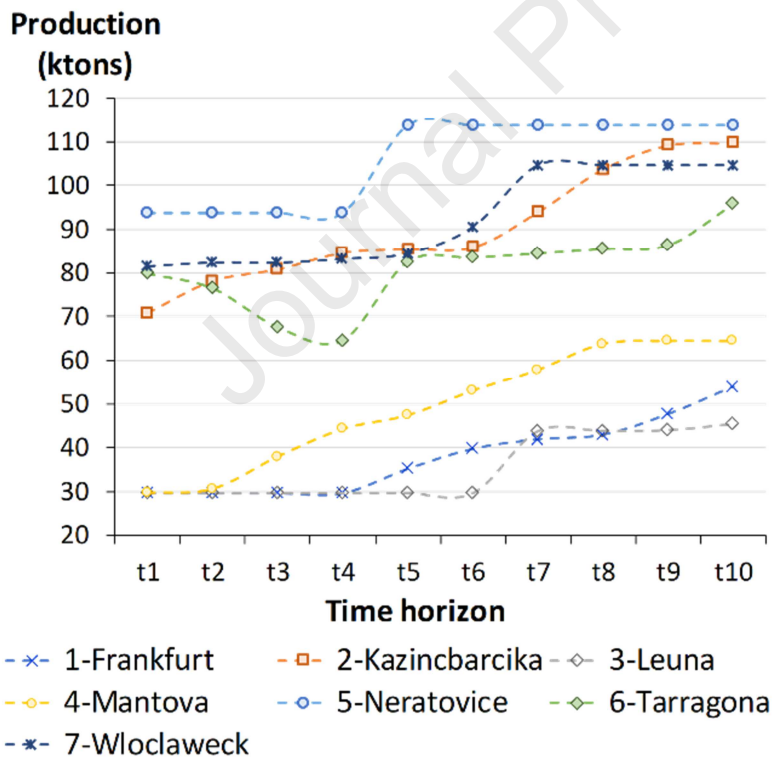


Figure 10. Total production of plants during the time horizon considered.

The production of all products at plants and sales of all products in markets for time periods 1, 5 and 10 are shown in Figure 11. In production charts, the blank bars represent the capacity of the technology and the colored ones indicate the actual production of each chemical. Similarly, in sales charts the blank bars represent the maximum demand of each products while the colored ones are the actual sales (note that at least 90 % of the maximum demand must be satisfied). Notice that, although acrylonitrile is the most sold product in all markets, the one with a highest production is cumene. This is because cumene is also used as raw material for the technology that produces acetone and phenol.

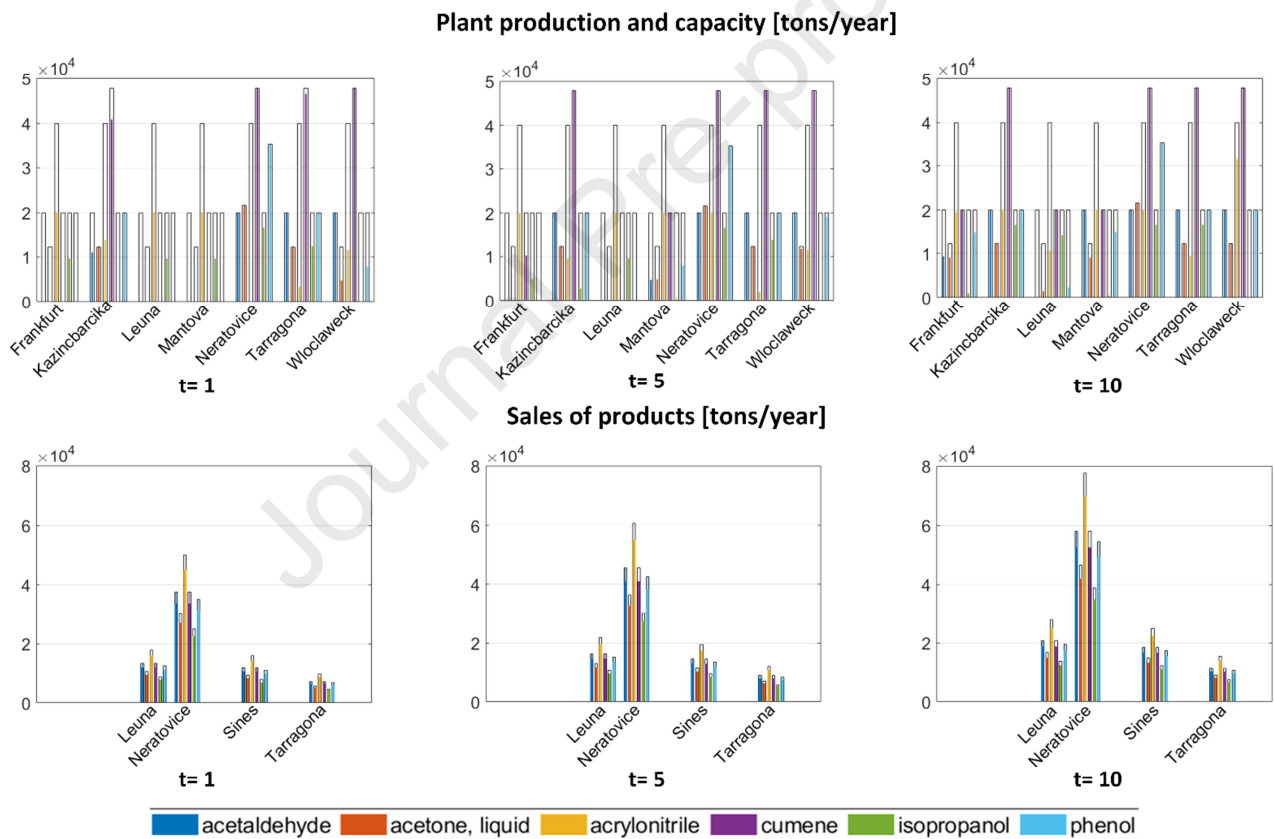


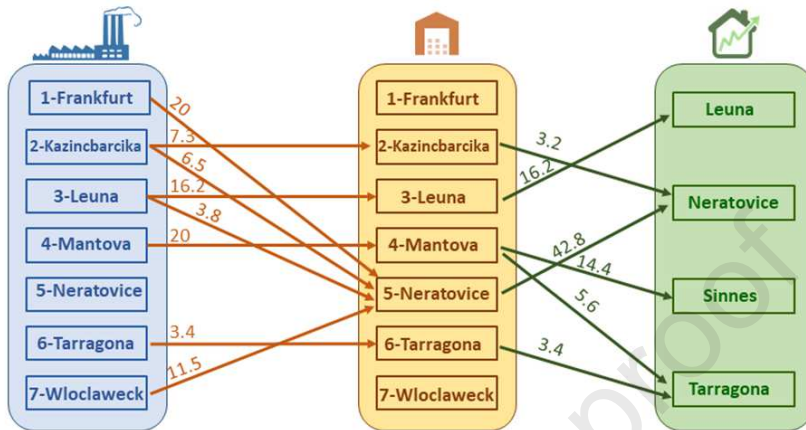
Figure 11. Maximum capacity (blank bar) and actual (colored bar) production of each technology (upper row), and demand upper bound (blank bar) and sales (colored bar) in markets for all chemicals (lower row) at time periods 1, 5 and 10.

Regarding the SC structure, as an example, Figure 12 presents the flows (ktons/year) between plants and warehouses and warehouses and markets corresponding to the

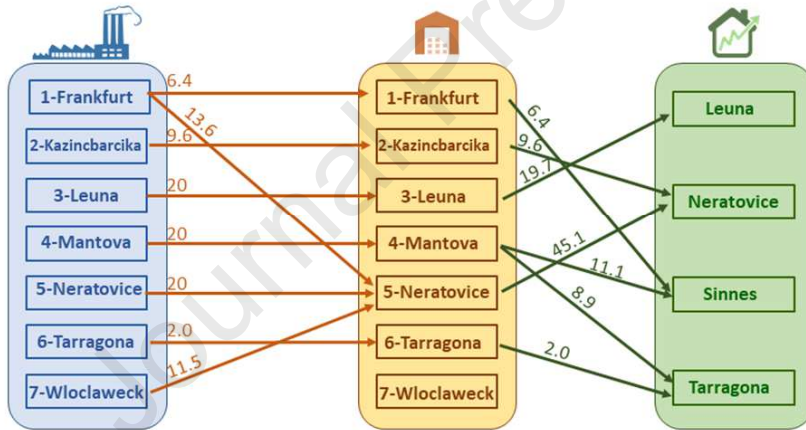
highest demanded chemical (see Table A.3), acrylonitrile, for the same time periods (1, 5 and 10).

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a) t=1



b) t=5



c) t=10

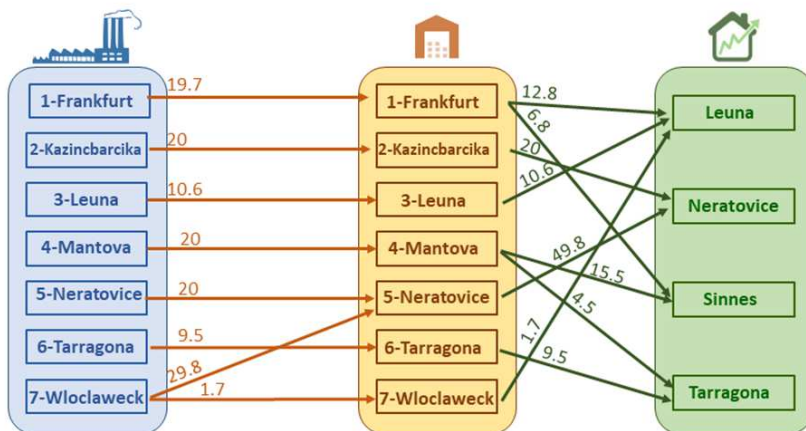


Figure 12. SC network and flows (ktons/year) for the highest demanded product (Acrylonitrile) in markets: a) time period 1, b) time period 5 and c) time period 10.

5.3 Sensitivity analysis

In this section, we present the most significant results of the sensitivity analysis carried out in order to study the effect of the CO₂ allowances price and the carbon cap reduction rate on the proposed cooperative game performance.

5.3.1 Effect of the CO₂ price

As explained in section 5.1, the ARIMA model predicts an evolution for the emission rights price within a confidence interval. In that range, different price evolutions (i.e., scenarios) have been forecasted using a Monte Carlo sampling. Particularly, in this study, we analyze the behavior of the 7-player game considering the upper and lower price scenarios predicted by ARIMA(4,1,4) and compare them with the results using the mean value prediction previously analyzed. The values of the maximum NPV attained by each company working individually and by the grand coalition, as well as their respective GWP for the upper and lower emission allowances price predictions, are shown in Table 5. Like in the base case analyzed before, the grand coalition turns out to be advantageous in both economic and environmental terms. The cooperation among companies increases the NPV, with respect to the overall NPV achieved by all companies working separately, around 50 % and 25 % for the predicted upper and lower prices, respectively. According to these results, the higher the price of the CO₂ allowances, the more economically efficient the grand coalition is (notice that for the predicted mean value of the allowances price, the NPV improvement is in between these two values, 28 %).

Table 5. NPV and GWP for each company acting separately and for the grand coalition, using the ARIMA upper and lower values predictions for the CO₂ allowances price.

Player n (company)	ARIMA upper prediction		ARIMA lower prediction	
	NPV_n (M€)	GWP_n^{total} (Mtons CO ₂ -eq)	NPV_n (M€)	GWP_n^{total} (Mtons CO ₂ -eq)
1	21.27	2.032	25.35	2.045
2	40.61	2.073	45.71	2.122
3	10.44	2.024	14.35	2.025
4	31.20	2.050	35.72	2.086

5	50.50	2.023	54.85	2.087
6	28.36	2.084	33.42	2.120
7	16.06	2.041	48.64	2.086
$\sum_n NPV_n$ $\sum_n GWP_n^{total}$	198.42	14.326	258.04	14.571
Grand coalition	296.65	14.018	323.23	14.236

As well as in the previous case, the next step is to apply the row generation algorithm of the cooperative game model to determine the core existence and a profit allocation within it, which assures the stability of the grand coalition. For these both instances, the respective game cores exist and the imputations found that meet the core conditions (Eq. (27)) are the following:

$$\pi_{ARIMAupper\ value}^* = \{31.68, 46.02, 25.14, 38.99, 60.94, 48.35, 45.53\}$$

$$\pi_{ARIMAlower\ value}^* = \{35.20, 51.77, 30.48, 41.58, 65.40, 47.61, 51.19\}$$

As can be seen, all companies improve their profit when they cooperate in the same SC to satisfy products demand in markets.

Regarding the environmental performance of the SC, when all companies cooperate in the grand coalition, the GWP decreases around 2 % with respect to the overall GWP generated by the non-cooperating companies. Although the emissions reduction rate achieved by the grand coalition is very similar for all instances analyzed, the CO₂ price does affect the absolute value of the GWP. The higher the price of the emission rights, the lower the environmental impact caused by the SC activity (see Table 2 and Table 5). If the GWP generated by the grand coalition is broken down into the different time periods through the time horizon considered (Figure 13), it can be observed that, as the cap is reduced over time (dotted line that represents the summation of the free allowances available for all companies), the price of the emission allowances has a growing impact on the CO₂ emissions. It is especially noticeable for time periods 4 to 6. For the last time periods (7 to 10), despite the price differences, the GWP is nearly constant since it is not possible to decrease the GWP and satisfy the high demand for products in markets simultaneously. On the other hand, for the first time periods (1 to 3), although the companies have enough free allowances to emit, the emissions are lower when the price of CO₂ allowances is higher so the companies can obtain greater benefit from emission rights surplus sales. In Figure 13, the first and last periods have been magnified in order to facilitate the visualization of the explained behavior.

The combination of three factors: the carbon cap reduction imposed by the government, the impossibility of a further emissions decrease due to the increasing products demand at markets with time and the CO₂ allowances price increase for the mean and upper values of ARIMA prediction, causes a dramatic rise in the expenditures of buying extra allowances at the last time periods, which cannot be compensated by the earnings due to the sales of allowances surplus during the initial periods of the time horizon, thus causing the NPV of the SC to decrease as the predicted CO₂ price increases (see Table 2 and Table 5).

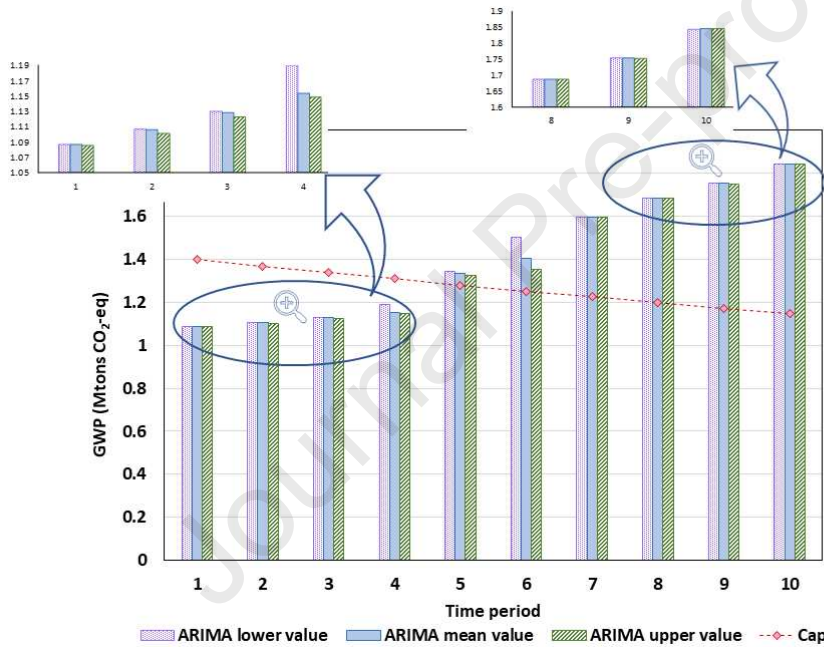


Figure 13. GWP generated at each time period for different ARIMA CO₂ price predictions.

This fact is clearly illustrated in Figure 14, where the net income related to the carbon trading for different ARIMA predictions through the time horizon are depicted. For the case of the lower prices predicted by the model, losses due to the purchase of allowances are almost constant despite the emissions growth with time (periods 7 to 10). This is due to the price decrease with time predicted by this particular ARIMA forecast (see Figure 7). In fact, considering the whole time horizon (10 years), the global net income due to carbon trading $\left(\sum_t Net_t^{CO_2} \right)$ is positive only in this case (ARIMA lower

value), with a value of 24.3 k€. For the mean and upper values predicted by the ARIMA model, the global net income due to carbon trading are -50 and -91.8 M€, respectively.

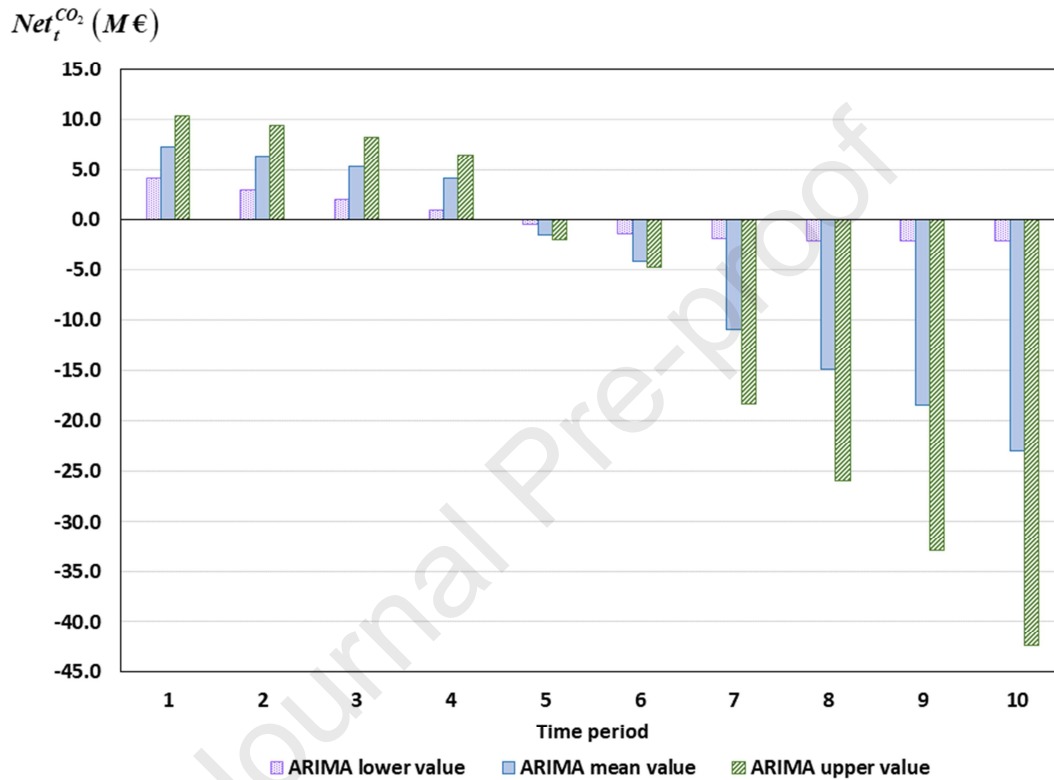


Figure 14. Net income due to the carbon trading for different ARIMA predictions.

5.3.2 Effect of the cap reduction rate

The results previously shown considered an annual decline in the cap value of 2.2%. In this section, we analyze the behavior of the cooperative SC if, for any reason, there is a change in the cap reduction policy. Specifically, we change the reduction rate in a range between 0 % and 50 % starting from the same initial value (2×10^8 kg CO₂-eq at $t=1$) and using the ARIMA mean value prediction as the CO₂ allowances price. We apply the same approach as in previous cases for 6 instances (cap reduction corresponding to 0 %, 2.2 %, 5 %, 10 %, 20 %, 50 %), that is, firstly we check whether the grand coalition achieves a better performance than that globally attained by the companies working

individually and then, we make use of the cooperative game theory to determine a profit share drawn from the core of the game, which ensures the stability of the grand coalitions established.

For all instances, the formation of the grand coalition has proved beneficial in terms of both economic and environmental performance and, for all games, the core constraints were met, thus the core exists. The imputations found that ensure the grand coalitions stability are displayed in Table.6.

Table.6. Profit share for the grand coalitions formed under different cap reduction rates.

% cap reduction	π^*
0	{35.96, 49.35, 32.97, 41.93, 58.32, 51.04, 54.07}
2.2	{33.83, 49.04, 26.87, 39.78, 62.91, 47.66, 48.49}
5	{31.39, 46.25, 26.67, 36.51, 59.39, 46.76, 44.73}
10	{27.86, 45.00, 21.04, 36.22, 59.37, 37.25, 40.14}
20	{20.97, 37.28, 7.90, 32.61, 49.51, 39.64, 44.43}
50	{16.55, 33.70, 9.85, 24.93, 48.60, 25.37, 28.85}

The convenience of working cooperatively can be clearly observed in Figure 15, where the NPVs (M€) obtained for the non-cooperating companies and for the grand coalitions are depicted.

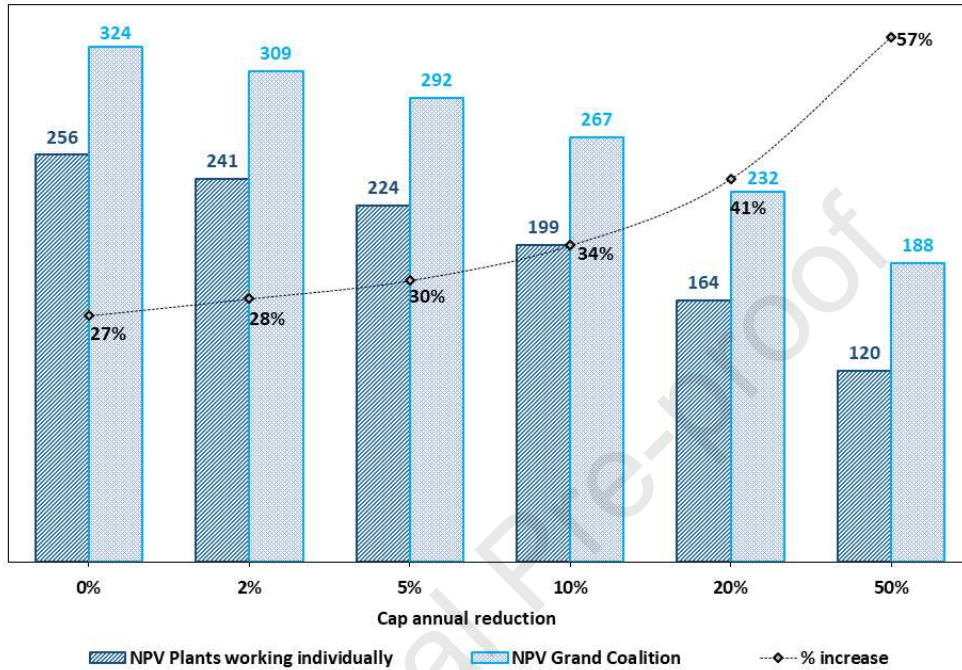


Figure 15. NPV (M€) achieved by the non-cooperating and the grand coalition for different cap reduction rates.

In addition, Figure 15 shows the increase ratio of the NPV corresponding to the grand coalitions with respect to the overall NPV achieved by all the companies if they worked individually, which ranges from 27 %, in the case that there is no annual cap reduction, to 57 %, in the case of the maximum reduction value considered in this study (50 % annual cap reduction). According to this ratio, the more restrictive the cap-and-trade policy is, the more incentivized the companies are to cooperate and share their resources.

Regarding the value of the GWP, for all cases the result was identical to that obtained for the base case (Table 2), regardless the cap annual reduction applied, thus indicating that the CO₂ allowances price has a higher impact on the SC emissions than the cap value. Obviously, the decrease of the free emission rights available is of a great significance for the NPV, as seen in Figure 14, since the companies must buy a greater number of allowances to cover their emissions, which cannot be reduced and satisfy their markets simultaneously.

6 Discussion

The results presented above unveil that cooperation is beneficial both in economic and environmental terms in all instances analyzed. To ensure the stability of the grand coalition (i.e., none of the players have any incentive to work alone or form smaller coalitions), the profit share among the companies must be advantageous for all participants. In this case, we made use of the core concept as sharing criterium, using a row generation algorithm to effectively find a core imputation.

The conditions taken as the base case correspond to the ARIMA mean value prediction (as forecasts have been obtained for different Monte Carlo scenarios) for the CO₂ allowances price and an annual reduction in the emissions cap corresponding to that planned for the phase 4 of the EU ETS (2.2 %). The sensitivity analysis carried out for these two features highlights that the more restrictive the carbon trade scheme is due to higher price or lower cap, the more economically efficient is to form the grand coalition (i.e. all plants working together in a cooperative SC). Regarding the environmental performance of the cooperative SC, the overall carbon emissions are more sensible to the CO₂ allowances price than to the emissions cap imposed by the government.

On the other hand, the proposed model also presents some limitations. For instance, like any MILP, as the number of binary variables increase, the combinatory complexity makes the problem harder to solve, and eventually for a given problem size the computation time is too high. For our case study of seven companies, the overall solution time is quite reasonable (approximately 10 s of CPU time). Obviously, for a case study where the number of companies involved in the game is higher enough, the problem would become intractable in terms of solution time. Other limitation of the model is the fault tolerance of the SC design. The proposed design does not consider the event of failure in the SC. However, our model has certain safeguards to mitigate unplanned disruptions. In case of a plant stops the scheduled production or a warehouse becomes unavailable (due to a disruptive event), as the companies cooperate, their common effort can counteract the decrease or even the cease of the target production of a plant, or the inoperative of an entity in the SC. Furthermore, each entity in the SC can individually act under unexpected events thanks to flexibility given to the model by allowing expansion capacity for plants and warehouses. In this way, as the solution design assigns a capacity value for each entity and for each period of time, it provides a gap between the current level and the capacity of an entity that could act as a risk management strategy by leveraging the new requirements due to a disruption occurring at a particular period of time.

7 Conclusions

Cooperative games theory has been successfully applied to the optimum design of sustainable SC management within the carbon trading policy framework. The key parameters for the carbon cap-and-trade model are the number of CO₂ free allowances assigned by the government (cap) and the price of the extra/surplus allowances to trade with. For the forecasting of CO₂ allowances price, the ARIMA model has been used based on the time series of the historic data. Despite the limitations of the model, ARIMA has proved to be a reliable and easy to apply method for this particular purpose. The proposed optimization model comprising the SC performance and the cap-and-trade model has been applied to a set of seven companies placed in different parts of Europe that must satisfy a minimum demand of six chemical products in four markets. The companies can act individually or cooperate in a collaborative SC, that is, forming the so called in cooperative game theory, grand coalition. The results highlight that cooperation is beneficial both in economic and environmental terms in all instances analyzed, and that CO₂ allowances price and cap influence equally in the economic performance of the cooperative SC, whereas the price has a higher impact than the cap in the environmental performance.

The importance of these results lies in the valuable information that they provide to decision makers for the SC management of companies regarding carbon market behavior and policies. On the other hand, governments can be aware of the impact of their decisions on the carbon cap value, which influences the collaborative actions of the companies that, in turn, can lead to a reduction in GHG emissions.

The main limitation of the model is that it does not consider the event of failure in the SC. Although the design presents some flexibility due to the expansion capacity of plants and warehouses, which can mitigate the effect of some unplanned events, the design would gain robustness by considering uncertainty in some parameters such as products demands or CO₂ allowances price. However, as the main objective of the present work is to prove the suitability of cooperative game theory to sustainable SC design and management, the incorporation of uncertainty would be aim of another future work.

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Notation

Sets / Indices

I/i technology

J/j plant

K/k warehouse

L/l market

N/n player

P/p product

S set of coalitions

Σ cumulative set of coalitions added to the Master Problem of the row generation algorithm

T/t time period

Subsets

$MP(i)$ set of main products of technologies

$IN(p)$ set of technologies that produce product p

$OUT(p)$ set of technologies that consume product p

Variables

Buy CO₂ allowances bought

C capacity of technologies/warehouses, tons

$CExp$ capacity expansion of technologies/warehouses, tons

CF cash flow, €

D	product demand in markets, tons
e	errors in ARIMA model
FCI	total fixed capital investment, €
$FTDC$	fraction of the total depreciable capital that must be paid in period t , €
GWP	Global Warming Potential, kg CO ₂ -Eq
INV	inventory of warehouses, tons
NE	net earnings, €
Net	net income due to carbon trading, €
NPV	Net Present Value, €
PU	purchases of products, tons
Q	product flows from plants to warehouses/from warehouses to markets, tons
SA	sales of products in markets, tons
$Sales$	CO ₂ allowances sold
W	input/output flow of products in plants, tons
x	binary variable for the transportation links between nodes of the SC
Y	predicted CO ₂ allowance price in time period t , €
y	binary variable for the occurrence of capacity expansion of technologies/warehouses
m	objective function value of the MILP subproblem of row generation algorithm, € (i.e. additional profit obtained by coalition S' when it deviates from the grand coalition)
n	characteristic function (profit attained by a player or coalition of players acting individually).
π	profit allocation vector

u binary variable that takes the value 1 when player n belongs to a coalition that violates the core constraint

w objective function value of the Master Problem of row generation algorithm, € (i.e. maximum additional profit obtained by a coalition S when it deviates from the grand coalition. If at any iteration $w > 0$, then the core is empty)

Parameters

Cap	free CO ₂ allowances given by the government to companies
\overline{CExp}	upper bound for the capacity expansion of technologies/warehouses, tons
\underline{CExp}	lower bound for the capacity expansion of technologies/warehouses, tons
$Cost$	cost of CO ₂ allowances bought, €
\overline{D}	maximum demand of products in markets, tons
\underline{D}	minimum demand of products in markets, tons
Imp^{EN}	Life cycle impact assessment (LCIA) result for the GWP indicator due to the consumption of 1 MJ of energy, kg CO ₂ -equivalents/MJ
Imp_p^{RM}	Life cycle impact assessment (LCIA) result for the GWP indicator due to the consumption of 1 kg of raw material p , kg CO ₂ -equivalents/kg of p
Imp^{TR}	Life cycle impact assessment (LCIA) result for the GWP indicator due to the transportation of 1 ton of mass 1 km of distance, kg CO ₂ -equivalents/(ton·km)
ir	interest rate, (dimensionless)
NT	number of time periods, dimensionless
$Price$	price of CO ₂ allowances sold, €
\overline{Q}	upper bound on the flows of materials, tons

\underline{Q}	lower bound on the flows of materials, tons
sv	salvage value of the network, dimensionless
α	fitting parameters for the autoregressive part of ARIMA
β	fitting parameters for the moving average part of ARIMA
h	energy consumed per unit product p produced by technology i in plant j , TOFOE (Tons of Fuel Oil Equivalent = 41.868 GJ)
λ	distance between SC entities, km
u	average value of the data set for ARIMA prediction
σ^2	variance in ARIMA model
t	minimum desired percentage of the technology capacity that must be used, dimensionless

Acronyms

ACF	Autocorrelation Function
AIC	Akaike information criteria
ARIMA	AutoRegressive Integrated Moving Average
BIC	Bayesian information criteria
ETS	Emissions Trading System
EU	European Union
GAMS	General Algebraic Modeling System
GHG	Green House Gas
ICAP	International Carbon Action Partnership
IPCC	Intergovernmental Panel on Climate Change

LCA	Life Cycle Assessment
LCIA	Life Cycle Impact Assessment
MP	Master Problem
PACF	Partial Autocorrelation Function
SC	Supply Chain

Superscripts

EN	energy
PL	plant
RM	Raw material
TR	transportation
WH	warehouse

Appendix A

Tables A.1 to A. 9 contain the input data for the case study.

Table A. 1. Distances (km) between plants and warehouses

	l_{jk}^{PL} (km)						
Plant/Ware.	Frankfurt	Kazincbarcika	Leuna	Mantova	Neratovice	Tarragona	Wloclaweck
Frankfurt	0	1138.34	370.12	817.02	551.36	1420.77	719.46
Kazincbarcika	1138.34	0	979.09	1086.16	695.51	2385.78	644.2
Leuna	370.12	979.09	0	870.12	295.45	1781.36	411.27
Mantova	817.02	1086.16	870.12	0	862.05	1183.24	1116.31
Neratovice	e	695.51	295.45	862.05	0	1855.47	277.14
Tarragona	1420.77	2385.78	1781.36	1183.24	1855.47	0	2110.37
Wloclaweck	719.46	644.2	411.27	1116.31	277.14	2110.37	0

Table A. 2. Distances (km) between warehouses and markets

	l_{kl}^{WH} (km)			
	Leuna	Neratovice	Sines	Tarragona
Frankfurt	370.12	551.36	2462.36	1420.77
Kazincbarcika	979.09	695.51	3614.54	2385.78
Leuna	0	295.45	2850.72	1781.36
Mantova	870.12	862.05	2357.76	1183.24
Neratovice	295.45	0	2970.72	1855.47
Tarragona	1781.36	1855.47	1212.82	0

Wloclaweck	411.27	277.14	3198.04	2110.37
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Table A. 3. Demand of chemicals at each market for $t=1$. An increase of 5% each time period is assumed.

	\overline{D}_{lpt} (ktons)			
	Leuna	Neratovice	Sines	Tarragona
Acetaldehyde	13.5	37.5	12	7.5
Acetone	10.8	30	9.6	6
Acrylonitrile	18	50	16	10
Cumene	13.5	37.5	12	7.5
Isopropanol	9	25	8	5
Phenol	12.6	35	11.2	7

Table A. 4. Price of chemical products (€/ton) at each market for $t=1$. An increase of 5% each time period is assumed.

	Leuna	Neratovice	Sines	Tarragona
Acetaldehyde	509.26	487.43	491.07	500.17
Acetone	432.87	414.32	417.41	425.14
Acrylonitrile	36.40	34.84	35.10	35.75
Cumene	401.23	384.04	386.90	394.07
Isopropanol	401.23	384.04	386.90	394.07
Phenol	709.88	679.45	684.52	697.20

Table A. 5. Variable investment cost coefficient (€ year/ ton) of technologies in plants for $t=1$.
An increase of 5% each time period is assumed.

	Frankfurt	Kazinbcarcika	Leuna	Mantova	Neratovice	Tarragona	Wloclaweck
Tech. 1	121.70	73.02	133.87	109.53	48.68	91.28	97.36
Tech. 2	124.58	74.75	137.04	112.12	49.83	93.43	99.66
Tech. 3	314.41	188.65	345.85	282.97	125.76	235.81	251.53
Tech. 4	139.64	83.78	153.60	125.68	55.86	104.73	111.71
Tech. 5	61.78	37.07	67.96	55.60	24.71	46.34	49.42
Tech. 6	220.78	132.47	242.86	198.70	88.31	165.59	176.63

Table A. 6. Fixed investment cost (M€) of technologies in plants for $t=1$. An increase of 5% each time period is assumed.

	Frankfurt	Kazinbcarcika	Leuna	Mantova	Neratovice	Tarragona	Wloclaweck
Tech. 1	11.08	6.65	12.18	9.97	4.43	8.31	8.86
Tech. 2	11.34	6.80	12.47	10.20	4.53	8.50	9.07
Tech. 3	28.61	17.17	31.47	25.75	11.45	21.46	22.89
Tech. 4	12.71	7.62	13.98	11.44	5.08	9.53	10.17
Tech. 5	5.62	3.37	6.18	5.06	2.25	4.22	4.50
Tech. 6	20.09	12.06	22.10	18.08	8.04	15.07	16.07

Table A. 7. Operating cost (€/ton) of technologies in plants for t=1. An increase of 5% each time period is assumed.

	Frankfurt	Kazincbarcika	Leuna	Mantova	Neratovice	Tarragona	Wloclaweck
Tech. 1	17.81	10.68	19.59	16.03	7.12	16.03	14.25
Tech. 2	48.56	29.14	53.42	43.71	19.43	43.71	38.85
Tech. 3	12.14	7.28	13.36	10.93	4.86	10.93	9.71
Tech. 4	30.76	18.45	33.83	27.68	12.30	27.68	24.61
Tech. 5	4.86	2.91	5.34	4.37	1.94	4.37	3.89
Tech. 6	30.76	18.45	33.83	27.68	12.30	27.68	24.61

Table A. 8. Energy consumption, h_{ijp}^{EN} , (FOET*/ton), of technologies in plants (Rudd, 1981)

	h_{ijp}^{EN}
Tech. 1	0.22
Tech. 2	0.6
Tech. 3	0.15
Tech. 4	0.38
Tech. 5	0.06
Tech. 6	0.38

* FOET: Fuel Oil Equivalent Tons

Table A. 9. Cost of raw materials (€/ ton) in plants for t=1. An increase of 5% each time period is assumed.

	Frankfurt	Kazincbarcika	Leuna	Mantova	Neratovice	Tarragona	Wloclaweck
Ethylene	274.91	233.68	302.40	247.42	233.68	247.42	219.93
Sulfuric acid	49.60	42.16	54.56	44.64	42.16	44.64	39.68
Hydrochloric acid	136.68	116.18	150.35	123.02	116.18	123.02	109.35
Hydrogen cyanide	551.15	468.47	606.26	496.03	468.47	496.03	440.92
Ammonia	165.34	140.54	181.88	148.81	140.54	148.81	132.28
Oxygen	35.27	29.98	38.80	31.75	29.98	31.75	28.22
Propylene	187.39	159.28	206.13	168.65	159.28	168.65	149.91

Table A. 10. Variable and Fixed Investment costs and Inventory costs associated with warehouses for t=1. An increase of 5% each time period is assumed.

	Variable cost (€/ ton)	Fixed cost (k€)	Inventory cost (€/ ton year)
Frankfurt	2.65	240.77	0.24

Kazincbarcika	1.59	144.46	0.14
Leuna	2.91	264.84	0.26
Mantova	2.38	216.69	0.22
Neratovice	1.06	96.31	0.10
Tarragona	2.38	216.69	0.22
Wloclaweck	2.12	192.61	0.19

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Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

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