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Research Article

Design of a Cooperative Sustainable Three-Echelon Supply Chain under Uncertainty in CO_2 Allowance

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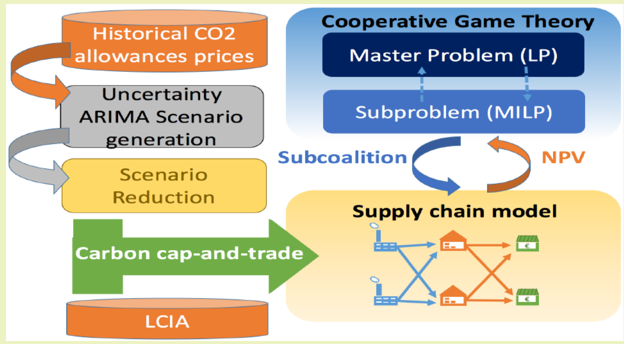
ABSTRACT: Driven by the growing concern regarding greenhouse gas emissions, in this work, we provide a robust stochastic model for the design of a cooperative supply chain (SC) under uncertainty in CO_2 allowance prices from the European Union Emissions Trading System (EU ETS). During the last years, CO_2 allowance prices have undergone unexpected changes, having strong impact on the design and management of optimal SC. The consideration of uncertainty in the allowance prices has therefore become more important. We use an autoregressive integrated moving average (ARIMA) model to predict future allowance prices. A full discretization of the underlying probability space leads to a number of scenarios far too large to be handled, so we compare two approaches to reduce the number of scenarios to a feasible maximum, the `ScenRed` algorithm and `K-means` clustering. The obtained results are compared with a deterministic approach that is widely studied in the literature, showing an increase in the benefits and a reduction of emissions.



KEYWORDS: *Uncertainty of CO_2 allowance prices, stochastic model, optimum supply chain management, cooperative game theory, ARIMA price prediction, scenario reduction, ScenRed, K-means*

■ INTRODUCTION

Nowadays, the reduction of greenhouse gas (GHG) emissions is gaining more relevance and should be taken into account when designing efficient supply chains. In order to reduce the GHG emissions, governments are adopting specific policies, resulting in changes in the optimal design of supply chains. This topic was addressed, for example, by Fareeduddin et al., who investigated a closed-loop supply chain model under the influence of a carbon tax, carbon caps, and carbon cap-and-trade system.[1] We follow the guidelines of the European Union Emissions Trading System (EU ETS), aiming to reduce GHG emissions by at least 40% by 2030.

In the design of an efficient supply chain (SC) and its management, each company must be aware of its participation in a globalized market when making decisions. In order to describe interactions between companies, game theory has been used extensively, modeling either cooperative or competitive behavior of the participants. The latter was, for example, studied by Du et al. in 2015, when they analyzed an emission-dependent SC based on a Stackelberg game approach under the impact of an emission cap-and-trade mechanism.[2]

In 2014, Yue and You presented a model for the design and planning of a noncooperative SC under a Stackelberg game and generalized Nash equilibrium.[3]

In 2020, Xia et al. investigated the impact of carbon trading on sales volume, sales profit, consumer surplus, and unit retail price in a SC modeled using a Stackelberg game.[4] A literature review from 2019 concluded that there is a scarcity of literature addressing green SC employing cooperative game concepts, and two years later, Salcedo Diaz et al. published an article describing the optimization of a multiperiod SC model incorporating a carbon trading policy and cooperative game theory.[5,6]

In most publications addressing the design of SC, a deterministic approach is taken, and uncertainties are not considered. The resulting designs are optimal for the chosen deterministic case but not robust to possible changes of the underlying parameters. Whenever stochastic approaches are used in literature, the focus most often lies on uncertainties in the demand, since satisfying the customer demand is the main driver of the supply chain. This was studied, for example, in 2021 by Khorshidvand et al., who presented a robust optimization model for a closed-loop SC with uncertain demand.[7] The authors also considered emission reduction and pointed out the benefit of a robust approach. Other papers, for

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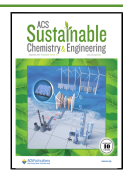

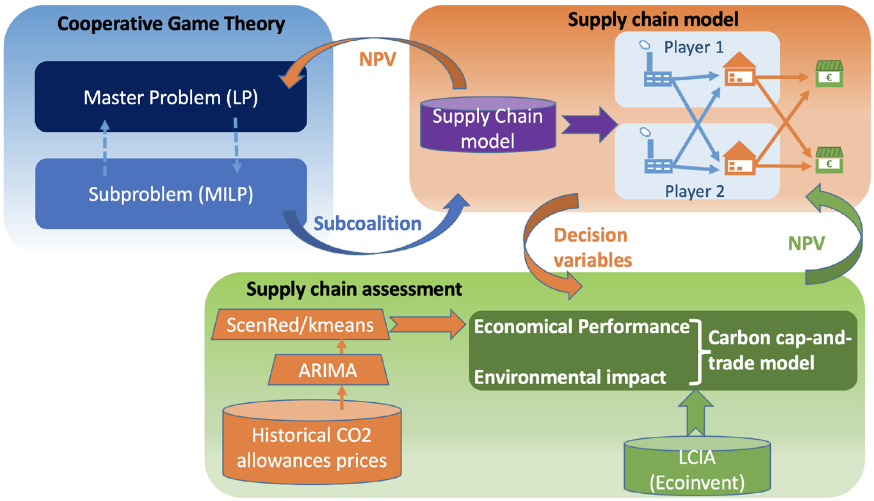

Figure 1. Scheme of the methodology applied in this work. Given the supply chain data, environmental data, and historical CO_2 allowances prices, a profit allocation is calculated using cooperative game theory for the supply chain model.

example, one by Zhitao et al. from 2022, additionally shows the importance of uncertainties in the carbon price.[8] Since the number of scenarios that must be considered for reliable results increases exponentially in the number of uncertain parameters, they also presented a method for scenario reduction, with the aim of being able to solve a two-stage stochastic model using popular commercial solvers.

In this paper, we use an autoregressive integrated moving average (ARIMA) model to forecast probable future CO_2 prices based on historical data. ARIMA models estimate parameters of the underlying probability distribution of a given time series, whenever the exact underlying distribution function is not known analytically. After fitting the model to the historical data, it can then be used to forecast future behavior of the time series (scenarios). The usage of ARIMA models for forecasting demand or prices has been studied and validated in the literature.[9,10]

The topics we investigate in this paper have been independently studied to some extent by various authors. However, to the best of our knowledge, none of them tried to investigate them conjointly. The work at hand fills this gap by presenting a robust stochastic model for a three-echelon supply chain that employs cooperative game theory to model the behavior of production plants. We consider the influence of uncertainty in carbon dioxide allowance prices and also study different scenario reduction methods together with the statistical information gap they cause, which we measure using the Jensen−Shannon distance.

The remainder of this work is structured as follows: We first present the problem statement, followed by the different methodologies applied. After that, we show numerical results and conclusions drawn from them.

PROBLEM STATEMENT

We study a three-echelon petrochemical supply chain superstructure which consists of production, storage, and market stages.[11,12] The cooperative supply chain consists of seven plants, representing seven European players from Frankfurt (Germany), Kazincbarcika (Hungary), Leuna (Germany), Mantova (Italy), Neratovice (Czech Republic), Tarragona (Spain), and Wloclawek (Poland). Each plant has an initial capacity of 20 kt/year and an annual expansion limit of 10−400 kt/year. We implement a cooperative game theory approach, in which all seven plants work together (as a grand coalition) to satisfy the demand.

Every plant can produce acetaldehyde, acetone, acrylonitrile, cumene, isopropanol, and phenol using one of six available technologies involving up to 18 different chemicals. To each plant, there is a corresponding warehouse with an initial capacity of 20 kt/year and an initial inventory of zero tons. The annual warehouse expansion limit is set between 5 and 400 kt/year. There is a limit on the annual purchases of raw materials of 32 kt/year, and it is not possible to buy final or intermediate products, preventing outsourcing.

We assume that each player satisfies an identical portion of the total market demand. Regardless of subcoalition formation, all players must be actively participating in the network to satisfy the total market demand. A minimum network demand satisfaction of 90% and an annual increase of 5% in market demand are assumed as well. There is a restriction on the material flow between plants and warehouses, as well as between warehouses and markets, of 5−500 kt/year.

We consider the environmental impact assessment through a calculation of the global warming potential, which includes the emissions from raw materials and energy consumption, as well as the emissions due to transportation between plants, warehouses, and markets.

The initial maximum amount of CO_2 allowances for each player is 2×10^8 kg CO_2 equivalent (eq), with a 2.2% annual reduction rate. This value is estimated according to the emissions right published by the Spanish government and according to phase 4 of the EU ETS.[6,12,13] Through the use of carbon caps and trade regulations, we can include the effect of carbon dioxide emissions on the profit of the network. It is expected that through cooperation of different companies the network is able to satisfy the market demand while reducing the total carbon dioxide emissions. The cooperative game theory approach yields a profit allocation, in which all players earn at least as much as in any smaller subcoalition, ensuring the stability of the grand coalition.[14]

We present a SC design and management, which is robust against uncertainty in future CO_2 allowance prices, by incorporating different possible price scenarios. We also address scenario reduction, being an important topic in

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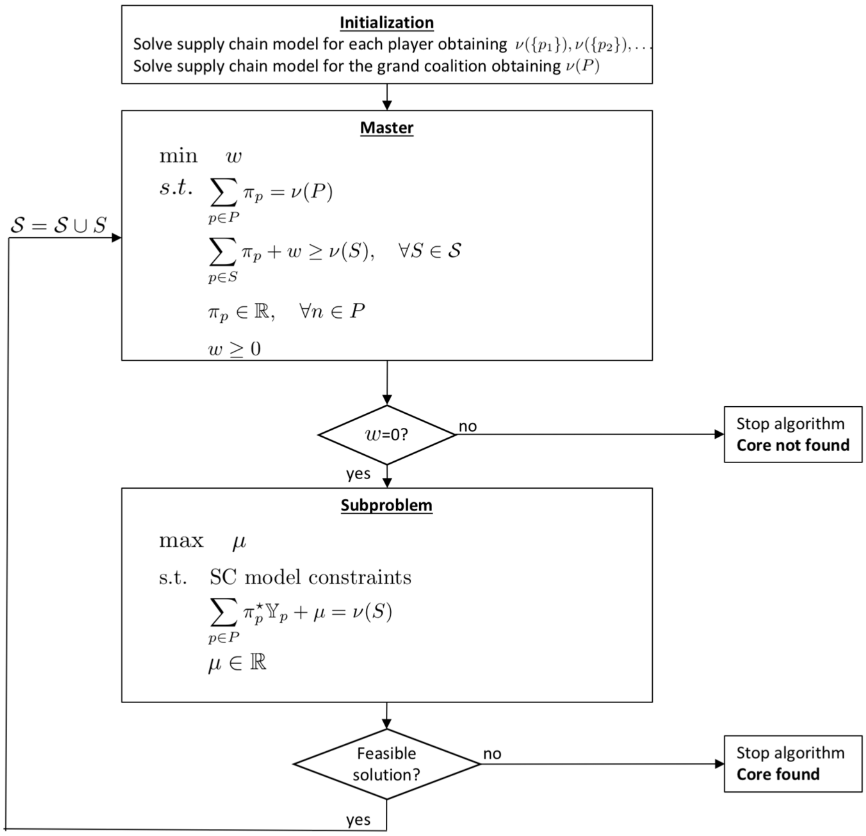

Figure 2. Flowchart of the row generation algorithm.

stochastic modeling due to computational limitations. In this paper, we present and compare two different methods to reduce the number of scenarios.

METHODOLOGY AND MATHEMATICAL FORMULATION

The methodology that is used in this work, its components, and the connection between them is presented in Figure 1.

The following types of data are needed for the computation: supply chain data; life cycle impact assessment (LCIA) data, required to determine the global warming potential (GWP); and historical CO_2 allowance prices, being the basis for scenario generation.

The goal is to find an optimal SC design and a profit allocation which ensures that at all considered times and for all players it is more profitable to work together with all other players than in smaller subcoalitions. The cooperative game theory approach is modeled by a numerical scheme that solves a master and a subproblem in an alternating manner. The master problem searches for a profit allocation among the players which ensures stability of the grand coalition. The subproblem searches for a subcoalition that could destabilize the cooperation, meaning that one or more players could earn more money in this subcoalition than in the grand coalition. If such a coalition is found, the master problem of the next iteration will take it into account when searching a new profit allocation for the grand coalition.

The supply chain model searches for a possible combination of expansion and transportation links that will ensure demand satisfaction while maximizing the profit. The carbon cap and trade model links the economic performance to the environmental impact by including net earnings from trading of the CO_2 allowances. To determine the global warming potential, we use data of the life cycle impact assessments from the Ecoinvent database. Using historical CO_2 allowance prices and an ARIMA model, a large number of scenarios are generated. We then reduce the number of scenarios using the `ScenRed` algorithm or `K-means` clustering, while measuring the corresponding information loss. The resulting stochastic problem with the reduced number of scenarios can then be solved using commercial software.

In the following subsections, we address each of the components of the methodology in detail.

Game Theory and Row Algorithm. A cooperative game model is based on a contract accepted by a group of players, who divide the total profit. Our goal is to find a profit allocation that makes the grand coalition the most profitable option for all players. The set of all such profit allocations is called the *core* and is defined mathematically as

$$C(P, \nu) = \left\{ \pi \in \mathbb{R}^{\mathrm{card}(P)} \,\middle|\, \sum_{p \in P} \pi_p = \nu(P) \text{ and } \sum_{p \in P} \pi_p \geq \nu(S),\ \forall\ S \subset P,\ S \neq \theta \right\} \tag{1}$$

The first constraint, known as efficiency property, states that the total profit of the grand coalition $\nu(P)$ must be equal to the sum of the profit shares of all players π_p. The second group of constraints forms the rationality property, stating that the profit of any subcoalition $S \subset P$, $\nu(S)$, must yield a smaller profit than the profit of the grand coalition, i.e., $\nu(S) \leq \nu(P)$. The rationality property consists of $2^{\mathrm{card}\ P}$ constraints, a

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number which grows exponentially in the number of players. In this work, we consider seven players, leading to $2^7 + 1$ subject to conditions in eq 1. We therefore have to solve 128 optimization problems to determine the benefit of each subcoalition in order to find a profit allocation from the core. Taking into account these optimization problems are possibly large-scale MILPs, and this could eventually be intractable. In order to simplify the computation, we use the row generation algorithm.[15] This allows us to solve the master problem with a reduced set of relaxed constraints that is initialized as

$$\mathcal{S} := \{P, \{p_1\}, \{p_2\}, ..., \{p_{\mathrm{card}P}\}\} \quad (2)$$

In each iteration, a subproblem is solved that identifies a new subcoalition which could violate the core, and adds it to the set $\mathcal{S}$. The iterative algorithm is shown in Figure 2.

Supply Chain Model. In this work, we address a multiperiod mixed integer linear program with the objective of maximizing the net present value (NPV) of a cooperative supply chain. The supply chain model is described by blocks of equations for mass balances, capacity constraints, environmental impacts, and economic assessments. Detailed information can be found in the Supporting Information (SI) under "Supply Chain", including the mass balance and capacity constraints, as well as the objective function of the problem.

Environmental Impact Assessment. The environmental impact of the supply chain is quantified by the global warming potential (GWP) indicator, which estimates the relative global warming contribution per kg of emitted gases over a period of time, compared to the contribution of 1 kg of carbon dioxide. We consider the emissions due to raw material consumption and transportation between plants and warehouses and between warehouses and markets, as well as emissions produced due to energy consumption. To calculate the total GWP, we used LCIA-data from the Ecoinvent database using a time horizon of 100 years. Further information and equations can be found in the SI under "Supply Chain" and "Environmental Impact Assessment".

Carbon Cap and Trade Model. Using the LCIA information, the global warming potential of a supply chain can be determined. Each plant of the network starts with an initial amount of CO_2 allowances. The trading system permits each plant to sell or buy its CO_2 allowances, influencing the total profit of the SC. The total network is subject to a maximum amount of possible emissions that will be reduced over the years. Hence, the price of CO_2 allowances is a parameter of uncertainty and has an influence on the design of the supply chain.[16] Further information and equations can be found in the SI under "Supply Chain" and "Objective Function".

ARIMA Model. In order to incorporate uncertainty into the CO_2 allowance prices, an autoregressive integrated moving average (ARIMA) model was used. Using the historical data from 2009 to 2021, the parameters p, d, and q of the model were identified using the Akaike and Bayesian information criteria.[17,18] We then generated $n_s = 1000$ different pricing scenarios using the models forecast ability.

The parameter p of the model determines the nonseasonal polynomial degree, that is, the number of lagged observations used. The parameter d is the order of differentiation used to remove seasonal trends from the time series data. Lastly, parameter q is the number of moving average terms used in the model. Detailed information can be found in the Supporting Information under "ARIMA Model".

Scenario Reduction. In the following, a scenario is a tuple of T values describing the CO_2 prices for the next T years. In this work, we take uncertainty of the CO_2 prices into account by solving a stochastic model, that should include a multitude of scenarios. The number of scenarios needs to be chosen in a way that leads to a good discretization of the underlying probability space. Since an analytical form of the probability distribution of the historical CO_2 prices is not known, we sample the distribution curve by a large number of scenarios and calculate the corresponding probabilities $P(s_i)$, s_i, $i = 1, ..., n_s$ using the histogram. We can now introduce a discrete probability distribution by weighting the probability of each scenario by the sum of the probabilities of all scenarios. The probability for s_i in this discrete distribution is denoted $P^d(s_i)$. See the Supporting Information for more details.

As described before, the number of samples n_s should be large. Unfortunately, this increases the number of equations and variables appearing in the stochastic linear optimization problem very fast. Hence, we must reduce the number of scenarios as much as possible, without losing significant statistical information contained in the variety of samples. At this point, we can follow different strategies on how to reduce n_s and how to measure the corresponding loss of information.

`ScenRed` Algorithm. The `ScenRed` algorithm was developed by Römisch et al.[19] Suppose, that a finite number of samples $\Omega^d = \{s_i\}_{i=1}^{n_s}$ and two discrete probability distributions P^d, Q^d: $\omega^d \to \mathbb{R}$ are given. The similarity of the distributions P^d and Q^d on a class of measurable functions $\mathcal{F} = \{f: \Omega^d \to \mathbb{R}, f \text{ measurable}\}$ is given by

$$d_{\mathcal{F}}(P^d, Q^d) = \sup_{f \in \mathcal{F}} \left| \sum_{i=1}^{n_s} f(s_i)P^d(s_i) - \sum_{i=1}^{n_s} f(s_i)Q^d(s_i) \right| \quad (3)$$

`ScenRed` was designed for the case of convex stochastic programs, which can mostly be written in the form of minimizing the expectation of a certain function f depending on a random variable and a spatial variable from a convex domain. A rather mild condition for the target function f is that it is continuous in the spatial variable. When restricting $\mathcal{F}$ to continuous functions, the distance (eq 3) is bounded from above by a Kantorovich functional which can be computed explicitly.[20] This explicit form of the Kantorovich functional can then be used to define the discrete values of the distribution Q^d on a smaller set of scenarios $n_s^{\mathrm{red}} \ll n_s$.

The problem at hand consists of a linear target function and subject to conditions with continuous as well as binary variables. For fixed binary (decision) variables, the problem is linear; convex and the target function is continuous. An application of `ScenRed` seems therefore reasonable. Unfortunately, with nonfixed binary variables, these analytical properties seem lost. A relaxation of the binary variables into continuous variables would be possible, and the large majority of variables is continuous itself (>95%). However, we nevertheless expect `ScenRed` to perform well for the problem under study.

`K-Means` Clustering. By an application of the `K-means` algorithm, the scenarios can be grouped into $n_s^{\mathrm{red}} \ll n_s$ clusters $c_1, ..., c_{n_s^{\mathrm{red}}}$.[21] The clusters satisfy

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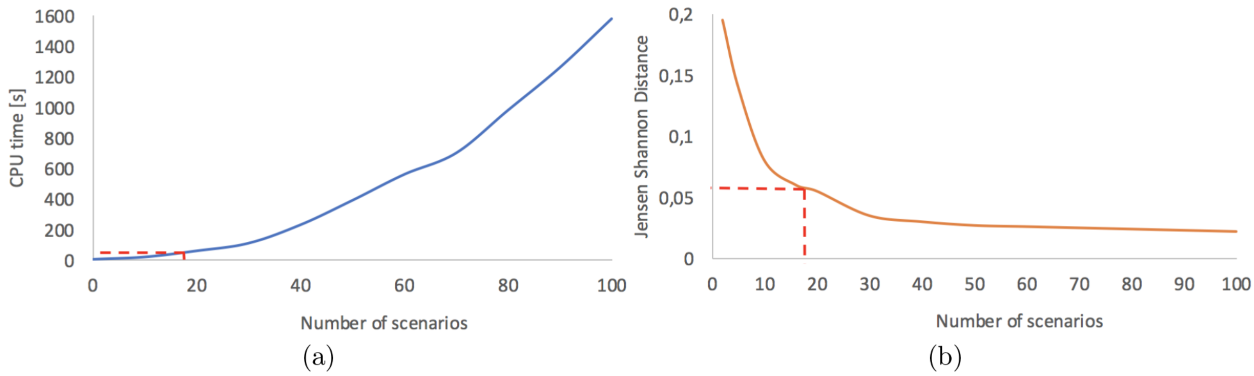

Figure 3. (a) CPU time for solving the stochastic problem for the grand coalition and different numbers of scenarios. (b) Jensen−Shannon distance $d_{JS,2}$ for changing number of reduced scenarios. This distance moves between 0 and 1 and is equal to 0 if and only if the two probability distributions are identical. As expected, it converges to zero for large numbers of scenarios. The dotted red line indicates the corresponding value for 16 reduced scenarios in both panels.

$$c_k \subset \Omega^d, \forall\, k = 1, \ldots, n_s^{\mathrm{red}}$$

$$\bigcup_{k=1}^{n_s^{\mathrm{red}}} c_k = \Omega^d$$

$$P^d\Big(\bigcup_{k=1}^{n_s^{\mathrm{red}}} c_k\Big) = \sum_{k=1}^{n_s^{\mathrm{red}}} P^d(c_k) := \sum_{k=1}^{n_s^{\mathrm{red}}} \sum_{s_i \in c_k} P^d(s_i) = \sum_{i=1}^{n_s} P^d(s_i) = 1 \tag{4}$$

By our definition of P^d, the probability of a cluster, $P^d(c_k)$, is defined as the sum of probabilities of samples in the cluster. We are now able to define a new probability distribution Q^d on the samples by assigning all scenarios in a cluster a fraction of the probability of the cluster. Since in clustering we forget about individual samples, no individual probabilities should be assigned either. Hence, it makes sense to define Q^d as

$$Q^d(c_k) = P^d(c_k) \overset{\mathrm{Def.}}{=} \sum_{s_i \in c_k} P^d(s_i),$$

$$Q^d(s_i) = \frac{P^d(c_k)}{\mathrm{card}(c_k)}, \forall\, s_i \in c_k, \forall\, k = 1, \ldots, n_s^{\mathrm{red}} \tag{5}$$

Jensen−Shannon Distance. We now have two probabilities for each scenario available, the initial $P^d(s_i)$ and the approximation $Q^d(s_i)$, for all i = 1, ..., n_s. In order to measure a distance between the distributions P^d and Q^d, we introduce the *Kullback−Leibler divergence*, which for any $b \in \mathbb{R}^+$ reads

$$D_{\mathrm{KL},b}(P^d, Q^d) := \sum_{i=1}^{n_s} P^d(s_i)\log_b \frac{P^d(s_i)}{Q^d(s_i)} \tag{6}$$

Note that $D_{\mathrm{KL},b}$ is not a metric, since it, for example, lacks symmetry. A straightforward symmetrization of the Kullback−Leiber divergence is the *Jensen−Shannon divergence*

$$D_{\mathrm{JS},b}(P^d, Q^d) := \frac{1}{2}D_{\mathrm{KL},b}\left(P^d, \frac{1}{2}(P^d + Q^d)\right) + \frac{1}{2}D_{\mathrm{KL},b}\left(Q^d, \frac{1}{2}(P^d + Q^d)\right) \tag{7}$$

and it can be easily checked that the square root of $D_{\mathrm{JS},b}$ defines a metric

$$d_{\mathrm{JS},b}(P^d, Q^d) := \sqrt{D_{\mathrm{JS},b}(P^d, Q^d)} \tag{8}$$

The metric $d_{\mathrm{JS,b}}$ is called a *Jensen−Shannon distance* for any value of $b \in \mathbb{R}_+$ to be fixed. The choice b = 2 implies the canonical bounds $0 \leq d_{\mathrm{JS},2}(P^d, Q^d) \leq 1$, where the expression is zero if and only if P^d is identical to Q^d. We use this distance in order to measure how much of the statistical information on the samples is lost as a result of a reduction algorithm applied. Measuring this information gap for n_s = 1000 samples and different numbers of clusters shows that taking $n_s^{\mathrm{red}} = 16$ clusters corresponds to an acceptable loss of statistical information of about 5%, as can be seen in Figure 3.

■ RESULTS AND DISCUSSION

All computational experiments were conducted on a MacBook Pro model 2020 with 16 GB Ram and macOS 11.2.1. All the models and solution algorithms have been written in GAMS 27.1. The solution algorithm used in GAMS is CPLEX running on eight threads. For the grand coalition and in the first iteration using 16 reduced scenarios, the subproblem consists of 249,050 equations, 379,981 continuous variables, and 7840 discrete variables. The master problem has 22 equations and nine variables.

In this paper, we present a design of a supply chain with cooperative game theory, as well as uncertainty in the CO_2 prices. The advantages of this approach are the reduction of emissions and increase of profit of the network. Fist, we must guarantee that the grand coalition is stable. In Table 1, we exemplarily compare the economic and environmental

Table 1. Net Present Value and Global Warming Potential for Grand Coalition and for Individual Companies Using ScenRed for Scenario Reduction

Player p (company)	NPV_p (M€)	$\mathrm{GWP}^{\mathrm{total}}$ (Mtons CO2-eq.)
1	25.36	2.03
2	43.38	2.07
3	14.86	2.02
4	34.93	2.05
5	52.87	2.02
6	31.53	2.08
7	47.57	2.04
All	$\sum_{p=1}^{7} \mathbf{NPV}_p = 250.50$	$\sum_{p=1}^{7} \mathrm{GWP}_p^{\mathrm{total}} = 14.32$
Grand coalition	324.52	13.99

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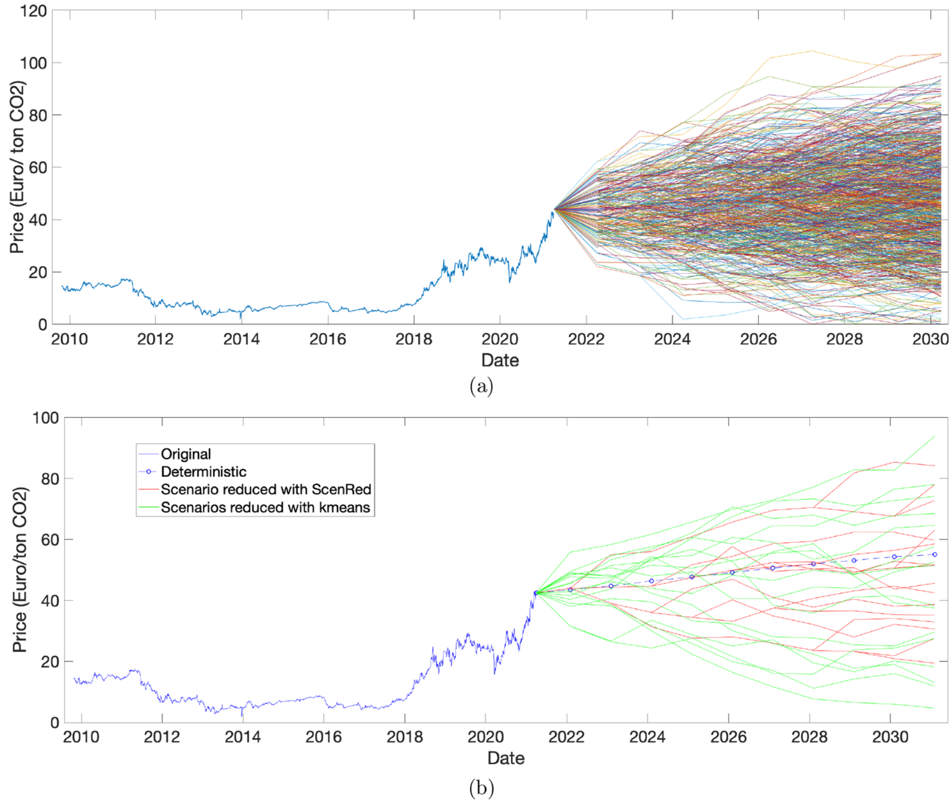

Figure 4. Representation of the historical CO_2 allowances prices between 2009 and 2021 and the forecasts. (a) Original 1000 sampled scenarios using the ARIMA (7, 1, 8) model are shown. (b) In blue is historical data, in dotted blue the deterministic scenarios, in red the `ScenRed` reduced scenarios, and in green the clustered scenarios due to `K-means`.

performance of the grand coalition against individual (one player) subcoalitions. As can be seen, the grand coalition results in an increased economic performance of 22.3%, as well as a reduction of 2% in emissions. One possible profit allocation that ensures stability of the grand coalition is Frankfurt 30.5%, Kazincbarcika 13.4%, Leuna 4.6%, Mantova 10.8%, Neratovice 16.3%, Tarragona 9.7%, and Wloclawek 14.7% of the total profit.

A stochastic model is harder to solve but provides a more robust result for the nonscenario-dependent variables to future changes in the CO_2 prices. To represent the uncertainty of the CO_2 allowance prices, a large number of scenarios is required and will be generated using an ARIMA model. The AIC and BIC information criteria show that the ARIMA model that best fits the historical CO_2 allowance prices between 2009 and 2021 is ARIMA ($p = 7$, $d = 1$, $q = 8$). This model is used to generate 1000 initial samples to predict the CO_2 price during the next 10 years. The original scenarios that were generated are represented in Figure 4(a). In order to reduce the number of scenarios to 16, we applied the `ScenRed` algorithm and the `K-means` clusterization. The reduced scenarios are shown in Figure 4(b).

A sensitivity analysis was carried out to ensure that the scenario generation and reduction provide good representations of the underlying probability space. The ARIMA model was run to generate 1000 initial scenarios, which were then reduced to different numbers of reduced scenarios using both `ScenRed` and `K-means`. The stochastic SC model was then solved using the reduced scenarios. This procedure was repreated 50 times. The range of deviation for the computed mean expected net present value (ENPV) is shown in Figure 5. It can be seen that a reduction of the original samples to only 16 reduced scenarios by both algorithms, `ScenRed` and `K-means`, only changing the overall outcome by ±1%.

When reducing scenarios using `ScenRed`, we obtained a 12% increase in economic performance, compared to a 5% increase when using `K-means`. This indicates that for the

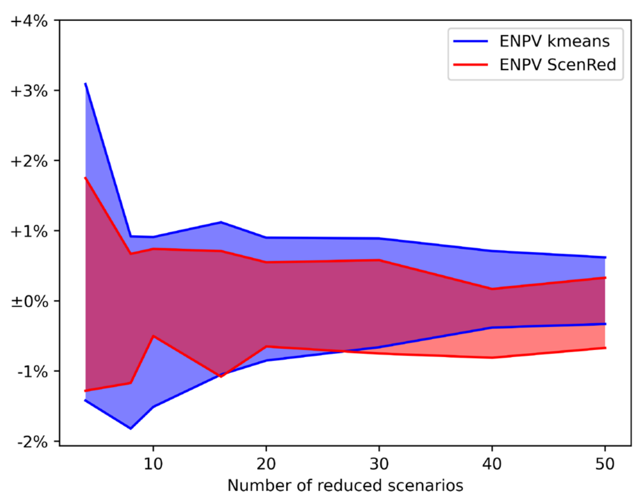

Figure 5. Range of relative deviation of the mean ENPV from the stochastic computation for different numbers of reduced scenarios for the grand coalition. The red area represents results obtained using `ScenRed`; the blue area represents results obtained using `K-means` clustering.

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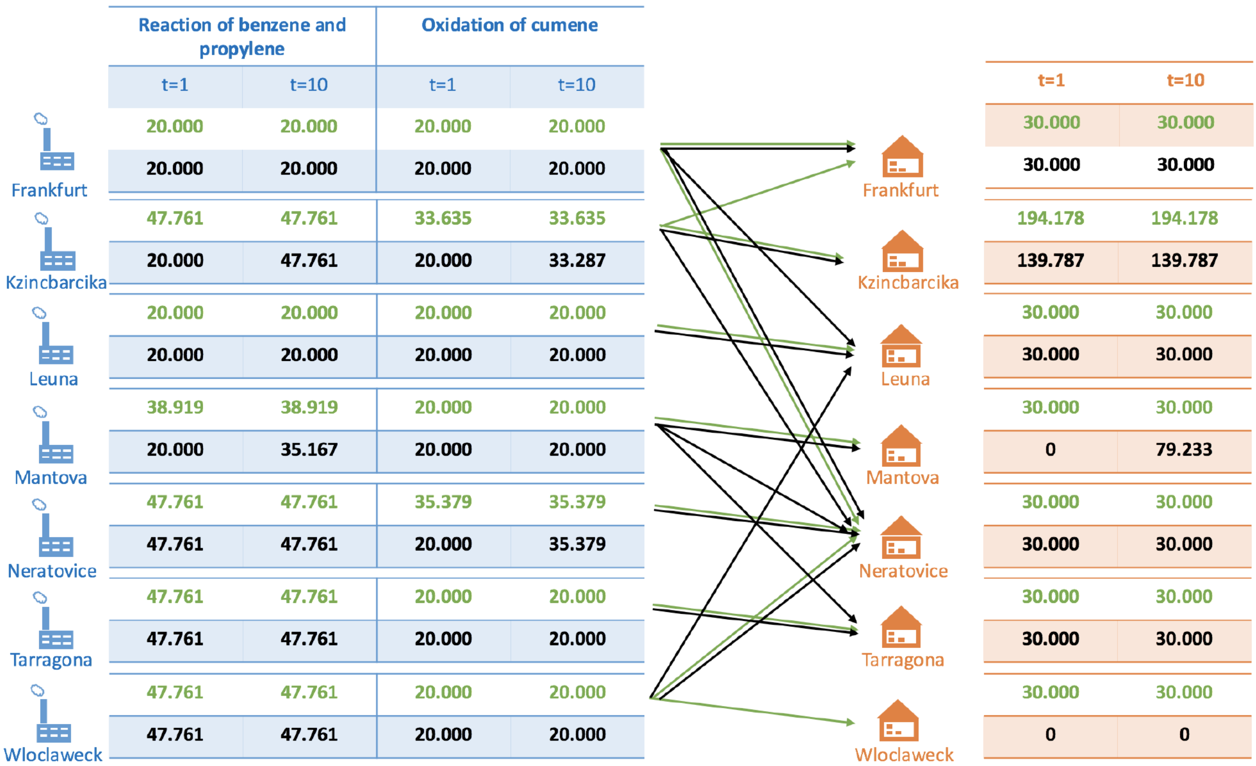

Figure 6. Capacity of the technologies reaction of benzene and propylene and oxidation of cumene, as well as the warehouse capacities for time periods 1 and 10. In green, the results for deterministic computations are shown, whereas black shows the values for the stochastic computation using the reduced scenarios by `ScenRed`. The transportation links for time period 10 between plants and warehouses are also represented.

problem under study `ScenRed` seems to be the better-suited algorithm for scenario reduction.

We observed that most publications apply a deterministic approach. It requires far less computational effort to solve the deterministic model, but unfortunately, the resulting supply chains are less robust when it comes to changes in the underlying parameters. To point out the importance of considering uncertainties in the parameters, we compared the supply chain design obtained from a deterministic approach with the one resulting from a stochastic approach. Figure 6 shows the capacities of the technologies (reaction of benzene and propylene, as well as oxidation of cumene) required to produce cumene, phenol, and acetone at all seven plants. It also shows the capacity of the warehouses for time periods t = 1 and t = 10 for the stochastic and the deterministic approach and the transportation links between plants and warehouses for time period 10. The deterministic design expands capacities of the plants and warehouses during the first year, while the stochastic design decides to expand them in later years. This can be seen, for example, in Kazincbarcika. Note that the supply chain design proposed by the stochastic model includes more transportation links.

Mantova is approximately located in the geographical center of the supply chain under study. Even though the stochastic as well as the deterministic model decide to expand the capacity of the Mantova plant, only the stochastic model includes transportation links to the warehouses in Neratovice and Tarragona. This decision provides the network with more flexibility to cope with big changes in demand, or changes in CO_2 price allowances, as in our case. Neratovice and Leuna are the markets with highest demand, and it can be seen that the stochastic model increases the number of transportation links to these markets. When considering the management of the SC, it is important to have enough flexibility to produce different products in different plants, while reducing the amount of CO_2 allowances that the network needs to buy in each time period. This can be accomplished through a meaningful amount and allocation of transportation links.

The stochastic model also changes some of the transportation links. It, for example, decides to transport some products from Kzincbarcika directly to the Neratovice warehouse, located directly beside the Neratovice market, instead of using the warehouse in Frankfurt.

We decided to restrict the possible structural changes of the SC through imposing a relatively high initial capacity for both plants and warehouses. This explains why the behaviors of some players in the deterministic and the stochastic approaches are identical, since the imposed initial capacity is enough to satisfy the growing demand already. Some plants and warehouses have a higher impact on emissions and profit of the total network, like Mantova and Kzincbarcika. This is due to the fact that they have relatively low production costs and are located close to the market with highest demand, Neratovice. Moreover, the stochastic approach does not operate the warehouse in Wloclawek.

After computing the deterministic and the stochastic SC designs, we exposed both of them to 1000 CO_2 price scenarios. The results show that the stochastic design leads to an increase of 12% in profit together with only negligible changes in emissions.

■ CONCLUSIONS

In this work, we presented a robust stochastic model for the design of a cooperative sustainable three-echelon supply chain

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formed by seven partners under uncertainties in CO_2 allowance prices. In order to discretize the underlying probability space, we simulated 1000 possible price scenarios using an ARIMA (7, 1, 8) model. Since a full stochastic computation exceeds the computational resources of ordinary computers, the number of scenarios needed to be reduced. Using the Jensen−Shannon distance for probability distributions, it turned out that the information loss using 16 scenarios, being a feasible amount for full stochastic computations, is less than 5%. This is an acceptable trade-off. We then considered a cooperative game strategy and checked its feasibility, meaning that no subcoalitions of players may be more profitable than the grand coalition of all players. When comparing the results of this grand coalition with the individual strategies, a profit increase by 22% is noted, together with a reduction in CO_2 emissions by 2.4%. Since the majority of articles from the literature use deterministic supply chain designs, we computed one for comparing our proposed stochastic supply chain design against it. To this end, we exposed both designs to the original 1000 CO_2 price scenarios. The experiment showed that the stochastic design leads to an increase of 12% in average profit.

All of these results show that supply chain designs resulting from a stochastic approach are much more robust to changes in the CO_2 prices. Since these prices oscillate and have been strongly increasing during the last years, it makes sense to consider them as a source of uncertainty.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acssuschemeng.2c01270.

> Description of the supply chain model (including all equations and variables), explanation of the ARIMA model and its parameters, and short explanation of AIC and BIC information criteria as well as background information regarding the scenario reduction (PDF)

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Notes

The authors declare no competing financial interest.

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