# Design of a three-echelon supply chain under uncertainty in demand and CO<sub>2</sub> allowance prices

F. L. Garcia Castro<sup>a</sup>, R. Ruiz-Femenia<sup>a</sup>, R. Salcedo-Diaz<sup>a</sup> and J. A. Caballero<sup>a</sup>

<sup>a</sup>Department of Chemical Engineering, Unviersity of Alicante, Apartado de Correos 99, Alicante 03080, Spain ruben.ruiz@ua.es

## Abstract

Nowadays there is a growing concern regarding greenhouse gas emissions and their consideration in the supply chain design. In this work we present a robust stochastic model for the design of a supply chain under uncertainty of CO<sub>2</sub>-allowance prices and market demand. The threeechelon petrochemical supply chain superstructure consists of four production plants in Europe, storage associated with these plants and four possible markets. At each plant different products can be produced according to the available technologies. The goal is to maximize the expected net present value (ENPV), while reducing the amount of CO<sub>2</sub> equivalent emissions. We implemented the carbon cap and trade model from the European Union emissions Trading System, whose goal is to reduce the emission cap over time in order to achieve a climate-neutral EU by 2050. We combine the environmental LCIA data, required to determine the global warming potential, with the forecast of CO<sub>2</sub> allowance prices. The problem involves a multi period mixedinteger linear program (MILP) formulation, which was implemented in Python using Pyomo and solved using IBMs CPLEX algorithm. To deal with uncertainty in market demand and CO2allowance prices, we implemented an ARIMA model and generated multiple scenarios. Since a full discretization of the resulting probability space leads to a number of scenarios that exceeds capacities of state of the art computers with ease, decomposition techniques are applied. The obtained results show an improvement of the economic performance when compared to the results from the deterministic approach that is being widely used in literature.

Keywords: CO<sub>2</sub> price uncertainty, stochastic model, optimum supply chain management, decomposition methods

## 1. Introduction

In a globalized world the efficiency of supply chains is gaining more importance. Supply chains integrate different activities, resources and institutions to ensure effective production, storage and distribution of products. Real world uncertainties can have a large impact on the design and efficiency of a supply chain. In this paper, we not only focus on uncertainties in the market demand (which have been studied extensively in the literature), but also on uncertainties in the CO<sub>2</sub> prices. In this work we will consider the European Union Emissions trading system, whose goal is to achieve a climate neutral EU by reduction of the maximum amount of allowed emissions over time, c.f. European Union (2016). The study of combined uncertainty in CO<sub>2</sub> prices and demand require the use of a huge number of scenarios for fully discretizing the underlying probability space. Since this exceeds capacities of modern day computer with ease, we combined various techniques to being able to obtain a supply chain design that takes these combined uncertainties into account.

We first generated a large number of scenarios and clustered them according to their economic and environmental performance. In order to solve the resulting stochastic mixed-integer linear program, we applied an Augmented Lagrangian Relaxation (ALR) scheme together with an alternating direction of multipliers to ensure separability of the problem into subproblems. The resulting subproblems could then be solved in parallel to reduce computational time. For more information regarding ALR see Boyd S., Parikh N., Chu E., Peleato B., Eckstein J. (2011); Conejo A. J., Castillo E., M'inguez R., Garc'ia-Bertrand R. (2006).

To the best of our knowledge, a combination of the beforementioned methods for the study of combined uncertainty in a European three-echelon petrochemical supply chain has never been used before.

#### Methodology

In this section, we briefly introduce the problem under study. Also, we review the different techniques that were combined in order to compute a stochastic supply chain model that adapts to the scenarios under study.

#### 2.1. Problem statement

The studied three-echelon petrochemical supply chain superstructure consists of 4 production plants in Europe: Kazincbarcika (Hungary), Leuna (Germany), Mantova (Italy) and Wloclaweck (Poland). Each plant has an expansion limit between 10 and 400 kt/year and an initial capacity of 20 kt/year, c.f. Guillen-Gos' albez, G., Grossmann, I.E. (2009). Each plant can produce acetalde-' hyde, acetone, acrylonitrile, cumene, isopropanol and phenol using one of 6 available technologies involving up to 18 different chemicals. Each plant has a warehouse with the same expansion limits and initial capacities associated to it. Initially, the inventory is empty. The material flow between plant and warehouses, as well as warehouses and markets, is limited to 500 kt/year. A minimum demand satisfaction of 30% is specified. The initial maximal amount of  $CO_2$  emissions is  $2 \cdot 10^8$  kg  $CO_2$  equivalent, with a 2.2% yearly reduction rate.

#### 2.2. Supply chain model

The model under study is composed of environmental impact, economical assessment, capacity constraints and mass balance equation blocks. The objective is to maximize the expected net present value, while satisfying all of these equation blocks. The cap-and-trade system provides a link between economic and environmental performance. Since a full description of the model would turn out to be quite long and considering the page limit, we refer the reader to Ruiz-Femenia et al. (2013) for more details on the model. The most important equations read Equation (1) describes the available emissions for the supply chain at each timestep *t* and scenario *s*, and consists of the maximum amount of emissions allowed by the system in each year, as well as the amount of bought as well as sold emissions. In equation (2), the economic impact of the emissions trading on the supply chain is calculated. We call this quantity NET<sub>CO2</sub>. This term is then taken into account when calculating the net earnings for a specific time and scenario, as described in equation (3).

$$GWP(t,s) \leq MAX_{CO2}(t) + BUY_{CO2}(t,s) - SALES_{CO2}(t,s), \quad \forall t,s$$
(1)

$$NET_{CO2}(t,s) = PRICE_{CO2}(t,s) \cdot SALES_{CO2}(t,s)$$
(2)

$$-\operatorname{COST}_{\operatorname{CO2}}(t,s) \cdot \operatorname{BUY}_{\operatorname{CO2}}(t,s), \quad \forall t,s$$

$$NETE(t,s) = (1 - TAX) \left[ EARNINGS(t,s) - EXPENSES(t,s) + NET_{CO2}(t,s) \right] (3) + TAX \cdot DEP(t), \quad \forall t, s$$

#### 2.3. Uncertainty in CO2 allowance prices and market demand

The scenarios for the CO<sub>2</sub> allowance prices were generated using an autoregressive integrated moving average (ARIMA) model. ARIMA models are defined by three parameters. The first parameter determines the non-seasonal polynomial degree. The second one is the order of differentiation used to remove seasonal trends. The third parameter is the number of moving average terms, which is related to the accuracy of approximations produced by an update of the parameters from fitting the model to the historical data. In Shumway and Stoffer (2000), details can be found.

Appropriate values of the parameters were identified by fitting the historical data from 2009 to 2021 and using the Akaike and Bayesian information criteria. In our case, the best-fitting model is ARIMA(7,1,8).

Random time series data for the demand of each chemical at each market were generated using a normally distributed random growth with a standard deviation of 7% to a given start value at time t = 0. We compared the environmental and economic performance of 1000 combined scenarios, and grouped them into 20 clusters using the K-means algorithm. The centroids of each cluster were then used as scenarios for the stochastic program. For an overview of clustering methods see Omran et al. (2007).

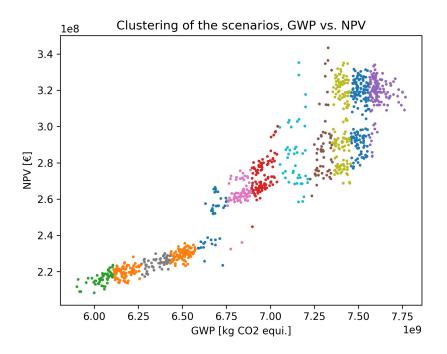


Figure 1: Economic and environmental performance of 1000 deterministic scenarios. The scenarios are clustered (colors).

#### 2.4. Augmented Lagrangian Relaxation

The aim of decomposition methods is to solve many easy-to-solve subproblems instead of one hard-to-solve full problem. For our supply chain model, the smallest subproblems result from a splitting of the full problem into subproblems containing information only on one scenario. The main difficulty then lies in the linking of the non-scenario dependent variables from each subproblem, since these should coincide. To do so, we included as many non-anticipative constraints to the model as there are non-scenario dependent variables. These non-anticipative

constraints represent the complicating constraints of the model, which have to be relaxed by introducing them as penalty terms into the objective, together with new multipliers. Since our objective is a linear function, we added additional quadratic penalty terms to ensure convergence of the method, resulting in the so called Augmented Lagrangian Relaxation of the problem. Because of the appearing products of variables from different scenarios in the quadratic penalty terms, the resulting objective is not decomposable into subproblems for each scenario anymore. To overcome this problem, the alternating direction method of multipliers is used. This method linearizes the product of variables from different scenarios using values of previous iterations for one of the appearing variables. The result is relaxed problem that is fully decomposable into subproblems only involving one scenario each.

A tolerance of 5% was set as stopping criteria for the ALR-loop. After each iteration, if the stopping criteria was not fulfilled, the multipliers will be updated according to the subgradient method and a new iteration is started, and we refer to Conejo A. J., Castillo E., M'inguez R., Garc'ia-Bertrand R. (2006) for details. The overall procedure is explained in fig. 2

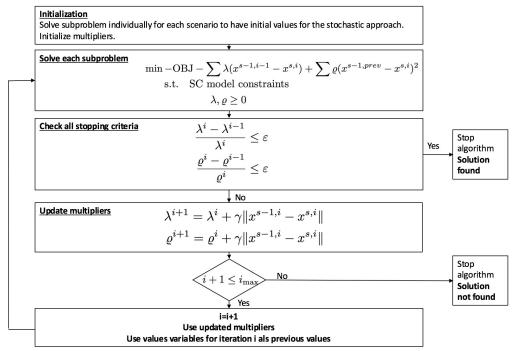


Figure 2: Schematic representation of the iterative solution algorithm. The problem has been separated into subproblems with additional coupling constraints, that appear as penalty terms in the objective functions. The multiplier update uses a subgradient method.

#### 3. Results

Numerical experiments were conducted on a MacBook Pro model 2020 with 16 GB Ram and macOS 11.2.1. The model has been implemented in Python using Pyomo and solved using IBMs CPLEX algorithm.

Thanks to the method of alternating direction of multipliers, each subproblem can be solved independently of the others. This allows for a massive speedup through parallelization, since in 5

the best case one processor only solves one or few subproblems per iteration. Since the solution time for each subproblem can vary, the solution times are measured and the subproblems are redistributed among the processors in the hope of balancing the solution time needed for the next iteration. This is the best a priory load balancing possible. In our case (on 6 processors), we could speedup the solution process by about 80% compared to sequential solving. The problem was moreover reformulated and the number of variables per subproblem could be reduced from about 27000 to 24000, further simplifying the solution process.

We validated our method by comparing the obtained stochastic supply chain design against its deterministic counterpart from a scenario with an average investment cost, which is typically the one chosen by companies. In average, the stochastic model yields to an increased net present value of approx. 927600 e while reducing the general warming potential by around 225000 tons of CO<sub>2</sub>-equivalent.

The resulting stochastic supply chain design has a net present value (NPV) of 254603229 e and a global warming potential (GWP) of 7624500 tons  $CO_2$  equi. In average, 580 tons of  $CO_2$  equivalent will be bought each year. In fig. 3, the capacities of the different technologies of each plant, as well as the warehouse capacitis for the last timestep. The figure also shows the total quantities transported between plants and warehouses, resp. warehouses and markets, in the last timestep.

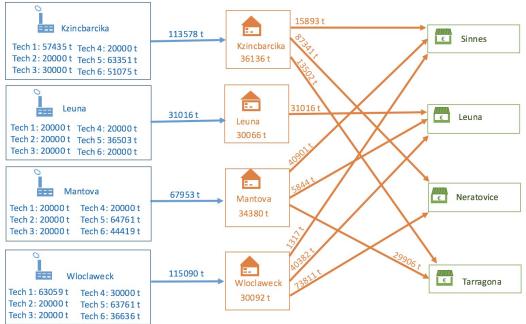


Figure 3: Stochastic supply chain design for the last timestep. On the left: Plants with corresponding capacities for each of the 6 available technologies. Center: Warehouses with corresponding capacities. Right: Markets. Arrows represent total transported quantities between the sites for the last timestep.

### 4. Outlook and further work

We are currently working on a supply chain design, which is able to repesent the penalties associated with a non-satisfaction of the demand. In this work, we studied the impact of uncertainty in market demand and CO<sub>2</sub> prices on the supply chain design. Nevertheless, a study for uncertainties in different parameters should be carried out, in order to recognize which

parameters possibly have a higher impact on the performane. We are also working on increasing the feasible number of scenarios and assess the information loss caused by the used clusterization. Considering the ALR loop, there are still many open questions regarding a robust choice and update of the multipliers for each iteration, which tend to have an enormous impact on the solvability of the stochastic model.

#### References

- Boyd S., Parikh N., Chu E., Peleato B., Eckstein J., 2011. Distributed Optimization and Statistical Learning via the Alternating Direction Method of Multipliers. Foundations and Trends in Machine Learning 3, 1–122.
- Conejo A. J., Castillo E., M'inguez R., Garc'ia-Bertrand R., 2006. Decomposition Techniques in Mathematical Programming. Springer-Verlag Berlin Heidelberg.

European Union, 2016. The EU Emissions Trading System (EU ETS).

URL https://ec.europa.eu/clima/sites/clima/files/factsheet ets en.pdf

- Guillen-Gos' albez, G., Grossmann, I.E., 2009. Optimal design and planning of sustainable chemical supply chains under' uncertainty. AIChE J. 55, 99–121.
- M. Omran, A. Engelbrecht, A. Salman, 11 2007. An overview of clustering methods. Intell. Data Anal. 11, 583-605.
- R. Ruiz-Femenia, G. Guillen-Gos' albez, L. Jim' enez Esteller, J. Caballero, 05 2013. Multi-objective optimization of environmentally conscious chemical supply chains under demand uncertainty. Chemical Engineering Science 95, 1–11.
- R. H. Shumway, D. S. Stoffer, 2000. Time Series Regression and ARIMA Models. Springer New York, New York, NY, pp. 89–212.

URL https://doi.org/10.1007/978-1-4757-3261-0\_2

6