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ORIGINAL RESEARCH

The profitability-sustainability trade-off in complex chemical value chains

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Abstract
The industry and transportation sectors account for more than 35% of global CO_2 emissions and there is increasing pressure on industry to reduce emissions. To remain competitive in their markets while reducing their emissions, companies need to re-optimise their entire value chain focusing not only on traditional costs, related to manufacturing and transport, but also on emission reduction targets. In this work, we propose a linear program to optimise a deterministic multi-objective value-chain problem aimed at minimising CO_2 emissions and maximising a company's total contribution margin. We test the model on a real-world dataset, provided by a multinational chemical company, to determine the main sources of emissions and their geographical distribution. Moreover, we analyse how much emissions can be reduced at a negligible impact on the total contribution margin and describe what the best strategies are to achieve the targeted emission reduction. We find that it is beneficial to move production to less polluting production sites, even when that increases the transportation in our setting. It is therefore advisable to jointly address the reduction of production- and transportation-related emissions, rather than separately.

Keywords Sustainable supply chain · Green supply chain · Production-distribution planning · Chemical industry · Multi-objective optimisation

1 Introduction

Greenhouse gas (GHG) emissions have a strong negative impact on our environment. They are one of the main causes for global warming. Several agreements have been made under

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the guidance of the United Nations (UN) in the last decades to limit and eventually lower the emissions of GHGs (Kyoto 1997 and Paris 2015 (UNFCCC, 2018)). In the European Green Deal (European Commission, 2021), the European Union strives for net-zero emissions of GHGs by 2050. According to a report by the European Environment Agency (European Environment Agency, 2021), the GHG emissions in the EU had already been reduced by 24% compared to 1990, as of 2019. The current objective is to further decrease the 2019 emissions by 44% within the next decade. In 2040, protection policies and regulations in Europe will be stricter than anywhere else in the world. For globally operating multinational companies, differences in environmental regulations across regions will have a clear impact on their decisions on where to produce their goods and how to organise their value chains.

One of the major GHGs emitted by human activity is carbon dioxide (CO_2) which accounts for more than 75% of global GHG emissions (EPA, 2022, 2023). Chemical companies are a major emitter of CO_2. In 2018, the chemical industry emitted 18% (1.5 gigatonnes) of all industrial emissions (cf. MacLeod and Matthey 2021 and IEA 2019).

A more recent report by the International Energy Agency (IEA, 2022) describes the chemical industry as the largest industrial energy consumer and the third largest industry subsector in terms of direct CO_2 emissions. Apart from European and global regulations imposing stricter limits on GHG emissions, the chemical sector faces increased pressure from society to improve in terms of sustainability (Keller et al., 2022). 'Chemophobia', the irrational fear of chemicals (Gribble, 2013; Saleh et al., 2019), is among the main reasons explaining the steep decrease shown by this industry in total shareholder return rate over the last decades (Gocke et al., 2021). Therefore, chemical companies have to re-design their value chains to incorporate these novel environmental aspects since they affect their profitability both directly (due to the imposed national/international regulations) and indirectly (due to the pressure from society to offer sustainable products).

The chemical industry is characterised by large multinational companies that have sites and customers worldwide. The geographical distribution of the production sites has a strong impact on costs and emissions. Some sites are equipped with more advanced technologies with relatively low manufacturing costs and emissions, but higher procurement costs (both in terms of raw materials and utilities). Other sites have relatively high manufacturing costs (e.g. due to dated machinery or production lines), but lower procurement costs (due to the proximity to raw materials or utilities suppliers). Moreover, cheaper and more sustainable sites may be located far from customer locations, which negatively impacts transportation costs and emissions. At each site, the production of chemical products involves a large number of processes in several production lines that require a diverse set of input materials and utilities. In order to properly account for costs and emissions, it is fundamental to carefully model all the value chain stages involved from raw materials procurement to final products delivery to customers. Since production and transportation are interconnected, they are both key factors for an efficient and sustainable chemical value chain.

The goal of our work is to analyse the profitability-sustainability trade-off in such a complex chemical value chain in order to provide insights that companies operating in this sector may use to make decisions that maximise their profitability while reducing their carbon footprint. Although the term 'sustainability' may have a broader meaning, in this work we use the definition provided by Keller et al. (2022) and restrict our attention to GHG emissions. We present a medium range production-planning model that optimises production and transportation plans for the existing value chain setup. For instance, we allow for a shift in production volumes between sites located in different regions. However, we do not consider measures such as an investment in a new production technology at a site or the increased purchase of green electricity certificates at sites where this has not been done in the past. We also do not consider the opening or closing of entire sites. While such aspects are worthwhile to take into account, our primary interest is to study options that are easily implementable in the short run and do not require any major investments. We also seek solutions that do not fundamentally alter volumes in markets currently served by the network to avoid unintended market disruptions. We make several contributions in this paper that we outline below.

1. We formulate a multi-objective problem for the end-to-end aggregate planning of a chemical value chain. This value chain encompasses procurement, multiple production stages and sites, and transportation of (semi-finished) goods. There are both costs and emissions associated with each activity in the value chain. This allows us to trade-off emissions of one type of activity (e.g. production) against another (e.g. transportation). This formulation is the most complete in literature so far as will be illustrated in the literature review (Sect. 2) and Table 1.
2. We show how to generate the Pareto frontier to evaluate the trade-off between profitability (e.g. the maximisation of the total contribution margin) and sustainability (e.g. the minimisation of the CO_2 emissions). This is a great managerial tool for decision makers, exceeds the state of the art which usually relies on single objective optimisation models.
3. We analyse the change in the cost and emission structure for different emission reduction targets and have several findings. First, it is possible to reduce emissions by a substantial amount with negligible effects on profitability. Second, the largest portion of the emission reduction is achieved by diminishing utility emissions. The relocation of the production to sites where more sustainable utilities are available allows to save up to 50% of the utility emissions and 10% of the total emitted CO_2. By contrast, it is difficult to reduce the emissions produced by raw materials and manufacturing. Finally, we observe that procurement is a strategic activity as a substantial part of emissions are associated with it.
4. We analyse the effect of different emission reduction targets on the geographical distribution of the production and emissions volumes. Different regions of the world have production equipment with different emission profiles. As a value chain reduces emissions, it shifts production volumes to regions with greener production equipment. This insight can be used to shift production volumes, and it can also inform investment decisions, as well as reactions to decisions by regional legislators.

The remaining part of the paper is structured as follows. In Sect. 2, we review the relevant literature. Section 3 describes characteristics of a chemical value chain and proposes a linear programming formulation to solve it. Section 4 outlines the studied scenario and proposes a solution approach to optimise the value chain. Section 5 provides managerial insights for decision makers to correctly address the profitability-sustainability trade-off derived from a numerical study based on a real-world dataset from a multinational chemical company. Conclusions and directions for future research are summarised in Sect. 6.

2 Literature review

The literature related to supply chain (or value chain) optimisation is vast. According to the review by Pourhejazy and Kwon (2016), over 380 articles published between 2005 and 2016 propose operations research techniques to address value chain problems. Moreover, several other reviews, which include earlier papers, are available in the literature. To mention only the most relevant and recent works, we refer to the reviews by Kallrath (2002b) and Fahimnia et al. (2013). Interestingly for the scope of this work, Kallrath (2002b) entirely focuses on planning and scheduling in the process industry. He classifies the literature according to the time horizon and the level of detail characterising the mathematical models: a medium-long time horizon and a low level of detail characterise production planning problems, while a short time horizon and a high level of detail characterise scheduling problems. A similar classification has also been proposed more recently by Chopra (2018). The production planning problem was addressed in Timpe and Kallrath (2000) and Kallrath (2002a), while the scheduling problem was addressed in González-Castaño et al. (2018) specifically for the process industry. A different classification of value chain optimisation problems, based on the degree of complexity, is proposed by Fahimnia et al. (2013). They identify seven categories depending on whether single or multiple products, plants, warehouses, customers, transport paths and time-periods are involved.

In the remainder of this section, we discuss some of the production-distribution papers in the literature that are most relevant to our work. Although there exist some rigorous models for integrated production-distribution planning, only a limited number of papers deal with the multi-product, multi-plant, multi-market and multi-time period setting (Perea-López et al., 2003; Tsiakis & Papageorgiou, 2008; Fahimnia et al., 2012; Manzini, 2012; Bashiri et al., 2012; Piewthongngam et al., 2013; Sarrafha et al., 2015; Klosterhalfen et al., 2019).

Until the beginning of the 2000s, costs and profits were the only key performance indicators (KPIs) considered. In contrast, in the last decade there has been an increasing interest in accounting for social, environmental and economic aspects in a single comprehensive model (Sindhwani et al., 2023). This approach has led to the concept of a sustainable (or green) value chain defined by Barbosa-Póvoa (2012) as:

> The operational structures that manage the raw materials and services from suppliers to costumers and back accounting for the explicit inclusion of social and environmental impacts.

Papers addressing sustainable value chain optimisation cover a wide range of topics: from game theory approaches to investigate the effects of an integrated or decentralised strategy in greening the value chain (Ghosha & Shahb, 2015; Basiri & Heydari, 2017; Madani & Rasti-Barzoki, 2017; Xia et al., 2022), to (mixed-)integer linear programming models to address multi-modal and reliable supply chain design (Kabadurmus & Erdogan, 2020), reverse logistics and closed-loop value chain setups (Sheu et al., 2005; Özceylan & Paksoy, 2013; Ramos et al., 2014; Govindan et al., 2015; Gaur et al., 2017; Miao et al., 2017; Lotfi et al., 2021; Sazvar et al., 2022). Since the literature on these topics is vast, we refer to the reviews provided by Barbosa-Póvoa (2012, 2014), Brandenburg and Rebs (2015), Eskandarpour et al. (2015) and Barbosa-Póvoa et al. (2018).

Sheu et al. (2005) provides a template model as a 5-layer (suppliers, plants, warehouses, distribution centers and customers) network design problem mainly focusing on transportation. Each layer in this network is modelled on an aggregated level that does not distinguish between different production lines and production recipes.

Sheu et al. (2005) consider recycling in supply chain management, but do not consider GHG emissions. In the remaining part of this section, we focus on papers that deal with multi-objective production-transportation planning optimisation in which the trade-off between financial KPIs and emission reduction is analysed. Articles that propose models for strategic or tactical decisions are listed in Table 1. Strategic models are characterised by the possibility to open or close facilities. Tactical models allocate production volumes within an existing network structure. All the papers in Table 1 consider transportation costs and emissions, some consider emissions associated with production but only one (Baud-Lavigne et al., 2014) considers emissions associated with procurement.

Table 1 Sustainable value chain literature: production-transportation planning models according to our key features

Author(year)	Opening facilities	Proc. costs	Proc. emissions	Prod. costs	Prod. emissions	Prod. multi Echelon	Transp. costs	Transp. emissions
Paksoy et al. (2011)	✗	✓	✗	✗	✗	✗	✓	✓
Paksoy and Özceylan (2014)	✗	✗	✗	✗	✗	✗	✓	✓
Baud-Lavigne et al. (2014)	✓	✓	✓	✓	✓	✗	✓	✓
Tognetti et al. (2015)	✗	✗	✗	✓	✓	✗	✓	✓
Brandenburg (2015)	✗	✓	✗	✓	✓	✗	✓	✓
Liotta et al. (2015)	✓	✗	✗	✓	✗	✗	✓	✓
Varsei and Polyakovskiy (2017)	✓	✓	✗	✓	✗	✗	✓	✓
Canales-Bustos et al. (2017)	✓	✗	✗	✗	✓	✗	✓	✓
Nurjanni et al. (2017)	✓	✗	✗	✓	✓	✗	✓	✓
Zhao et al. (2017)	✓	✓	✗	✓	✓	✗	✓	✓
Jabbarzadeh et al. (2019)	✗	✗	✗	✓	✓	✓	✓	✓
Mohebalizadehgashti et al. (2020)	✓	✓	✗	✗	✗	✗	✓	✓
Fragoso and Figueira (2021)	✓	✓	✗	✓	✓	✗	✓	✓
Sadjady Naeeni and Sabbaghi (2022)	✓	✗	✗	✗	✓	✗	✓	✓
Hashmi et al. (2022)	✗	✓	✗	✓	✓	✗	✓	✓
This work	✗	✓	✓	✓	✓	✓	✓	✓

The abbreviations are "proc." for procurement, "prod." for production and "transp." for transportation

Fahimnia et al. (2013) also provide a review and classification of production and transportation planning models. Their classification is based on traditional supply chain criteria such as: number of plants, warehouses and distribution centers, products, customers, time periods and methods to deliver products to customers. Table 1 uses different classification criteria to also distinguish the emission sources considered by the different models. The table highlights that our work is among the first to consider procurement costs and emissions and one of very few papers to consider production emissions.

Papers that include facility location decisions often omit important cost or emission sources. Liotta et al. (2015) omit production emissions and procurement emissions and costs; Mohebalizadehgashti et al. (2020) omit procurement emissions and production emissions and costs; Canales-Bustos et al. (2017) and Sadjady Naeeni and Sabbaghi (2022) include production emissions but not costs. The most comprehensive models are by Baud-Lavigne et al. (2014), Varsei and Polyakovskiy (2017), Nurjanni et al. (2017), Zhao et al. (2017) and Fragoso and Figueira (2021), who include both production and transportation costs and emissions in their objectives. Relative to these papers, our model includes procurement costs and emissions as well as multiple echelons in the supply chain, although we have no facility location decision.

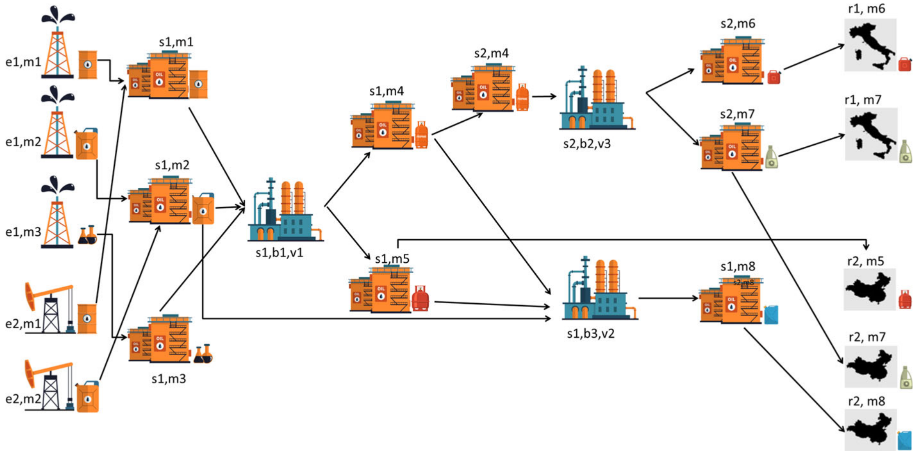


Fig. 1 Example of a chemical value chain. From left to right: two external suppliers (e1, e2) dispatch products m1, m2, m3 to raw materials warehouses at site s1. Raw materials warehouses feed production line b1 running recipe v1 at site s1. The production line produces two output products (m4, m5) stored in output warehouses. Products m4 and m5 together with m2 are used internally at site s1 to run production line b3 using recipe v2 to produce m8. Product m4 is also dispatched to site s2 to be used as input material to produce products m6 and m7. Products m5, m6, m7 and m8 are dispatched and sold in two different markets

Papers that do not include facility location decisions usually consider both production and transportation costs and emissions except for Paksoy et al. (2011) and Paksoy and Özceylan (2014). Brandenburg (2015); Tognetti et al. (2015); Jabbarzadeh et al. (2019) and Hashmi et al. (2022) provide relatively comprehensive models. Our model adds procurement costs and emissions as well as multiple echelons compared to these papers.

The above mentioned literature deals with value chains of at most 5-echelons, each one with a limited number of sites, warehouses or customers. By contrast, our model can accommodate a complex value chain consisting of numerous external suppliers and multiple production stages. We model several production lines located at different sites spread worldwide. Table 1 shows that our paper provides the most complete model setup yet. The final goal of our article is to analyse the profitability-sustainability trade-off of a complex value chain and to optimise its production-transportation planning in a short-medium time horizon (∼1 year).

3 Optimisation of complex chemical value chains

3.1 Terminology and notation

In this section, we describe the complex value chain setup as it occurs in the chemical industry, as well as in the broader process industry. In the following, we will use the word product for the output of any production process regardless of whether this output is a semi-finished or finished product. Figure 1 provides an example of the type of value chain we consider.

A chemical value chain is comprised of sites $s \in S$. Each site has several production lines denoted B_s and the set of all production lines is $B = \cup_{s \in S} B_s$. Associated with each production line $b \in B$ is a set of recipes N_b that can be prepared on production line b. To simplify the notation, we define the set $S_v = \{s\}$ as a singleton containing the site s where recipe ν is available. We let M denote the set of all input and output products. Production with recipe $\nu \in N_b$ requires inputs contained in $\Phi^-(\nu)$ and delivers outputs contained in $\Phi^+(\nu)$. Therefore, the sets of all required inputs and outputs for recipes that can be run on production lines at site s are provided by (1a) and (1b), respectively.

$$\Pi^-(s) = \bigcup_{\nu \in \cup_{b \in B_s} N_b} \Phi^-(\nu) \tag{1a}$$

$$\Pi^+(s) = \bigcup_{\nu \in \cup_{b \in B_s} N_b} \Phi^+(\nu) \tag{1b}$$

Outputs and inputs of a recipe ν can be both materials and utilities. The set S_{sm} contains those sites to which product $m \in M$ may be delivered from site $s \in S$. The annual maximum operating time for each production line $b \in B$ is provided by $\overline{U}_b$.

We let E denote the set of suppliers where inputs can be procured. As a supplier may provide several inputs, the set $\Phi^+(e)$ contains all the inputs available from supplier $e \in E$ (which is an output for the supplier $e \in E$). Sites which may procure input $m \in M$ from supplier $e \in E$ are are contained in the set S_{em}.

Final products are sold to different markets $r \in R$. We let Ω_r denote the set of products sold in the market $r \in R$. Each product $m \in \Omega_r$ has a demand in market r (Q_{rm}) that the value chain must deliver. The set R_{sm} contains those markets $r \in R$ where product $m \in M$ available at site $s \in S$ is sold.

3.2 Network representation

Figure 1 shows that a value chain can be modelled as a directed graph $G(V, A)$, where nodes represent suppliers, warehouses, production sites and markets and arcs represent operations that transform goods. (Such a transformation may be chemical (manufacturing) or in location (transportation).) The set of nodes V is composed of five different types of nodes v, as shown in Fig. 2.

The set $V^E = \{(e, m) : e \in E, m \in \Phi^+(e)\}$ contains a node for each supplier-input pair from supplier $e \in E$. The sets $V^- = \{(s, m) : s \in S, m \in \Pi^-(s)\}$ and $V^+ = \{(s, m) : s \in S, m \in \Pi^+(s)\}$ contain all the nodes representing input and output warehouses, respectively. The set $V^R = \{(r, m) : r \in R, m \in \Omega_r\}$ contains the markets that the value chain supplies. Each node $v \in V^R$ represents a market $r \in R$ where product $m \in M$ is sold. Note that each recipe $\nu \in N$ is also a a transformation process. Thus, the set of all vertices is given by $V = V^E \cup V^- \cup N \cup V^+ \cup V^R$.

We can now introduce arcs for network $G(V, A)$. The arc set A is the union of the following five sets of arcs:

$$A^E = \{((e, m), (s, m)) \in V^E \times V^- : s \in S_{em}, m \in \Pi^-(s)\} \tag{2}$$

$$A^{in} = \{((s, m), \nu) \in V^- \times N : m \in \Phi^-(\nu), s \in S_\nu\} \tag{3}$$

$$A^{out} = \{(\nu, (s, m)) \in N \times V^+ : m \in \Phi^+(\nu), s \in S_\nu\} \tag{4}$$

$$A^{ts} = \{((s, m), (s', m)) \in V^+ \times V^- : s' \in S_{sm}\} \tag{5}$$

$$A^R = \{((s, m), (r, m) \in V^+ \times V^r : r \in R_{sm}\} \tag{6}$$

The set A^E contains arcs that connect supplier product pairs $(e, m) \in V^E$ with input warehouses $(s, m) \in V^-$. The arc $((e, m), (s, m)) \in A^E$ exists only if site s is in set S_{em}. A^{in} contains arcs that connect input warehouses of site $s \in S$ with recipes $\nu \in \cup_{b \in B_s} N_b$. A^{out}

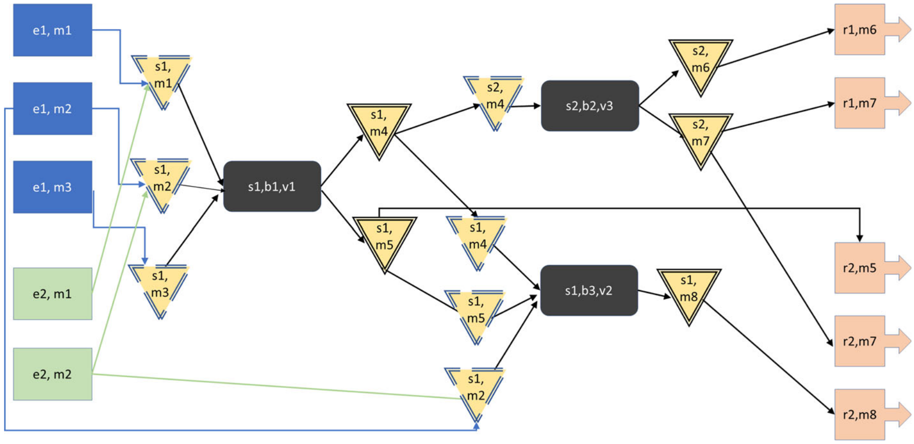


Fig. 2 Network representation of the value chain example: rectangles represent external materials' suppliers, triangles represent warehouses, if with a double-dashed line are input materials' warehouses, otherwise are output materials' warehouses, smooth rectangles represent specific production lines b at site s using a specific recipe ν, rectangles with an arrow on the right-hand side represent the different divisions, operating in a country, selling and dispatching final products to customers

contains arcs that connect the recipes to output warehouses at the same site. A^{ts} contains arcs that connect output and input warehouse nodes (at different or identical sites). The arc $((s, m), (s', m))$ exists if and only if s' is in the set S_{sm}. Thus A^{ts} contains internal transportation arcs. A^R contains arcs that connect warehouses of finished products with the markets to which these finished products are sold. The arc $((s, m), (r, m))$ exists only if r is in the set R_{sm}.

To summarise, the network $G(V, A)$ is given by:

$$V = V^E \cup V^- \cup N \cup V^+ \cup V^R$$
$$A = A^E \cup A^{in} \cup A^{out} \cup A^{ts} \cup A^R.$$

Each recipe $\nu \in N$ requires a certain amount of input of each of the inputs in $\Phi^-(\nu)$ to run the recipe for one unit of time on a production line. This amount of input consumed by a recipe is denoted by τ_a^c for each $a \in A^{in}$. Analogously, each recipe $\nu \in N$ produces a certain amount of each output in $\Phi^+(\nu)$ when the recipe is run for one time unit on a production line. This amount is denoted by τ_a^p for each $a \in A^{out}$. We define the coefficients $-c_a$ as the cost associated with traversing arc $a \in A \setminus A^{in}$. For any $a \in A^E$, c_a should be interpreted as the cost that site s faces to buy one unit of material m from supplier e for $a = ((e, m), (s, m))$. For $a \in A^{out}$, $-c_a$ should be interpreted as the manufacturing cost to produce one unit of material $m \in \Phi^+(\nu)$ using recipe $\nu \in N$ for $a = (\nu, (s, m))$. For $a \in A^{ts}$, it represents the cost to ship product $m \in \Phi^+(\nu)$ from output warehouse $(s, m) \in V^+$ to input warehouse $(s, m) \in V^-$. When $a \in A^R$, c_a represents the difference between the price and the transportation cost to move one unit of product m from site s to market r for $a = ((s, m), (r, m))$. Finally, for $a \in A^{ts}$, $-c_a$ is the cost of transporting one unit of product m from site s to site s' for $a = ((s, m), (s', m))$. Expressions for c_a are given in (7) which contains some additional generic notation from Table 2. In analogous fashion, we define the coefficient g_a to account for emissions (8). Further details regarding costs and emissions are provided in Table 2.

$$c_a = \begin{cases} P_a - C_a^{TR}, & \forall a \in A^R \\ -C_a^{TS}, & \forall a \in A^{ts} \\ -C_a^{M}, & \forall a \in A^{out} \\ -C_a^{E}, & \forall a \in A^E \end{cases} \tag{7}$$

$$g_a = \begin{cases} G^{TR}, & \forall a \in A^R \\ G^{TS}, & \forall a \in A^{ts} \\ G^{M}, & \forall a \in A^{out} \\ G^{E}, & \forall a \in A^E \end{cases} \tag{8}$$

3.3 Contribution margin optimisation

In this section, we present the linear program (LP) which relies on the graph $G(V, A)$ described in Sect. 3.2.

The main variables of our model are of two types: Those associated with nodes, accounting for the time that each production line $b \in B$ operates running a specific recipe $\nu \in N$; those associated with arcs, accounting for the quantity of inputs provided by suppliers, the quantity of produced outputs and the quantity of transported goods between sites and from sites to customers.

We define the variable $x_\nu \in \mathbb{R}^+$ as the amount of time spent running recipe $\nu \in N$. We define variables $q_a \in \mathbb{R}^+$ as the quantity of materials that are produced, consumed or transported along arc $a \in A$. Table 3 provides a detailed description of the involved variables.

Objective

To optimise the profitability of our complex value chain, we maximise the company's total contribution margin (cm). Traditionally, it is provided by (9) deducting transportation costs (10), manufacturing costs (11), and procurement costs (12) from revenues (13).

$$cm = R - TC - MC - PC \tag{9}$$

$$TC = \sum_{a \in A^{ts}} C_a^{TS} q_a + \sum_{a \in A^R} C_a^{TR} q_a \tag{10}$$

$$MC = \sum_{a \in A^{out}} C_a^{M} q_a \tag{11}$$

$$PC = \sum_{a \in A^{E}} C_a^{E} q_a \tag{12}$$

$$R = \sum_{a \in A^{R}} P_a q_a \tag{13}$$

It is possible to re-write the objective as:

$$cm = \sum_{a \in A \setminus A^{in}} c_a q_a \tag{14}$$

with the notation in (7).

Table 2 Types of costs and emissions (per units) considered within the model

Param	Arc a	Origin	Destination	Meaning
P_a	$(s, m), (r, m)$	Output warehouse	Customer	Unit price of product m in market r
C_a^{TR}	$(s, m), (r, m)$	Output warehouse	Customer	Unit cost to transport product m from site s to market r
C_a^{TS}	$(s, m), (s', m)$	Output warehouse	Input warehouse	Unit transportation cost of material m from site s to site s'
C_a^{M}	$(\nu), (s, m)$	Prod. line running recipe ν	Output warehouse	Unit manufacturing cost to produce material m at prod. line b running recipe ν
C_a^{E}	$(e, m), (s, m)$	Supplier	Input warehouse	Unit cost of input m from supplier e
G_a^{TR}	$(s, m), (r, m)$	Output warehouse	Customer	Unit emission to transport product m from site s to market r
G_a^{TS}	$(s, m), (s', m)$	Output warehouse	Input warehouse	Unit emission to transport material m from site s to site s'
G_a^{M}	$(\nu), (s, m)$	Prod. line running recipe ν	Output warehouse	Unit manufacturing emissions to produce material m at prod. line b running recipe ν
G_a^{E}	$(e, m), (s, m)$	Supplier	Input warehouse	Unit emission associated with input m procured from supplier e

Column 'Arc a' shows for which arcs in the graph G(V,E) these parameters are defined

Table 3 Description of the variables utilised in the model

Variable	Node ν/Arc a	Origin	Destination	Meaning
x_ν	ν	—	—	Running time of recipe ν
q_a	$(s, m), (r, m)$	Output warehouse	Customer	Quantity of product m delivered to market r from site s
q_a	$(s, m), (s', m)$	Output warehouse	Input warehouse	Quantity of material m transported from site s to site s'
q_a	$(\nu), (s, m)$	Prod. line running recipe ν	Output warehouse	Quantity of material m produced using ν
q_a	$(s, m), (\nu)$	Input warehouse	Prod. line running recipe ν	Quantity of material m utilised running recipe ν
q_a	$(e, m), (s, m)$	Supplier	Input warehouse	Quantity of input m procured from supplier e

Column 'Node ν/Arc a' shows for which nodes/arcs in the graph G(V,E) these variables are defined

Table 4 List of all parameters required to describe the model

Param	Defined for	Meaning
c_a	$a \in A \setminus A^{in}$	Price/Cost
g_a	$a \in A \setminus A^{in}$	Emissions
τ_a^c	$a \in A^{in}$	Consumption rate
τ_a^p	$a \in A^{out}$	Production rate
Q_v	$v \in V^R$	Demand of product m requested from market r
$\overline{U}_b$	$b \in B$	Maximum operating time for production line b

Constraints

The LP models a production-transportation planning problem. Therefore, there are two types of constraints: those related with production and those related with transportation.

We first describe production-related constraints: Constraint (15) guarantees that each production line does not exceed the maximum (annual) operating time ($\overline{U}_b$). Note that we need to sum over all recipes in N_b, since a production line can run several recipes. Constraints (16) and (17) link the production decisions (x_ν) with the product flows (q_a) through the production and consumption rates (τ^p and τ^c respectively).

$$\sum_{\nu \in N_b} x_\nu \leq \overline{U}_b \qquad \forall b \in B \tag{15}$$

$$x_\nu = \tau_a^c q_a \qquad \forall \nu \in N, \forall a \in \delta^-(v) \tag{16}$$

$$x_\nu = \tau_a^p q_a \qquad \forall \nu \in N, \forall a \in \delta^+(v) \tag{17}$$

The notation $\delta^-(v)$ ($\delta^+(v)$) defines the set of all incoming (outgoing) arcs of node v, i.e. $\delta^-(v) = \{a \in A \mid a = (v, v')\}$ and $\delta^+(v) = \{a \in A \mid a = (v', v)\}$ for any $v \in V$.

Transportation-related constraints ensure that the flow conservation between warehouses (either at the same or different locations) is guaranteed. Flow-conservation is imposed by (18), while demand fulfilment is guaranteed by (19).

$$\sum_{a \in \delta^+(v)} q_a \leq \sum_{a \in \delta^-(v)} q_a \qquad \forall v \in V^- \cup V^+ \tag{18}$$

$$\sum_{a \in \delta^-(v)} q_a = Q_v \qquad \forall v \in V^R \tag{19}$$

Table 4 summarises all the parameters required to construct the LP.

3.4 Emissions optimisation

To analyse the profitability-sustainability trade-off, we need to consider the CO_2 emissions-related objective.

Objective

We minimise the CO_2 emissions (co_2) associated with the procurement of inputs (PE), the manufacturing of goods (ME) and transportation (TE). They are computed using (21), (22), and (23), respectively. These equations use the notation in Table 2.

$$co_2 = PE + ME + TE \tag{20}$$

$$PE = \sum_{a \in A^E} G_a^E q_a \tag{21}$$

$$ME = \sum_{a \in A^{out}} G_a^M q_a \tag{22}$$

$$TE = \sum_{a \in A^{ts}} G_a^{TS} q_a + \sum_{a \in A^R} G_a^{TR} q_a \tag{23}$$

With the notation in (8), we can write the objective as

$$co_2 = \sum_{a \in A \setminus A^{in}} g_a q_a. \tag{24}$$

4 The profitability-sustainability trade-off

4.1 Methodological approach

We compute a set of Pareto-efficient points to properly analyse the profitability-sustainability trade-off. A Pareto efficient point is a non-dominated solution in that there are no other solutions such that the contribution margin increases without an increase in emissions, or such that the emissions decrease without a decrease in the contribution margin. All Pareto points together constitute the so-called Pareto frontier.

We use a revised version of the ϵ-constrained method (Haimes et al., 1971; Mavrotas, 2009) to generate points of the Pareto frontier. The ϵ-constrained method is an iterative method that solves a single objective model at each iteration in which one of the competing objectives is set as the objective, and the other objective is constrained to meet a minimum value ϵ. Details regarding the implementation of algorithms to solve a generic multi-objective problem are available in Mavrotas (2009). In Sect. 4.2, we describe how we computed the first Pareto-efficient point that we use as a benchmark. Then, we explain how we implemented the ϵ-constrained method to solve our specific problem in Sect. 4.3. Figure 3 shows a diagram of the proposed methodological approach.

4.2 Lexicographic approach as a benchmark

In the lexicographic approach, a decision maker first optimises the highest priority objective and then seeks to optimise lower priority objectives without sacrificing performance on higher priority objectives. In our value chain optimisation problem, the highest priority objective of the decision maker is the maximisation of the company's total contribution margin. Subsequently, the decision maker considers the minimisation of the emissions due to procurement, production and transportation.

In our analysis, we consider a deterministic lexicographic multi-objective linear programming model in which the objective with the higher priority is the total contribution margin (9) and the one with the lower priority is the total CO_2 emissions (20).

A lexicographic multi-objective model is solved in two stages:

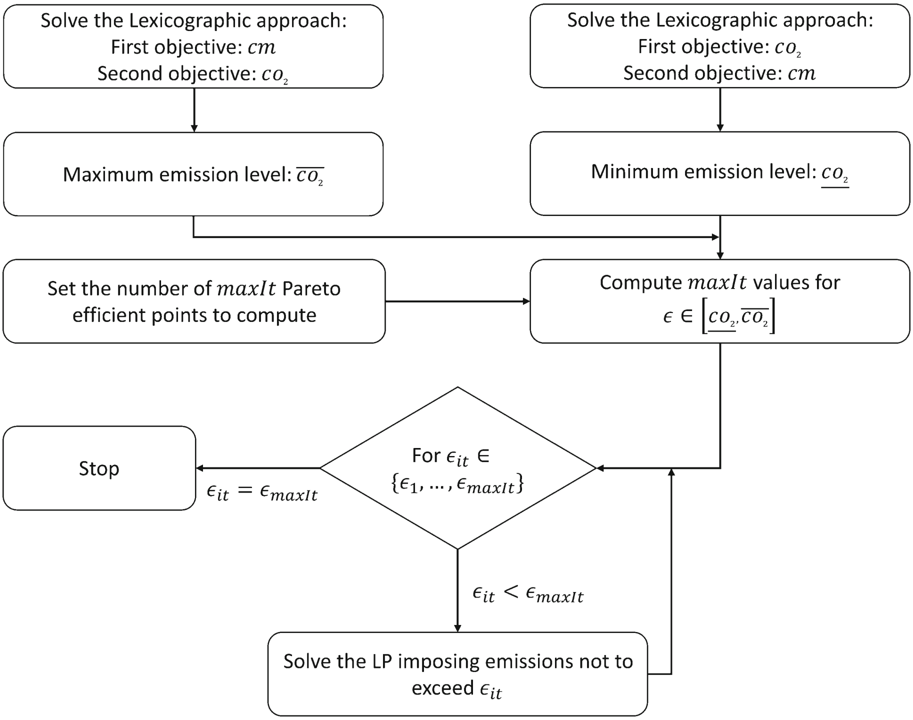


Fig. 3 Diagram of the implemented methodology

- Solve problem $\mathcal{P}_1$:

$$cm^* = \max \sum_{a \in A \setminus A^{in}} c_a q_a$$
$$\text{s.t.}(15) - (19)$$
$$x_\nu \in \mathbb{R}^+ \qquad \forall \nu \in N \tag{25}$$
$$q_a \in \mathbb{R}^+ \qquad \forall a \in A \tag{26}$$

- Solve problem $\mathcal{P}_2$:

$$co_2^* = \min \sum_{a \in A \setminus A^{in}} g_a q_a$$
$$\text{s.t.}(15) - (19)$$
$$(25) - (26)$$
$$\sum_{a \in A \setminus A^{in}} c_a q_a \geq cm^* \tag{27}$$

The lexicographic solution provides a useful initial operating suggestion, but it does not allow the decision makers to trade off the competing objectives of sustainability and profitability. The next section provides an approach for that.

4.3 Pareto frontier

To initialize the ϵ-constrained method we need a first non-dominated point and then a criteria to generate a (large) set of efficient points. By construction, the solution (cm^*, co_2^*) obtained using the lexicographic approach is Pareto-efficient. Therefore, we can use it as a benchmark for further analysis on the profitability-sustainability trade-off. In the remaining part of this section we describe the procedure to generate the other non-dominated points using the ϵ-constrained method.

In our implementation, we use the contribution margin as the single objective and constrain the CO_2 emissions to not exceed ϵ for different choices of ϵ.

First, we compute a lower bound and an upper bound for the total contribution margin (cm) and the CO_2 emissions (co_2). The upper bound for the contribution margin is computed by solving problems $\mathcal{P}_1$ and $\mathcal{P}_2$ omitting any constraints on emissions. We define the solution of the above described problems $(\overline{cm}, \overline{co}_2)$ as the contribution margin and emissions upper bounds, respectively. The lower bounds $(\underline{cm}, \underline{co}_2)$ are computed by reversing the lexicographic approach used to obtain the benchmark. That is, we first minimise the CO_2 emissions and then maximise the contribution margin without increasing the first objective. We define these new problems as $\mathcal{P}_1^{LB}$, $\mathcal{P}_2^{LB}$.

- $\mathcal{P}_1^{LB}$:

$$\begin{aligned} \underline{co}_2 = \min \sum_{a \in A \setminus A^{in}} g_a q_a \\ \text{s.t.}(15) - (19) \\ (25) - (26) \end{aligned}$$

- $\mathcal{P}_2^{LB}$:

$$\begin{aligned} \underline{cm} = \max \sum_{a \in A \setminus A^{in}} c_a q_a \\ \text{s.t.}(15) - (19) \\ (25) - (26) \\ \sum_{a \in A \setminus A^{in}} g_a q_a \leq \underline{co}_2 \end{aligned} \tag{28}$$

To construct the entire frontier, we generate $maxIt$ efficient points. Point $i \in \{1, \cdots, maxIt\}$ is generated by solving problems $\mathcal{P}'_1$, obtained by adding constraint (29) to problem $\mathcal{P}_1$, and $\mathcal{P}'_2$, obtained by replacing constraint (27) with (31) in $\mathcal{P}_2$.

$$\sum_{a \in A \setminus A^{in}} g_a q_a \leq \epsilon_{it} \tag{29}$$

where

$$\epsilon_{it} = \overline{co}_2 - \Delta(it - 1), \quad \text{and} \quad \Delta = \frac{\overline{co}_2 - \underline{co}_2}{maxIt - 1} \tag{30}$$

$$\sum_{a \in A \setminus A^{in}} c_a q_a \geq cm^*_{it} \tag{31}$$

The solution to problem $\mathcal{P}_1^{'}$ is the maximum achievable contribution margin if the CO_2 emissions can be no greater than ϵ_{it}. However, solving this problem does not guarantee that the pair $(cm^*_{it}, \epsilon_{it})$ is Pareto-efficient. To provide this guarantee, it is necessary to solve $\mathcal{P}_2^{'}$. Note that solving this latter problem may produce only two types of solutions: it proves that $(cm^*_{it}, \epsilon_{it})$ is Pareto-efficient or it finds a Pareto-efficient point $(cm^*_{it}, co2^*_{it})$, where $co2^*_{it} \in [\epsilon_{it+1}, \epsilon_{it}]$.

5 Real-world application

5.1 Chemical value chain characteristics

The model described in Sect. 4.3 is tested on real-world data provided by a multinational chemical company. The value chain considered is a subpart of its global operations. It involves around 20 sites (about 40% located in North America (NA), 30% in the region "Europe, Middle-East and Africa" (EMEA) and the remaining equally distributed between Latin America (LATAM) and Asia Pacific (APAC)) producing around 30 final products and more than 250 intermediate products using approximately 400 inputs, among which 50% may be procured from external suppliers. Overall, the sites are composed of more than 250 production lines running over 400 recipes. This complex value chain leads to a model involving around 5000 variables and 4000 constraints. All the parameters required by the model are obtained from the company's planning and reporting systems. In the context of a chemical supply chain, the emissions generated in the manufacturing phase are determined using the chemical reactions involved and the consumption of utilities required for operating the production lines. Similarly, emissions associated with raw materials are either provided directly by the company's external suppliers, who may employ a similar approach as the one described above, or an estimate from a specialised third-party data provider (https://sphera.com/). Transportation emissions are determined according to the GLEC framework (Greene & Lewis, 2019).

In all the experiments, we build and solve the LP using Gurobi 9.5.2 (Gurobi Optimization LLC, 2023).

5.2 Objectives of the analysis

The analysis of the Pareto frontier allows us to answer four business and research questions:

- By how much can the emissions be reduced at a negligible impact on the total contribution margin?
- What is the best strategy to achieve the targeted emissions reduction?
- How are the emissions geographically distributed for different CO_2 reduction targets?
- What are the main sources of emissions?

For a proper assessment of the answers to these questions provided in the upcoming sections, it is important to recall that our model allows for the exploitation of CO_2 reduction measures that are available within the existing production network and value chain setup only. That means, our mathematical model formulation does not consider, e.g., the opening/closing of entire sites, a potential investment in a new production technology at a site, or the increased purchase of green electricity certificates at sites where this has not been done in the past. Instead, we only consider the available options within the status quo. While the other aspects are interesting avenues for future work, our current approach facilitates the short-term implementation of the insights gained as they do not require any major investment.

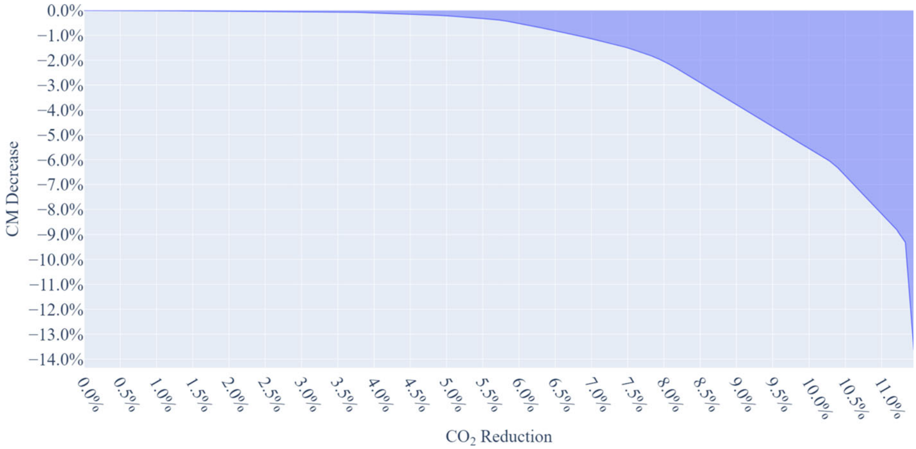


Fig. 4 Contribution margin decrease for an increasing CO_2 emissions reduction in the fixed market share optimisation approach

5.3 Emissions reduction impact on the company's profitability

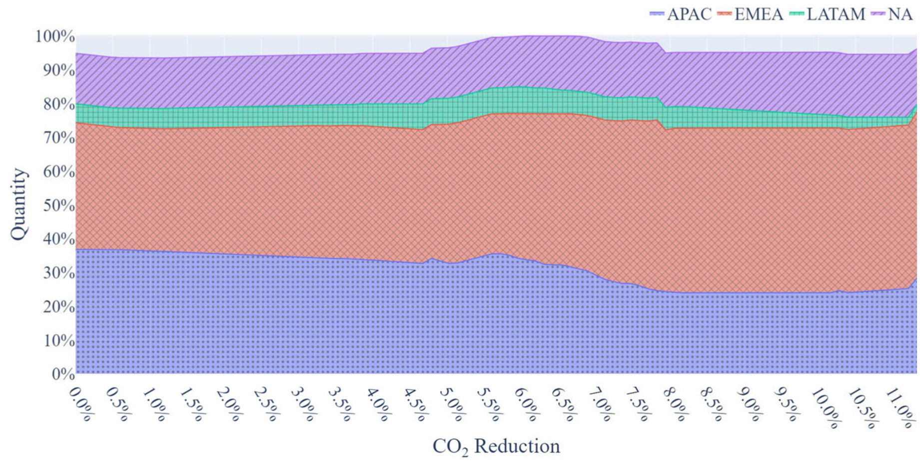
In this section, we answer the question regarding the amount of CO_2 emissions that can be reduced at a negligible impact on the total contribution margin. Figure 4 shows the Pareto frontier. We observe a drastic decrease in the total contribution margin once the requested CO_2 reduction is larger than 40%. This high reduction in the CO_2 emissions can reduce the gap by 25% with the objective stated by the European Green Deal in a single year. However, the profitability reduction required to reach this objective amounts to around 14%. This is not negligible, but rather excessive. To interpret our results we define a profitability reduction of less than 1% as negligible.

Figure 4 shows that the contribution margin is more heavily impacted once the targeted CO_2 emissions decrease exceeds 8%. The maximum achievable CO_2 reduction that has a negligible impact on the total contribution margin is at around 7%. Interestingly, a 5% savings in CO_2 emissions may be achieved by only sacrificing 0.2% of the contribution margin.

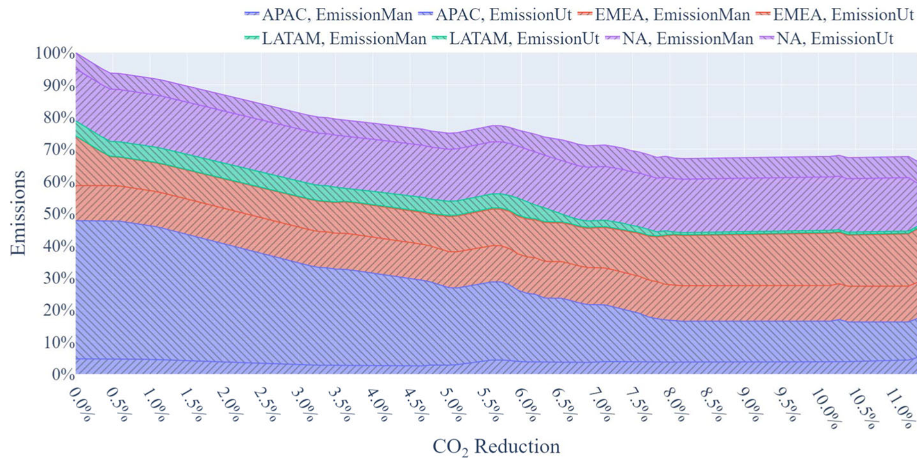
5.4 Strategies to achieve targeted emission reductions

In this section, we analyse what are the best strategies to achieve the targeted CO_2 emissions reduction. Figure 5 shows that, as the CO_2 emission reduction increases, the best strategy for the company involves the relocation of production either within the same region or between different regions. From Fig. 5a, we find that it is possible to reduce CO_2 emissions by 3% simply by relocating production within the same region. This emissions reduction is achieved primarily by reducing the emissions associated with utilities (cf. Fig. 5b). A reduction of utility emissions by 18% can cut the overall CO_2 emissions by 3%. To reach this goal, the company starts to use more expensive but environmentally friendly and efficient production lines. The relocation of production within the same region is enough to achieve this lower reduction target.

In order to achieve a slightly higher CO_2 reduction target (between 3 and 6%), it is necessary to partially shift the production from APAC to EMEA and LATAM. More specifically, if



(a) Quantities produced per region (in percentage of the highest production volume)



(b) Emissions due to manufacturing and utilities' consumption by region

Fig. 5 Variation of production quantities and emissions by region

the target is lower than 4.5%, the production can be moved from APAC to EMEA. Otherwise, if the goal is to reach a 6% reduction, it is necessary to increase the production in LATAM.

If the emissions reduction target is between 6% and 9%, it is necessary to decrease production in APAC and increase production in NA. For a target higher than 7.5%, it is not necessary to increase the production in LATAM; production lines in NA and EMEA are more efficient to cover the production drop in APAC. Up to this emission target, the largest part of the demand that is no longer produced in APAC and LATAM, is produced in EMEA. This trend changes when a CO_2 decrease above 9% is required. In this case, the reduced utilisation of plants in APAC and LATAM is covered by a drastic increase in the operations in NA. Table 5 summarises the four different strategies according to the emissions' target that the company may seek to achieve.

Table 5 Suggested strategy depending on CO_2 reduction target

CO_2 reduction target	CO_2 reduction range	Suggested production location strategy
Extremely low	(0, 3%]	Use the benchmark geographical distribution, choose more efficient production lines in APAC and EMEA
Low	(3%, 4.5%]	Reduce production in APAC, increase production in EMEA
	(4.5%, 6%]	Reduce production in APAC, increase production in EMEA and LATAM
Moderate	(6%, 7.5%]	Reduce production in APAC, increase production in EMEA, LATAM and (slightly) in NA
	(7.5%, 9%]	Reduce production in APAC, increase production in EMEA and (slightly) in NA
High	(9%, 12%]	Reduce the production in APAC and LATAM and increase it in EMEA and (mainly) NA

Overall, the common characteristic of the strategies is the need to transfer the production from the APAC region to EMEA. NA and LATAM play a supporting role. The proposed strategies only involve a geographical relocation of the production and a re-optimisation of the transportation plan. Therefore, they may be implemented in practice since they do not involve further investments or complex and high-level decisions such as entirely leaving a market or accepting a drastic drop in profitability.

5.5 Geographical distribution of CO_2 emissions

In this section, we analyse the geographical distribution of the emissions under different CO_2 reduction targets. Figure 6 illustrates the emissions' distribution by region. If the company focuses only on its profitability, emissions are mainly located in APAC and EMEA. These regions produce around 74% of the overall emissions, 40% and 34% respectively. The remaining emissions are mainly produced in NA accounting for around 20%. LATAM emits around 7% of the total CO_2 emissions. By contrast, if the main focus of the company is on lowering the emissions, EMEA is the first region by CO_2 emissions producing around 55% of the overall emissions. The remaining emissions are almost entirely produced in NA and APAC.

Note, however, that as the model seeks to reduce the *global* CO_2 footprint, it moves production to facilities with low emissions per unit produced. Thus, investment in green production facilities will actually attract more production to these facilities. In accordance with Figs. 5, 6 shows that under a low CO_2 reduction target, the emissions are cut in EMEA using more expensive but more sustainable and efficient production plants. When the target consists in a low or moderate reduction, the production shifts from APAC to EMEA and LATAM diminishing the emissions in APAC while increasing the emissions in EMEA and

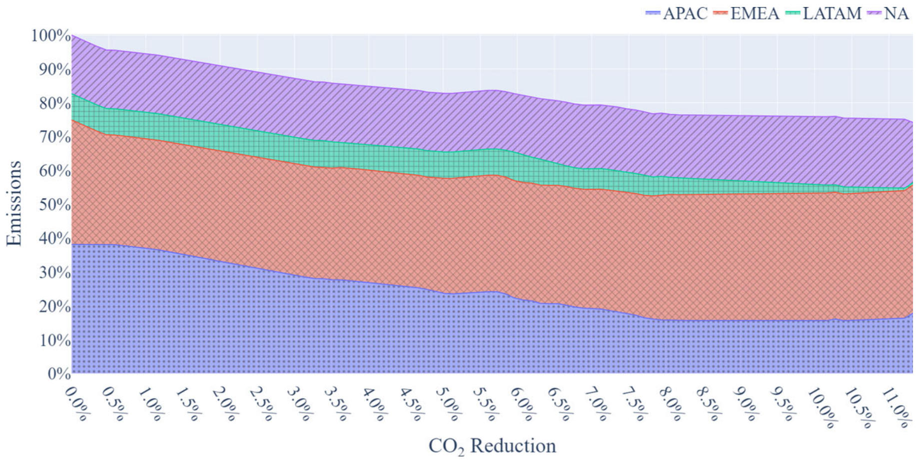


Fig. 6 Manufacturing, utilities and raw materials emissions variation (by region) by the CO_2 reduction

LATAM. For higher emission reduction targets, the CO_2 emissions in LATAM vanish while they drastically increase in EMEA and NA.

Figure 6 highlights an interesting insight. Europe, which as a region is probably the most committed to cut its emissions within the next 30 years, may see an increase in its absolute GHG emissions due to the comeback of production from APAC and LATAM for companies that seek to reduce their global (as opposed to local) CO_2 footprint. Thus local taxes on CO_2 emissions may either increase global emissions or make investment in other regions more attractive. Policy makers that seek to incentivise companies to reduce the global CO_2 footprint should be aware of this. Especially in the short-term, companies that have to drastically cut their emissions are willing to move their production to more sustainable plants. Since stricter GHG regulations have been imposed in Europe since the end of the 90 s, these sustainable plants are mainly located in Europe.

5.6 Main sources of CO_2 emissions

In the previous section, we have analysed how the company should act to reach different CO_2 emission reduction targets with minimal negative effects on profitability. In this section, we analyse what the main sources of emissions are to inform how companies can lower their CO_2 footprint. We distinguish between five different sources of emissions: raw materials procurement, manufacturing, utilities consumption, internal transportation between company sites and external transportation to customers.

Figure 7 shows the variation in emissions (by source) as the required CO_2 reduction target increases. If the company focuses only on its profitability, raw materials are the largest source of emissions. They account for around 50% of the total emissions. Manufacturing constitutes the second largest source of emissions, at around 21%. Utilities follow at 20%. This runs against the widespread idea that transportation is one of the most important sources of emissions. In our value chain, transportation emissions play only a minor role. Transportation accounts for around 5% of the overall CO_2 emissions with an almost equal contribution given by internal and external transportation. The distribution of emissions by source does not vary as the required CO_2 reduction increases. Interestingly, the largest portion of the emission

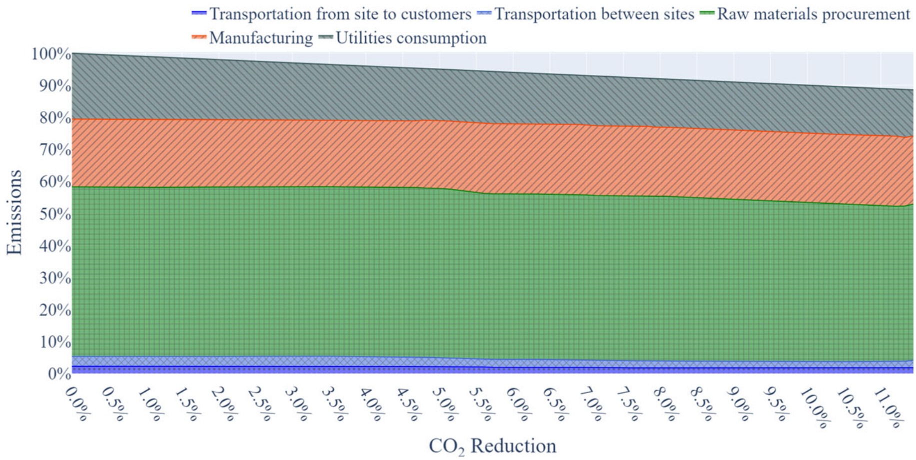


Fig. 7 Emissions variation (by source) at the increase of the CO_2 reduction

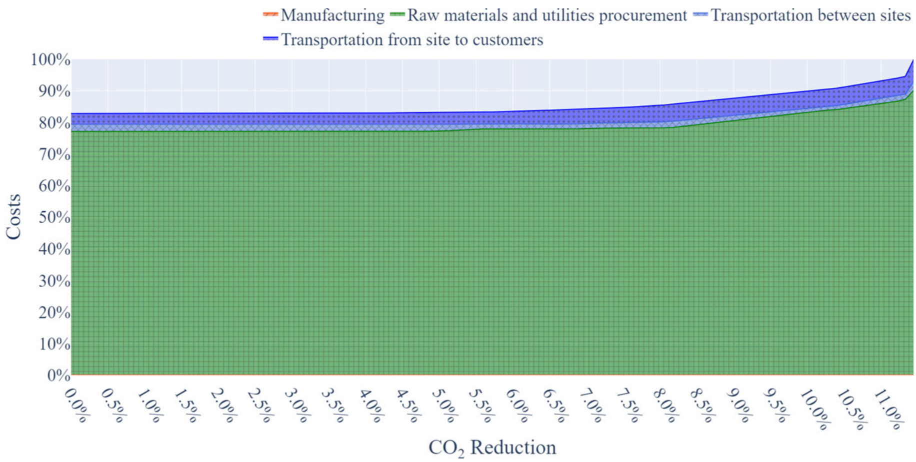


Fig. 8 Costs variation (by source) at the increase of the CO_2 reduction

savings is achieved by diminishing utility emissions. The relocation of the production to sites where more sustainable utilities are available allows up to 50% of the utility emissions and 10% of the total emitted CO_2 to be saved. In contrast, it is difficult to reduce the emissions produced by raw materials and manufacturing.

Figure 8 shows that the largest part of the costs are related to the procurement of raw materials from external suppliers. These account for more than 85% of all considered costs. Interestingly, when there is an increase in the request to reduce CO_2 emissions, the company increases its expences in raw materials to procure more sustainable inputs. Costs due to transportation within different sites of the company and to customers remain constant, always accounting for 7–8% of total costs. Interestingly, manufacturing costs are negligible since they account for less than 1%. Note that in the manufacturing costs, we do not include assets depreciation.

Figures 7 and 8 show that raw materials are the main source of costs and emissions. This implies that procurement decisions are strategic both to reduce costs and emissions. The main objective should be to negotiate contracts with external suppliers to improve their sustainability and to invest in research on more sustainable and efficient production processes.

6 Conclusions and future research

In the present work, we propose a simple approach based on the ϵ-constrained method to analyse the profitability-sustainability trade-off in a complex chemical value chain. This approach provides an easily understandable output (the Pareto frontier) that may be used by decision makers to reduce the CO_2 footprint of their company's value chain. Moreover, this work is the first to consider all the main sources of costs and emissions (i.e., procurement, production and transportation) and to solve a large scale supply chain optimisation problem using an efficient solution approach based on a linear programming model. The proposed methodology may be easily adapted to other different production and transportation planning problems arising not only in the chemical industry but in the entire process industry. This model may also be revised to address the product specific carbon footprint problem, in which the carbon footprint of individual products are constrained. However, such an extension leads to a non-linear model. The model in this paper has the advantage of tractability, especially given the scale of the problem.

In our real-world case study from the chemical industry, we have analysed the Pareto frontier and identified four different possible CO_2 reduction targets and proposed tailored strategies to relocate production operations for each scenario. Our findings demonstrate that transportation is not a key factor in the reduction of CO_2 emissions for the considered chemical value chains. In fact, it may be possible to reduce the overall emissions by increasing transport emissions. In chemical value chains, utilities are the main lever to lower CO_2 emissions while preserving financial profitability. Moreover, our results point out that raw materials are the main source of costs and emissions, but currently there are limited options to find more sustainable suppliers capable to support the company in lowering the products' CO_2 footprint. Therefore, strategic procurement and supplier development should be key ingredients in sustainability plans to reach the target of the European Green Deal.

Future research can consider uncertainty in demand as well as supply processes. This uncertainty can be modelled with a stochastic model (which may yield a stochastic programming problem), or through uncertainty sets (leading to a robust optimisation model). In addition, it may be valuable to track and thus assign the carbon emissions to final sales products or different regions. This enables companies to meet targets set by local legislators or to target a reduction in the footprint of specific products or product families.

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Data Availibility Statement Due to the nature of the research, due to legal and commercial reasons, supporting data is not available.

Declarations

Conflicts of interest The authors declare the following financial interests/personal relationships which may be considered as potential Conflict of interest: Matteo Cosmi reports financial support was provided by BASF. Steffen Klosterhalfen reports a relationship with BASF that includes: employment. Figure 1 has been designed using assets from Freepik.com. Those assets are shared under free licence.

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