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Sustainable supply chain optimisation: An industrial case study ☆

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ABSTRACT

Sustainability plays a key role in the management of a successful and responsible business. When trying to improve the sustainability performance of a business, there are three major challenges that need to be addressed. First, assessment of sustainability requires consideration of not just economic, but also environmental and social impacts. Second, we need to find appropriate sustainability indicators and gather the necessary data in order to quantify sustainability performance. Finally, sustainability has to be seen in the context of the whole system, i.e. it has to include all activities along the supply chain. In this work, we consider all three aspects and propose a multi-objective optimisation framework for the optimisation of a sustainable supply chain. Three sustainability indicators have been considered, namely the total cost, GHG emissions and lead time. We apply this framework to an industrial test case using real-world data drawn from a Dow Chemical business. The results show clear trade-offs between the three different objectives. However, we can also observe that typically a considerable decrease in GHG emissions or lead time can already be achieved by only a relatively small increase in cost. The proposed framework enables us to determine such trade-off relations and consequently make decisions that improve the sustainability performance of the supply chain.

1. Introduction

"Sustainability means making every decision with the future in mind." This is the concise definition of sustainability given by The Dow Chemical Company. Sustainability is critical to the long-term success of a business and increasingly requires consideration of not just the economic but also the environmental and social impacts associated with all the company's activities (Mahler, 2007). Traditionally, the responsibility for ensuring sustainability lies with a company's individual organisational units, which attempt to optimise their performance only in their own sphere of competence. However, this approach often leads to decisions that are optimal for an individual unit but suboptimal for the whole system. Therefore, a key opportunity and challenge now is to take a more holistic approach by essentially trying to optimise the entire supply chain, which includes all stages from procurement to production to distribution, in a single framework (Linton, Klassen, & Jayaraman, 2007).

In terms of environmental sustainability, the need to look broadly at potential impacts is clear in efforts such as the Carbon Disclosure Project (Accenture for CDP, 2013), the Global Reporting Initiative (GRI, 2012), and the Greenhouse Gas Protocol (GHG Protocol, 2011). All these efforts encourage businesses to understand, report and improve not only what is in their direct control, but what they can influence or choose in both upstream and downstream supply chains for their products and activities. Dow's preliminary estimates of the "cradle to grave" greenhouse gas (GHG) emissions, using the principles described by the GHG Protocol, suggest that 30% of the emissions come from Dow's direct activities, with the rest occurring upstream or downstream (Mazor, Muellerweiss, Helling, & Behr, 2012). Therefore, better insights into how the supply chain structure and operation can influence emissions could lead to significant opportunities to improve performance across the supply chain.

Supply chain optimisation has usually considered cost as the key performance metric. The concept of sustainability, however, also requires consideration of other dimensions, such as greenhouse gas emissions and other potential environmental impacts, as well as customer service metrics like responsiveness and resiliency (Papageorgiou, 2009; Shah, 2005). Inclusion of additional metrics greatly increases the complexity of the problem and requires the collection of data that are often not readily

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Nomenclature

Indices

- c customers
- i, j chemicals
- k equipment units
- m, n production plants
- p, q production stages
- s raw material suppliers

Sets

- $I^{FED}_{m,p}$ set of chemicals fed into stage p of plant m
- $I^{PRO}_{m,p}$ set of chemicals produced in stage p at plant m
- $I^{PTP}_{m,n}$ set of chemicals that can be transported from plant m to plant n
- $I^{SAL}_{m,c}$ set of chemicals produced at plant m that can be sold to customer c
- $I^{SU}_{m,p,k}$ set of chemicals that unit k in stage p at plant m can produce or can be set up to produce
- $I^{SUP}_{s,m}$ set of chemicals that can be purchased from supplier s for plant m
- $K_{m,p}$ set of units in stage p at plant m
- M^{new} set of plants that can be added to the existing network
- P_m set of stages at plant m

Parameters

- $CF_{i,j,m,p,k}$ conversion factor for conversion of chemical i into chemical j in unit k of stage p at plant m
- $CIUP_{i,m,p,k}$ maximum increase in amount of chemical i that can be produced in unit k of stage p at plant m [t]
- $\overline{CIUP}_m$ maximum increase in amount of chemicals that can be produced at plant m [t]
- $CIUP^T_{m,p,k}$ maximum increase in processing time for unit k of stage p at plant m [h]
- $CLO_{i,m,p,k}$ minimum amount of chemical i to be produced in unit k of stage p at plant m if unit k is producing chemical i [t]
- $CUP_{i,m,p,k}$ maximum amount of chemical i that can be produced in unit k of stage p at plant m [t]
- $\overline{CUP}_m$ maximum amount of chemicals that can be produced at plant m [t]
- $CUP^T_{m,p,k}$ maximum processing time for unit k of stage p at plant m [h]
- $D_{i,c}$ amount of chemical i ordered by customer c [t]
- $DIS^{PTP}_{m,n}$ distance between plant m and plant n [km]
- $DIS^{SAL}_{m,c}$ distance between plant m and customer c [km]
- $DIS^{SUP}_{s,m}$ distance between supplier s and plant m [km]
- EF^{EC}_m GHG emission factor associated with energy consumed at plant m [kg CO_2e/kWh]
- $EF^{PRO}_{i,m,p,k}$ GHG emission factor for producing chemical i in unit k of stage p at plant m [kg CO_2e/t]
- $EF^{SUP}_{i,s}$ GHG emission factor for supplier s producing chemical i [kg CO_2e/t]
- $EF^{TRPTP}_{i,m,n}$ GHG emission factor for transporting chemical i from plant m to plant n [kg CO_2e/(t km)]
- $EF^{TRSAL}_{i,m,c}$ GHG emission factor for transporting chemical i from plant m to customer c [kg CO_2e/(t km)]
- $EF^{TRSUP}_{i,s,m}$ GHG emission factor for transporting chemical i from supplier s to plant m [kg CO_2e/(t km)]
- $EF^{WT}_{i,m,p,k}$ GHG emission factor for treatment of waste generated from producing chemical i in unit k of stage p at plant m [kg CO_2e/t]
- $FCO^{CI}_{i,m,p,k}$ fixed cost for increasing capacity of producing chemical i in unit k of stage p at plant m [$]
- $\overline{FCO}^{CI}_m$ fixed cost for increasing production capacity at plant m [$]
- $FCO^{CIT}_{m,p,k}$ fixed cost for increasing maximum processing time in unit k of stage p at plant m [$]
- FCO^{INV}_m one year investment cost associated with the construction of plant m [$]
- $FCO^{PRO}_{i,m,p,k}$ fixed cost for producing chemical i in unit k of stage p at plant m [$]
- $FCO^{SU}_{i,m,p,k}$ fixed cost for setting up production of chemical i in unit k of stage p at plant m [$]
- $FCO^{WT}_{i,m,p,k}$ fixed cost for treatment of waste generated from producing chemical i in unit k of stage p at plant m [$]
- $FUP^{PTP}_{i,m,n}$ maximum amount of chemical i that can be transported from plant m to plant n [t]
- $FUP^{SAL}_{i,m,c}$ maximum amount of chemical i that can be transported from plant m to customer c [t]
- $FUP^{SUP}_{i,s,m}$ maximum amount of chemical i that can be transported from supplier s to plant m [t]
- GHG^{CON}_m one year GHG emission associated with the construction of plant m [kg CO_2e]
- $R_{i,m,p,k}$ rate of producing chemical i in unit k of stage p at plant m [t/h]
- $TT^{PTP}_{i,m,n}$ time required to transport chemical i from plant m to plant n [h]
- $TT^{SAL}_{i,m,c}$ time required to transport chemical i from plant m to customer c [h]
- $TT^{SUP}_{i,s,m}$ time required to transport chemical i from supplier s to plant m [h]
- $UCO^{CI}_{i,m,p,k}$ unit cost for increasing capacity of producing chemical i in unit k of stage p at plant m [$/t]
- $\overline{UCO}^{CI}_m$ unit cost for increasing production capacity at plant m [$/t]
- $UCO^{CIT}_{i,m,p,k}$ unit cost for increasing maximum processing time in unit k of stage p at plant m [$/h]
- $UCO^{PRO}_{i,m,p,k}$ unit cost for producing chemical i in unit k of stage p at plant m [$/t]
- $UCO^{SUP}_{i,s}$ unit cost for purchasing chemical i from supplier s [$/t]
- $UCO^{TRPTP}_{i,m,n}$ unit cost for transporting chemical i from plant m to plant n [$/t]
- $UCO^{TRSAL}_{i,m,c}$ unit cost for transporting chemical i from plant m to customer c [$/t]
- $UCO^{TRSUP}_{i,s,m}$ unit cost for transporting chemical i from supplier s to plant m [$/t]
- $UCO^{WT}_{i,m,p,k}$ unit cost for treatment of waste generated from producing chemical i in unit k of stage p at plant m [$/t]
- $UEC_{i,m,p,k}$ unit energy consumption for producing chemical i in unit k of stage p at plant m [kWh/t]

Continuous variables

- $CI_{i,m,p,k}$ increase in amount of chemical i that can be produced in unit k of stage p at plant m [t]
- $\overline{CI}_m$ increase in amount of chemicals that can be produced at plant m [t]
- $CI^T_{m,p,k}$ increase in processing time for unit k of stage p at plant m [h]
- $FED_{i,m,p,k}$ amount of chemical i fed into unit k of stage p at plant m [t]
- $PRO_{i,m,p,k}$ amount of chemical i produced in unit k of stage p at plant m [t]
- $\overline{PRO}_{i,m,p,q}$ amount of chemical i flowing from stage p to stage q at plant m [t]
- $\overline{PTP}_{i,m,n}$ amount of chemical i transported from plant m to plant n [t]

$PTP^{in}_{i,m,p}$	amount of chemical i from other plants fed into stage p at plant m [t]
$PTP^{out}_{i,m,p}$	amount of chemical i produced in stage p at plant m transported to other plants [t]
$SAL_{i,m,p}$	amount of chemical i produced in stage p at plant m to be sold [t]
$\overline{SAL}_{i,m,c}$	amount of chemical i produced at plant m sold to customer c [t]
$SUP_{i,m,p}$	amount of chemical i purchased for stage p at plant m [t]
$\overline{SUP}_{i,s,m}$	amount of chemical i purchased from supplier s for plant m [t]
TCO	total cost [$]
$TGHG$	total GHG emission [kg CO_2e]
TLT	total lead time [h]

Binary variables

$Y_{i,m,p,k}$	1 if chemical i is produced in unit k of stage p at plant m
$\overline{Y}_m$	1 if plant m is built
$Y^{CI}_{i,m,p,k}$	1 if capacity for producing chemical i in unit k of stage p at plant m is increased
$\overline{Y}^{CI}_m$	1 if capacity for plant m is increased
$Y^{CIT}_{m,p,k}$	1 if processing time for unit k of stage p at plant m is increased
$Y^{PTP}_{i,m,n}$	1 if chemical i is transported from plant m to plant n
$Y^{SAL}_{i,m,c}$	1 if chemical i is transported from plant m to customer c
$Y^{SUP}_{i,s,m}$	1 if chemical i is transported from supplier s to plant m

available, which is especially true with regards to environmental data. However, a multidimensional analysis can reveal trade-offs between different objectives and therefore increases the likelihood that a given solution will have farther-reaching and longer-lasting benefits.

A holistic approach to supply chain management requires a general optimisation framework incorporating multiple dimensions and capable of solving industrial-scale problems. In this paper, we propose a framework which supports decisions dealing with supply chain planning, expansion and design problems, and clearly quantifies the trade-offs between economic, environmental, and responsiveness performance. An industrial test case drawn from a Dow business demonstrates the applicability of the approach to real-world problems.

This paper is organised as follows. In Section 2, we present a state-of-the-art literature review on the incorporation of environmental impact quantification methods into process and particularly supply chain optimisation. Section 3, which provides the general problem statement, is followed by Section 4, which presents the mathematical model that allows the optimisation of the tactical planning of a supply chain in terms of economic, environmental, and responsiveness performance. Section 5 describes the solution method used to obtain Pareto optimal solutions. In Section 6, we apply the proposed framework to the Dow case and elaborate on the insights drawn from the optimisation results. Extensions of the model necessary for solving plant and network expansion problems are considered in Section 7. Finally, in Section 8, we close with a summary of the main results and some concluding remarks.

2. Literature review

With growing ecological awareness, the design and operation of more environmentally sustainable processes become increasingly relevant for the chemical and process industry. Yet before we can start taking actions to improve the environmental performance of a process, we first need to answer one fundamental question: How do we quantify the environmental performance of a process?

This question has led to the development of a number of environmental impact quantification methodologies over the last few decades. While Ness, Urbel-Piirsalu, Anderberg, and Olsson (2007) and Singh, Murty, Gupta, and Dikshit (2009) give comprehensive reviews on sustainability assessment methods, in this literature review, we specifically focus on works considering optimisation with environmental assessment.

In the following, we first introduce the concept of Life Cycle Assessment (LCA), which has turned out to be the most widely used environmental impact quantification method in supply chain optimisation, and then review works that explicitly incorporate the quantification of environmental impacts into optimisation frameworks and in particular into supply chain optimisation.

2.1. Life cycle assessment

LCA is a sustainability assessment method that considers environmental impacts throughout the entire life cycle of a product. A complete life cycle consists of all life cycle stages, which are acquisition, production, distribution, use, and disposal. LCA follows a general framework in which environmental impacts are identified, quantified and interpreted. It comprises four phases: Goal and Scope Definition, Inventory Analysis, Impact Assessment, and Interpretation (ISO, 2006a). As shown in Fig. 1, the first three phases are consecutive whereas the Interpretation phase occurs at all LCA stages. In fact, the one-headed arrows in Fig. 1 can be replaced by two-headed arrows to indicate that LCA is always an iterative process.

In the first phase, the Goal and Scope Definition phase, the boundaries of the life cycle system to be examined and a functional unit are defined, with the functional unit being a reference unit which quantifies the performance of the system.

Based on the specifications from the Goal and Scope Definition phase, Inventory Analysis involves the construction of a flow model of the system, the collection of data, and the calculation of pollutant emissions and resource consumptions in relation to the functional unit. Data collection is often the most labour- and time-intensive part of an LCA study. Over the last two decades, many LCA databases have been developed by governmental bodies, industries, and consultancies. These databases are often incorporated into LCA software tools. An overview of LCA databases is given by Finnveden et al. (2009).

The third phase is Impact Assessment, which takes the results from the Inventory Analysis phase and translates them into numerical indicators in order to assess the significance of the calculated environmental impacts. The Impact Assessment phase consists of six steps: selection of impact categories, classification, characterisation, normalisation, grouping, and weighting.

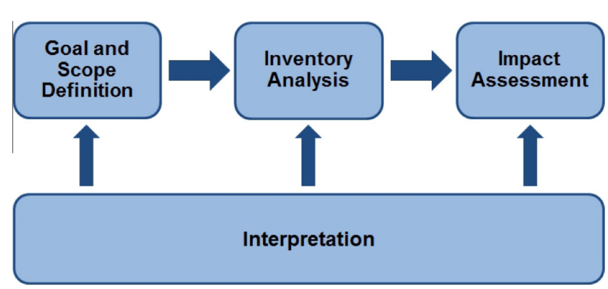


Fig. 1. The graph shows the four phases of Life Cycle Assessment.

According to the international standard (ISO, 2006a, 2006b), the first three steps – selection of impact categories, classification, and characterisation – are mandatory whereas normalisation, grouping, and weighting are optional. Here, the characterisation step, in which cause-effect characterisation models are used to calculate the environmental indicator values, is the most critical one. In fact, characterisation modelling is still an area in need of considerable research (Baumann & Tillman, 2004; Bare, 2010). There exist different characterisation methods, yet comparisons reveal that results from different methods can differ significantly (Dreyer, Niemann, & Hauschild, 2002; Renou, Thomas, Aoustin, & Pons, 2008). This is mainly due to the lack of knowledge about certain environmental mechanisms.

Finally, in the Interpretation phase, one identifies the most significant impacts and evaluates the data from the previous phases. The data are evaluated in terms of completeness, consistency in assumptions and methods, and sensitivity to model uncertainties (Crawford, 2011).

Comprehensive reviews on LCA are given by Rebitzer et al. (2004), Pennington et al. (2004), and Finnveden et al. (2009). The holistic approach of LCA makes it attractive to both academics and practitioners. This is especially true in the process optimisation community, as shown in the remaining of this literature review.

2.2. Environmental impact quantification in process optimisation

The first process optimisation frameworks involving systematic quantification of environmental impacts have been proposed in the 1990s. Stefanis, Livingston, and Pistikopoulos (1995, 1997) developed a method called Methodology for Environmental Impact Minimization (MEIM) which measures environmental impacts associated with the system according to the LCA approach and integrates them into the optimisation framework. This method has been applied to continuous as well as batch processes. One characteristic of MEIM is that in addition to the process plant, the system boundaries also enclose all processes related to raw material acquisition and energy generation. Different environmental impacts such as air pollution, water pollution, and global warming are examined in this framework, which leads to multi-objective optimisation problems. Stefanis et al. (1997) use the ϵ-constraint method (Hwang & Masud, 1979) to create Pareto curves showing the trade-off between cost efficiency and environmental impact abatement. Since Stefanis et al. (1995, 1997), other works using MEIM have been conducted, applying the method to various processes (Buxton, Livingston, & Pistikopoulos, 1997, 1999; Pistikopoulos & Stefanis, 1998).

After the international standard for LCA (ISO, 1997) has been established, the potential of the application of LCA in process selection, design and optimisation has been examined in greater detail (Azapagic, 1999). With LCA, the paradigm in environmental system management has shifted from process-specific evaluation to a more holistic approach that considers the entire material and energy supply chain. Azapagic and Clift (1999a, 1999b, 1999c) particularly focus on the application of LCA in process optimisation and introduce a framework referred to as Optimum LCA Performance (OLCAP). Compared to MEIM, OLCAP puts more emphasis on the Impact Assessment phase of LCA. Here, quantities acquired in the Inventory Analysis phase are aggregated into environmental impacts using appropriate coefficients, and also the weighting of environmental impacts has been considered. Unlike previous process optimisation frameworks with environmental considerations, in which waste minimisation is the primary objective, an approach such as OLCAP minimises the actual environmental impacts. In fact, OLCAP case studies have shown that waste minimisation, e.g. by re-use and recycling, often does not lead to the optimal environmental performance (Azapagic, 1999).

To this day, a number of LCA optimisation frameworks have been established at the plant level (Alexander, Barton, Petrie, & Romagnoli, 2000; Eliceche, Carvalán, & Martínez, 2007; Guillén-Gosálbez, Caballero, & Jiménez, 2008; Vince, Marechal, Aoustin, & Bréant, 2008) and for energy systems (Carvalho, Serra, & Lozano, 2011; Gebreslassie, Guillén-Gosálbez, Jiménez, & Boer, 2010; Liu, Pistikopoulos, & Li, 2010; Pietrapertosa, Cosmi, Macchiato, Salvia, & Cuomo, 2009). The most recent review of those works is provided by Pieragostini, Mussati, and Aguirre (2012).

2.3. Environmental impact quantification in supply chain optimisation

In contrast to process design at the plant level, supply chain management needs to make decisions concerning a broader spectrum of business units, such as procurement, production, and distribution. Hugo and Pistikopoulos (2005) present one of the first works that incorporate LCA into supply chain optimisation. It applies a relatively detailed LCA by using the Eco-indicator 99 method (Pré Consultants, 2001) to model the potential environmental damages. In the Goal and Scope Definition phase, the following five life cycle stages are defined: foreground production process, transportation of raw materials, transportation of products, generation and supply of utilities, and production of raw materials. Data required from the Inventory Analysis phase are obtained from the material and energy balances of the supply chain model. For Impact Assessment, ten relevant impact indicators are identified, quantified, normalised, weighted and finally aggregated into one single impact index. For the weighting process, Eco-indicator 99 provides three different perspectives based on Cultural Theory principles. These perspectives are Hierarchist, Individualist, and Egalitarian, which lead to different sets of weighting factors. As a result, a multi-objective optimisation problem can be formulated, with the two objectives being the maximisation of the net present value (NPV) and the minimisation of the environmental impact index.

Hugo and Pistikopoulos (2005) apply their optimisation framework to the design of a vinyl chloride monomer and ethylene supply chain. The results show the trade-off between the economic and the ecological objectives. However, different network designs have been found that have nearly the same environmental impact, but differ significantly in their economic performance. It is also shown that the environmental performance strongly depends on the chosen perspective, i.e. the weighting of the environmental impacts.

Similar to Hugo and Pistikopoulos (2005), Guillén-Gosálbez, Mele, and Grossmann (2010), Pinto-Varela, Barbosa-Póvoa, and Novais (2010) and Mele, Kostin, Guillén-Gosálbez, and Jiménez (2011) also make use of the Eco-indicator 99 method in their supply chain optimisation frameworks. Bojarski, Laínez, Espuña, and Puigjaner (2009) utilise the IMPACT 2002+ method (Humbert, Margni, & Jolliet, 2005) and incorporate CO_2 emissions trading into their supply chain model. The application of this framework to a maleic anhydride supply chain reveals that CO_2 trading favours the use of the more environmentally damaging benzene over butane. This is due to the fact that CO_2 trading schemes do not explicitly consider aspects like human health and resource depletion, which raises questions about the general suitability of such environmental regulations.

Apart from integrating LCA methodology into supply chain optimisation using Eco-indicator 99, Guillén-Gosálbez and Grossmann (2009, 2010) consider the aspect of uncertainty. Whereas in their first work, Guillén-Gosálbez and Grossmann (2009) deal with uncertainties associated with the life cycle inventory, uncertainties related to the characterisation model are considered in the subsequent paper (Guillén-Gosálbez & Grossmann, 2010). The uncertainties have been incorporated into the supply chain model by using chance constraint programming methods. Solution algorithms have been developed and applied to case studies, which include supply chain design as well as expansion problems. The results show that the proposed framework can be used to optimise the performance of the system in the space of uncertain parameters.

An LCA with full Impact Assessment requires reliable data for the characterisation model. For many processes, these data do not exist in high quality or are not readily accessible. According to Slade, Bauen, and Shah (2009), this is especially true for biofuel systems. For this reason, it is often preferred to use the amount of GHG emissions occurring in the whole life cycle as the environmental performance indicator (Hugo, Rutter, Pistikopoulos, Amorelli, & Zoia, 2005; Slade et al., 2009; You & Wang, 2011; Zamboni, Bezzo, & Shah, 2009, 2011).

In addition to considering the amount of GHG emissions as the environmental indicator, You, Tao, Graziano, and Snyder (2011) incorporate social impacts into their supply chain optimisation framework. An input–output approach focusing on the aspect of job creation is proposed. A case study is conducted for the design of a biofuel supply chain for the state of Illinois. The obtained Pareto curves show the trade-off between economic and ecological performances as well as the trade-off between economic and social performances. Moreover, it can be observed that whereas the economic-ecological Pareto relationship is approximately exponential, the relationship between Pareto optimal social impacts and total costs is almost linear.

The subjective nature of the weighting process in the LCA Impact Assessment phase is often criticised. However, omitting this step also means that we have to deal with more than one single environmental impact index. This leads to an increased number of objectives and requires greater computational effort to solve the multi-objective optimisation problem. To tackle this problem, Pozo, Ruíz-Femenia, Caballero, Guillén-Gosálbez, and Jiménez (2012) use Principal Component Analysis (PCA), which is a dimensionality reduction method, to analyse correlations between environmental indicators and, based on this analysis, reduce the number of indicators taken as objectives. In their case studies, Pozo et al. (2012) have shown that the proposed approach effectively reduces the dimensionality of the objectives and thereby reduces the computational effort while still preserving the optimal Pareto structure to a large extent.

Table 1 lists the reviewed works on supply chain optimisation which specifically claim contribution to the improvement of the sustainability performance of the examined supply chain. For each reference, the table shows which objectives have been considered for the optimisation, which kind of supply chain optimisation problem has been solved and which environmental impact quantification method has been used.

By examining Table 1, one can observe that most optimisation frameworks have only been applied to the design of new supply chain networks. The sole optimisation of supply chain operations and the optimisation of supply chain expansion problems have rarely been considered. This is mostly due to the fact that the examples presented do not deal with real-world cases. In real-world industrial applications, the goal is usually to optimise the planning of an existing supply chain network or to explore the benefits of expanding the existing network. We further find that both LCA applying a full assessment of different impacts and LCA only taking the GHG emissions into account are applied in supply chain optimisation. The choice mainly depends on the availability of reliable data.

Finally, Table 1 indicates that supply chain optimisation incorporating environmental sustainability indicators is a fairly new research area and not many works have been conducted on this topic so far. Especially large-scale real-world case studies are scarce. This has motivated us to contribute to this subject by developing our own optimisation framework and applying it to a real-world industrial case study. The next sections describe the results of this research effort, starting with the general problem statement based on which the mathematical model is derived.

3. Problem statement

We consider a supply chain network consisting of raw material suppliers, production plants, and customers, as illustrated in Fig. 2. A set of raw materials is purchased and transported to each production plant, which transforms them into products. Intermediate products can be transported to other plants whereas final products are distributed to the customers in order to fulfil specified demands.

Table 1
The list is an overview of the reviewed works on supply chain optimisation incorporating environmental impact quantification and their key characteristics.

	Economic objective	Ecological objective	Tactical planning	Supply chain expansion	Supply chain network design	LCA, full impact assessment	LCA, GHG emissions
Hugo and Pistikopoulos (2005)	✓	✓			✓	✓	
Hugo et al. (2005)	✓	✓			✓		✓
Quariguasi Frota Neto et al. (2008)	✓	✓	✓			✓	
Guillén-Gosálbez and Grossmann (2009)	✓	✓		✓	✓	✓	
Bojarski et al. (2009)	✓	✓			✓	✓	
Slade et al. (2009)	✓	✓			✓		✓
Zamboni et al. (2009)	✓	✓			✓		✓
Guillén-Gosálbez et al. (2010)	✓	✓			✓	✓	
Guillén-Gosálbez and Grossmann (2010)	✓	✓		✓		✓	
Pinto-Varela et al. (2010)	✓	✓			✓	✓	
Mele et al. (2011)	✓	✓			✓	✓	
Zamboni et al. (2011)	✓	✓			✓		✓
You and Wang (2011)	✓	✓			✓		✓
You et al. (2011)	✓	✓			✓		✓
Pozo et al. (2012)	✓	✓		✓	✓	✓	

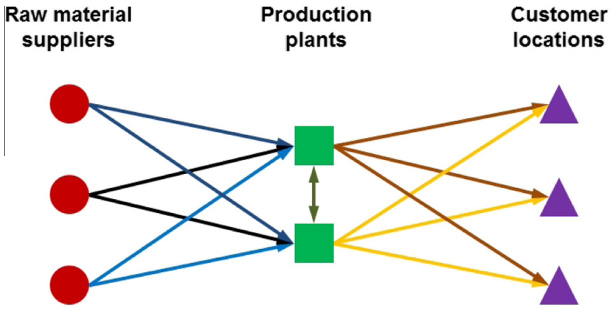


Fig. 2. The schematic shows the structure of a supply chain network connecting suppliers, plants, and customers.

The production process at each plant is considered to be a batch process and can consist of different stages, e.g. multiple sequential reactions in separate reactors. In each stage, there can be multiple units, e.g. reactors and blenders, operating in parallel.

Given are raw material supplier, plant, and customer locations, potential transportation routes, customer demands, production and transportation capacities, processing times, transportation distances and times, fixed and variable costs as well as environmental impact factors associated with all relevant supply chain operations. The goal is to optimise the tactical planning of such a supply chain for a single time period, which is typically one year, while satisfying all customer demands. The decision variables here are

- the amounts of raw materials to be purchased from each raw material supplier,
- the allocation of products to plants and units,
- the amounts of products to be produced in each unit,
- the material flows from suppliers to plants, between plants, and from plants to customers.

The overall objective can be the minimisation of total cost, the minimisation of total environmental impact, the optimisation of responsiveness, or to seek a balanced solution considering two or all of these three objectives.

4. Mathematical formulation

The optimisation problem stated in the previous section can be formulated as an MILP problem involving continuous and binary variables. In the following, we present the mathematical formulation of this MILP model. Note that all continuous variables used in this model are constrained to be nonnegative. A list of indices, sets, parameters, and variables is given in the Nomenclature section.

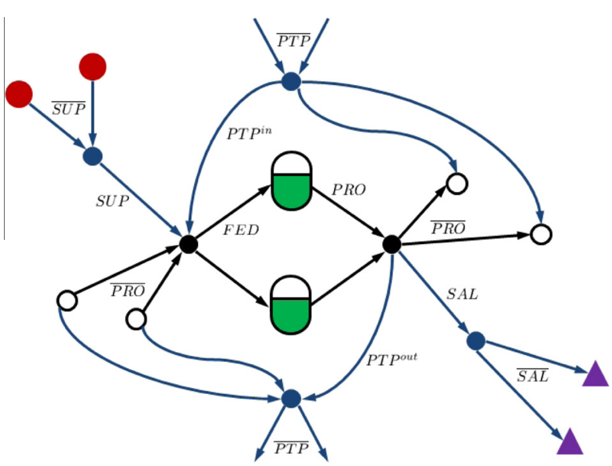


Fig. 3. The graph shows the mass flows involved in each production stage. Mass balances are performed at each filled node. For the sake of better readability, the indices accompanying the variables are omitted in the figure.

4.1. Mass balances

The mass balances are performed at each stage p of each plant m for every chemical i. The schematic in Fig. 3 shows how this is achieved.

$FED_{i,m,p,k}$, which is the amount of chemical i fed into unit k of stage p at plant m, consists of flows coming from the previous stage, suppliers and other production plants. In unit k, $FED_{i,m,p,k}$ is converted into products $PRO_{j,m,p,k}$ with the corresponding conversion factors $CF_{i,j,m,p,k}$. The products from each stage can then be distributed to the next stage, customers and other plants. These mass balances are given by Eq. (1).

$$SUP_{i,m,p} + \sum_{q \in P_m} \overline{PRO}_{i,m,q,p} + PTP^{in}_{i,m,p} = \sum_{k \in K_{m,p}} FED_{i,m,p,k} \quad \forall m, p \in P_m,\ i \in I^{FED}_{m,p} \tag{1a}$$

$$FED_{i,m,p,k} = \sum_{j \in I^{PRO}_{m,p}} CF_{i,j,m,p,k} PRO_{j,m,p,k} \quad \forall m,\ p \in P_m,\ k \in K_{m,p},\ i \in I^{FED}_{m,p} \tag{1b}$$

$$\sum_{k \in K_{m,p}} PRO_{i,m,p,k} = \sum_{q \in P_m} \overline{PRO}_{i,m,p,q} + PTP^{out}_{i,m,p} + SAL_{i,m,p} \quad \forall m,\ p \in P_m,\ i \in I^{PRO}_{m,p} \tag{1c}$$

Eqs. (2), (3) and (4) state the mass balance equations concerning supplies, flows between plants, and sold products delivered to customers.

$$\sum_{s} \overline{SUP}_{i,s,m} = \sum_{p \in P_m} SUP_{i,m,p} \qquad \forall m, i \tag{2a}$$

$$\overline{SUP}_{i,s,m} = 0 \qquad \forall s, m, i \notin I^{SUP}_{s,m} \tag{2b}$$

$$\sum_{n} \overline{PTP}_{i,n,m} = \sum_{p \in P_m} PTP^{in}_{i,m,p} \qquad \forall m, i \tag{3a}$$

$$\overline{PTP}_{i,m,n} = 0 \qquad \forall m, n, i \notin I^{PTP}_{m,n} \tag{3b}$$

$$\sum_{p \in P_m} PTP^{out}_{i,m,p} = \sum_{n} \overline{PTP}_{i,m,n} \qquad \forall m, i \tag{3c}$$

$$\sum_{p \in P_m} SAL_{i,m,p} = \sum_{c} \overline{SAL}_{i,m,c} \qquad \forall m, i \tag{4a}$$

$$\overline{SAL}_{i,m,c} = 0 \qquad \forall m, c, i \notin I^{SAL}_{m,c} \tag{4b}$$

$$\sum_{m} \overline{SAL}_{i,m,c} = D_{i,c} \qquad \forall i, c \tag{4c}$$

4.2. Capacity constraints

There are capacity constraints both on the production and transportation operations. Eqs. (5a) and (5b) set bounds on the product amounts whereas Eq. (5c) restricts the processing time of each unit.

$$CLO_{i,m,p,k} Y_{i,m,p,k} \leqslant PRO_{i,m,p,k} \leqslant CUP_{i,m,p,k} Y_{i,m,p,k} \quad \forall m, p \in P_m, k \in K_{m,p}, i \in I^{PRO}_{m,p} \tag{5a}$$

$$\sum_{p \in P_m} \sum_{k \in K_{m,p}} \sum_{i \in I^{PRO}_{m,p}} PRO_{i,m,p,k} \leqslant \overline{CUP}_m \qquad \forall m \tag{5b}$$

$$\sum_{i \in I^{PRO}_{m,p}} \frac{PRO_{i,m,p,k}}{R_{i,m,p,k}} \leqslant CUP^{T}_{m,p,k} \qquad \forall m, p \in P_m, k \in K_{m,p} \tag{5c}$$

The transportation capacity constraints are given by (6) in terms of maximum amount of products that can be transported via each route.

$$\overline{SUP}_{i,s,m} \leqslant FUP^{SUP}_{i,s,m}\, Y^{SUP}_{i,s,m} \quad \forall s,m,i \in I^{SUP}_{s,m} \tag{6a}$$

$$\overline{PTP}_{i,m,n} \leqslant FUP^{PTP}_{i,m,n}\, Y^{PTP}_{i,m,n} \quad \forall m,n,i \in I^{PTP}_{m,n} \tag{6b}$$

$$\overline{SAL}_{i,m,c} \leqslant FUP^{SAL}_{i,m,c}\, Y^{SAL}_{i,m,c} \quad \forall m,c,i \in I^{SAL}_{m,c} \tag{6c}$$

4.3. Objective functions

In our multi-objective framework, we use three different objective functions which are measures for the economic, environmental, and responsiveness performance of a supply chain.

As the economic performance indicator, we use the total cost as given in Eq. (7), in which *FCO* and *UCO* denote fixed and unit cost, respectively. The total cost is the sum of all costs associated with raw material purchase, production, waste treatment, scale-up, supplier-to-plant transportation, plant-to-plant transportation, and plant-to-customer transportation. Here, we refer to scale-up as the process of adjusting an equipment unit such that it can produce a product that it is not currently producing. Fixed costs can arise from various sources, e.g. from fixed required manpower, equipment maintenance, or asset depreciation. In the case of scale-up, the fixed cost is primarily associated with the cost of modifying the corresponding piece of equipment.

$$\begin{aligned} TCO = & \sum_s \sum_m \sum_{i \in I^{SUP}_{s,m}} UCO^{SUP}_{i,s}\, \overline{SUP}_{i,s,m} \\ & + \sum_m \sum_{p \in P_m} \sum_{k \in K_{m,p}} \sum_{i \in I^{PRO}_{m,p}} \Big(FCO^{PRO}_{i,m,p,k}\, Y_{i,m,p,k} + UCO^{PRO}_{i,m,p,k}\, PRO_{i,m,p,k} \\ & + FCO^{WT}_{i,m,p,k}\, Y_{i,m,p,k} + UCO^{WT}_{i,m,p,k}\, PRO_{i,m,p,k} \Big) \\ & + \sum_m \sum_{p \in P_m} \sum_{k \in K_{m,p}} \sum_{i \in I^{SU}_{m,p,k}} FCO^{SU}_{i,m,p,k}\, Y_{i,m,p,k} \\ & + \sum_s \sum_m \sum_{i \in I^{SUP}_{s,m}} UCO^{TRSUP}_{i,s,m}\, \overline{SUP}_{i,s,m} \\ & + \sum_m \sum_n \sum_{i \in I^{PTP}_{m,n}} UCO^{TRPTP}_{i,m,n}\, \overline{PTP}_{i,m,n} \\ & + \sum_m \sum_c \sum_{i \in I^{SAL}_{m,c}} UCO^{TRSAL}_{i,m,c}\, \overline{SAL}_{i,m,c} \end{aligned} \tag{7}$$

As the environmental performance indicator, we take the impact of GHG emissions on global warming. Conceptually, other environmental impacts can be quantified in a similar way. The emission factors are typically a combination of case-specific performance data and characterisation factors from LCA analyses. As indicated by Eq. (8), the total GHG emissions can be associated with raw material, production, waste treatment, energy consumption, and transportation. Note that energy consumption is related to power generated off-site.

$$\begin{aligned} TGHG = & \sum_s \sum_m \sum_{i \in I^{SUP}_{s,m}} EF^{SUP}_{i,s}\, \overline{SUP}_{i,s,m} + \sum_m \sum_{p \in P_m} \sum_{k \in K_{m,p}} \sum_{i \in I^{PRO}_{m,p}} \Big(EF^{PRO}_{i,m,p,k} \\ & + EF^{WT}_{i,m,p,k} + EF^{EC}_m\, UEC_{i,m,p,k} \Big) PRO_{i,m,p,k} \\ & + \sum_s \sum_m DIS^{SUP}_{s,m} \sum_{i \in I^{SUP}_{s,m}} EF^{TRSUP}_{i,s,m}\, \overline{SUP}_{i,s,m} \\ & + \sum_m \sum_n DIS^{PTP}_{m,n} \sum_{i \in I^{PTP}_{m,n}} EF^{TRPTP}_{i,m,n}\, \overline{PTP}_{i,m,n} \\ & + \sum_m \sum_c DIS^{SAL}_{m,c} \sum_{i \in I^{SAL}_{m,c}} EF^{TRSAL}_{i,m,c}\, \overline{SAL}_{i,m,c} \end{aligned} \tag{8}$$

As a measure for responsiveness, we consider the total lead time, which we define as the sum of all processing and transportation times, as given in Eq. (9).

$$\begin{aligned} TLT = & \sum_m \sum_{p \in P_m} \sum_{k \in K_{m,p}} \sum_{i \in I^{PRO}_{m,p}} \frac{PRO_{i,m,p,k}}{R_{i,m,p,k}} + \sum_s \sum_m \sum_{i \in I^{SUP}_{s,m}} TT^{SUP}_{i,s,m}\, Y^{SUP}_{i,s,m} \\ & + \sum_m \sum_n \sum_{i \in I^{PTP}_{m,n}} TT^{PTP}_{i,m,n}\, Y^{PTP}_{i,m,n} + \sum_m \sum_c \sum_{i \in I^{SAL}_{m,c}} TT^{SAL}_{i,m,c}\, Y^{SAL}_{i,m,c} \end{aligned} \tag{9}$$

This completes the mathematical model that forms the centrepiece of our multi-objective supply chain optimisation framework. It gives a relatively detailed representation of the production processes by using a multistage model. This allows the distinction between different processes and the modelling of plant-to-plant transportation of intermediates. More important, unlike most cost minimisation models, this formulation includes two additional objective functions depicting the total GHG emission and the total lead time.

5. Solution method

In this work, we use the ϵ-constraint method (Haimes, Lasdon, & Wismer, 1971) to solve the multi-objective optimisation problem. In the following, we present the ϵ-constraint algorithm that we are using after giving a formal definition of Pareto optimality (Pareto, 1906).

5.1. Pareto optimality

We consider a multi-objective optimisation problem in the following form:

$$\begin{aligned} \min \quad & \boldsymbol{f}(\boldsymbol{x}) = \left[f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \ldots, f_p(\boldsymbol{x})\right]^T \\ \text{s.t.} \quad & \boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0} \\ & \boldsymbol{g}(\boldsymbol{x}) \leqslant \boldsymbol{0} \\ & \boldsymbol{x} \in X \end{aligned} \tag{10}$$

Definition 1. A point $\boldsymbol{x}^* \in X$ is Pareto optimal (also referred to as efficient or non-dominated) if and only if there does not exist another point $\boldsymbol{x} \in X$ such that $\boldsymbol{f}(\boldsymbol{x}) \leqslant \boldsymbol{f}(\boldsymbol{x}^*)$ and $f_i(\boldsymbol{x}) < f_i(\boldsymbol{x}^*)$ for at least one objective function f_i.

This means that, compared to a Pareto optimal solution, one cannot find another solution that further decreases one objective function without increasing any of the other objective functions. Hence, Pareto optimal solutions depict trade-off relationships between different objectives. If we plot all Pareto solutions on an objective plane, we usually obtain a clear front, which is called

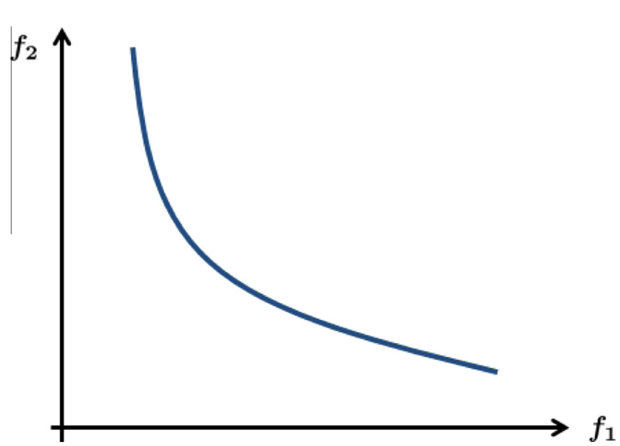


Fig. 4. The Pareto front for a bi-objective optimisation problem shows the trade-off relationship between the two objectives.

the Pareto optimal front or simply Pareto front. Fig. 4 shows such a Pareto front resulting from a bi-objective optimisation. Every point below the Pareto curve is infeasible and every solution found above it is not Pareto optimal.

5.2. ϵ-Constraint algorithm

To apply the ϵ-constraint method, we reformulate the multi-objective optimisation problem (10) into the following single-objective optimisation problem:

$$\begin{aligned} \min \quad & f_j(\boldsymbol{x}) \\ \text{s.t.} \quad & f_i(\boldsymbol{x}) \leqslant \epsilon_i \quad \text{for } i = 1, 2, \ldots, p \text{ with } i \neq j \\ & \boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}, \quad \boldsymbol{g}(\boldsymbol{x}) \leqslant \boldsymbol{0}, \quad \boldsymbol{x} \in X \end{aligned} \tag{11}$$

where ϵ_i are chosen constants.

Theorem 1. *$\boldsymbol{x}^* \in X$ is Pareto optimal if it is a unique optimal solution of problem (11) for any given upper bound vector $\boldsymbol{\epsilon} = [\epsilon_1, \ldots, \epsilon_{j-1}, \epsilon_{j+1}, \ldots, \epsilon_p]^T$.*

We apply Theorem 1, which has been proved by Chankong and Haimes (1983), and present an algorithm using the ϵ-constraint method to solve a multi-objective optimisation problem, i.e. obtaining Pareto optimal solutions, with three performance indicators. The proposed algorithm is as follows.

Step 1: Find the maximum and minimum values for ϵ_2 by solving

$$\begin{aligned} \min \quad & f_i(\boldsymbol{x}) \\ \text{s.t.} \quad & \epsilon_2 = f_2(\boldsymbol{x}) \\ & \boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}, \quad \boldsymbol{g}(\boldsymbol{x}) \leqslant \boldsymbol{0}, \quad \boldsymbol{x} \in X, \quad \epsilon_2 \in \mathbb{R} \end{aligned} \tag{12}$$

for $i = 1, 2, 3$ and thereby obtaining $\epsilon_2^1, \epsilon_2^2$, and ϵ_2^3, respectively. Set upper bound $\epsilon_2^U = \max(\epsilon_2^1, \epsilon_2^3)$ and lower bound $\epsilon_2^L = \epsilon_2^2$.
Step 2: Discretise ϵ_2 and select a sequence of N grid points, $\epsilon_{2,1}, \epsilon_{2,2}, \ldots, \epsilon_{2,N}$, between ϵ_2^L and ϵ_2^U. Set counter $n = 1$.
Step 3: Set $\epsilon_2 = \epsilon_{2,n}$.
Step 4.1: Find the maximum and minimum values for ϵ_3 by solving

$$\begin{aligned} \min \quad & f_i(\boldsymbol{x}) \\ \text{s.t.} \quad & f_2(\boldsymbol{x}) \leqslant \epsilon_2, \quad \epsilon_3 = f_3(\boldsymbol{x}) \\ & \boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}, \quad \boldsymbol{g}(\boldsymbol{x}) \leqslant \boldsymbol{0}, \quad \boldsymbol{x} \in X, \quad \epsilon_3 \in \mathbb{R} \end{aligned} \tag{13}$$

for $i = 1, 3$ and thereby obtaining ϵ_3^1 and ϵ_3^3, respectively. Set upper bound $\epsilon_3^U = \epsilon_3^1$ and lower bound $\epsilon_3^L = \epsilon_3^3$.
Step 4.2: Discretise ϵ_3 and select a sequence of M grid points, $\epsilon_{3,1}, \epsilon_{3,2}, \ldots, \epsilon_{3,M}$, between ϵ_3^L and ϵ_3^U. Set counter $m = 1$.
Step 4.3: Set $\epsilon_3 = \epsilon_{3,m}$.
Step 4.4: Obtain Pareto optimal point by solving:

$$\begin{aligned} \min \quad & f_1(\boldsymbol{x}) \\ \text{s.t.} \quad & f_2(\boldsymbol{x}) \leqslant \epsilon_2, \quad f_3(\boldsymbol{x}) \leqslant \epsilon_3 \\ & \boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}, \quad \boldsymbol{g}(\boldsymbol{x}) \leqslant \boldsymbol{0}, \quad \boldsymbol{x} \in X \end{aligned} \tag{14}$$

Step 4.5: Set $m = m + 1$. Go to Step 5 if $m > M$, otherwise go back to Step 4.3.
Step 5: Set $n = n + 1$. Stop algorithm if $n > N$, otherwise go back to Step 3.

If we want to obtain Pareto optimal solutions in terms of two of the three objectives, we only have to apply the inner loop (Steps 4.1–4.5) for the corresponding objectives.

6. Case study

We now apply the optimisation model presented in Section 4 to a real-world industrial case study for which the data are provided by The Dow Chemical Company. The given supply chain consists of 17 raw material suppliers providing 11 raw materials, 7 production plants producing 270 products, and customers aggregated into 268 customer regions. Given are the raw material supplier, production plant, and customer locations, the available transportation links, the supplier, reactor, plant, and transportation capacities, and the forecast customer demands for one year.

At each plant, we have a three-stage production process, which is illustrated in Fig. 5. We refer to the three stages as reaction 1, reaction 2, and blending. The purpose of reaction 1 is to produce chemicals that can be used as reactants in reaction 2. Products from reaction 2 then enter the blending process through which the final products are formed. Each reactor can produce a certain set of products, which may include both products from reaction 1 and reaction 2, i.e. reaction 1 and reaction 2 can take place in the same reactor if the reactor is suited for both reactions.

For the formulation of the economic performance indicator, we are given the fixed and unit costs for transportation, production, waste treatment, and scale-up. The cost for purchasing raw materials is assumed to be a constant and is therefore not considered in the optimisation. The transportation times and reactor processing times, which are required to calculate the total lead time, are also given. Not directly given are the emission factors needed to calculate the GHG emissions, which means that further data have to be collected for the estimation of the emissions. Therefore, in Section 6.1, we first explain which data and methods we use to quantify GHG emissions in this case study.

6.1. Quantification of GHG emissions

First, we define the boundaries of our system, i.e. we decide which GHG emissions to take into account. Ideally, we would consider emissions from all processes associated with the supply chain. However, this is often difficult due to the lack of accurate data. The model for this case study includes GHG emissions.

- generated at the production plants,
- associated with energy consumption, i.e. from off-site power generation,
- from off-site waste treatment,
- and from transportation.

We do not consider emissions associated with the production of the raw materials since accurate supplier-specific data are not available. Note that GHG emissions resulting from the production of the raw materials can be significant. However, since here we are essentially assuming that all suppliers are equally emission intensive, the corresponding amount of GHG emissions is a

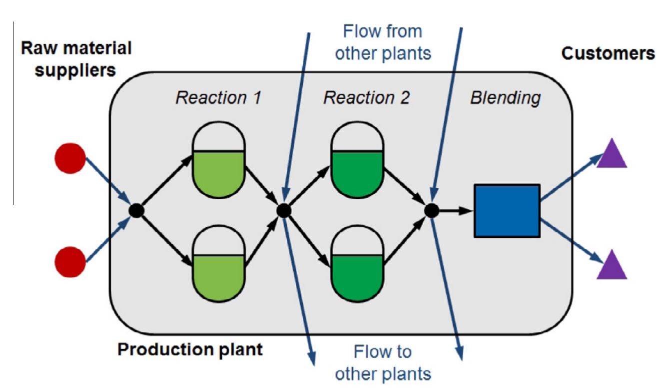


Fig. 5. The schematic illustrates the three-stage model of the production plants in the case study.

constant and therefore does not affect the optimisation. In the following, we elaborate on how each of the above mentioned emissions is quantified.

6.1.1. GHG emissions associated with production

GHG emissions generated at the production plants can be estimated by using company reports that list the annual GHG emissions and total amount of products produced in the most recent year at each plant. The major GHGs emitted from the plants are CO_2, CO, N_2O, and CH_4. The various GHGs differ in their global warming potentials. To take this into account, we use the GWP100 characterisation factors (Forster et al., 2007) shown in Table 2 to convert the amount of emissions into a common unit, kg CO_2e (CO_2 equivalent). For instance, the characterisation factor for N_2O indicates that its impact on global warming is 300 times as high as CO_2's.

Using this information, we obtain plant-specific GHG emission factors given in kg CO_2e emitted per tonne reactor product produced.

6.1.2. GHG emissions associated with energy consumption

We know the annual total product amount and total energy consumption for the previous year. From this, we can estimate the plant-specific unit energy consumption in kWhr energy consumed per tonne reactor product produced. Note that here, the available data for energy consumption include both heat and power.

In terms of GHG emissions, detailed information on energy generation for each plant is not readily available. In fact, this kind of information is very difficult to obtain since one would have to trace back all the energy transformation paths incorporated in the energy grid. Therefore, since the plants in our network are located in different countries, we use emission factors for electricity and heat generation on a national level (IEA Statistics, 2011) as an estimate. This gives us GHG emission factors in kg CO_2e emitted per kWhr energy used.

6.1.3. GHG emissions associated with waste treatment

In the company reports, the amounts of waste from each plant are listed along with the dedicated waste treatment methods. From this information, we can estimate the GHG emissions associated with the treatment of the wastes from the production plants. The three major waste treatment methods are combustion, landfill, and wastewater treatment. The estimation of the corresponding emissions is explained in the following.

6.1.3.1. Combustion. In order to estimate the GHG emission from combustion, we first calculate the carbon content of a waste compound typical for the plants in our supply chain. This waste consists of 30% of a mixture of different polymers and 70% of water. Assuming complete combustion, we can determine the CO_2 emission from the combustion of this waste mixture. This way, we obtain an emission factor given in kg CO_2e per kg waste combusted. The validity of this estimate is confirmed by comparing it to values from literature (EpE, 2010).

6.1.3.2. Landfill. A large portion of the wastes from the production plants is disposed in landfills. After being placed in a landfill, the waste is first decomposed by aerobic bacteria. Anaerobic bacteria begin to consume the remaining waste once the available oxygen is depleted. Biogas, which contains primarily CO_2 and CH_4, is emitted through the fermentation process. It is commonly assumed that 50% of the carbon content in the waste will be converted to CO_2 and the remaining 50% to CH_4 (RTI International, 2010).

The complete degradation of solid wastes in landfills can take many years and thus generates GHGs over a long period of time. To simulate the degradation process, we apply a model proposed by IPCC (2006, chap. 3), which uses the following first-order decay equations:

$$W_t = LC_{t-1}\left(1 - e^{-k}\right) \tag{15a}$$

$$C_t = C_{t-1}\, e^{-k} \tag{15b}$$

where the index t indicates the year, W is the annual amount of CH_4 generated from decomposable material, L is the CH_4 generation potential, C is the amount of decomposable degradable organic carbon (DDOC) accumulated in the waste material, and k is the reaction constant.

The CH_4 generation potential and the amount of DDOC in the waste compound are characteristics of the specific waste disposed. In the framework of the IPCC tool, we choose industrial waste as an estimate and calculate the GHG emissions over 50 years since, according to the model, this is the amount of time required for over 95% of the DDOC to degrade. We obtain a GHG emission factor of 1.69 kg CO_2e per kg solid waste disposed. A similar value is obtained by using LandGEM (EPA, 2005), another commonly used landfill gas emissions model.

6.1.3.3. Wastewater treatment. The GHG emission factor for wastewater treatment that we use, which is 0.0027 kg CO_2e per kg of wastewater, is taken from Bani Shahabadi, Yerushalmi, and Haghighat (2009). For their estimation, Bani Shahabadi et al. (2009) have built models of on-site as well as off-site processes. Also, nutrient removal and different wastewater treatment methods have been taken into account. Similar values can be found in other literature, such as Snip (2009).

6.1.4. GHG emissions associated with transportation

Knowing the distances between the locations and the corresponding transportation modes, we can calculate the GHG emissions from transportation by applying emission factors given in kg CO_2e per tonne chemical transported per km distance travelled. We use transportation emission factors specifically provided for the chemical industry by CEFIC (2011).

6.2. Optimisation results

Now using the available input data and applying the model presented in Section 4, we obtain an MILP with 533,093 continuous variables, 529,970 binary variables, and 1,125,966 constraints. We implement the model in the modelling environment AIMMS and solve it using CPLEX 12.4. Please note that in this paper, we do not show any results on the computational performance since we want to focus on the insights from the optimisation results. However, we can report that in average, one problem can be solved within a few minutes with an integrality gap of less than 0.1%.

We first perform a cost minimisation, a GHG emission minimisation, and a lead time minimisation separately, and compare the solutions of these three optimisation problems. We refer to these three cases as base cases. Fig. 6 shows the breakdown of the total cost in those base cases. For all three solutions, plant-to-customer transportation contributes the most to the total cost, followed by supplier-to-plant transportation and production. Obviously, the total cost for the minimum cost solution is lower than the ones

Table 2
The GWP100 characterisation factors depict the different global warming potentials of various GHGs.

GHG	CO_2	CO	N_2O	CH_4
Characterisation Factor	1	1.57	300	25

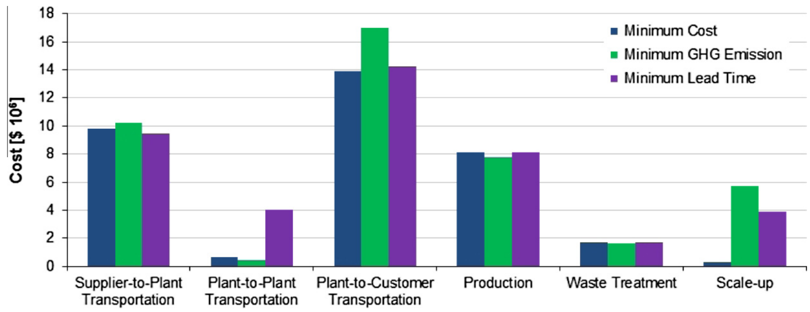


Fig. 6. By solving the tactical planning problem, one obtains this breakdown of the total cost for the three base cases.

for the other two solutions. However, it is remarkable that, in both the case of minimum GHG emission and the case of minimum lead time, the total cost is almost 30% higher than the total cost achieved by cost minimisation. Fig. 6 further indicates that large amounts of intermediates have to be transported between the plants in order to minimise the total lead time. Also, scale-up procedures are expensive and are therefore minimised in a cost minimisation. This is very different in an emission or lead time minimisation in which costs are not taken into account.

The GHG emission breakdown shown in Fig. 7 indicates that the largest contribution of emissions originates from energy generation. The minimum cost and minimum lead time solutions lead to approximately the same total GHG emission. Compared to these two cases, the minimum GHG solution reduces the total GHG emission by almost 10%.

Fig. 8 shows the product allocation scheme, i.e. the amount of products produced at each plant, for the three base cases. The first observation we make is that the production at plant P1 and P7 is almost the same for all three solutions. The reason for this is that most of the customers served by each of these two plants either cannot be served by any of the other plants in our network or distribution of products from other plants to these customers would come with disproportionately high cost and transportation time.

Compared to the minimum cost solution, P3's and P5's production has increased whereas P4's and P6's has decreased in the minimum GHG emission solution. In fact, the production at plant P6 drops to zero. This is due to the fact that P4 and especially P6 have lower energy efficiencies and at the same time are located in countries with carbon-intensive energy grids. Therefore, these plants generate more GHG per unit product produced. Since all customers served by P4 and P6 can also be reached by P3 and P5, the production is shifted to the latter two plants. The only reason why P4's production has not also dropped to zero in the minimum GHG solution is that P3 and P5 have already reached their maximum production capacities.

In the minimum lead time configuration, the production at plant P2 is zero. This solution is not intuitive and unexpected at first glance since P2 is located very closely to all its customers. However, for the production of the demanded products, P2 requires raw materials and intermediates produced at other plants. The transportation of these chemicals to P2 comes with long transportation times. Therefore, the minimum lead time solution suggests producing all products at the other plants and only using P2 as a distribution hub, which means that instead of shipping various raw materials and intermediates to P2, only the final products are transported to P2 and then distributed from there to nearby customers.

Figs. 6–8 show the three limiting solutions since each of them solely minimises one of the objective functions. Now we examine the relationship between each two of the three objectives by determining the corresponding Pareto fronts. This results in three Pareto curves which are shown in Fig. 9.

All three Pareto curves show trade-off relationships between the respective objectives. All three curves have similar shapes, each expressing three distinct parts. With increasing one objective function, the other one experiences a steep decrease in the first part of the curve. It then decreases almost linearly in the second part before the curve reaches the last part in which almost no further improvement can be achieved. In the first part of the curve, the Pareto optimal solutions suggest structural changes in the supply chain network, hence the sharp decrease in one of the objective functions while only slightly increasing the other one. In the second part, incremental changes are made depending on the upper bound constraint on the value of one of the objective functions, which leads to an almost linear relationship. Finally, the curve becomes flat in the last part when limitations of the supply chain network are reached.

After examining two objectives at a time, we now apply our multi-objective framework to the optimisation problem considering all three objectives. As a result, we obtain a 3-dimensional Pareto front depicted by the contour plot in Fig. 10. It illustrates the trade-off relationship between all three objectives and shows that, in order to decrease one objective function, at least one of the other two has to be increased.

For the evaluation and visualisation of single Pareto solutions, we use a spider diagram as shown in Fig. 11 in which each triangle

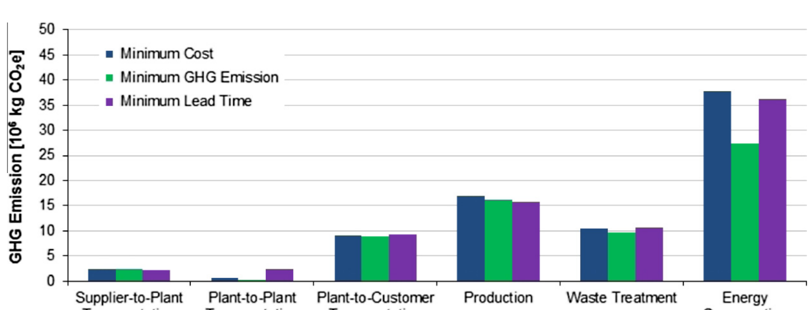


Fig. 7. By solving the tactical planning problem, one obtains this breakdown of the total GHG emission for the three base cases.

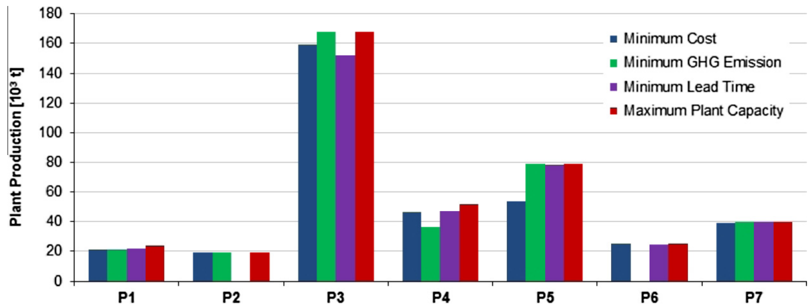


Fig. 8. The graph shows the optimal product allocation in the three base cases obtained by solving the tactical planning problem. The maximum plant capacity for each plant is used as a reference to indicate the level of capacity utilisation.

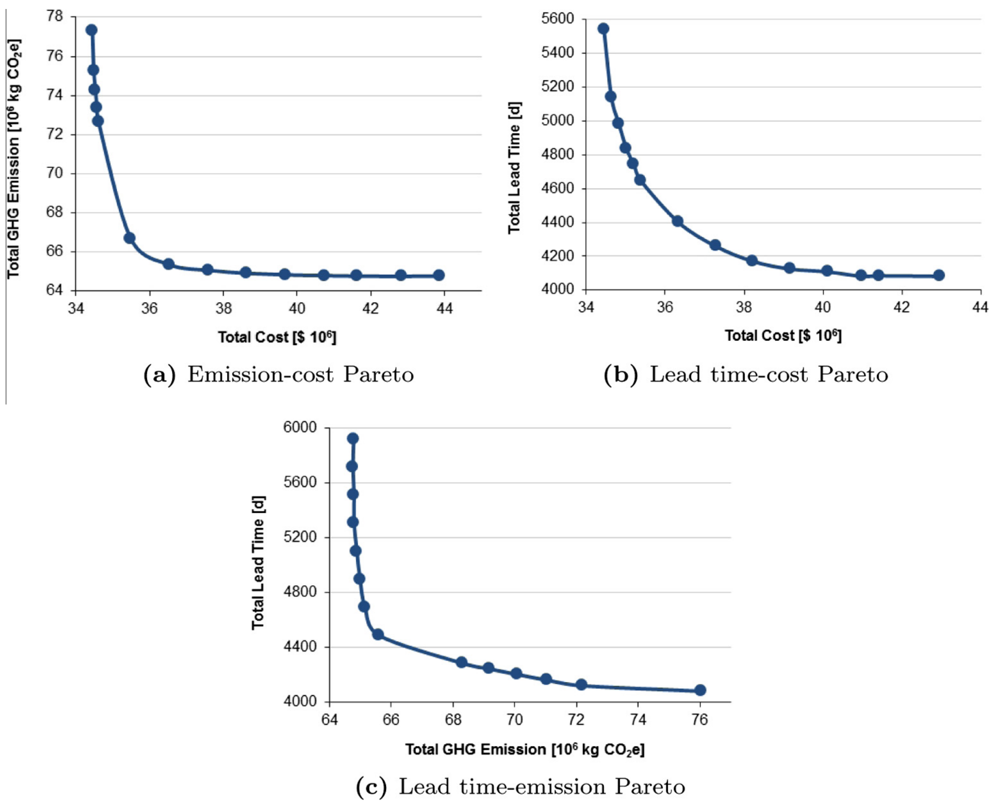


Fig. 9. Each plot shows a Pareto curve that shows the trade-off relationship between two of the three objectives.

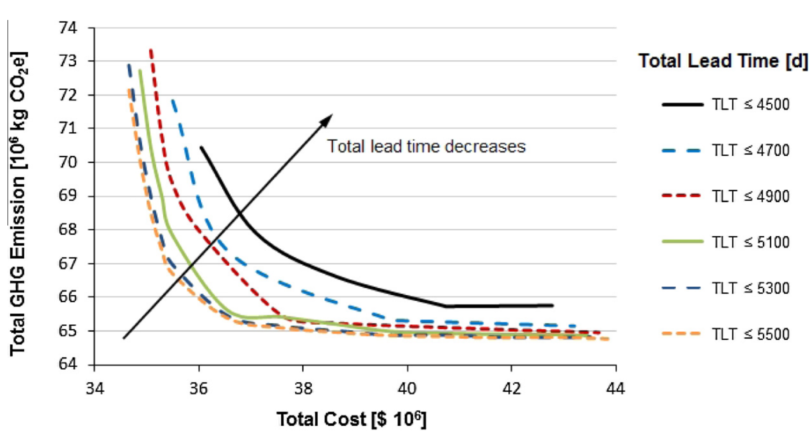


Fig. 10. The contour plot shows Pareto optimal solutions with respect to all three objectives.

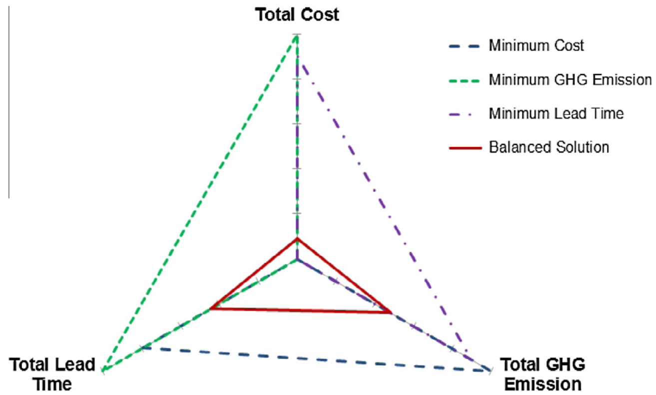


Fig. 11. The spider diagram shows the comparison between the base case solutions and one more balanced Pareto optimal solution.

represents one Pareto point. The diagram has three axes depicting the three objective functions. We use normalised scales, i.e. the value 1 on the scale corresponds to the maximum and 0 corresponds to the minimum objective function value found among all Pareto solutions.

Fig. 11 shows four different Pareto solutions. The first three are solutions to the three base cases. One can see that in each of those cases, we perform optimally in terms of one objective but very badly with respect to the other two. The fourth Pareto solution shown in Fig. 11 depicts a solution that is more balanced between the three objectives. In this case, the total cost is slightly higher than the minimum value, but the other two objective functions have been decreased considerably.

7. Model extensions

The model presented in Section 4 is suited for optimising the tactical planning of a supply chain and we have demonstrated its applicability with our industrial case study. The model can be extended such that it can also be used to solve plant and network expansion problems. In the following, we describe these model extensions and apply them to expansion problems based on the same supply chain used in our case study.

Note that unlike in Section 6, the additional data used in this section are not directly drawn from existing plants. However, these are realistic values since they are estimated from available real data. With the results, we are able to demonstrate the capability of the proposed optimisation framework to solve such problems and illustrate potential impacts on the supply chain system.

7.1. Plant expansion

In some of the solutions presented in Section 6, we see some plants reaching their maximum production capacities. This indicates that the performance of the supply chain could be further improved if those plants had higher capacities. To explore the potential benefits of increasing plant capacities, we integrate this into our supply chain model from Section 4 by replacing constraints (5) with

$$CLO_{i,m,p,k}\, Y_{i,m,p,k} \leqslant PRO_{i,m,p,k} \leqslant CUP_{i,m,p,k}\, Y_{i,m,p,k} + CI_{i,m,p,k} \quad \forall m, p \in P_m, k \in K_{m,p}, i \in I^{PRO}_{m,p} \tag{16a}$$

$$\sum_{p\in P_m}\sum_{k\in K_{m,p}}\sum_{i\in I^{PRO}_{m,p}} PRO_{i,m,p,k} \leqslant \overline{CUP}_m + \overline{CI}_m \quad \forall m \tag{16b}$$

$$\sum_{i\in I^{PRO}_{m,p}} \frac{PRO_{i,m,p,k}}{R_{i,m,p,k}} \leqslant CUP^T_{m,p,k} + CI^T_{m,p,k} \quad \forall m, p \in P_m, k \in K_{m,p} \tag{16c}$$

$$CI_{i,m,p,k} \leqslant CIUP_{i,m,p,k}\, Y^{CI}_{i,m,p,k} \quad \forall m, p \in P_m, k \in K_{m,p}, i \in I^{PRO}_{m,p} \tag{16d}$$

$$\overline{CI}_m \leqslant \overline{CIUP}_m\, \overline{Y}^{CI}_m \quad \forall m \tag{16e}$$

$$CI^T_{m,p,k} \leqslant CIUP^T_{m,p,k}\, Y^{CIT}_{m,p,k} \quad \forall m, p \in P_m, k \in K_{m,p} \tag{16f}$$

where CI denotes capacity increase and $CIUP$ the corresponding upper bound.

To take costs associated with capacity increase into account, we add the following term to Eq. (7):

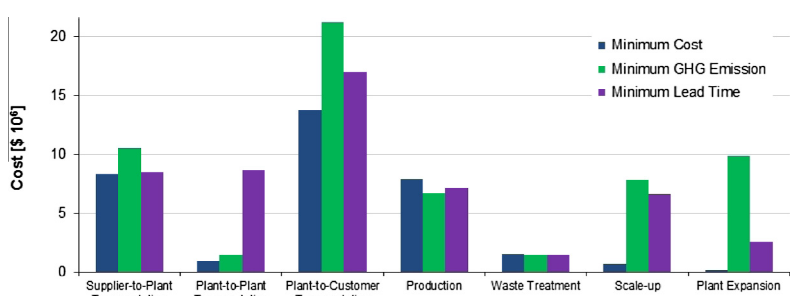


Fig. 12. By solving the plant expansion problem, one obtains this breakdown of the total cost for the three base cases.

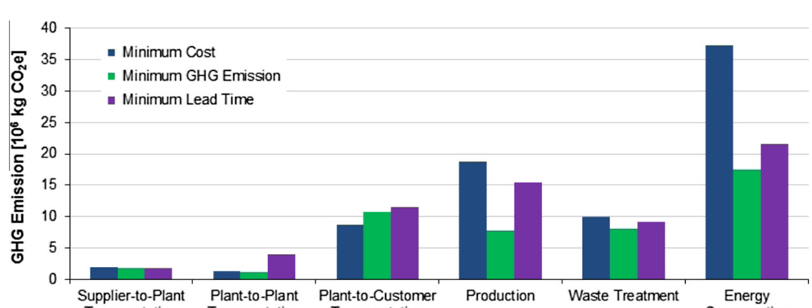


Fig. 13. By solving the plant expansion problem, one obtains this breakdown of the total GHG emission for the three base cases.

$$\sum_m \sum_{p\in P_m} \sum_{k\in K_{m,p}} \sum_{i\in I^{PRO}_{m,p}} \left(FCO^{CI}_{i,m,p,k} Y^{CI}_{i,m,p,k} + UCO^{CI}_{i,m,p,k} CI_{i,m,p,k}\right)$$
$$+\sum_m \left(\overline{FCO}^{CI}_m \overline{Y}^{CI}_m + \overline{UCO}^{CI}_m \overline{CI}_m\right) \qquad (17)$$
$$+\sum_m \sum_{p\in P_m} \sum_{k\in K_{m,p}} \left(FCO^{CIT}_{m,p,k} Y^{CIT}_{m,mp,k} + UCO^{CIT}_{m,p,k} CI^{T}_{m,p,k}\right)$$

Since we want to examine the maximum potential benefits from plant expansion, we do not limit plant capacity increases in the following problem. From solving the three base cases, we obtain the cost breakdowns, GHG emissions breakdowns, and product allocation schemes shown in Fig. 12–14, respectively. In Fig. 14, capacity increase is depicted by production higher than the pre-expansion plant capacity. It can be observed that while the minimum cost solution only suggests a relatively small capacity increase, we obtain a high overall capacity increase for the minimum GHG emission as well as for the minimum lead time solution.

In the minimum cost solution, the capacities at P3 and P6 are increased. Interestingly, the reason for this is not that P3 and P6 are the most inexpensive plants in terms of production. The preferred product allocation to these plants rather results from their large product portfolios and advantageous locations.

In the minimum GHG emission solution, the capacity at plant P5 almost triples due to the plant's low carbon intensity. The production at P2, P4 as well as P6 is zero since their customers are now served by P5. The production at P1 and P7 remains the same due to their relatively limited product portfolios and remote locations.

In terms of minimising lead time, it is advantageous to produce at as few plants as possible since it minimises the number of plants to which raw materials have to be shipped. Hence, in the minimum lead time solution, about 85% of the production occurs at P3 and P5 whereas production at P2, P4, and P6 is very small and P7 produces some products that can only be produced there. The latter four plants mainly act as distribution hubs for customers that cannot be directly reached by P3 or P5.

The Pareto relationships obtained from optimisation considering plant expansion are shown in Fig. 15. Compared to the Pareto

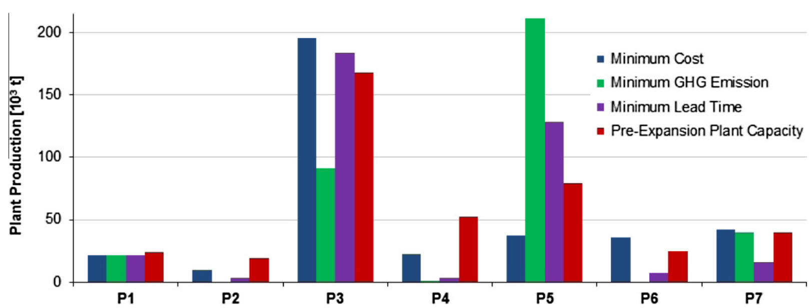
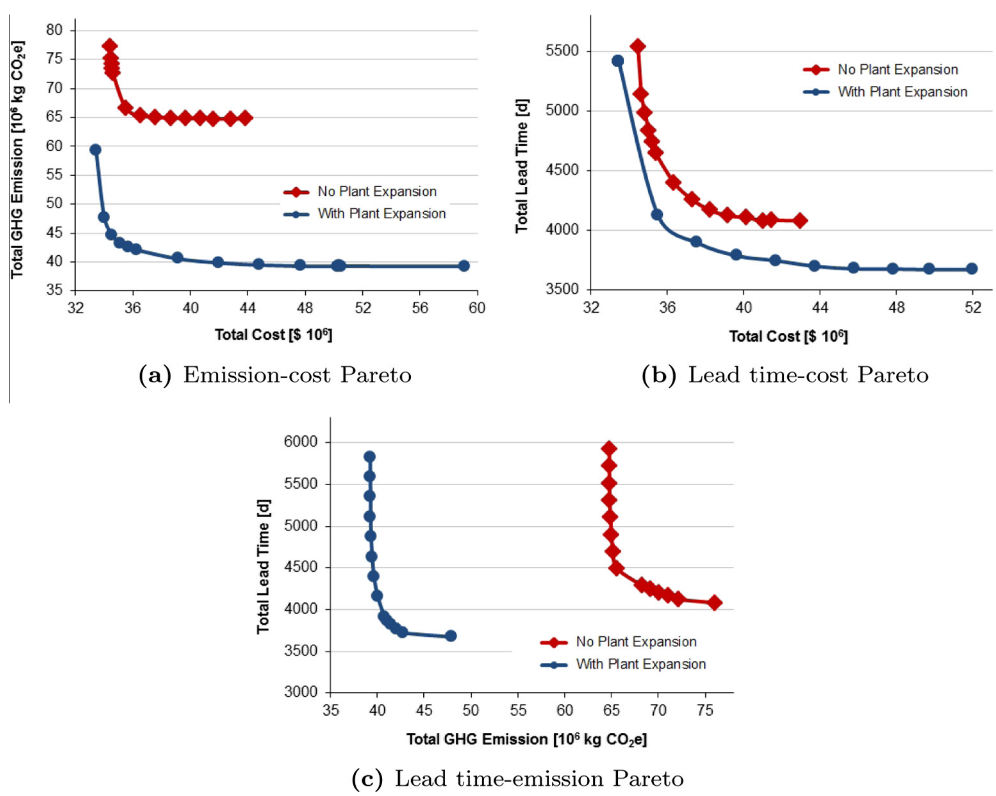


Fig. 14. The graph shows the optimal product allocation in the three base cases obtained by solving the plant expansion problem.



(a) Emission-cost Pareto

(b) Lead time-cost Pareto

(c) Lead time-emission Pareto

Fig. 15. The three plots compare the Pareto curves obtained from solving the problem allowing and not allowing plant capacity increase.

curves obtained in Section 6, the trade-off relationships have improved. For instance, the emission-cost Pareto curve in Fig. 15a indicates that, with the same cost, considerably more GHG emissions can be reduced by allowing plant capacity increase.

7.2. Network expansion

Suppose we have already exhausted all plant capacity increase potential in the existing supply chain network. Now one way to further improve the supply chain is to expand the network by e.g. adding new production plants. To include this in our model from Section 4, we merely have to add the costs and GHG emissions associated with the construction of new plants to the formulation. To achieve this, we introduce the new binary variables $\overline{Y}_m$, add the constraint

$$Y_{i,m,p,k} \leqslant \overline{Y}_m \quad \forall m \in M^{new}, p \in P_m, k \in K_{m,p}, i \in I^{PRO}_{m,p} \tag{18}$$

where M^{new} is the set of plants that can be added to the existing network. Furthermore, we add the terms (19) and (20) to (7) and (8), respectively.

$$\sum_{m \in M^{new}} FCO^{INV}_m \overline{Y}_m \tag{19}$$

$$\sum_{m \in M^{new}} GHG^{CON}_m \overline{Y}_m \tag{20}$$

$\overline{Y}_m$ is 1 if plant m is built and 0 otherwise. Since we calculate costs and emissions for a fixed period of one year, FCO^{INV}_m and GHG^{CON}_m are distributed one year investment costs and one year construction related GHG emissions, respectively. These are estimated by taking the total investment and GHG emission associated with the construction of the new plant and divide the values by the plant's expected lifetime in years. Moreover, the scale-up costs for new plants are zero since these are assumed to be already included in the investment costs.

In the following, we consider one plant, P8, that can be potentially added to the existing supply chain network. We assume P8 to be a state-of-the-art plant, i.e. compared to most of the existing plants, P8 is more energy and cost efficient, generates less waste, and has lower GHG emissions. Plant P8 has a large product portfolio and would be located at the same place as some of the raw

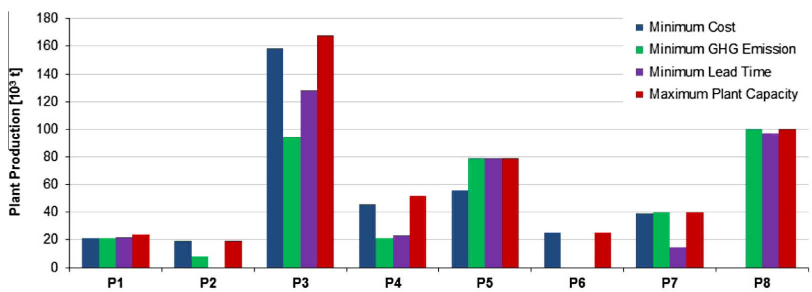
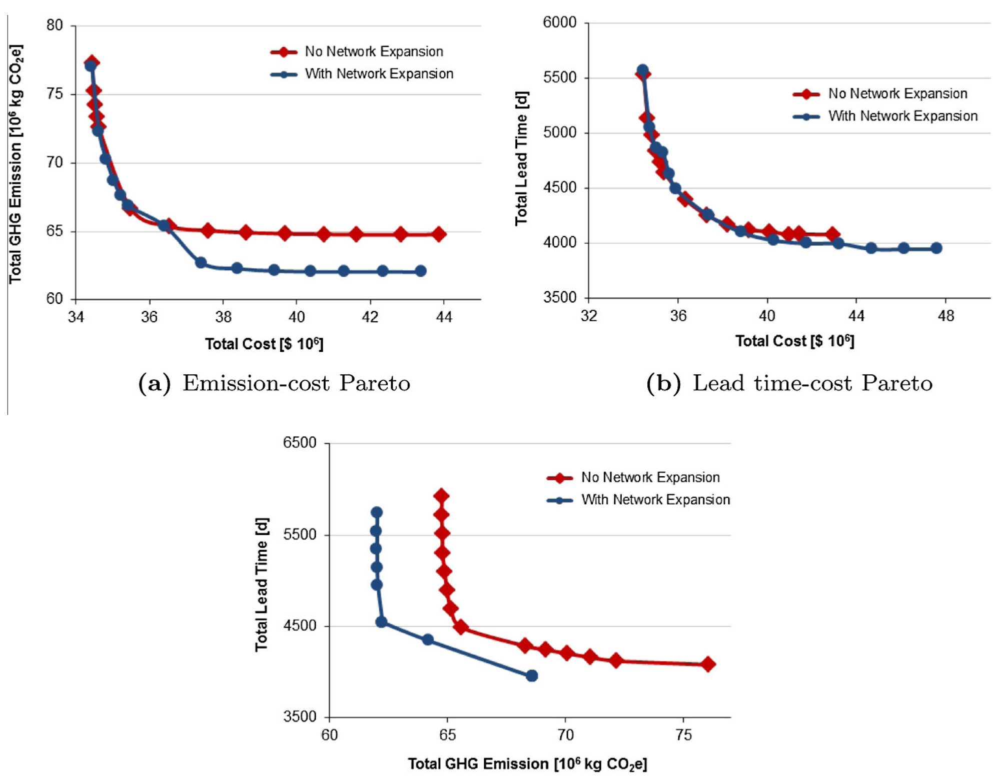


Fig. 16. The graph shows the optimal product allocation in the three base cases obtained by solving the network expansion problem.



(a) Emission-cost Pareto

(b) Lead time-cost Pareto

(c) Lead time-emission Pareto

Fig. 17. The three plots compare the Pareto curves obtained from solving tactical planning problem and the network expansion problem.

material suppliers. By applying our optimisation framework to this network expansion problem, we obtain the product allocation schemes and Pareto curves shown in Fig. 16 and 17, respectively.

Fig. 16 shows that the minimum cost solution does not suggest building P8, which indicates that the reduction of operational costs by including P8 in the network does not exceed the investment cost. The minimum GHG emission solution adds P8 to the existing network. Comparing it to the solution from Section 6 (c.f. Fig. 8), one can see that a significant part of P3 and P4's production is shifted to P8 resulting in P8 reaching its maximum capacity. The minimum lead time solution also includes P8. Here, most of the production is allocated to P3, P5, and P8.

Similar to the plant expansion problem, Fig. 17 shows that the Pareto relationships obtained from solving the network expansion problem have improved in comparison to the results from Section 6. Also, the shapes of the Pareto curves have changed. We see clear kinks in the curves which indicate significant changes in the network structure. For instance, in the emission-cost Pareto curve shown in Fig. 17a, the existing network remains the same in the Pareto solutions that have a cost of $\$34.4 \times 10^6 - \$36.4 \times 10^6$. For a total cost higher than $\$36.4 \times 10^6$, plant P8 is added to the network. We conclude that a solution balancing all three objectives could benefit from adding plant P8 to the supply chain network although it is not suggested by the minimum cost solution.

8. Conclusions

This paper addresses the optimal design and planning of sustainable industrial supply chains considering three key performance indicators: total cost, total GHG emission, and total lead time. A multi-objective optimisation framework incorporating these sustainability indicators has been developed and applied to an industrial test case drawn from a Dow business.

The results show clear trade-off relationships between the three objectives. This provides information on how much impact a certain increase in cost would have on the performance of the supply chain with respect to those different indicators. In particular, the shapes of the Pareto curves indicate that a considerable decrease in GHG emissions or lead time can already be achieved by a small increase in cost.

We have further shown the utility of the proposed approach on plant and network expansion problems. We have therefore demonstrated that the proposed optimisation framework can be used to solve various types of supply chain problems of large scales.

The emphasis of this work lies on the application of the proposed framework to a large-scale industrial case study with real data. At this point, we want to emphasise the importance of collecting accurate data, which has been a major challenge in this work. With the required data, the proposed framework can be applied to a wide range of supply chains in the chemical and process industry. Moreover, the model can be used as a basis for further extensions such as multiperiod supply chain optimization considering time-dependent demand and inventory constraints.

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