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A general optimization framework for the design and planning of energy supply chain networks: Techno-economic and environmental analysis

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Highlights

- A unified modeling representation (E-STN) for material and energy supply chains.
- General optimization model for the design/planning of material and energy supply chains.
- Optimization of capacity expansion, energy mix, techno-economic & environmental aspects.
- Emissions caps are more effective measures for emissions reduction than emissions costs.
- Cost versus emissions study via sensitivity analysis and multi-objective optimization.

Abstract

A general spatial optimization framework that relies on the use of a modified state-task network representation for design and planning problems in material and energy supply chain networks is presented. In brief, the proposed optimization framework considers for the tasks and states of the network: (i) the optimal selection and sizing of conversion, transfer and storage technologies, (ii) the capacity expansion for each technology over time, (iii) the inventory levels for storable states, (iv) the quantities of states converted or transferred through tasks, and (v) the optimal energy mix. Several variations of an illustrative design and planning problem of a mixed material and energy supply chain network have been solved effectively to study the trade-off between costs and emissions levels and different emissions regulation policies. A sensitivity analysis study with respect to alternative emissions caps and a multi-objective optimization example considering the conflicting objectives of total cost and emissions are also presented. The case studies showed that a more efficient way for emissions reductions is through regulation and emissions caps rather than increased emissions costs (i.e., 3.3% emissions reductions). Overall, the proposed optimization framework could be used to integrate various types of material and energy supply chain operations using a unified modeling representation towards the more efficient management of such interdependent networks under techno-economic and environmental aspects.

Keywords

Capacity expansion; Optimal energy mix; Emissions; Optimization; Multi-objective; Sustainability

1. Introduction

Modern energy networks have been continuously improving towards reducing their environmental footprint by introducing low-carbon technologies, improving energy efficiency of the overall system and securing energy resources for their long-term sustainable operation. The main challenge in energy systems lies on how to systematically improve energy supply and demand side by considering environmental sustainability and efficient economic performances. Environmental sustainability may involve integration of clean technologies into the conventional energy system to tackle the effects of greenhouse gas emission. This integration should result in solutions that are characterized by both reduced environmental footprint and improved economical and operational performance targets. Towards these targets, an integrated energy supply chain network should consider the capacity expansion of the involved technologies and the optimal generation and flow of resources within the whole network to achieve a cost-effective energy supply chain network design, with reduced emissions levels while ensuring the demand satisfaction of the end users.

In recent years, Energy Systems Engineering has been emerged as an excellent means of providing systematic approaches that could quantify different levels of complexity of such systems (i.e., technology, plant, energy supply chain network). More specifically, Energy Systems Engineering provides a solid methodological scientific framework to arrive at integrated solutions to complex energy systems problems, by adopting a holistic systems-based approach for optimization, simulation and control problems of energy supply chains networks. Energy systems engineering approaches have been presented for subjects related to design and control modeling (Diangelakis and Pistikopoulos, 2017), integrated operational and maintenance planning (Zulkafli and Kopanos, 2016), and low-carbon energy systems (Corbetta et al., 2016). The abovementioned works studied and developed state-of-the-art methodologies and tools for energy systems planning, design, operation and control from various levels in process plant to supply chain and system-wide levels as covered in a recently published book (Kopanos, Liu and Georgiadis, 2017).

A good number of energy systems engineering research works on the subject can be found in the open literature. For example, Kim et al. (2011) studied the optimal design of biomass supply chain networks for biofuels. Fernandes et al. (2013) proposed mixed integer linear programming model for the strategic design and planning of petroleum supply chains. Hasan et al., (2014) presented a mathematical model for the optimization of nationwide, regional, and statewide carbon capture, utilization, and sequestration supply chain networks. Koltsaklis et al., (2014) developed an optimization model for the design and operational planning of energy networks based on combined heat and power units. Guerra et al. (2016) presented optimization frameworks for the integrate design and planning of water networks and shale gas supply chains. In addition, Arredondo-Ramírez et al. (2016) presented optimal infrastructure planning approaches for shale gas supply chain networks. Ng and Maravelias, (2017) proposed an optimization model for the design of biofuel supply chains with variable regional depot and biorefinery locations. Gao and You (2017) developed a modeling framework and computational algorithm for hedging against uncertainty in sustainable supply chain design using life cycle optimization. Calderón et al., (2017) presented an optimization framework for the design of synthetic natural gas supply chains.

For material-based supply chain networks, Grossmann, (2005) discussed the need for enterprise-wide approaches for the integrated management of supply, production and transportation activities. Shah (2005) and Papageorgiou (2009) provided excellent reviews on the design and planning considering uncertainty, business and sustainability aspects. Most of the suggestions and conclusions drawn in these works apply to the energy supply chain case. Although there is a large number of works in the open literature that cope with different types of material or energy supply chains, there is a lack of a unified modeling representation for dealing with combined material and energy supply chain networks under an integrated optimization framework.

The focus of this study is on material and energy supply chain networks that consist of several types of interdependent and interconnected technologies that could be located in different geographical regions and perform various process, such as exploitation of energy resources from natural reservoirs, transformation of resources into intermediate and final products, transfer of energy or material resources to end users of other downstream technologies of the overall network. A general modeling representation is proposed in this study for the unified modeling of material-based and energy-based supply chains. Based on the proposed modeling representation, a general optimization framework is developed that could be used for the modeling of several types of energy supply chains design and planning problems (e.g., oil and gas industries, power industries, and renewable energy industries etc.). This general modeling representation is proposed as a means for the integrated management of material and energy supply chain networks within a single optimization framework, and constitutes the main contribution of this study.

The paper is structured as follows. In Section 2, the proposed modeling approach for the design and planning of energy supply chains is described. The problem statement of the study is formally defined in Section 3. The proposed optimization framework is then presented in Section 4, followed by the description and discussion of the results of the case studies in Section 5. Finally, some concluding remarks are provided in Section 6.

2. Proposed Modeling Approach: Energy State Task Network (E-STN)

In this work, we present a general representation for modeling operations in energy supply chains inspired by the State Task Network (STN) representation for chemical processes (Kondili et al., 1993). The STN is a directed graph that consists of three key elements: (i) state nodes that represent the feeds as well as intermediate and final products, (ii) task nodes that stand for the process operations which transform material from one or more input states into one or more output states, and (iii) arcs that link state and task nodes indicating the flow of materials. In this representation, state and task nodes are denoted by circles and rectangles, respectively (see Figure 1). The salient characteristic of the STN representation is that distinguishes the process operations from the resources that may be used to execute them, and therefore provides a means for describing very general process recipes. The STN representation has been broadly used in process scheduling problems with some applications to material-based supply chain networks (Lainez et al., 2009) and biomass supply chains (Pérez-Fortes et al., 2012).

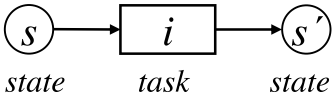


Figure 1. Typical State Task Network (STN) representation.

In the context of energy supply chain networks, we show how the definition of states and tasks of the original STN representation should be modified so as to be able to model the set of operations performed in such environments. That way, a unified modeling framework for the operations in energy supply chains is developed. In addition, our modeling representation is based on a spatial approach that divides the overall geographical region of interest (e.g., a country) into a finite number of zones. The formal definition of the states and nodes as well as the types of technology considered in the proposed Energy supply chain STN (E-STN) representation follows.

2.1. Definition of states in energy supply chain operations

In this work, we propose the classification of state nodes into energy material resources, energy forms, and undesired substances; as shown in Figure 2.

- **Energy material resources states** represent material resources, non-renewable primary or secondary energy material resources, "renewable" biomass materials (wood, energy crops, forest or agricultural residues, municipal solid waste, etc.) and biofuels (e.g., bioethanol, biodiesel). Primary energy material resources include fossil fuels (such as coal, petroleum, natural gas) and nuclear fuels (such as Plutonium-239 and Uranium-235). Secondary energy material resources comprise chemical fuels such as diesel, ethanol, propane, butane, gasoline and hydrogen.
- **Energy forms states** represent secondary energy, such as electrical energy and heat as well as primary renewable energy such as solar, wind, geothermal energy and energy from water (excluding biomass and biofuels). In contrast to energy material resources states, energy form states are not tangible.
- **Undesired substances states** represent unwanted elements that can contaminate or have a harm effect in the natural environment. Contaminants and pollutants of different forms (i.e., solid particles, liquid droplets, or gases) as well as greenhouse gases, such as CO_2 and NO_x, are typically the main undesired by-product substances in energy supply chain networks.

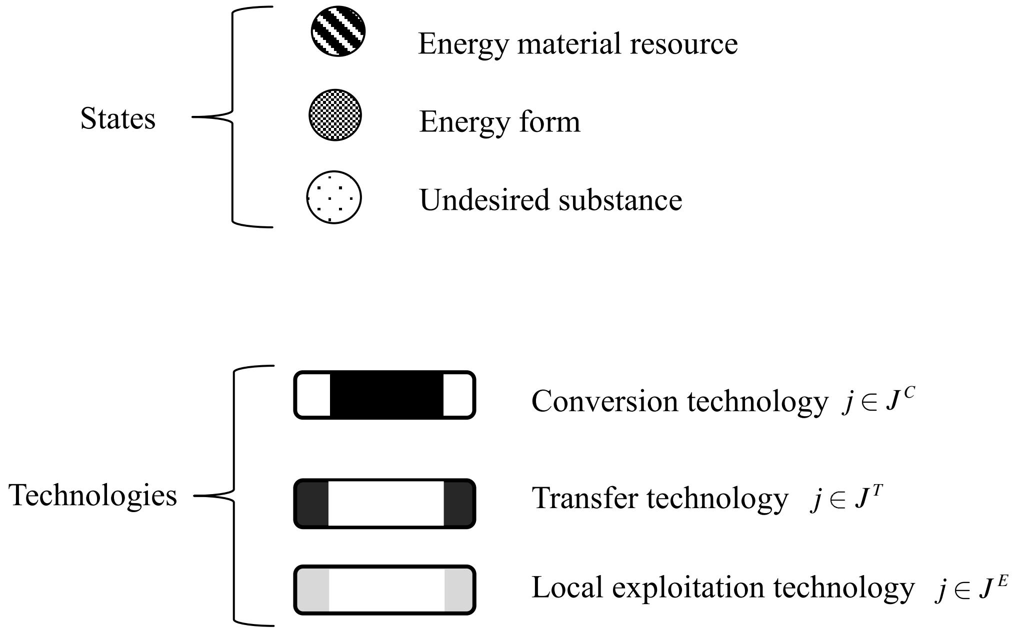


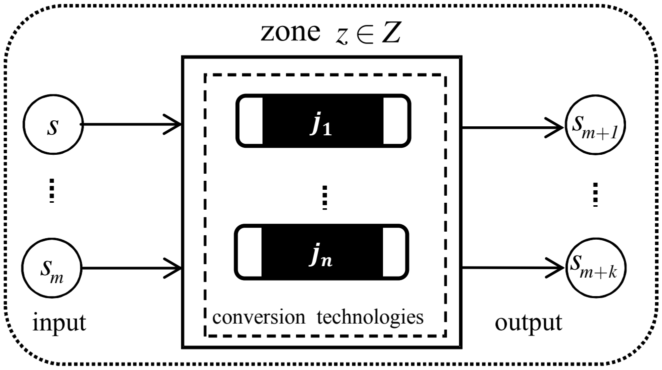
Figure 2. E-STN representation: states and technologies.

2.2. Definition of tasks in energy supply chain operations

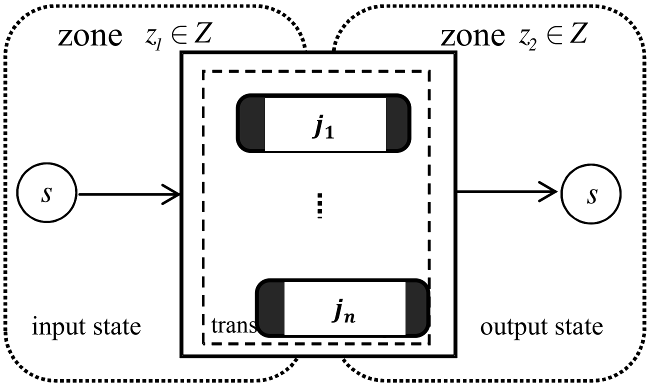
The task nodes are categorized into conversion tasks, transfer tasks and local exploitation tasks, as described below.

- **Conversion tasks** represent tasks that can transform a set of any type of states into a different set of states, as shown in Figure 3a. For instance, a conversion task (e.g., combustion) may transform energy material resources states (e.g., coal) into energy forms states (e.g., electricity and heat) and undesired substances states (CO_2, etc.). A conversion task (e.g., photovoltaic effect) could transform energy forms (e.g., solar energy) into other energy forms (e.g., electricity). In addition, a conversion task (e.g., fermentation) may transform energy material resources states (e.g., sugarcane, wheat or corn) into other material resources states (e.g., bioethanol). Even a conversion task (e.g., scrubbing for carbon capture) may transform undesired substances states (e.g., flue gas) into other undesired substances states (e.g., CO_2). Many other combinations of input and output states in conversion tasks exist.
- **Transfer tasks** represent tasks that can transfer a given state (of any type) from one zone to another. As Figure 3b depicts, the output state of the transfer task is the same with the input state; although the quantity may be different (e.g., due to losses). Once again, our definition of transfer tasks is very general. For instance, a transfer task using a proper transfer technology (e.g., railroad, ship, trucks) may transport an energy or material resource state (e.g., coal). We also consider that an energy form (e.g., electricity) could be transferred by a transfer task through a transfer technology (e.g., power grid). Our approach also allows the representation of transfer operations for undesired substances states. Depending on the nature, the type and other particular characteristics of the state different transfer technology options may exist. Notice that not all states (e.g., solar or wind energy) can be transferred.
- **Local exploitation tasks** represent tasks that can exploit locally available (in given capacity) energy or material resources states, referred to as raw materials states. These tasks are considered as imaginary transfer tasks and technologies as shown in Figure 3c. Local exploitation tasks may involve minerals or fossil fuel sources (e.g., extraction of coal or

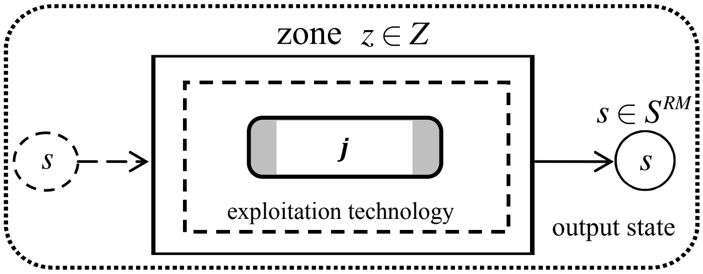
crude oil) or exploitation of available renewable energy sources (e.g., solar radiation, wind, etc.). Notice that transfer of available locally states from one zone to another could also take place through transfer tasks as long as the state is transferable.



(a) Conversion task.



(b) Transfer task.



(c) Local exploitation task.

Figure 3. E-STN representation: tasks.

2.3. Definition of types of technologies in energy supply chain operations

We consider the following main types of technologies: conversion, transfer, and local exploitation, as displayed in Figure 2.

- **Conversion technologies** could perform conversion tasks. The definition of conversion technologies may include energy generation technologies from combustion (power plants, combined heat and power), electrochemical (e.g., fuel cells) or nuclear (e.g., fusion or fission) conversion to biomass pretreatment units and technologies for energy generation from primary renewables (e.g., photovoltaics, wind turbines, etc.). Technologies that transform a set of states to another set of states are considered as conversion technologies. An example of such technologies is the reformer of a fuel cell system that extracts hydrogen (output state) from natural gas (input state). Technologies (e.g., scrubbers) used to capture undesired substances states are also considered as conversion technologies.
- **Transfer technologies** could perform transfer tasks. The definition of transfer technologies used here is very broad. For example, transfer technology could be any type of transportation modes (e.g., railroad, ship, road), pipelines networks (e.g., for natural gas or transfer of hot water or steam) and electrical grids.
- **Local exploitation technologies** could perform local exploitation tasks**.** For example, the local exploitation technology could be of any type of exploitation mode such as crude oil extraction, natural gas extraction, coal exploitation, wind energy exploitation through wind turbines, solar energy exploitation through photovoltaic panels, etc.

We also define storage technologies that could store any type of storable states (e.g., storage tanks to store energy material resources states, heat buffer tanks or batteries to store energy form states). Storage technologies are not displayed in the E-STN, since storage is not defined as a task.

3. Problem Statement

This study focuses on the modeling representation of material and energy supply chains under design, planning and economic constraints. The problem under study considers a geographical region that has a number of material and energy sources and is characterized by varied material and energy needs throughout a given long-term time horizon. The supply chains problem is formally defined in term of the following items:

- A given planning horizon divided into a number of equally-length time periods $t \in T$.

- A set of zones $z \in Z$ that is divided into internal zones ($z \in Z^{in}$) and external zones ($z \in Z^{ex}$).
- A set of energy forms and energy material resources states $s \in S$ that are classified by raw material states ($s \in S^{RM}$) with maximum amount of available raw material states $\omega_{(z,s,t)}$, product states ($s \in S^{FP}$) with known demand profiles $\zeta_{(z,s,t)}$, storable states ($s \in S^{B}$) with minimum $\beta^{\min}_{(z,s,t)}$ and maximum $\beta^{\max}_{(z,s,t)}$ inventory levels and disposable states ($s \in S^{D}_{z}$).
- A set of tasks $i \in I$ that could perform by a number of technologies $j \in J$ and can consume or produce states. These tasks are categorized to local exploitation tasks ($i \in I^{RM}_{s}$), input and output tasks ($i \in I^{-}_{s}$ and $i \in I^{+}_{s}$), and transfer tasks ($i \in I^{T}_{s}$).
- A number of technologies $j \in J$ that are categorized into local exploitation technology ($j \in J^{E}$), conversion technology ($j \in J^{C}$), transfer technology ($j \in J^{T}$) and, storage technology ($j \in J^{B}$). For each conversion, local exploitation and storage technology, the lower $\gamma^{\min}_{(z,j,t)}$ and upper $\gamma^{\max}_{(z,j,t)}$ bound of the capacity expansion are defined. Similarly, the lower $\gamma^{\mathrm{T,min}}_{(z,z',t)}$ and upper $\gamma^{\mathrm{T,max}}_{(z,z',t)}$ bound of the capacity expansion for transfer technology is also defined.
- For every conversion, local exploitation and transfer technology, the lower and upper bound of available capacity are given as $\alpha^{\min}_{(z,z,i,j,t)}$ and $\alpha^{\max}_{(z,z,i,j,t)}$, respectively.
- Given investment cost to establish the respective technology $\varepsilon^{0}_{(z,j,t)}$ and investment cost to expand the capacity of its technology $\varepsilon_{(z,j,t)}$.
- Given fixed operating cost $\delta_{(z,j,t)}$, raw materials cost $\psi^{E}_{(z,s,i,j,t)}$, production cost $\pi_{(z,s,i,j,t)}$, inventory cost $\lambda_{(z,s,t)}$, transfer cost $\varphi_{(z',z,s,i,j,t)}$ and disposable cost $\lambda^{D}_{(z,s,t)}$.

The additional considerations of the problem under study are the following: (i) the demands for products states should be fully satisfied; and (ii) the states can be disposed per time period especially the undesired substances states, the disposal of energy material resources and energy form states can be avoided by putting high values of disposable cost.

For every time period, the key decisions to be made by the optimization model are:

- the selection of technology for each task;

- the amount of capacity expansion and total installed capacity for each technology;
- the inventory level for storable states in its respective storage technology;
- the quantity of states converted or transferred through tasks that can be performed by its respective technology.

The objective is to minimize the cost of the energy supply chain design and planning that includes:

- fixed assets costs that include investment cost to establish and expand conversion, local exploitation and storage technologies;
- fixed transfer cost to establish and expand transfer technology;
- fixed operating cost on the total installed capacity of the conversion technologies;
- variable costs which include production, inventory and transfer cost; and
- disposable cost for the release of states to the environment (e.g., emissions cost).

4. Optimization Framework

In this section, a mixed integer programming model based on the proposed E-STN representation is presented for the design and planning problem of energy supply chains. The whole set of constraints of the proposed mathematical model is categorized into: (i) design constraints, (ii) design-planning linking constraints, (iii) planning constraints, (iv) economics equations, and (v) the objective function. The description of the proposed model follows.

4.1. Design Constraints

4.1.1. Establishment and capacity expansion for technologies.

In order to model the installation status of the energy supply chains operations, the following set of binary variables is introduced:

$$W_{(z,j,t)} = \begin{cases} 1 & \text{if conversion or local exploitation technology } j \text{ is established in zone } z \text{ in time period } t, \\ 0 & \text{otherwise.} \end{cases}$$

$$Y_{(z,j,t)} = \begin{cases} 1 & \text{if capacity of conversion or local exploitation technology } j \text{ begins installing in zone } z \text{ in time period } t, \\ 0 & \text{otherwise.} \end{cases}$$

$$W^{B}_{(z,s,j,t)} = \begin{cases} 1 & \text{if storage technology } j \text{ for state } s \text{ is established in zone } z \text{ in time period } t, \\ 0 & \text{otherwise.} \end{cases}$$

$$Y^B_{(z,s,j,t)} = \begin{cases} 1 \text{ if capacity of storage technology } j \text{ for state } s \text{ begins installing in zone } z \text{ in time period } t, \\ 0 \text{ otherwise.} \end{cases}$$

$$Y^T_{(z,z',j,t)} = \begin{cases} 1 \text{ if capacity of transfer technology } j \text{ begins installing in zone } z \text{ in time period } t, \\ 0 \text{ otherwise.} \end{cases}$$

Constraints (1) ensure that the establishment of each conversion or local exploitation ($j \in J^{CE}_z$) and storage technology ($j \in J^B_{(s,z)}$) could take place at most once in any internal zone ($z \in Z^{in}$) throughout the time horizon considered. The establishment of a technology represents first-time investment decisions often related to fundamental infrastructure construction. Constraints (2) and (3) link the binary variables that represent the establishment and the capacity expansion of technologies. A technology establishment could only take place if and only if a capacity expansion occurs at the same time period, as defined by constraints (2), and at the same time there has been no establishment in the previous time periods, as modeled by constraints (3).

$$\begin{aligned} &\sum_{t\in T} W_{(z,j,t)} \le 1 \quad \forall z \in Z^{in}, j \in J^{CE}_z \\ &\sum_{t\in T} W^B_{(z,s,j,t)} \le 1 \quad \forall z \in Z^{in}, s \in S, j \in J^B_{(s,z)} \end{aligned} \tag{1}$$

$$\begin{aligned} &W_{(z,j,t)} \le Y_{(z,j,t)} \qquad \forall z \in Z^{in}, j \in J^{CE}_z, t \in T \\ &W^B_{(z,s,j,t)} \le Y^B_{(z,s,j,t)} \quad \forall z \in Z^{in}, s \in S, j \in J^B_{(s,z)}, t \in T \end{aligned} \tag{2}$$

$$\begin{aligned} &W_{(z,j,t)} \ge Y_{(z,j,t)} - \sum_{t'<t} W_{(z,j,t')} \qquad \forall z \in Z^{in}, j \in J^{CE}_z, t \in T \\ &W^B_{(z,s,j,t)} \ge Y^B_{(z,s,j,t)} - \sum_{t'<t} W^B_{(z,s,j,t')} \quad \forall z \in Z^{in}, s \in S^B_z, j \in J^B_{(s,z)}, t \in T \end{aligned} \tag{3}$$

4.1.2. Total capacity installed and expansion for technologies.

For each zone and time period, the total installed capacity for each conversion or local exploitation technology ($F_{(z,j,t)}$), storage technology ($F^B_{(z,s,j,t)}$), and transfer technology ($F^T_{(z,z',j,t)}$) are modeled by the following set of constraints:

$$\begin{aligned} &F_{(z,j,t)} = \varphi_{(z,j)} + F_{(z,j,t-1)} + E_{(z,j,t)} \qquad \forall z \in Z^{in}, j \in J^{CE}_z, t \in T : t = 1 \\ &F_{(z,j,t)} = F_{(z,j,t-1)} + E_{(z,j,t)} \qquad \forall z \in Z^{in}, j \in J^{CE}_z, t \in T : t > 1 \end{aligned} \tag{4}$$

$$\begin{aligned} &F^{B}_{(z,s,j,t)} = \varphi^{B}_{(z,s,j)} + F^{B}_{(z,s,j,t-1)} + E^{B}_{(z,s,j,t)} && \forall z \in Z^{in}, s \in S^{B}_{z}, j \in J^{B}_{(s,z)}, t \in T : t = 1 \\ &F^{B}_{(z,s,j,t)} = F^{B}_{(z,s,j,t-1)} + E^{B}_{(z,s,j,t)} && \forall z \in Z^{in}, s \in S^{B}_{z}, j \in J^{B}_{(s,z)}, t \in T : t > 1 \end{aligned} \tag{5}$$

$$\begin{aligned} &F^{T}_{(z,z',j,t)} = \varphi^{T}_{(z,z',j)} + E^{T}_{(z,z',j,t)} && \forall z \in Z^{in}, z' \in Z^{T}_{z'}, j \in J^{T}_{(z,z')}, t \in T : t = 1 \\ &F^{T}_{(z,z',j,t)} = F^{T}_{(z,z',j,t-1)} + E^{T}_{(z,z',j,t)} && \forall z \in Z^{in}, z' \in Z^{T}_{z'}, j \in J^{T}_{(z,z')}, t \in T : t > 1 \end{aligned} \tag{6}$$

Parameters $\varphi_{(z,j)}$, $\varphi^{B}_{(z,s,j)}$ and $\varphi^{T}_{(z,z',j)}$ stand for the initial installed capacity of each technology per zone.

For each technology and zone, variables $E_{(z,j,t)}$, $E^{B}_{(z,s,j,t)}$ and $E^{T}_{(z,z',j,t)}$ represent the corresponding capacity expansion taking place per time period, as defined by:

$$\begin{aligned} &\gamma^{\min}_{(z,j,t)} Y_{(z,j,t-\mu_{(z,j,t)})} \le E_{(z,j,t)} \le \gamma^{\max}_{(z,j,t)} Y_{(z,j,t-\mu_{(z,j,t)})} && \forall z \in Z^{in}, j \in J^{CE}_{z}, t \in T \\ &\gamma^{\min}_{(z,j,t)} Y^{B}_{(z,s,j,t-\mu_{(z,j,t)})} \le E^{B}_{(z,s,j,t)} \le \gamma^{\max}_{(z,j,t)} Y^{B}_{(z,s,j,t-\mu_{(z,j,t)})} && \forall z \in Z^{in}, s \in S^{B}_{z}, j \in J^{B}_{(s,z)}, t \in T \end{aligned} \tag{7}$$

$$\gamma^{\mathrm{T,min}}_{(z,z',t)} Y^{T}_{(z,z',j,t-\mu^{T}_{(z,z',j,t)})} \le E^{T}_{(z,z',j,t)} \le \gamma^{\mathrm{T,max}}_{(z,z',t)} Y^{T}_{(z,z',j,t-\mu^{T}_{(z,z',j,t)})} \qquad \forall z \in Z^{in}, z' \in Z^{T}_{z'}, j \in J^{T}_{(z,z')}, t \in T \tag{8}$$

The γ parameters provide lower and upper bounds to the capacity expansion for each technology while parameters $\mu_{(z,j,t)}$ (or $\mu^{T}_{(z,z',j,t)}$) represent the necessary installation duration after which a technology capacity expansion becomes available.

4.2. Linking Constraints for Design and Planning

For each zone and time period, design and planning decisions are connected by the following set of constraints that provide lower and upper bounds on the operational level ($P_{(z,z',i,j,t)}$) of each conversion, local exploitation and transfer technology through the total installed capacity of the corresponding technology:

$$\alpha^{\min}_{(z,z,i,j,t)} F_{(z,j,t)} \le P_{(z,z,i,j,t)} \le \alpha^{\max}_{(z,z,i,j,t)} F_{(z,j,t)} \qquad \forall z \in Z^{in}, s \in S_{z}, i \in I^{+}_{s}, j \in (J^{CE}_{z} \cap J_{i}), t \in T \tag{9}$$

$$\begin{aligned} &\alpha^{\min}_{(z,z',i,j,t)} F^{T}_{(z,z',j,t)} \le P_{(z,z',i,j,t)} \le \alpha^{\max}_{(z,z',i,j,t)} F^{T}_{(z,z',j,t)} \\ &\qquad\qquad \forall z \in Z, z' \in Z^{T}_{z'}, s \in S_{z}, i \in I^{T}_{s}, j \in (J^{T}_{(z,z')} \cap J_{i}), t \in T \end{aligned} \tag{10}$$

Parameters $\alpha^{\min}_{(z,z',i,j,t)}$ and $\alpha^{\max}_{(z,z',i,j,t)}$ are expressed as percentages and represent minimum and maximum availability factors of the total installed capacity of each technology, respectively.

For each zone and time period, bounds on the storage level ($B_{(z,s,t)}$) for each storable state are also imposed through the total installed capacity of the corresponding storage technology, as given by:

$$\beta^{\min}_{(z,s,t)} \sum_{j \in j \in J^{B}_{(s,z)}} F^{B}_{(z,j,t)} \le B_{(z,s,t)} \le \beta^{\max}_{(z,s,t)} \sum_{j \in j \in J^{B}_{(s,z)}} F^{B}_{(z,j,t)} \qquad \forall z \in Z^{in}, s \in S^{B}_{z}, t \in T \tag{11}$$

Parameters $\beta^{\min}_{(z,s,t)}$ and $\beta^{\max}_{(z,s,t)}$ are expressed as percentages and represent safety inventory levels and maximum availability of storage capacity, respectively.

4.3. Planning Constraints

4.3.1. Raw materials states availability.

In this study, we define 'raw materials' states $s \in S^{RM}_{z}$, which correspond to principal input states (any type of states), categorized into renewables and non-renewables ($s \in S^{NR}$). For each renewable state per zone and time period, the amount of the renewable state consumed by tasks $i \in I^{RM}_{s}$ through local exploitation technologies $j \in J^{E}_{z}$ plus the amount of the renewable state transferred to other zones cannot exceed the maximum available amount of this state $\omega_{(z,s,t)}$, according to:

$$\sum_{i \in I^{RM}_{s}} \sum_{j \in (J^{E}_{z} \cap J_{i})} P_{(z,z,i,j,t)} + \sum_{i \in I^{T}_{s}} \sum_{j \in (J^{T}_{(z,z')} \cap J_{i})} \sum_{z' \in Z^{T}_{z'}} P_{(z,z',i,j,t)} \le \omega_{(z,s,t)} \qquad \forall z \in Z, s \in S^{RM}_{z} : s \notin S^{NR}, t \in T \tag{12}$$

For each zone, the total availability for each non-renewable raw material state ($\omega^{NR}_{(z,s)}$) throughout the whole time horizon is constrained by:

$$\sum_{t \in T} \sum_{i \in I^{RM}_{s}} \sum_{j \in (J^{E}_{z} \cap J_{i})} \sum_{t \in T} P_{(z,z,i,j,t)} \le \omega^{NR}_{(z,s)} \qquad \forall z \in Z^{in}, s \in (S^{RM}_{z} \cap S^{NR}) \tag{13}$$

4.3.2. States connection and balance.

Constraints (14) express the states connection and balance in each zone at the end of each time period. According to these constraints, the inventory level of storable states $s \in S^{B}_{z}$ at the end of each time period per zone depend on: (i) the inventory at the end of the previous time period $B_{(z,s,t-1)}$ considering some losses $\eta_{(z,s,t)}$, (ii) the given demand, if any, (iii) the lost sales, (iv) the disposed amount, (v) the amount produced from local exploitation tasks (if the state is a raw material state), (vi) the inlet or outlet transferred amount, and (vii) the amount produced by task $i \in I_s^+$ or consumed by task. For any state that cannot be stored ($s \notin S_z^B$), the state balance considers only: (i) the given demand, if any, (ii) the lost sales, (iii) the disposed amount, (iv) the amount produced from local exploitation tasks (if the state is a raw material state), (v) the inlet or outlet transferred amount, and (vi) the amount produced by task $i \in I_s^+$ or consumed by $i \in I_s^-$.

$$\begin{aligned}
B_{(z,s,t)} = {} & (1-\eta_{(z,s,t)})B_{(z,s,t-1)} - \zeta_{(z,s,t)} + L_{(z,s,t)} - D_{(z,s,t)} + \overbrace{\sum_{i\in I_s^{RM}} \sum_{j\in(J_z^E \cap J_i)} P_{(z,z,i,j,t)}}^{\text{production: local exploitation tasks}} \\
& + \overbrace{\sum_{z'\in Z_{z'}^T} \sum_{i\in I_s^T} \sum_{j\in(J_{(z',z)}^T \cap J_i)} \kappa_{(s,i,j)}^+ P_{(z',z,i,j,t)}}^{\text{inlet flow from transfer tasks}} - \overbrace{\sum_{z'\in Z_{z'}^T} \sum_{i\in I_s^T} \sum_{j\in(J_{(z,z')}^T \cap J_i)} \kappa_{(s,i,j)}^- P_{(z,z',i,j,t)}}^{\text{outlet flow from transfer tasks}} \\
& + \overbrace{\sum_{i\in I_s^+} \sum_{j\in(J_z^C \cap J_i)} \kappa_{(s,i,j)}^+ P_{(z,z,i,j,t)}}^{\text{production from conversion tasks}} - \overbrace{\sum_{i\in I_s^-} \sum_{j\in(J_z^C \cap J_i)} \kappa_{(s,i,j)}^- P_{(z,z,i,j,t)}}^{\text{consumption from conversion tasks}} \quad \forall z \in Z, s \in S_z, t \in T \qquad (14)
\end{aligned}$$

$$\begin{aligned}
& B_{(z,s,t=0)} = \beta_{(z,s)}^0 && \forall z \in Z, s \in S_z^B \\
& B_{(z,s,t)} = 0 && \forall z \in Z, s \notin S_z^B, t \in T \\
& D_{(z,s,t)} = 0 && \forall z \in Z, s \notin S_z^D, t \in T
\end{aligned}$$

Parameters $\beta_{(z,s)}^0$ correspond to the initial inventory of each storable states $s \in S_z^B$. Losses coefficients are set to zero for all storable states in the first time period. Parameters $\kappa_{(s,i,j)}^{+/-}$ represent coefficients related to conversion and transfer tasks. Inventory levels of non-storable states and disposal levels for non-disposable states are set to zero.

4.4. Economics Equations

In this part, the major cost equations for the design and planning problem of a general energy supply chain are presented.

Fixed assets costs for conversion, local exploitation and storage technologies: correspond to the investment required for establishing and expanding the technologies, as given by:

$$FA_t = \sum_{z \in Z^{in}} \sum_{j \in J_z^{CE}} (\varepsilon^0_{(z,j,t)} W_{(z,j,t)} + \varepsilon_{(z,j,t)} E_{(z,j,t)}) + \sum_{z \in Z^{in}} \sum_{s \in S^B} \sum_{j \in J^B_{(s,z)}} (\varepsilon^0_{(z,j,t)} W^B_{(z,s,j,t)} + \varepsilon_{(z,j,t)} E^B_{(z,s,j,t)}) \quad \forall t \in T \qquad (15)$$

Fixed assets costs for transfer technologies: correspond to the total investment for creating a transfer network between two zones and is associated with the fixed investment required to install a transfer technology and the investment required (per unit) for increasing the capacity of transfer technology:

$$FA^{TS}_t = \sum_{z \in Z^{in}} \sum_{z' \in Z^T_{z'}} \sum_{j \in J^T_{(z',z)}} (\varepsilon^{T0}_{(z,z' j,t)} Y^T_{(z,z',j,t)} + \varepsilon^T_{(z,z',j,t)} E^T_{(z,z',j,t)}) \quad \forall t \in T \qquad (16)$$

Fixed operating costs: are considered to be proportional to the total capacity of all conversion and local exploitation technologies installed, according to:

$$FOC_t = \sum_{z \in Z^{in}} \sum_{j \in J_z^{CE}} \delta_{(z,j,t)} F_{(z,j,t)} \quad \forall t \in T \qquad (17)$$

Variable costs: consist of costs related to raw materials, production, inventory, transfer, disposal and lost sales costs:

$$VOC_t = RC_t + PC_t + IC_t + TC_t + DC_t + LS_t \quad \forall t \in T \qquad (18)$$

The raw materials cost consists of the cost required for the consumption of raw material states by tasks through local exploitation technologies:

$$RC_t = \sum_{z \in Z^{in}} \sum_{s \in S_z^{RM}} \sum_{i \in I_s^{RM}} \sum_{j \in (J_z^E \cap J_s \cap J_i)} \psi_{(z,s,i,j,t)} P_{(z,z,i,j,t)} \quad \forall t \in T \qquad (19)$$

The production cost is associated to the cost needed for producing states through local exploitation or conversion technologies:

$$PC_t = \sum_{z \in Z^{in}} \sum_{s \in S_z} \sum_{i \in I_s^+} \sum_{j \in (J_z^{CE} \cap J_i)} \pi_{(z,s,i,j,t)} P_{(z,z,i,j,t)} \quad \forall t \in T \qquad (20)$$

The inventory cost for storable states is given by:

$$IC_t = \sum_{z \in Z^{in}} \sum_{s \in S_z^B} \lambda_{(z,s,t)} B_{(z,s,t)} \quad \forall t \in T \qquad (21)$$

The transfer cost includes the transfer cost of any state (including states with demands or not as well as raw material states) that could be transferred between any pair of zones:

$$TC_t = \sum_{z' \in Z} \sum_{z \in Z_{z'}^T} \sum_{s \in (S_z \cap S_{z'})} \sum_{i \in I_s^T} \sum_{j \in (J_{(z',z)}^T \cap J_i)} \vartheta_{(z',z,s,i,j,t)} P_{(z',z,i,j,t)} \qquad \forall t \in T \tag{22}$$

The disposal cost represents the corresponding cost for disposing the disposable states $s \in S_z^D$ to the environment (e.g., carbon tax or other emissions related costs) or other destinations:

$$DC_t = \sum_{z \in Z^{in}} \sum_{s \in S_z^D} \lambda_{(z,s,t)}^D D_{(z,s,t)} \quad \forall t \in T \tag{23}$$

Lost sales represents the associated costs for the unsatisfied demand of demand-states $s \in S_z^{FP}$:

$$LS_t = \sum_{z \in Z^{in}} \sum_{s \in S_z^{FP}} \lambda_{(z,s,t)}^L L_{(z,s,t)} \quad \forall t \in T \tag{24}$$

4.5. Objective Function

The optimization goal is the minimization of the total cost that involves fixed assets costs for technologies, and fixed and variable operating costs, as defined in the previous subsections:

$$min \sum_{t \in T} (FA_t + FA_t^{TS} + FOC_t + VOC_t) \tag{25}$$

4.6. Remarks

Note that the proposed mathematical model can readily address other objective functions, such as the net present value, or multi-objective optimization problems through the use of relevant methods (e.g., ε-constraint method). It should be also mentioned that the definition of zones and the duration of each time period is problem specific and depends on the associated decision maker. For instance, in the national power grid case, the power system is divided in zones according to the division of the transmission lines network and major producers and consumers. This is usually a geographical division, but it could be done following other criteria as well. Regarding the length of the time periods, in the design problem it is common to consider yearly periods, since these problems correspond to major strategic decisions. The total time horizon for design problems usually varies for 15 to 30 years. For planning problems, the length of the time periods can be months, weeks or even days. The same applies to the total time horizon for planning problems.

5. Case Studies

In this section, three cases for the design and planning problem of a mixed material-based and energy supply chain network are presented in order to highlight the special features of the proposed optimization framework. More specifically, the first case introduces the baseline energy supply chain design problem. The effect on the design of the energy supply chain network by increasing the emissions costs and by imposing bounds on the generated emissions levels are studied in the second and third case, respectively. In the last part of this section, to highlight the some types of analyses that the proposed approach could be used, we presented a sensitivity analysis study with respect to alternative emissions caps and a multi-objective optimization example considering the conflicting objectives of total cost and emissions. All problem instances have been solved by the proposed optimization framework in GAMS/CPLEX 12 in an Intel(R) core i7 under standard configurations and a zero optimality gap. All solutions have been found in negligible computatonal times.

5.1. Case A: Design and Planning of an Energy Supply Chain Network

5.1.1. Description of Case A

The system under consideration consists of nine states ($s1$ - $s9$), among of which three states ($s1,s3,s4$) are raw material states, two states ($s5,s9$) are energy form states, three states ($s2,s6,s8$) are energy material resources states and one state ($s7$) is an undesired substance state. The energy material resources states can be stored in their respective storage tanks or can be disposed. The energy form states cannot be stored but they could be disposed to the environment. There are a total of eight tasks ($i1$ - $i8$) in the network representation. The network consists of three conversion tasks ($i2,i4,i5$), two transfer tasks ($i3,i6$) and three local exploitation tasks ($i1,i7,i8$). For each task, there are associated technologies ($j1$ - $j11$) are shown in Figure 4. There are also storage technologies for each storable state ($js1$ - $js8$).

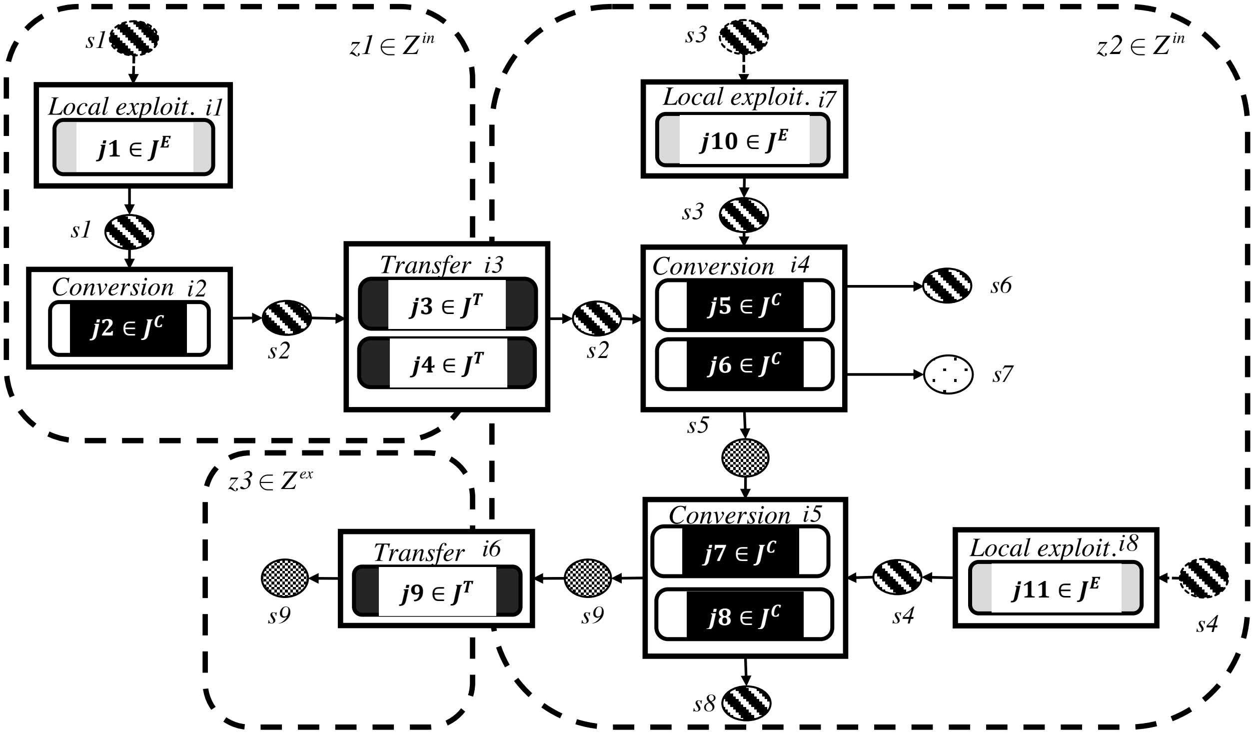


Figure 4. E-STN representation for the energy supply chain network considered.

According to Figure 4, the raw material state $s1$ is converted into energy material resource state $s2$ by conversion task $i2$ that can be performed by conversion technology $j2$. The energy material resource state $s2$ is transferred through transfer task $i3$ which includes two transfer technology $j3$ and $j4$. Then, energy material resource state $s2$ reacts with raw material state $s3$ in conversion task $i4$ that can be performed by conversion technologies $j5$ and $j6$ to produce energy material state $s6$, energy form state $s5$ and undesired substances states $s7$. This type of conversion task can be a typical steam methane reforming plant, in which methane reacts with water to produce hydrogen, heat and carbon dioxide. Meanwhile, in conversion task $i5$ that could be performed by two conversion technologies $j7$ and $j8$, utilizes the energy form state $s5$ and reacts with raw material state $s4$ to produce energy material resource state $s8$ and energy form state $s9$. The energy form state $s9$ in zone 2 can be sold and transferred to the external energy network (e.g., zone 3) through transfer task $i6$. The available storage technology per state and zone is displayed in Table 1.

Table 1. Available storage technologies per state and zone

Storable States	$z1$	$z2$

s1	*js1*	-
s2	*js2*	*js2*
s3	-	*js3*
s4	-	*js4*
s6	-	*js6*
s8	-	*js8*

The minimum ($\alpha^{min}_{(z,z',s,i,j,t)}$) and maximum ($\alpha^{max}_{(z,z',s,i,j,t)}$) availability percentage of output states from task $i \in I_s^+$ is equal to 0 and 1, respectively. For the states that can be stored, the minimum inventory level ($\beta^{min}_{(z,s,t)}$) is equal to 0.5 and maximum inventory level ($\beta^{max}_{(z,s,t)}$) is equal to 1. The coefficients for the input states of task $i \in I_s^-$ and output states of task $i \in I_s^+$ that can be performed by technology *j* are given in Table 2 and Table 3, respectively.

Table 2. Coefficients $\kappa^-_{(s,i,j)}$ for input states for tasks $i \in I_s^-$ that can be performed by technologies j .

State	Task	*j2*	*j3*	*j4*	*j5*	*j6*	*j7*	*j8*	*j9*
s1	*i2*	1	-	-	-	-	-	-	-
s2	*i3*	-	1	1	-	-	-	-	-
s2	*i4*	-	-	-	0.5	0.5	-	-	-
s3	*i4*	-	-	-	0.5	0.5	-	-	-
s4	*i5*	-	-	-	-	-	1	1	-
s5	*i5*	-	-	-	-	-	1.5	1.5	-
s9	*i6*	-	-	-	-	-	-	-	1

Table 3. Coefficients $\kappa^+_{(s,i,j)}$ for output states for tasks $i \in I_s^+$ that can be performed by technologies j .

State	Task	*j2*	*j3*	*j4*	*j5*	*j6*	*j7*	*j8*	*j9*

s2	*i2*	1	-	-	-	-	-	-	-
s2	*i3*	-	1	1	-	-	-	-	-
s5	*i4*	-	-	-	1	1	-	-	-
s6	*i4*	-	-	-	1	1	-	-	-
s7	*i4*	-	-	-	5	10	-	-	-
s8	*i5*	-	-	-	-	-	1	1	-
s9	*i5*	-	-	-	-	-	1	1	-
s9	*i6*	-	-	-	-	-	-	-	1

The necessary installation time ( ) for conversion and local exploitation technology is equal to one period while for storage technologies is considered zero.

Table 4 provides the investment cost, fixed operating cost and production cost with minimum and maximum capacity installed per technology. As the number of time period increases, the investment cost to establish the technology $\varepsilon^{0}_{(z,j,t)}$ increases by a factor of 1.01 to 1.5 from the cost of the previous time period. The investment cost to establish storage technology is 1,000 (m.u./unit) and increases by a factor of 1.005 from the cost of the previous time period. The investment cost to establish local exploitation technology increases over time period by this expression: $1,000(1.02t)$. The investment cost $\varepsilon_{(z,j,t)}$ for increasing the capacity of a technology varies within a certain range. In addition, the initial inventory cost $\lambda_{(z,s,t)}$ for all states $s \in S^B$ is 0.1 m.u./unit and increases by a factor of 1.05 from the cost of the previous time period. The initial emissions cost $\lambda^{D}_{(z,s,t)}$ for undesired substances state $s7$ is 18 m.u./unit, and increases over time by this expression: $1+0.05\ \lambda^{D}_{(z,s,t-1)}$. The initial disposable costs $\lambda^{D}_{(z,s,t)}$ for other states are very high at about 500 m.u./unit and increases by a factor of 1.1 from the costs of the previous time period. The disposable costs for other states are fixed to high values to avoid energy material resources or energy form states to be disposed to the environment. The necessary installation time ($\mu_{(z,j,t)}$) for conversion and local exploitation technology is equal to one period while for storage technologies is considered zero.

Table 4. Investment cost, fixed operating cost and production cost with minimum and maximum capacity installed per technology.

Technology	γ^{min}	γ^{max}	$\varepsilon^{0}_{(z,j,t)}$ (m.u./unit)	$\varepsilon_{(z,j,t)}$ (m.u./unit)	$\delta_{(z,j,t)}$ (m.u./unit)	$\pi_{(z,s,i,j,t)}$ (m.u./unit)
j1	50	50	(1,326-1,820)	(1,122-1,540)	-	-
j2	5	50	20,000	(1,300-2,000)	15	12
j5	10	40	28,000	(3,800-4,200)	20	20
j6	10	40	25,000	(2,500-3,200)	40	25
j7	5	30	20,000	(1,900-2,200)	30	30
j8	5	30	26,000	(1,800-2,200)	25	40
j10	50	50	(1,326-1,820)	(1,122-1,540)	-	-
j11	50	50	(1,326-1,820)	(1,122-1,540)	-	-
j3	0	30	2,000	(1,000-1,300)	0	0
j4	0	30	2,000	(1,000-1,300)	0	0
j9	0	50	2,000	(800-1,000)	0	0

A total planning horizon of 20 time periods is considered. It is assumed that the energy supply chain network did not exist before the beginning of the planning horizon of interest, therefore there is no initial state (i.e., $f^{0}_{(z,j)}, f^{B0}_{(z,s,j)}, f^{T0}_{(z,z',j)}$) that is taken into account for this case study. Figure 5 displays the normalized demand profiles for states ($s \in S^{FP}$) per zone by having as a reference the highest demand observed for each state throughout the planning horizon.

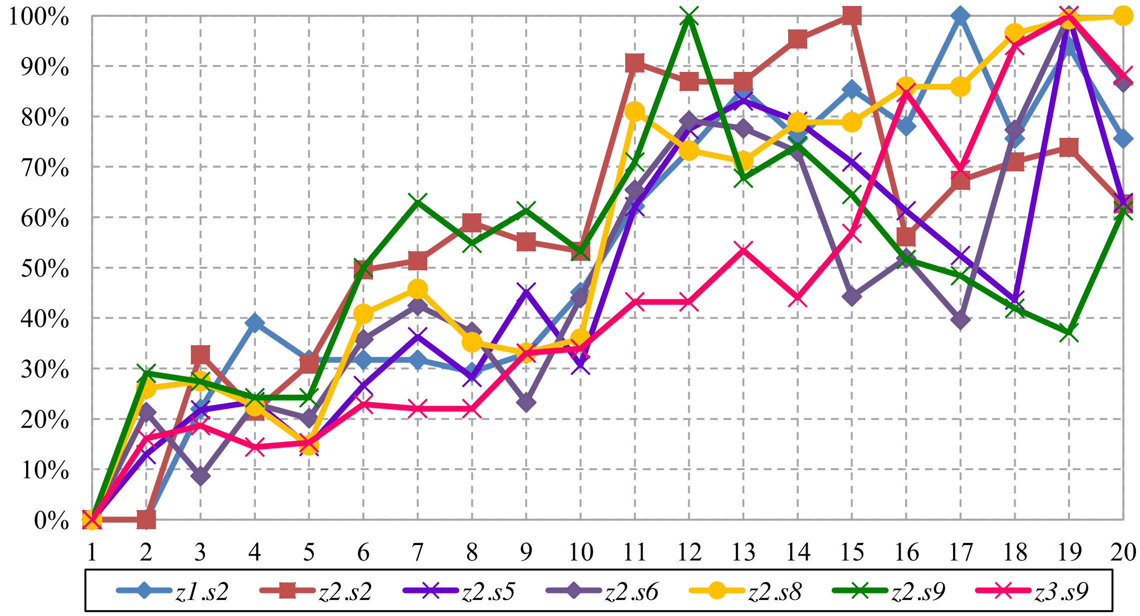


Figure 5. Demand profiles for states $s \in S^{FP}$ for all case studies.

5.1.2. Results of Case A

Figure 6 displays the optimal capacity expansion planning for conversion ($j3, j4, j9$), local exploitation ($j1, j10, j11$), transfer ($j3, j4, j9$) and storage technologies ($js2, js6, js8$) for the planning horizon of interest (i.e., binary variables Y, Y^T, Y^B). All local exploitation, conversion and transfer technologies are established in the first time period because there was no initial installed capacity for any of the technologies, there are demands for states from the second time period and on, and the establishment costs for these technologies are lower in the first time periods. Since in this example, we consider a construction time for these technologies equal to one time period, most storage technologies are established in next time periods when production of storable states could occur. For instance, storage technology $js2$ in $z1$ is first established in the third time period while storage technologies $js2$, $js6$ and $js8$ in $z2$ are established in the second, third and fifth time period (see Figure 6).

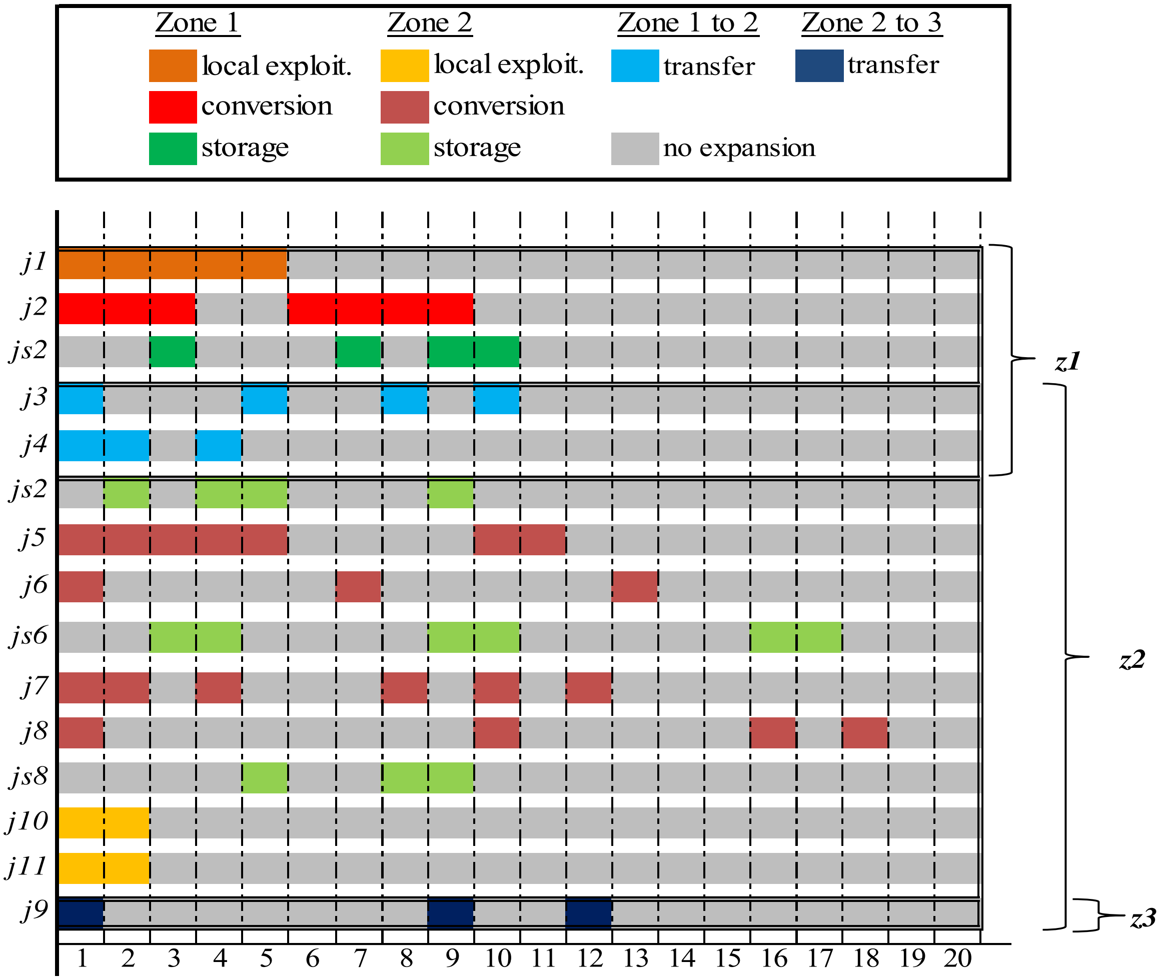


Figure 6. Case A: Capacity expansion planning per technology, zone and time period.

The capacity expansion for each technology usually takes place in early time period (from time period 1 to time period 16) because the investment costs to establish the technology ($\varepsilon^{0}_{(z,j,t)}$) and investment cost to increase the capacity of technology ($\varepsilon_{(z,j,t)}$) are generally cheaper in earlier time periods than in the later time periods (time period 17 onwards). For example, the latest time period to establish transfer technologies are not more than 16 time period (e.g., $j9$ is established by the latest time period 12) because the investment cost to increase the capacity of its transfer technology ($\varepsilon_{(z,j,t)}$) starts to increase in time period 17. Similarly, the capacity expansion of conversion technologies also occurs in early time periods. Observe that there is a capacity expansion for conversion technology $j8$ in later time periods (e.g., time period 16 and 18) in order to meet higher demand for state $s8$ in the following time periods 17 to 20 (see Figure 5).

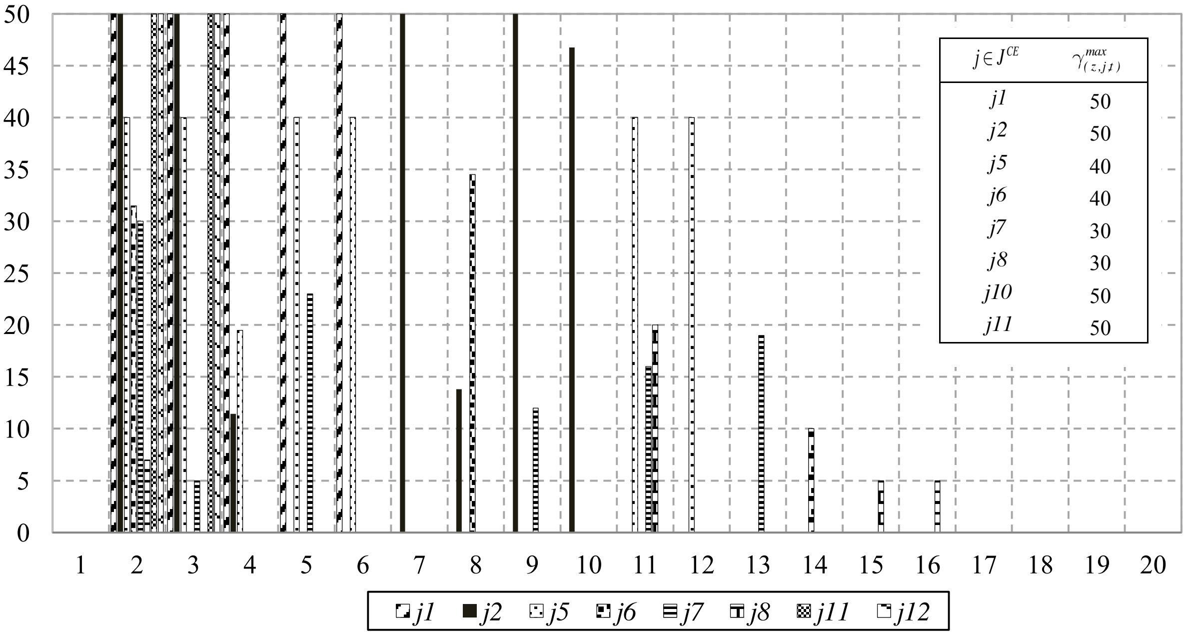


Figure 7. Case A: Capacity expansion for local exploitation and conversion technologies per time period.

Figure 7 shows the capacity expansion levels for local exploitation and conversion technologies per time period of planning horizon. Recall that the installation time to construct each conversion technology is one time period. For example, local exploitation technologies $j1, j10, j11$ and conversion technologies $j2, j5, j6, j7, j8$ are established in time period 1 (refer Figure 6). These capacity expansions are available in the next time period (e.g., time period 2). The higher capacity expansion for technologies is observed in time period 2 for $j1, j2, j5, j7, j10$ and $j11$ due to cheaper investment costs to establish the local exploitation and conversion technology ($\varepsilon^{0}_{(z,j,t)}$) in early time period in comparison to the later time period. The investment cost to increase the capacity of established technologies ($\varepsilon_{(z,j,t)}$) also varies over time.

The capacity expansion of conversion technology $j5$ is more preferable than that of conversion technology $j6$ for conversion task $i4$, which is in time period 3 to 6, 11 and 12. This is because the emissions cost for conversion technology $j5$ is lower than that of conversion technology $j6$. The reason is that, the coefficients of undesired substances state $s7$ for output task $i4$ that can perform conversion technology $j5$ have half the values of the coefficients of undesired substances state $s7$ for conversion technology $j6$ (refer to Table 3). In addition, the capacity expansion investment cost for conversion technology $j5$ is lower in these time periods. There is capacity expansion of conversion technology $j6$ in time periods 8 and 14, because there is moderate production of undesired substances state $s7$ in these time periods and the capacity expansion investment cost of conversion technology $j6$ is lower than that of conversion technology $j5$. In addition, there is a higher installed capacity for conversion technology $j7$ than that of $j8$ for performing conversion task $i5$, because of the lower investment costs of conversion technology $j7$ in comparison to those of $j8$.

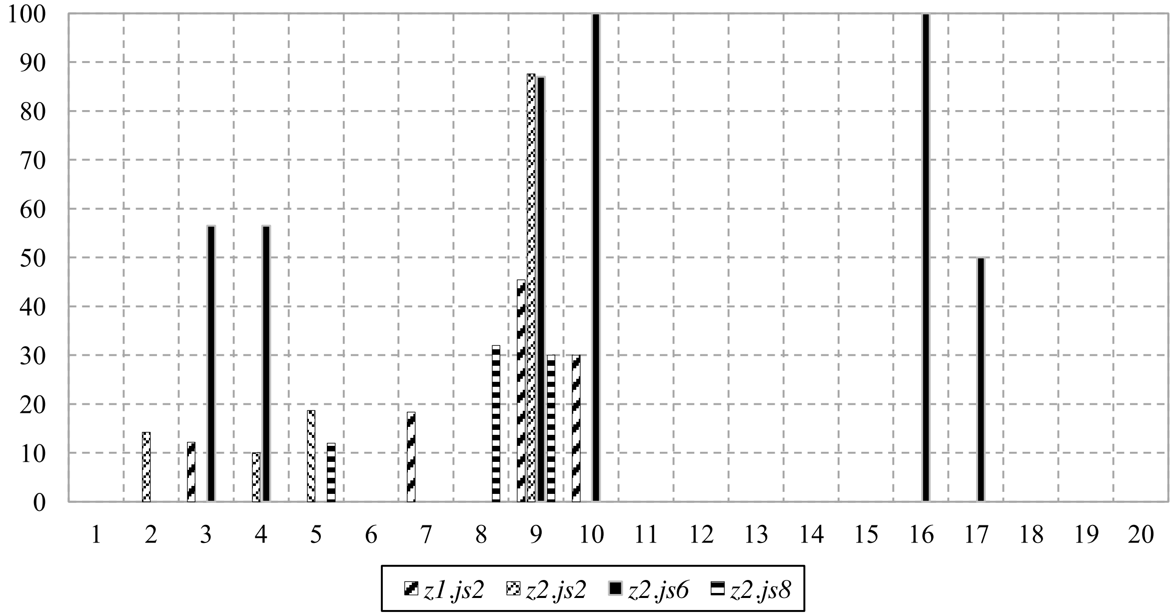


Figure 8. Case A: Capacity expansion for storage technologies $j \in J^B$ per zone and time period.

Figure 8 displays the capacity expansion profiles for storage technologies for the whole planning horizon. The expansion capacity for storage technology is assumed to be available at the same time period the storage technology is installed (see Figure 6 and Figure 8). There highest capacity expansion of storage technology $js6$ is observed in time period 10 and 16, because of the high demand for state $s6$ in the following time periods (refer to Figure 5).

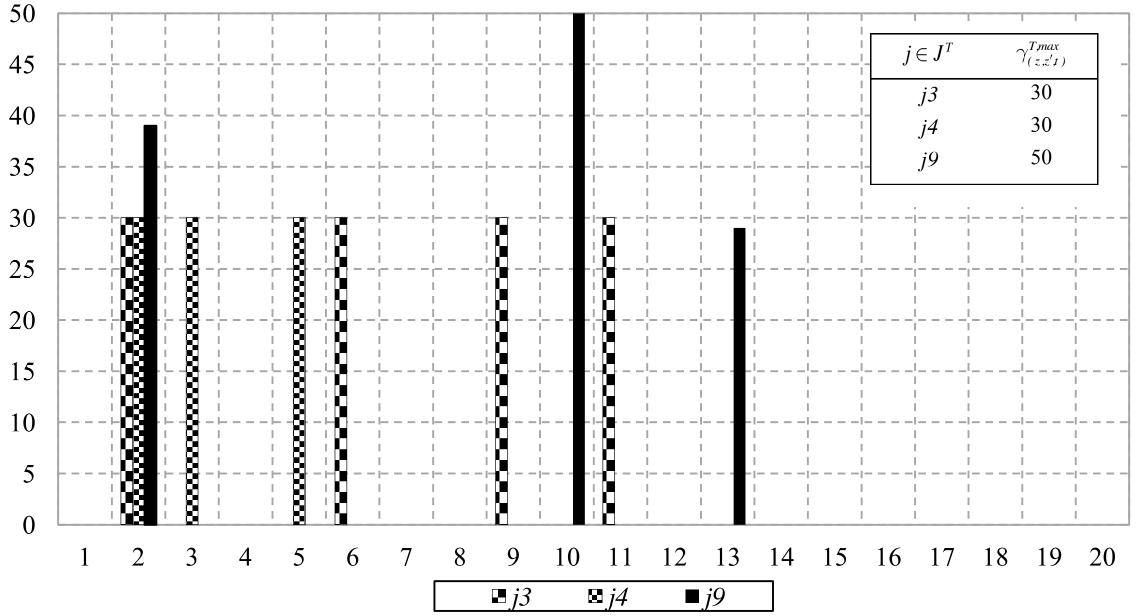


Figure 9. Case A: Capacity expansion for transfer technologies $j \in J^T$ per time period.

Figure 9 shows the capacity expansion for transfer technologies for the whole planning horizon. The installation time to construct each transfer technology is 1 time period. Similarly to local exploitation and conversion technologies, the expanded capacity for transfer technologies is available after one time period of the beginning of their installation (see Figure 6 and Figure 9). The highest capacity expansion for transfer technologies $j3$ and $j4$ to perform transfer task $i3$ are observed in time period 2 because the investment cost to establish and to increase the capacity of transfer technology in early time periods is lower than that of the later time periods. The expansion capacity for transfer technology $j9$ in time period 2 is 39 units. The quantity of state $s9$ that is transferred through transfer technology $j9$ from time period 2 until time period 9 must be less than or equal to 39. In time period 10, the expansion of transfer technology $j9$ is needed to increase the transferred quantity of state $s9$ to zone 3 from time period 10 to 12. In this case, the capacity of transfer technology $j9$ increases to 89 units in time period 10. Then, there is another capacity expansion in time period 13 to further increase the transferred quantity of state $s9$ to zone 3 from time period 13 and onwards.

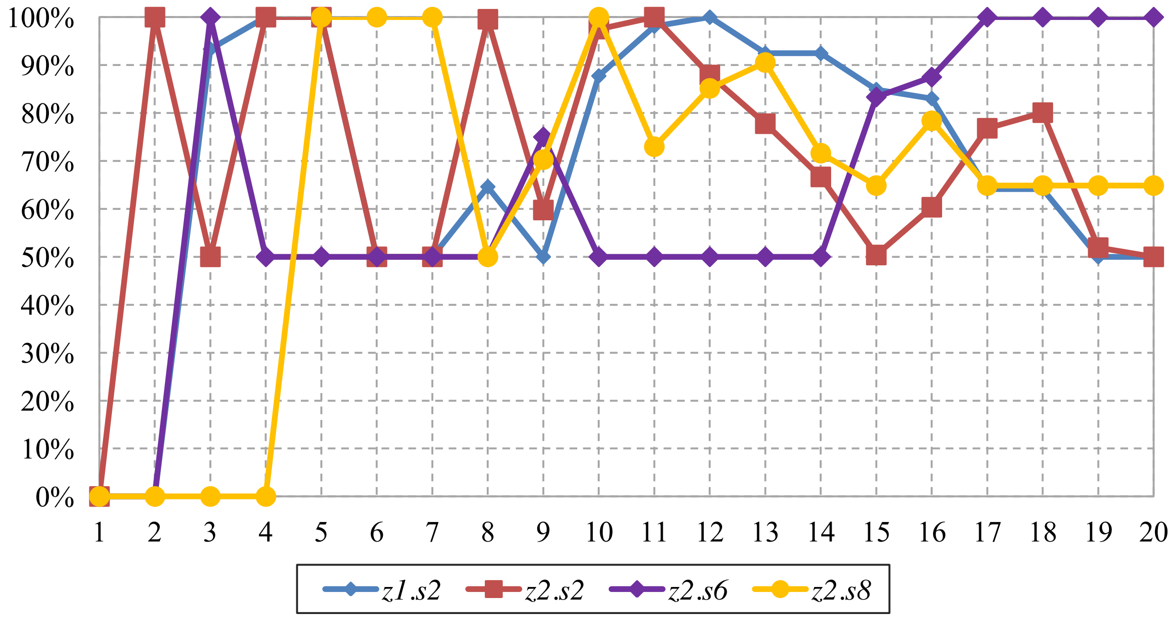


Figure 10. Case A: Inventory profiles for states $s \in S^B$ per zone and time period.

Figure 10 shows the normalized inventory profiles for storable states. The reference values are the total installed capacity of storage technology that can store its respective states per time period. It is expected to observe that lower inventory levels occur in time periods with high demands for states. For example, a low inventory level for $s2$ in $z2$ is observed in time period 15 because there is a very high demand for $s2$ in $z2$ in this time period (see Figure 5).

The inventory level of state $s6$ from time period 17 to 20 reaches its maximum because of: (i) the expansion of storage technology $js6$ in time period 16 and 17 (see Figure 8), (ii) the relatively low demand for state $s6$ in time period 17, and (iii) the high demand for state $s8$ in the last periods of the planning horizon. Although the demand for state $s6$ increases from period 18 to 20, the inventory level is still at the maximum because the amount of state $s6$ that is produced from task $i4$ satisfies directly its demand. Finally, notice that there is no inventory level for state $s8$ from time period 1 until 4 because the storage technology for $s8$ (i.e., $js8$) has not been established yet in these periods (see Figure 6).

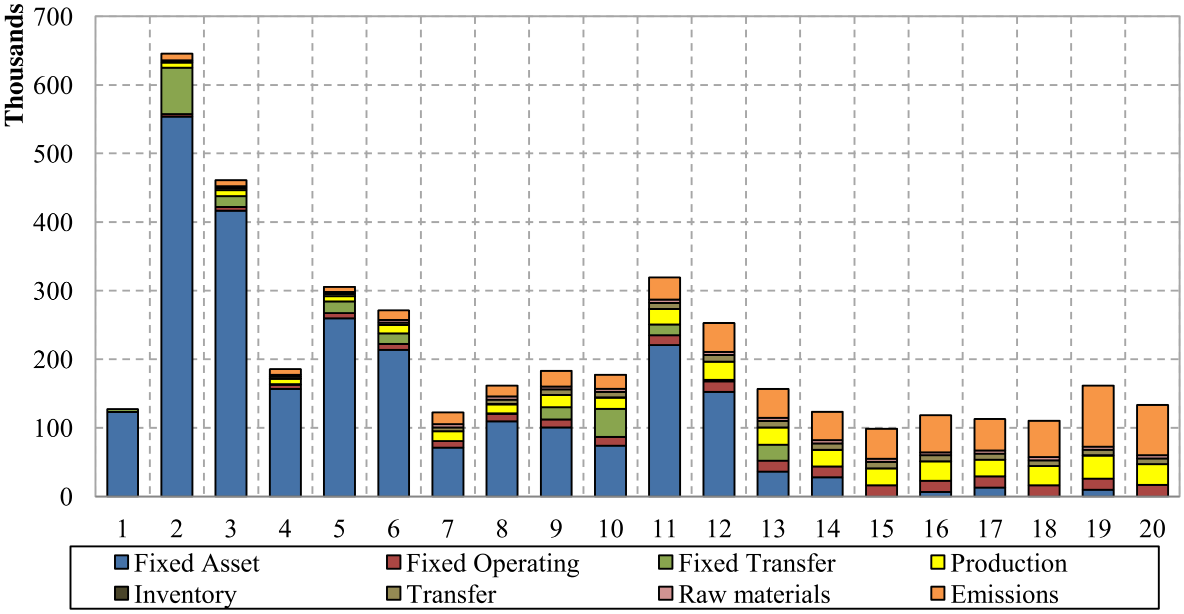


Figure 11. Case A: Cost term breakdown throughout the planning horizon.

Figure 11 shows the breakdown of the total cost per associated cost and time period. The optimal solution reports a total cost of 4,226,906 rmu (relative money units). This total cost includes the following terms: (i) fixed asset cost (i.e., investment cost to establish and expand local exploitation, conversion and storage technologies), (ii) fixed operating cost (i.e., total capacity cost), (iii) fixed transfer cost (i.e., investment cost to establish and expand transfer technologies), (iv) production cost (i.e., cost for producing states through conversion technologies), (v) inventory cost (i.e., cost for storable states through storage technologies), (vi) transfer cost (i.e., cost for transferring states through transfer technologies), (vii) raw materials cost (i.e., cost for transferring raw materials states from local exploitation technologies), and (viii) emissions cost (i.e., carbon tax for the release of emission to the environment). Fixed assets and transfer costs are higher in earlier periods while fixed operating, production and emissions costs become higher as demands and the corresponding production of states increases over time. The highest fixed asset cost is observed in time period 2 because the investment cost to establish technologies ($\varepsilon^{0}_{(z,j,t)}$) and investment cost to increase the capacity of technologies ($\varepsilon_{(z,j,t)}$) is lower than the investment costs in later time periods. Emissions cost increases over the time because of: (i) the expansion of conversion technologies $j5$ and $j6$ due to higher demands for states $s5$ and $s6$, and (ii) the increase of the emission cost coefficient over time.

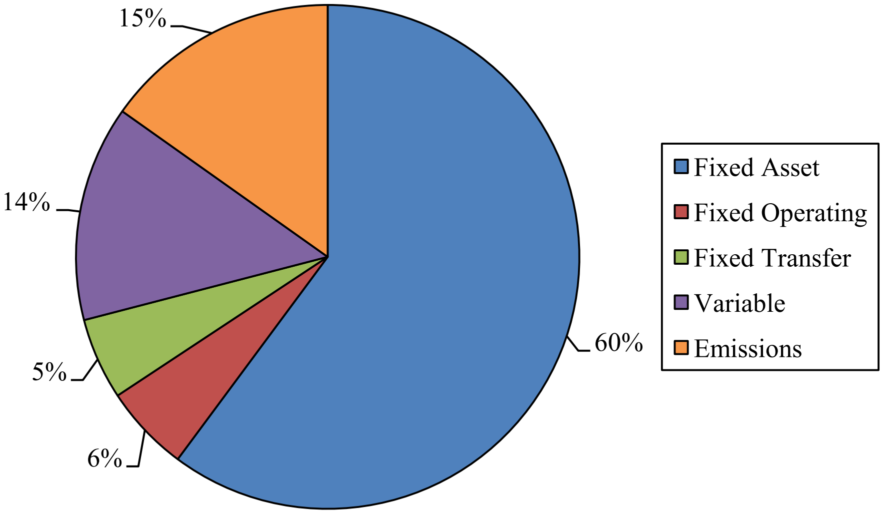


Figure 12. Case A: Total cost breakdown (percentage).

Figure 12 shows the total cost breakdown for the problem under consideration. The fixed asset cost is the highest cost term at about 60% of the total cost. The second highest cost is the emissions cost at around 15% of the total cost followed by variable costs at 14%. Finally, the fixed operating and transfer cost count for the 6% and 5% of total cost, respectively.

5.2. Case B: Design and Planning of an Energy Supply Chain Network: the effect of increasing the emissions cost (carbon tax)

5.2.1. Description of Case B

In this example, a slightly modified version of the previous case study is considered. All parameters and costs values are the same as before. The main difference is that the emissions costs $\lambda^{D}_{(z,s,t)}$ (e.g., carbon tax prices) for undesired substance state $s7$ is increasing over time. Case B is divided into two subcases: (i) Case B.1 (emission cost is two times the emission cost of Case A), and, (ii) Case B.2 (emission cost that is three times the emission cost of Case A).

5.2.2. Results of Case B

Figure 13 displays the normalized cost comparison of the solutions of all cases (Case A, Case B.1 and Case B2). Percentages are calculated by dividing each cost term with the highest total costs of the cases (i.e., that of Case B.2). Emissions costs are not included in this figure because different coefficients are used for each problem instance. The results do not show big differences in variable, fixed transfer and operating costs among the different cases. The main differences observed, but still small, are in the fixed assets cost with Case B.2 having a slightly higher fixed assets cost that the other two cases. This is because of the higher levels of capacity expansion of more expensive but lower-emissions conversion technology $j5$ in Case B.2 in comparison to that installed in Case B.1 and Case A. Consequently, the amount of states produced from task $i4$ using conversion technology $j5$ increases over the time, resulting in lower emissions generation than in other cases. The total installed capacity for conversion technology $j5$ in Case B.1 and Case B.2 is more than that for conversion technology $j6$ in Case A (see Figure 17).

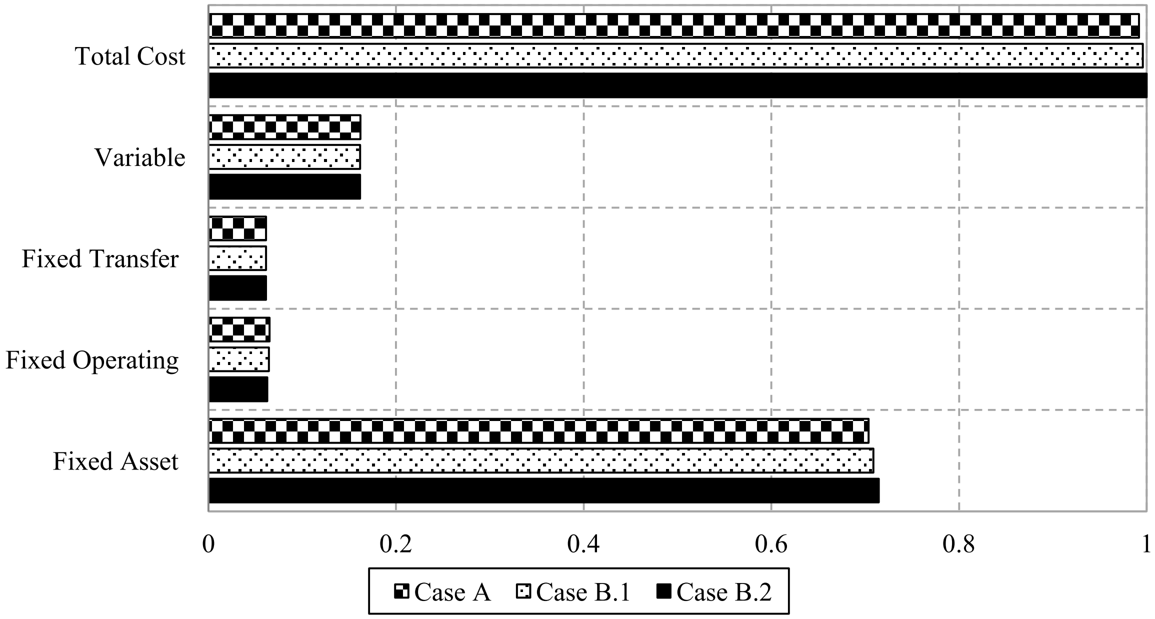


Figure 13. Cost terms comparison for cases A, B.1 and B2 (percentage).

Figure 14 shows the aggregated total emissions for Case A, Case B.1 and Case B.2. As expected, Case A reports higher emissions levels than the other cases. Generally speaking, the higher the emissions costs, the lower the total emissions levels. Differences among the emissions levels of the different cases start being more visible from time periods that feature high demands for the states that can be produced by the task that has as by-product the undesired state (emissions). At the end of the time horizon considered, the differences in aggregated total emissions in comparison to Case A is 268 units for Case B.1 and 423 units for Case B.2. Overall, small reduction in the emissions levels have been observed by imposing higher emissions costs and the overall design of the energy supply chain network has not been affected much. Increasing more dramatically the emissions costs is expected to have a higher effect on the optimal design of the network but from the practical point of view this could most probably result to unrealistically high emission costs.

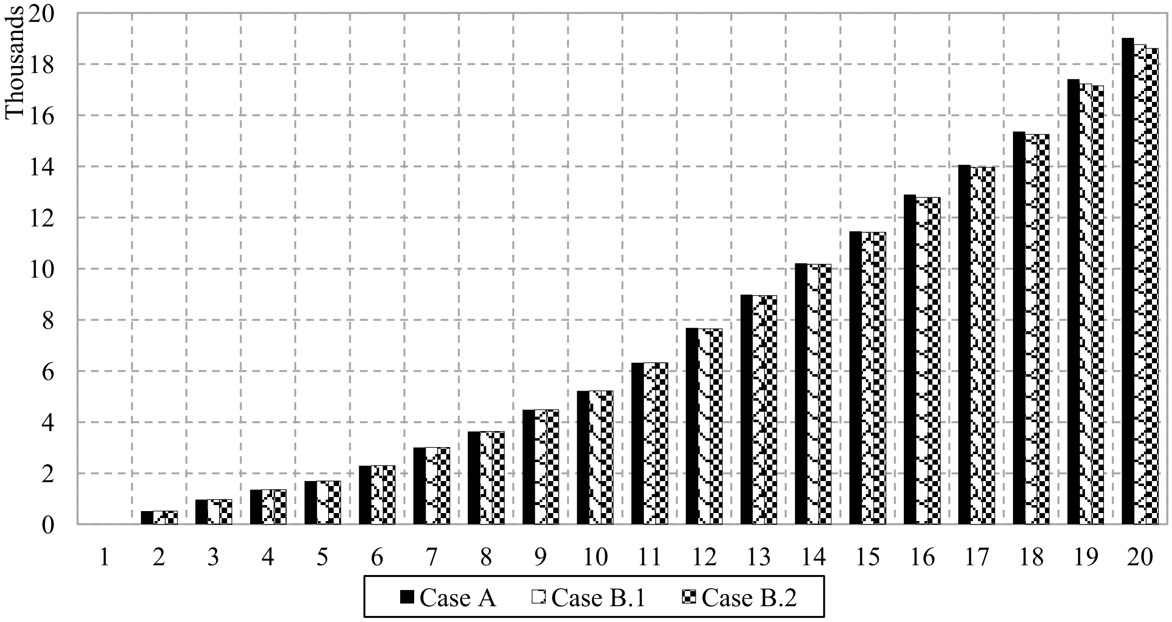


Figure 14. Aggregated total emissions per time period.

5.3. Case C: Design and Planning of an Energy Supply Chain Network: the effect of emissions levels caps.

5.3.1. Description of Case C

In this example, a slightly modified case study of Case A is considered by imposing an upper bound on the disposed amount of the states ($D_{(z,s,t)}$) for disposable state $s \in S_z^D$ (i.e., emissions levels limits). The maximum amount of emissions per time period in the solution of Case A was 2,057.5 units. Here, in Case C, an upper bound of 1,700 units on the emissions per period is set.

5.3.2. Results of Case C

Figure 15 displays the percentage of cost comparisons for Case A and Case C. The emissions cost for Case C is 0.01m.u lower than the emission cost for Case A. This is because the amount of disposed states is more limited through the emissions levels cap. However, the fixed asset cost for Case C increases to 0.04m.u in comparison to the fixed asset cost for Case A. In this case, the expansion to install conversion technology $j5$ (more expensive but cleaner technology than conversion technology $j6$) is more frequent than the conversion technology $j6$ to perform task $i4$. This is a direct result of imposed upper bound on the emissions levels in Case C.

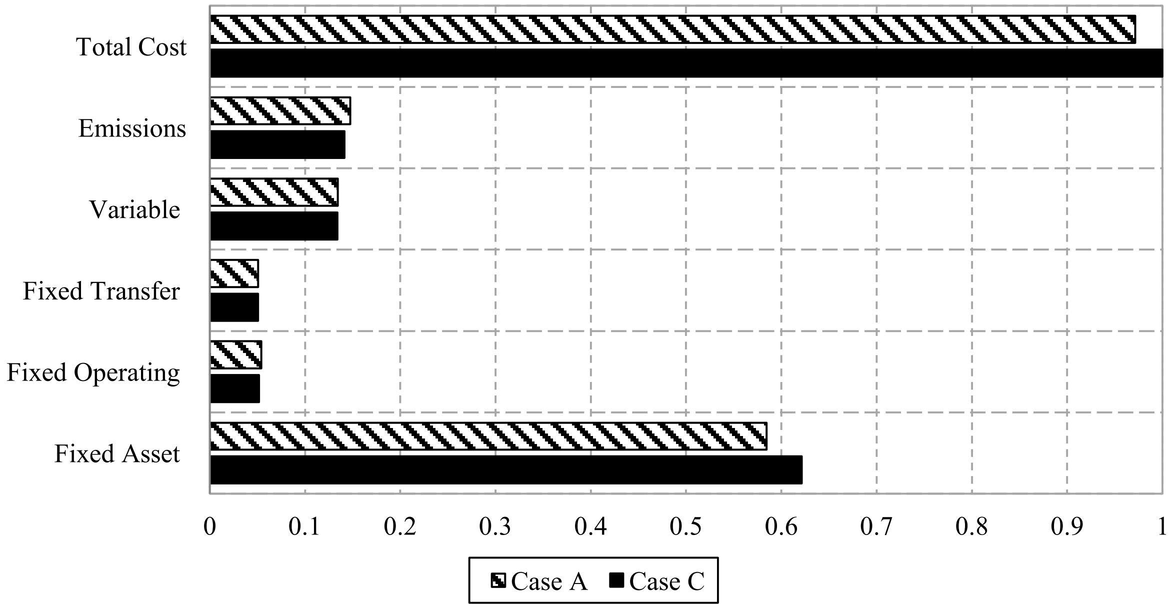


Figure 15. Cost term comparison between Case A and C.

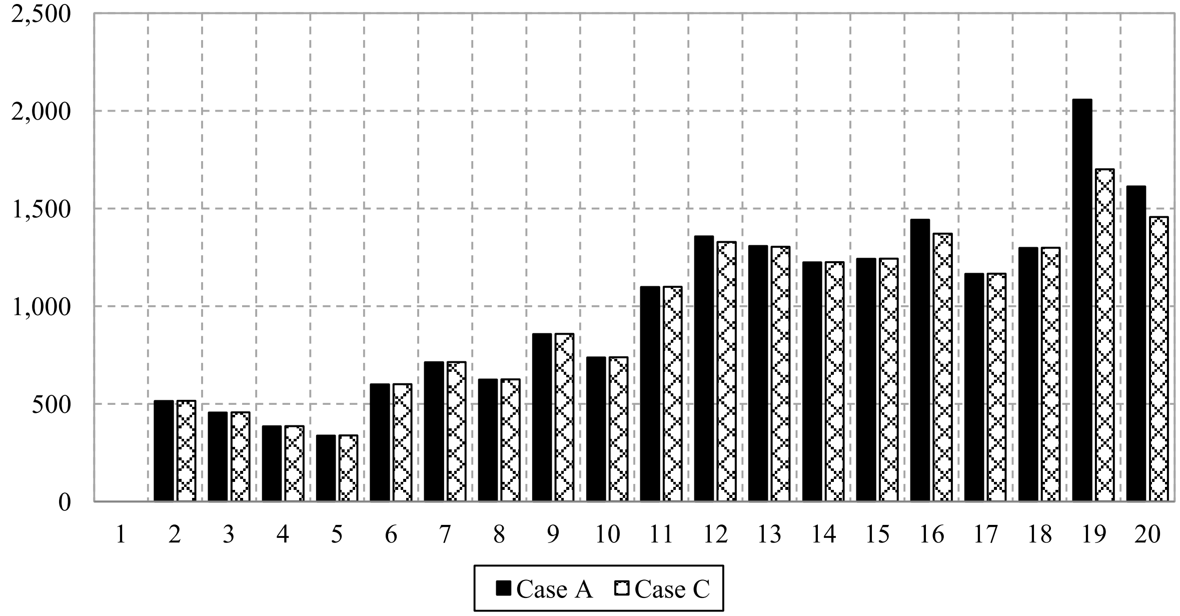


Figure 16. Comparison of amount of disposable state $s7$ (emissions) per time period between Case A and Case C.

Figure 16 shows the emissions level throughout the planning horizon. In this case, the disposable state is the only undesired substances state $s7$ (emissions). There is reduction in emissions level in time period 12, 16,19 and 20 for Case C in comparison to Case A. This is because, for task $i4$ in Case C, conversion technology $j5$ has converted higher amounts of output states compared to conversion technology $j6$ in these time periods compared to the solution of Case A. It is observed that a total emissions reduction of 3.3% in Case C with respect to Case A.

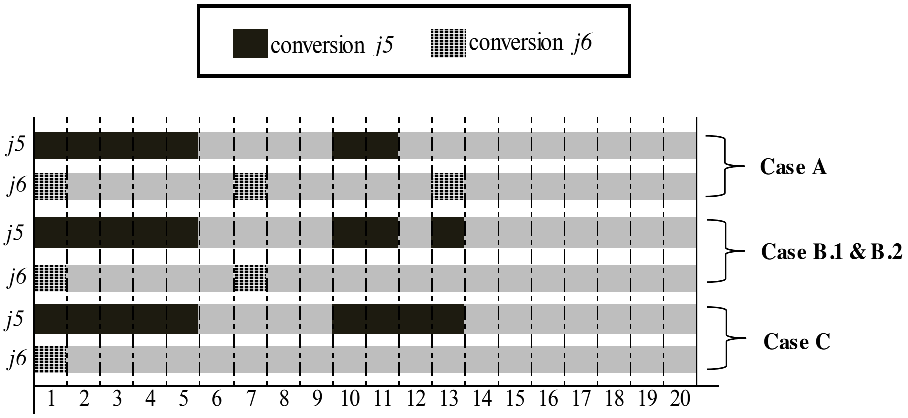


Figure 17. Comparison of capacity expansion planning for conversion technologies $j5$ and $j6$ per time period for all cases.

Figure 17 shows the comparison of the capacity expansion planning for conversion technologies $j5$ and $j6$ per time period for all cases. As it has been discussed previously, there are more capacity expansions for conversion technology $j5$ than that of conversion technology $j6$ for Case C in comparison to Case A and Case B. In Case B.1 and Case B.2, the capacity expansion planning for these technologies is the same (i.e., variables Y). However, a higher capacity expansion for conversion technology $j5$ is reported in Case B.2 than in Case B.1. This case shows that emissions can be reduced imposing upper bounds on their generated levels (emissions caps by regulations).

Overall, through the case studies considered it is evident that for emissions reduction, specified emissions limits (e.g., carbon limits through regulations) are more effective that increasing the emissions cost. However, lower emissions limits would result in an increase in total costs due to the need for installing lower-carbon technologies that are typically more expensive than most conventional technologies at this time.

5.4. Further Analyses: Sensitivity Analysis and Multi-objective Optimization

In this part, we present some further illustrative analyses that could be performed by the proposed optimization framework. Figure 18 displays a sensitivity analysis for total emissions and costs with respect to alternative emissions caps, while Figure 19 presents total emissions reduction and cost increase (with respect to the emissions unconstrained case, i.e., Case A) per emissions caps scenario considered. These two figures give a complete picture of the trade-offs between total emissions and cost under varied emissions caps. It is observed that: (i) total cost increases significantly for emissions caps below 1,850 metric units, and (ii) the descrease rate for total emissions is higher for emissions caps above 1,900 metric units. It has been found that the minimum emissions cap possible is 1,678 metric units, since below this emissions cap value the resulting optimization problem becomes infeasible (i.e., some demands for states cannot be satisfied completely). With respect to the emissions unconstrained case, the different emissions caps considered can achieve emissions reductions from 0.18% to 3.27% resulting to total cost increases from 0.01% to 2.95%, respectively. In practice, an emissions cap around 1,850 metric units could be considered as a good choice, since it would reduce emissions by 2.36% requiring a moderate cost increase by 0.48%.

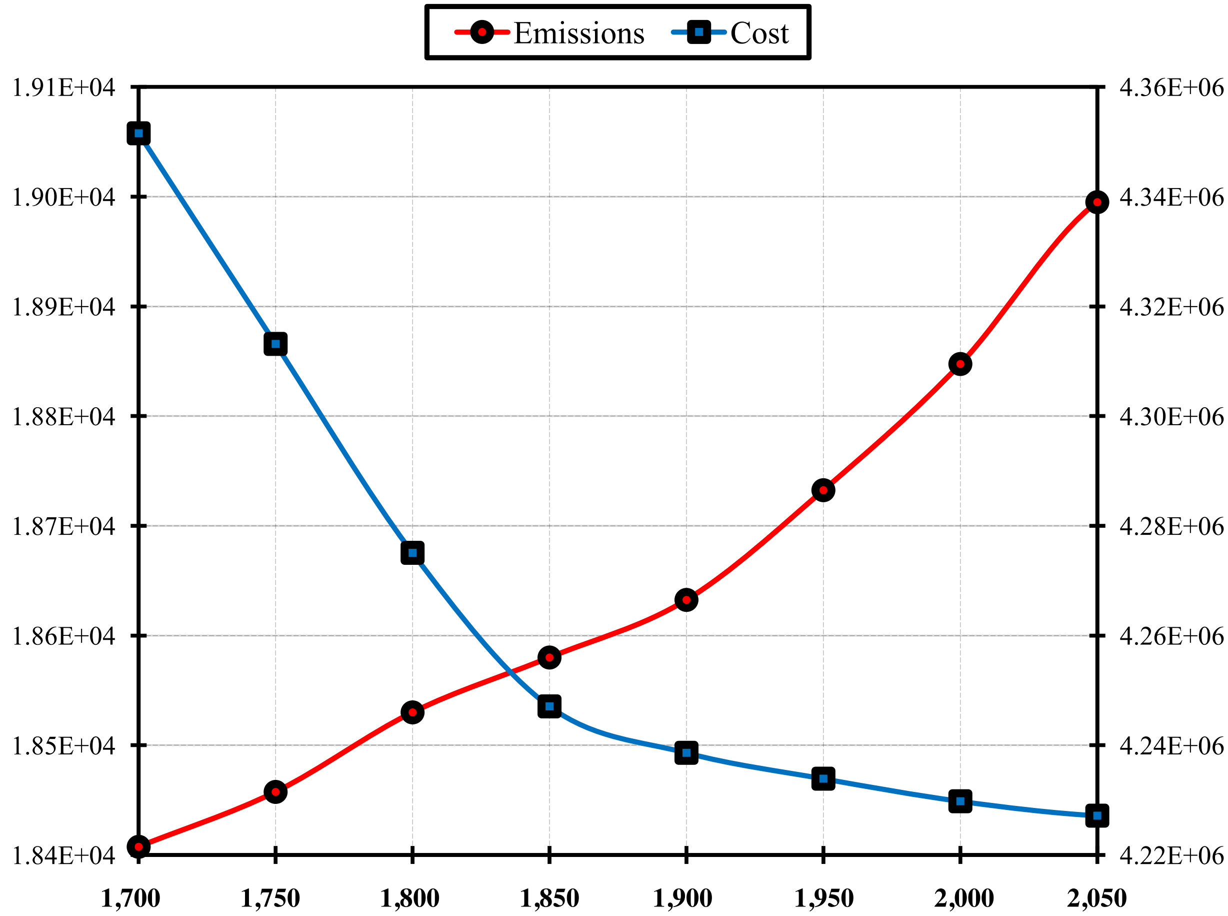


Figure 18. Sensitivity analysis for total emissions and cost under different emissions caps.

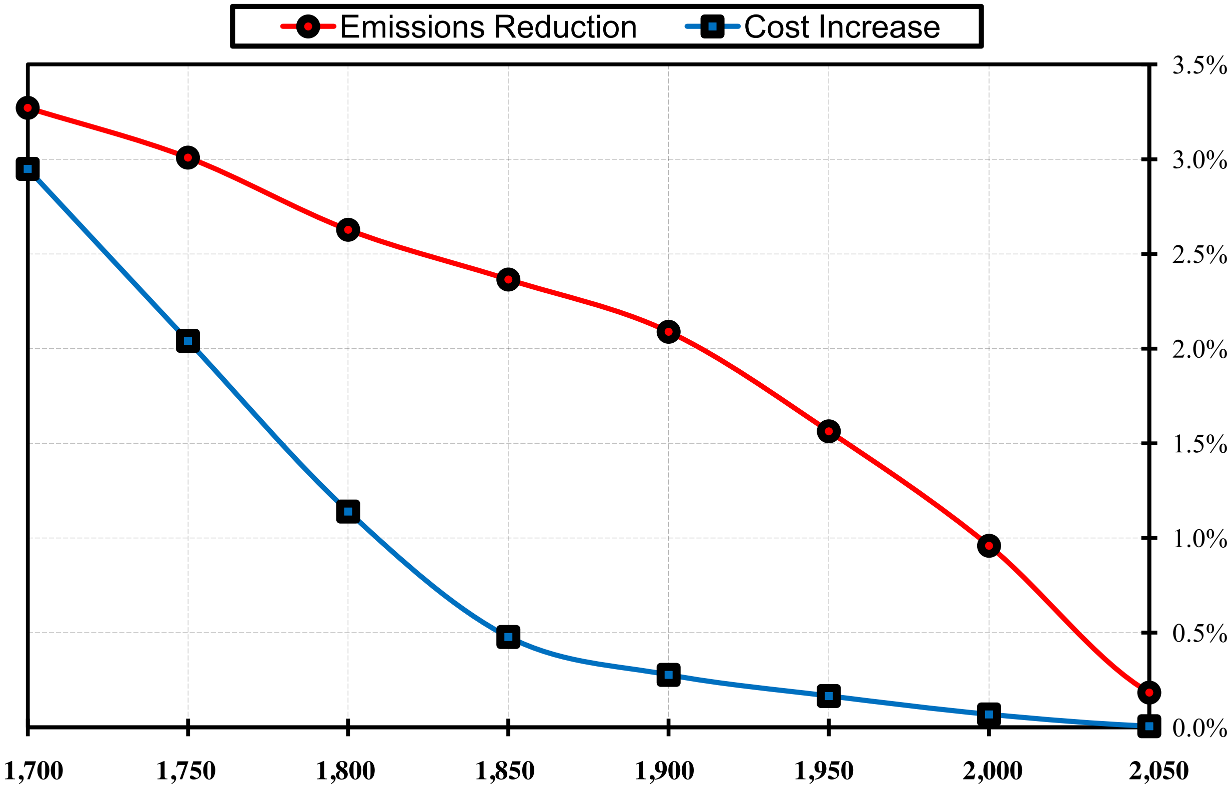


Figure 19. Total emissions reduction and cost increase under different emissions caps (with respect to the emissions unconstrained case, i.e., Case A).

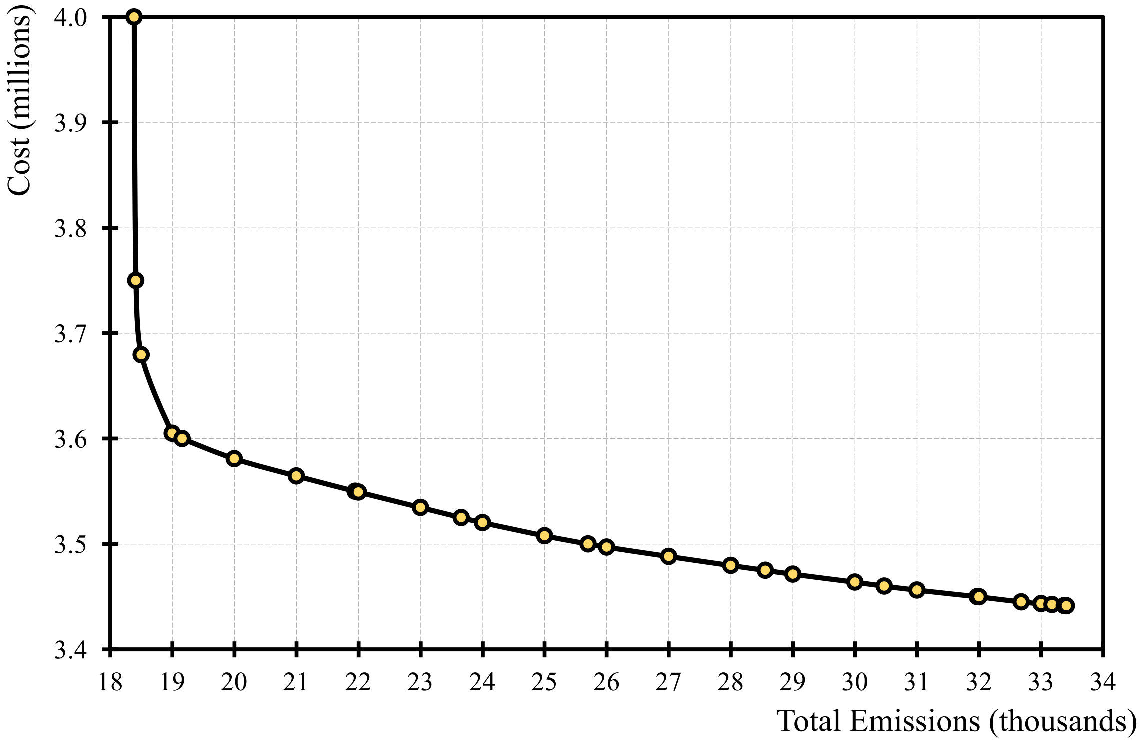


Figure 20. Multi-objective optimization: Pareto frontier for total emissions and cost.

Finally, the proposed optimization model has been used in a multi-objective optimization framework through the ε-constraint method. Total emissions and costs are the two objectives considered. Figure 20 displays the Pareto frontier found. The Pareto frontier shows clearly the trade-offs between the two conflicting objectives. Notice that any solution point: (i) below this Pareto frontier would be infeasible, and (ii) above this Pareto frontier is suboptimal. Figure 20 shows that the total cost grows exponentially to achieve reduction in total emissions below 19,000 metric units. In practice, a decision maker would most probably select a solution point within the second interval of the x-axis of Figure 20 (i.e., total emissions from19,000 to 20,000 metric units).

6. Conclusions

In this study, the Energy State Task Network (E-STN) representation has been introduced as a means for modeling the main operations in material and energy supply chain networks in a unified fashion for design and planning problems of such systems. The illustrative cases presented demonstrate the main features and the applicability of the general optimization framework developed for techno-economic and environmental analysis studies. The case studies solved demonstrated that a more efficient way for emissions reductions is through regulation and emissions caps rather than increased emissions costs; a reduction of 3.3% in emissions has been reported. It has been shown how the proposed model can be used effectively to study the trade-off between costs and emissions levels and different environmental policies (i.e., emissions costs and caps) under sensitivity analysis and multi-objective optimization studies. The proposed optimization framework could be used to integrate various types of material and energy supply chain operations using a unified modeling representation. Overall, the proposed design and planning model can address an extensive range of energy supply chain networks. Introduction of problem-specific constraints may be required in some cases. Ongoing and future research activities focus on the modeling of more complex material and energy supply chain networks and the incorporation of uncertainty in the resulting optimization frameworks.

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NOMENCLATURE

Indices/Sets

$i \in I$	tasks (conversion, transfer)
$j \in J$	technologies (conversion, transfer, storage)
$s \in S$	states (material resources, energy forms, undesired substances)
$t \in T$	time periods
$z \in Z$	internal and external zones

Subsets

J^C	conversion technologies
J^T	transfer technologies
J^E	local exploitation technologies
J^B	storage technologies
J_i	technologies that could perform task i
J_s	technologies that involve state s
J_z	technologies that could be installed in zone z
J_z^E	local exploitation technologies in zone z
J_z^{CE}	conversion and local exploitation technologies in zone z
$J_{(z,z')}^T$	transfer technologies that can transfer states from zone z to z'
$J_{(s,z)}^B$	storage technologies for state s in zone z
I_s^-	tasks that consume state s (input state)
I_s^+	tasks that produce state s (output state)
I_s^T	tasks that could transfer state s
I_s^{RM}	tasks that involve raw material state s
S_z	states that are present in zone z

S_z^{RM}	‘raw materials’ states in zone z (principal states)
S^{NR}	non-renewable raw materials states
S_z^{FP}	states s that have demand in zone z (demand states)
S_z^{B}	storable states s of zone z
S_z^{D}	disposal states s of zone z
Z^{in}	internal zones of the energy supply chain network
Z_z^{T}	zones that are connected to zone z (transfer of states to zone z)

Superscripts

max	maximum
min	minimum
+	output
-	input

Parameters

$\alpha_{(z,z,i,j,t)}$	bounds on the available capacity for conversion and transfer task
$\beta_{(z,s,t)}^{\min}$	bounds on the inventory level for states that can be stored $s \in S^B$
$\gamma_{(z,j,t)}$	bounds on the capacity expansion for conversion and storage technologies
$\gamma_{(z,z',t)}^{\mathrm{T}}$	bounds on the capacity expansion for transfer technology $j \in J^T$
$\delta_{(z,j,t)}$	fixed operating cost for the total installed capacity of technology j
$\varepsilon_{(z,j,t)}^{0}$	investment cost required to establish a technology
$\varepsilon_{(z,j,t)}$	investment cost required to increase the capacity of a technology
$\zeta_{(z,s,t)}$	demand for final product states $s \in S^{FP}$ in zone z in time period t
$\eta_{(z,s,t)}$	losses coefficient for states that can be stored $s \in S^B$
$\vartheta_{(z',z,s,i,j,t)}$	cost for transferring the states that are considered as final products $s \in S^{FP}$
$\kappa_{(s,i,j)}$	coefficient for input/output states for tasks i that can perform technology j
$\lambda_{(z,s,t)}$	inventory cost for the states that can be stored

$\lambda^{D}_{(z,s,t)}$	penalty cost for the release of the materials/energy/undesired substances states states to the environment
$\mu_{(z,j,t)}$	necessary installation time for technology j in zone z, if its construction starts in time period t
$\mu^{T}_{(z,z',j,t)}$	necessary installation time for transfer technology j that connects zone z and z', if its construction starts in time period t
$\pi_{(z,s,i,j,t)}$	cost for producing states by performing conversion tasks through conversion technology
$\psi_{(z,s,i,j,t)}$	raw materials cost
$\omega_{(z,s,t)}$	maximum available amount of raw material states

Parameters (initial status of the overall system)

$\beta^{0}_{(z,s)}$	initial inventory level for states
$\varphi_{(z,j)}$	initial installed capacity for conversion technology $j \in J^{C}$ and local exploitation technology $j \in J^{E}$ in zone z
$\varphi^{B}_{(z,s,j)}$	initial installed capacity for storage technology $j \in J^{B}$ in zone z
$\varphi^{T}_{(z,z',j)}$	initial installed capacity for transfer technology $j \in J^{T}$ that connects two zones

Continuous Variables (non-negative)

$D_{(z,s,t)}$	quantity of states that can be disposed
$F_{(z,j,t)}$	total capacity of conversion technology j in zone z in time period t
$E_{(z,j,t)}$	increase of capacity for conversion technology j in zone z in time period t
$F^{B}_{(z,s,j,t)}$	total capacity of storage technology j that can store state s in zone z in time period t
$E^{B}_{(z,s,j,t)}$	increase of capacity for storage technology j that can store state s in zone z in time period t
$F^{T}_{(z,z',j,t)}$	total capacity of transfer technology j that can transfer from zone z to zone z' in time period t

$E^{T}_{(z,z',j,t)}$	increase of capacity for transfer technology j that can transfer from zone z to zone z' in time period t
$P_{(z,z',i,j,t)}$	quantity of states converted or transferred through task i using technology j from zone z to zone z' in time period t
$B_{(z,s,t)}$	inventory of state s in zone z at the end of time period t
FA_t	investment on fixed assets in time period t
FA^{TS}_t	investment cost for transfer network in time period t
FOC_t	fixed operating cost in time period t
VOC_t	variable operating cost in time period t (includes production & inventory & transportation & state purchases)
RC_t	raw material states cost
PC_t	production cost for final product states in time period t
IC_t	inventory cost for material states in time period t
TC_t	transfer cost for final product states within internal zones and external sales of final product states to external zones
DC_t	penalty cost for the states that is disposed to the environment(e.g., emissions cost)
LS_t	penalty cost for lost sales for states whose demand is not met

Binary Variables

$W_{(z,j,t)}$	= 1, if conversion or local exploitation technology j is established in zone z in time period t
$W^{B}_{(z,s,j,t)}$	= 1, if storage technology j for state s is established in zone z in time period t
$Y_{(z,j,t)}$	= 1, if capacity of conversion or local exploitation technology j begin installing in zone z in time period t
$Y^{B}_{(z,s,j,t)}$	= 1, if capacity of storage technology j for state s begin installing in zone z in time period t
$Y^{T}_{(z,z',j,t)}$	= 1, if capacity of transfer technology j starts installing in zone z in time period t

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