

Resource Integration Across Processing Clusters: Designing a Cluster of Clusters

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ABSTRACT

Achieving worldwide sustainable development is a practical challenge that demands an efficient management of resources across their entire value chains. This practical task requires the optimal selection of pathways for extracting, processing, and transporting resources to meet the demands in different geographic regions at minimal economic cost and environmental impact. This work addresses the challenge by proposing a systematic framework for designing resource-processing networks that can be applied to resource management problems. The framework considers the integration and resource exchange within and across multiple processing clusters. It allows for the life cycle assessment of the environmental and economic impacts of the defined value chains, and design accordingly the different processing and transport systems from extraction to final use. The proposed representation and optimization model are demonstrated in a case study to assess the impact of energy transition under decarbonization constraints on long-distance energy supply chains. The objective is to identify optimal cluster designs and interconnecting transportation networks for decarbonized energy supply between energy exporters and importers.

Keywords: Optimization, Supply Chain, Energy, Carbon Dioxide, Life Cycle Analysis

INTRODUCTION

Population growth is associated with increased demand for resources (water, energy, food, products...), fuel combustion, emissions levels, and waste production. Addressing these challenges requires effective resource management to ensure economic prosperity and avoid environmental disasters. Achieving the goals of sustainable development globally requires a life cycle view of the resource management problem.

Process systems engineering has provided different methods and approaches to manage material and energy resources through optimal integration. Heat [1] and mass [2] integration have been implemented at the chemical process scale to minimize feedstock intake and waste generation while meeting a defined production level. The scope of integration has been extended through total site analysis [3] to include exchanging resources between different plants within close vicinity.

Process Integration has been the basis for designing integrated systems, where different plants can exchange specified resources to achieve defined objectives

(economic or environmental). Many problems in this field are developed as mathematical programming models whose solutions yield the optimal outcomes for the defined problems. For example, Almansoori and Shah [4] proposed a mixed integer linear programming (MILP) model for optimizing the design and operation of H₂ supply chains. Alnouri et al. [5] proposed an optimization model for water integration and optimal brine management. Al-Mohannadi et al. [6] proposed a mixed integer linear programming model for integrating CO₂ across sources and sinks to optimize the design of CO₂ capture, utilization, and sequestration (CCUS) systems. These are some applications among many of the Process Integration approaches that have been widely described and reviewed [7]. Many of these approaches focus on a specific number of resources, which limits the scope of such approaches. Expanding the scope would then require developing new models that account for the missing opportunities.

To address this gap, new methods have been proposed that consider more holistic sets of resources by incorporating more materials. For example, the C-H-O

approach balances carbon, hydrogen, and oxygen elements in integrated processing clusters [8]. Different energy streams have been considered in multi-sectoral energy systems design through simulations and linear programming [9]. Although such approaches provide more generic frameworks than the direct applications described earlier, they still lack the comprehensiveness of integrated designs needed when considering different raw materials, intermediates, waste, and emissions streams. Ahmed et al. [10] proposed a resource integration representation of a processing cluster and a MILP model for maximizing the profit of the integrated system while abiding by environmental constraints. The flexible representation allows a complete accounting of all material and energy resources. The framework considers the specifications and conditions at which resources can be exchanged, with an inclusive accounting for the economics of processes and flows. However, this resource integration representation allows resource extraction, production, use, and reuse only within a defined system, which is limiting when it comes to life-cycle assessment considerations or representing the interactions across geographic locations.

Some of the energy systems modeling tools have considered the spatial aspect of the integration problem [11]. In such approaches, the transportation network is an infrastructure dedicated to one of the energy vectors (like a pipeline that transports H_2 from location A to location B). Besides the fact that such models are limited to the energy systems they present (by the resource and process selection), the representation of the transportation network does not allow the consideration of multiple options that may impact the processing in different locations. This work proposes a framework for simultaneous resource integration within and across multiple processing clusters. The novel approach builds on Ahmed et al.'s [4] representation and expands the scope to include multiple systems with supply chains for exchanging resources. The transportation networks and processing clusters have similar generic representation which allows the consideration of multiple technologies for processing and transportation of the resources. A MILP model is proposed to minimize the integrated system's costs. This is the first generic framework for resource integration that yields optimal value chains under environmental limitations while considering transportation networks as processing clusters. An illustration of the model is presented by considering the problem of decarbonizing the energy supply chain between an energy importer and an energy exporter, including long-distance shipping of energy carriers and CO_2 . The case study considers the emissions across the energy value chain in the different systems, as well as different decarbonization pathways, to propose cost-optimal strategies for achieving decarbonization targets at the global level.

PROBLEM STATEMENT

Given is a system characterized by multiple processing clusters and different resources that can be processed and exchanged within and across the clusters. Each cluster is characterized by a set of processing options that can consume, produce, and convert the resources accessible by the cluster. The aim is to find the optimal capacities of the processing options that result in minimizing the net cost of the overall system while meeting the defined demands of resources in each cluster and abiding by defined footprint limitations.

The proposed representation allows for considering generic systems representing resources' value chains. Each processing cluster can be attributed to a geographic location or a transportation network. This allows the consideration of resource or process availability that may vary across geographic regions. Supply chains or transportation networks can access resources in different geographic locations, which allows for considering different modes of transport, each of which can be characterized as a processing option within the supply chain cluster. Integrating supply chains into the design of processing networks allows accounting for all possible opportunities to determine optimal configurations that meet defined demands at constrained footprint impacts. For example, when designing energy vectors for long-distance shipping, while some pathways may be considered better for shipping (due to high energy density, for example), they might produce more emissions or require higher costs for processing with respect to other less energy-dense carriers. Hence, considering the different processing and transportation options of the various resources simultaneously allows the identification of the synergies and trade-offs to support efficient decisions.

This work proposes a generic approach for considering integrated value chains, giving the user flexibility in defining the specifics of the problem. The aim is to determine the optimal processing options, their location, and their capacity by designing low-cost, low-footprint value chains.

CLUSTER-OF-CLUSTERS REPRESENTATION

Figure 1 illustrates an example of a superstructure considered in the proposed framework. Each resource that can be consumed, produced, or exchanged within each system is characterized and tracked along the corresponding resource line. Each resource line is characterized by its physical properties (temperature, pressure, composition, AC/DC power, frequency, etc.) and geographic location. The characterization builds upon common infrastructures for energy and material transmission (like power, feedstock, waste, etc.).

Different resources can be imported to each system as fresh feedstock or energy/power inputs, or exported as products, by-products, waste streams, etc. The processes shown in the representation act as conversion units with connections to each resource line. These conversion processes account for any processing a resource line must go through to change its location or specifications. The units are characterized by their costs and capacity limitations, allowing full economic accounting across the entire systems.

The proposed methodology provides a comprehensive scope for considering the integration and resource exchange within and across multiple processing clusters. Each cluster is defined based on accessibility to the available processes and resources. This incorporates the spatial dimensions into the planning framework. The proposed representation considers the supply chains as systems with different transport modes that can exchange resources between different geographic locations. By considering the exchange of resources between multiple clusters, the entire value chain can be assessed, and the impact of transportation modes on resource production and utilization in different systems can be evaluated.

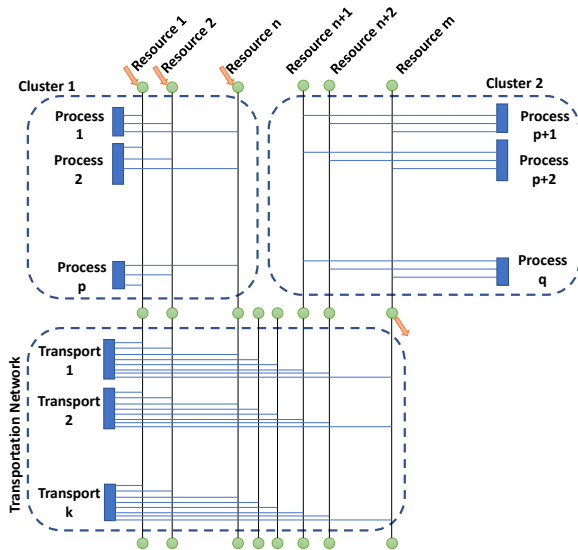


Figure 1. Resource integration across multiple clusters.

OPTIMIZATION MODEL

Given are a set of resources $R = \{r_1, r_2, \dots, r_n\}$, a set of processes $P = \{p_1, p_2, \dots, p_n\}$, a set of components $C = \{c_1, c_2, \dots, c_n\}$, and a set of systems (or clusters) $S = \{s_1, s_2, \dots, s_n\}$. Note that the transportation units are considered in the proposed representation as “processes” since they “convert” resource lines from one location to another. Cost, capacity limits, and environmental impact characterize each processing and transportation unit. The proposed framework uses MILP to select the

processing and transportation units to minimize the system's cost under defined constraints on resource imports and exports (resource availability, demand, environmental constraints, etc.). The optimization variables are: the capacities of the different processes (and transportation options) in each system, the resources imports and exports flow rates into and out of each system, the flows of resources exchanged between systems, and the binary variables that activate each of the processes in each system.

The parameters used for characterizing the processes and resource lines are as follows: the conversion parameters, which are defined as the ratio of the flow rate of resource r produced by process p in system s relative to $F_{p,s}$, the composition of each component in each resource line in each system, the minimum and maximum capacity of each process in each cluster, the minimum and maximum resource import and export flowrate from each system, and the minimum and maximum resource flow rates of resources exchanged across the different systems.

The following parameters are considered in establishing the economic model to formulate the objective function: the capital expenditure of the processing units in each system is represented as the ratio of the annualized capital costs relative to the capacity of the units, the operating costs of the processing units in each system are represented as the ratio of the operating costs relative to the capacity of the units, and the selling and buying prices of each resource at each system. Economies of scale may result in cost advantages at high production capacities, leading to a non-linear relationship between the capital cost and the capacity. However, when the capacities are high enough, the impact of the economies of scale diminishes, which justifies the linear relation assumed in this work.

The model is set by defining the following constraints that ensure the applicability of the solution and its abidance to mass and energy balances and technical and environmental constraints defined by the user:

- Resource balance: resource balances are defined for each resource line to ensure mass and energy conservation across exports, imports, exchanges, and process conversions.
- Capacity limits: the lower and upper limits on the capacity of each considered process are introduced to ensure the applicability of the solutions based on the process's technical limitations.
- Flowrates limits: the limits on the flowrates of resource imports, exports, and exchanges between the different clusters are introduced to allow the user to define resource demands, consider resource availability, and account for any

limitation on the exchanges between systems.

- Components limits: the limits on the components in the resource exports and imports are defined to allow for the consideration of environmental limitations (such as emissions reduction targets, waste discharges, toxicity limits, etc.).

The total net cost of the overall system (the cluster of all clusters) is determined by accounting for the costs of installing and operating the processing (and transportation) units, the costs of acquiring the resources in the different clusters, and the revenues from selling the resources in each system. The objective function is developed by defining the net cost based on all the accounted costs and revenues to minimize it.

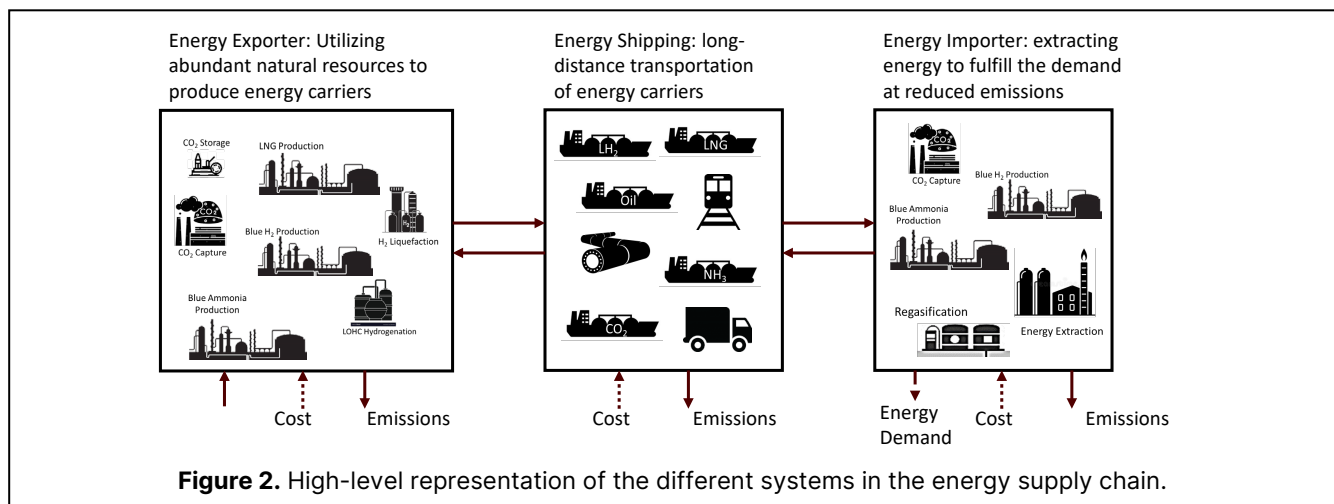
Considering the spatial dimension coupled with the ability to exchange resources across the clusters allows a holistic vision of the interactions between the systems, where the decisions in one system affect the entire value chain. The MILP model can efficiently screen through all possible combinations to give real-time solutions and suggestions on the optimal technology mix of the whole supply chain (from production to transportation, to final use). Note that all the optimization runs performed in the case study (the following section) gave solutions in less than 1 second.

CASE STUDY: DECARBONIZING LONG-DISTANCE ENERGY SUPPLY CHAIN

The framework applies to analyzing energy supply chains, which can be represented by three systems: an energy importer, an energy exporter, and energy shipping. Figure 2 shows a high-level representation of the considered systems. The energy exporter utilizes abundant natural resources to produce energy carriers that an energy importer can store, transport, and use to supply a defined demand. The case study presented here is based on exporting energy between an energy importer and an

energy exporter 8000 nautical miles apart. The base case corresponds to exporting Liquefied Natural Gas (LNG). This case establishes a performance benchmark for supply chain costs and emissions against which decarbonization is assessed. The emissions from the supply chain can be reduced either through CO₂ capture, shipping, and storage to decarbonize the LNG-based energy supply chain, or by replacing natural gas with alternative hydrogen fuels and carriers. Applying the proposed framework to the described problem allows determining the processes to be implemented in each system (importer, exporter, and shipping) and their capacities, and the flowrates of the different resources imported, exported, and exchanged across the systems. These variables directly relate to key decisions for the optimal supply chain design, which include the following: What are the cost-optimal supply chain decarbonization pathways? Where can decarbonization technologies be applied to reduce targeted supply chain emissions? Which energy carriers should be produced and shipped? Where to produce alternative fuels? How will the cost-optimal decarbonization affect the direct costs and emissions incurred by each system? Considering all the systems constituting the supply chain simultaneously in this design process allows accounting for the impact each of the considered pathways has on the others. For example, transitioning to H₂ based fuels at the importer would decrease the LNG production level at the exporter, given that the energy demand to be supplied at the importer is fixed. This would affect the scale of CO₂ capture and storage from the LNG production process, and the shape of the required shipping fleet (type and number of ships).

The different decisions are considered by defining energy carriers' production processes at the exporter and the corresponding shipping and processing units in the remaining systems. The energy carriers considered are LNG (base case), H₂, which can either be directly shipped as a liquid or loaded on a liquid organic H₂ carrier (LOHC), and Ammonia. An additional case is investigated



considering LNG as an energy carrier (EC) and decarbonizing the supply chain by capturing the CO₂ at the exporter and the importer. The captured emissions at the importer are shipped back to the exporter to be stored, as CO₂ sequestration may result in safety concerns in some locations [12]. An option for decarbonizing the ships using the shipped alternative fuels (H₂ and NH₃) as fuel for shipping instead of heavy fuel oil (HFO) is

considered.

Defining the energy supply chain problem in the cluster-of-clusters framework requires introducing the following resources: energy carriers (H₂, NH₃, LNG), the processed H₂ conditioned for shipping (liquid or loaded on LOHC), forms of direct energy, CO₂ footprint (from each of the processes), and CO₂ streams in the supply chain (captured, compressed, and liquified CO₂).

Table 1: Key parameters characterizing energy carriers' production and processing units at the exporter.

Process	Cost (\$/GJ)	Natural Gas Intake (GJ NG/GJ)	Power Intake (MWh/GJ)	CO ₂ emissions (kgCO ₂ /GJ)
LNG production	2.61	1.17	0	17.8
Blue H ₂ Production	4.54	1.46	0	10
H ₂ Liquefaction	5.82	0	59	0
LOHC Hydrogenation	0.40	0	0.58	0
Blue NH ₃ production	13.90	1.52	24	2.2

Table 2: Key parameters characterizing energy carriers' processing units at the importer.

Process	Cost (\$/GJ)	EC Usage for heat (%)	Power Intake (kWh/GJ)
LNG Regasification	0.34	1.5%	0.10
H ₂ Regasification	0.14	0%	1.2
LOHC Dehydrogenation	1.28	21%	2.3

Table 3: Key parameters characterizing energy carriers' ships in the shipping system.

Process	Cost (\$/GJ)	EC loss (%)	CO ₂ emissions (kgCO ₂ /GJ)
LNG Ships	1.66	6.21%	3.13
H ₂ Ships	7.59	7.31%	10.7
LOHC Ships	5.15	0.00%	12.4
NH ₃ Ships	3.23	0.15%	7.22
H ₂ -fueled LOHC ships	3.44	16.3%	0
NH ₃ -fueled NH ₃ ships	2.25	9.64%	0

Table 4: Key parameters characterizing the different units across the CO₂ supply chain.

System	Process	Cost (\$/tCO ₂)	Natural Gas Intake (GJ/tCO ₂)	Power Intake (kWh/tCO ₂)	CO ₂ emissions (tCO ₂ /tCO ₂)
Exporter	CO ₂ capture and compression	60	3	108	0.11
	CO ₂ Processing	3.26	0	4	0
	CO ₂ Storage	10	0	0	0
Shipping	CO ₂ Ships	70	0	-	0.12
	LNG Fueled CO ₂ ships	61	1.05	-	0.09
Importer	CO ₂ Capture	48	3	28.7	0.11
	CO ₂ Liquefaction	8.5	0	83.1	0

The system contains a three clusters, 24 resources, and 25 processes. The resources and processes are defined within each cluster based on availability, cost, energy requirements, and CO₂ emissions levels. The systems incorporate two major supply chains for shipping energy and CO₂. The optimization problem aims to find the optimal configuration that supplies the energy demand for the importer at minimum cost while abiding by a defined supply chain emissions level. The energy demand at the importer is set to 140 million GJ/y.

Tables 1 through 4 summarize the data used in setting up the case study. The data on LNG production is based on Katebah et al. [13] and Raj et al. [14]. LNG regasification parameters are estimated based on Hafner and Luciani [15] and Park et al. [16]. The data on blue H₂ production is based on the integrated process reported by Katebah et al. [17]. The parameters characterizing the blue ammonia production process are based on the description of the ammonia process in Ullmann's Encyclopedia [18] and on data reported by Wang et al. [19] and Pfromm [20] on the ammonia process and CO₂ capture [21]. The studies reported by Raab et al. [22] and Niermann et al. [23] were used to estimate the data for H₂ liquefaction and LOHC hydrogenation and dehydrogenation. CO₂ capture data are based on the parameters of CO₂ capture from a natural gas combustion flue gas [24]. The costs of CO₂ sequestration are based on a report by the Global CCS Institute [25], assuming 10 \$/tCO₂ storage and transportation costs. The parameters characterizing CO₂ liquefaction, processing, and CO₂ ships are based on a report published by Element Energy Limited [26] in collaboration with Brevik Engineering, Polarconsult, TNO, and SINTEF. Note that the parameters shown in the tables are used to define the conversions of the different processes based on the intake and production levels of the different resources with respect to their capacities. This allows defining clear boundaries for each process to avoid double counting. For example, the power requirements parameter is defined as zero for some processes. This means that the process does not require importing the resource "power" from the integrated cluster. Power may be produced and consumed within the process boundaries, which may impact the conversion factors of the resources like cost and CO₂ emissions (which are also stated in the tables).

Table 1 shows the key parameters that define the energy carrier's production (from natural gas) and processing units in the cluster representing the energy exporter. The parameters are reported based on LHV energy content in the fuels produced and processed by each unit. Note that the reported costs do not include the cost of natural gas or power, which are considered as resources imported into the cluster as fresh feeds. The power is assumed to be obtained from natural gas-fired power plants with an emissions factor of 0.54

kgCO₂/kWh. The power price at the exporter is assumed to be 0.032 \$/kWh, and the natural gas cost is 4 \$/GJ. Table 2 shows the parameters used to characterize the processing units at the importer. These units treat the received energy carriers from the ships to be at conditions suitable for energy extraction (through combustion). The heat requirements of these units are covered by the corresponding energy carriers, which is accounted for through the inefficiency or the EC loss parameter. LOHC dehydrogenation is an endothermic process that results in high energy requirements covered by the shipped H₂. The power is assumed to be covered by a natural gas power plant at a price of 0.19 \$/kWh. Natural gas combustion at the importer (from the case of shipping LNG) produces 50.3 kgCO₂/GJ. Table 3 presents the parameters characterizing the shipping fleets. The reported costs include heavy fuel oil (HFO), used as the fuel for H₂ ships, LOHC ships, and NH₃ ships. Energy carriers' losses from the ships are due to EC evaporation (LNG and H₂ and NH₃) or due to utilizing the shipped EC as shipping fuels (H₂-fueled and NH₃-fueled ships). The evaporated energy carriers are recovered and used onboard to supply power to the ship's engine (with HFO). CO₂ emissions from the ships are due to the combustion of the shipping fuels (HFO and LNG). The costs of the decarbonized ships are determined by assuming a 20% increase in the ship's capital costs. The cost reduction is due to not utilizing HFO on the decarbonized ships. The trade-off is between avoiding the HFO cost or reducing the energy efficiency of the supply chain by using the energy carriers as fuels. Table 4 shows the parameters that characterize the different units along the CO₂ supply chain. CO₂ is captured from the LNG production, compressed, and stored at the exporter. The CO₂ captured from natural gas combustion at the importer is treated and shipped back to the exporter, where it is processed and stored. The heating requirements for CO₂ capture are covered by burning the natural gas in the supply chain. Two options for fueling the CO₂ ships are considered: HFO or LNG (produced at the exporter) as shipping fuels. Natural gas power is assumed to cover the power requirements of CO₂ processing units.

RESULTS

The optimization model, based on the defined system, contains 870 constraints and 654 variables. The model is set up in Python and solved using Gurobi. The optimal scenario with the highest emissions flow rate was obtained by running the optimization model at relaxed emissions constraint. This scenario corresponded to producing LNG at the exporter and exporting it on LNG carriers to the importer, where it is regasified, and natural gas is combusted to cover the 140 million GJ/y energy demand. The corresponding emissions level in that

scenario is 10.23 MMtCO₂/y (26% from the exporter, 69% from the importer, and 5% from the ships).

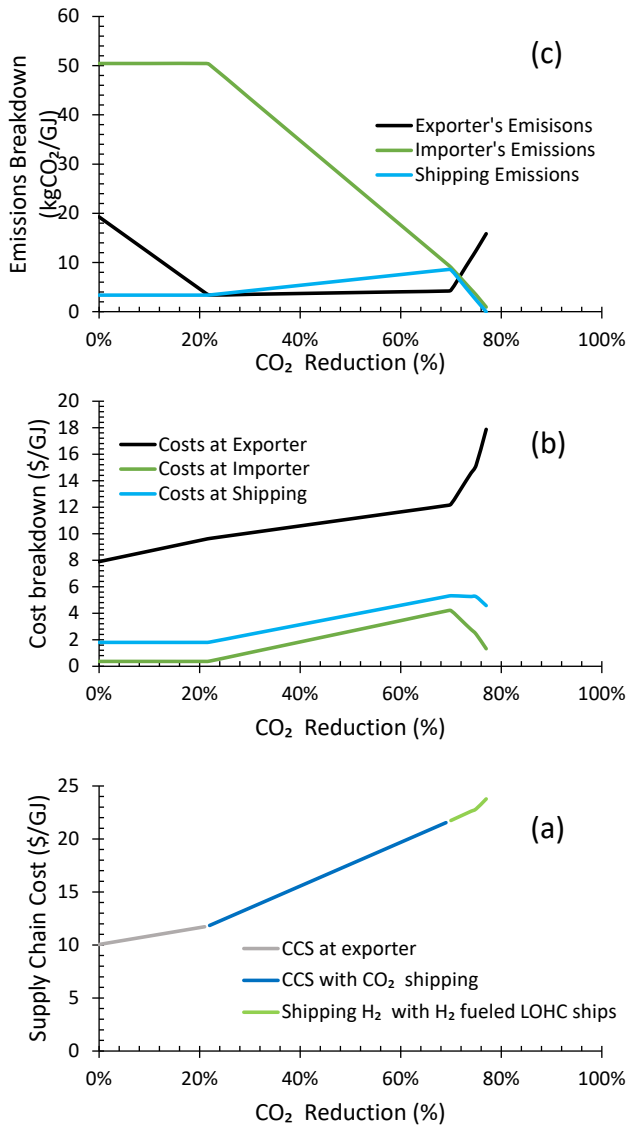


Figure 3. The total supply chain cost (a) and the breakdown of costs (b) and emissions (c) across the three systems at different CO₂ reduction levels.

The emissions limit constraint was then introduced by setting an upper limit on the CO₂ exports across all the systems. The CO₂ emission limit was reduced from 10.23 MMtCO₂/y to 2.35 MMtCO₂/y. Further CO₂ reduction was not attainable considering the described technologies. The supply chain cost and the costs and CO₂ emissions of each considered system are tracked. Figure 3 shows the results obtained at varying CO₂ emissions reduction. Three different system configurations were identified as the CO₂ emissions reduction target increased. Low emissions reduction levels (up to 21%) could be achieved by capturing the emissions from LNG production and storing

them at the exporter. This results in maintaining the cost and emissions level in the shipping system and at the importer, as no changes in the designs are required. The emissions at the exporter drop while the cost increases due to the investment in CO₂ capture and storage (CCS).

Emissions reduction between 21% and 69% can be achieved by capturing the emissions of the exporter and the importer and storing them at the importer. The captured emissions from the importer are shipped back to the exporter on CO₂ ships. This configuration increased the costs for all three systems due to the investments required in CO₂ capture, shipping, and storage. The emissions at the exporter were maintained at the same level achieved in the previous configuration as all the emissions were captured. The importer's emissions level dropped significantly, while the level of emissions from shipping increased. The rise in the shipping energy level is due to introducing a new shipping fleet that burns fuel onboard. Going beyond 69% emissions reduction requires a transition in the energy system at the importer from LNG to H₂. The optimization solution showed that blue H₂ would be produced and loaded on LOHC at the exporter and then shipped to the importer on oil tankers fueled by H₂. This scenario reduces the cost and emissions level in the shipping system and at the importer due to burning a fuel mix with less carbon content in both systems. The cost and emissions level increase at the exporter. This is because of the higher cost of blue H₂ production relative to LNG production. Moreover, a high amount of CO₂ is captured from the H₂ production, resulting in high emissions due to the capture inefficiency. The results indicate a variation in the performance of the systems as the emissions reduction target increases. An option that achieves global emissions reduction may increase emissions at a singular system level. At the same time, an option that results in global cost reduction may require an unevenly distributed investments. This indicates the necessity for fair crediting of CO₂ reduction to promote efficient implementation globally.

CONCLUSIONS

This work presented a methodology for cost-optimal integration of different resources within and across multiple systems. The representation allows tracking energy and material streams based on their defined specifications. The generic representation of resources and processes gives the user flexibility in defining the problem by considering multiple material and energy resources that can be integrated across different processing units. The model allows full economic accounting by considering the cost of processes and transportation pathways, the cost of imported resources, and revenues from selling the exports. A comprehensive environmental accounting is allowed by considering multiple footprints.

Considering the design of multiple processing systems simultaneously results in insightful decision-making that accounts for the impact of systems interactions. The method can be applied to a wide range of problems like circular value chains, industrial symbiosis beyond eco-industrial parks, and the net-zero transition. This study presented an application of the framework for decarbonizing the energy supply chain by defining three systems: an energy carrier, an energy importer, and an energy exporter. Such a problem has been addressed in literature by analyzing one or two supply chains, but no work has considered multiple options simultaneously in an optimization framework. In this work, different technologies are considered for decarbonizing the different systems, and the interconnectivity of the decision-making was accounted for in the proposed method. The results showed that cost-optimal decarbonization starts with CO₂ capture and storage at the exporter (reducing 21% of the emissions), followed by CO₂ capture at the importer (with CO₂ shipping, which reduces up to 69% of the emissions), and energy transition to H₂ is activated at high CO₂ emissions reduction targets, which allows for 77% emissions reduction. The CO₂ marginal abatement cost increases from 110 \$/tCO₂ to 250 \$/tCO₂ as the reduction targets rise. The analysis showed that the environmental and economic impact of the decarbonization transition on the different systems varies with the targeted reduction levels. Hence, the implementation of an optimal transition calls for fair crediting of emissions reduction (environmentally and economically) across the systems.

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