AMERICAN UNIVERSITY OF BEIRUT

THE INVESTIGATION OF MULTIPLE AND BLENDED FUEL OPTIONS IN CARBON-CONSTRAINED INDUSTRIAL CLUSTERS

by
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ABSTRACT

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With the increasing climate change concerns, governments around the world are working on setting targets to mitigate its upsurge. Greenhouse gases (GHG), more specifically carbon dioxide (CO_2), are the highest contributors to global warming. As a result, strict restrictions on GHG emissions are being set worldwide to a limit. Industrial sectors rely extensively on fossil fuels, the highest carbon emitters, and in turn face many challenges towards the compliance of the set emission standards. Therefore, finding solutions that would both meet the environmental requirements while satisfying the industries' energy and fuel demands has been the focus of several studies over the years.

The integration of biomass, or a renewable source of energy as an alternative to fossil fuels, has been previously investigated by many. Other works involved the development of carbon utilisation strategies to reduce carbon footprints. However, few studies targeted the incorporation of more than one type of fossil fuel with biomass and/or renewable energy in a carbon constrained industrial cluster. Therefore, this thesis proposes a carbon reduction optimisation-based technique that integrates more than one source of energy with carbon utilisation technologies and assesses both its economic and environmental feasibilities.

A systematic optimization-based model is introduced to develop sustainable utilization strategies to meet a cluster's product requirements, while meeting the set CO_2 emission limits and maximizing associated financial returns. A Mixed Integer Nonlinear Program (MINLP) was developed to select the optimal allocation of the different types of fuels, the optimal source to sink mapping and carbon utilization configuration to meet the mentioned targets.

Five case studies consisting of a natural gas cluster, a coal cluster, a biomass cluster, a blended fuel cluster, and a multiple fuel cluster, were conducted to illustrate the proposed model. The multiple fuel case study resulted in the lowest post-capture emissions with 9469 t CO_2/d generating a high-end profit of $907.16 million/y. Two sensitivity analyses were conducted on the multiple fuel case study to assess the effect of varying the net carbon capture rate (NCCR) and the renewable percentage on the previously mentioned variables. It was further proven that at higher carbon capture rates, the reliance on fossil fuels decreased and the switch to renewable energy was favoured.

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ABBREVIATIONS

ATM	Automated Targeting Model
CCUS	Carbon Capture Utilization and Storage
CO_2	Carbon Dioxide
FFDE	Fossil Fuel Derived Energy
GHG	Greenhouse Gases
LCA	Life Cycle Assessment
NCCR	Net Carbon Capture Rate
ROC	Renewables Obligation Certificates

CHAPTER 1

INTRODUCTION

The world's energy demand is expected to increase by 45% between the years 2015 and 2030, and by more than 300% by the end of 2100 (Chalvatzis & Ioannidis, 2017). This upsurge in global energy requirement has led growing industries to rely extensively on fossil fuels. The latter is considered the primary source of 85% of the current global energy consumption, making them the world's dominant power and energy supply and the largest contributors to greenhouse gas (GHG) emissions (Hasan, First, Boukouvala, & Floudas, 2015; Valkila & Saari, 2010). Furthermore, fossil fuels can be monetized and utilized in various processes. From the production of power to their conversion to value-added products, the industrial sector has long depended on these types of fuel to increase its end profit (Vora, 2012).

In recent years, the development of industrial clusters as a means to gain competitive advantage and reduce costs has witnessed an upsurge in various sectors around the world (Liu, Geng, Zhang, Dong, & Liu, 2014). Generally, a cluster can be considered a network of plants, firms, or even institutions located within a geographic region that allows the exchange of materials and energy among its entities (Porter, 1998). The inter-linked symbiosis and synergies that industrial clustering offers create opportunities for economic growth and expansion; however, at the expense of the environment. Because of the abovementioned monetization of fossil fuels, the reliance of this sector on fossil fuel-derived energy (FFDE) has caused a drastic increase in its carbon footprint, accounting for over 28% of global carbon dioxide (CO_2) emissions (IPPC, 2018).

With the alarming rise in global warming, major climate change concerns are being raised with regard to the increasing anthropogenic GHG emissions. Following the aforesaid industrial trends and human activities, the global average temperature, which has already observed an elevation of 1 ℃, is estimated to reach a rise of 1.5 ℃ by 2040 (IPPC, 2018). The global GHG emissions reached a yearly increase of 1.3%, striking a new record of 50.9 gigatons of CO_2 equivalent (Olivier & Peters, 2018). As a result, the Paris Climate Agreement established in 2015 has set global targets to reduce GHG emissions by a factor of 80-95% by 2050 (de Pee et al., 2018). This has pushed governments all around the world to enforce carbon taxes on industrial clusters and set CO_2 emission limits in compliance with the targets imposed by the Paris Agreement. Therefore, the need to satisfy the rising energy demands, while conforming to the set emission bounds, has pushed researchers to seek mitigation techniques that could be implemented in industrial clusters.

This study introduces a new carbon reduction strategy that focuses on choosing the best allocation of different fossil fuels, biomass, and blended fuels to an industrial cluster with set carbon constraints. The challenge in designing such a cluster falls with identifying the most optimal selection of fossil fuels, their utilization and monetization techniques, and the different carbon management methods, all while developing synergies between fossil fuel conversion and CO_2 emission mitigation. The complexity of this problem calls for a strong systematic approach that can assess the feasibilities of all the possible options according to the set constraints and define the most optimal configuration that would yield a low carbon emission-fuel utilization strategy that any industrial cluster can apply.

This work aims to introduce a new carbon reduction method that targets both the environmental and economic aspects. The analysis consists of a superstructure optimization-based model that develops sustainable utilization strategies to meet a carbon-constrained cluster's product requirements at the highest possible profit. The model aims at finding the optimal allocation of different types of fuel either for the production of value-added products or the power generation, the percentage of renewable energy to be integrated and the optimal carbon utilization techniques as a means to reduce the GHG emissions.

The following thesis consists of five chapters. Chapter two covers a detailed literature review on the available approaches to carbon mitigation techniques in an industrial cluster. Chapter three describes the methodology followed in this research by introducing the design problem, the tools used for its implementation, and the conducted case studies. Chapter four discusses the results that were obtained, presents sensitivity analyses, and assesses the limitations of the study with future recommendations. Finally, chapter five concludes by presenting the main findings of the research.

CHAPTER 2

LITERATURE REVIEW

Over the past centuries, fossil fuels, namely oil, coal, and gas, have been dominating the world's industrial sector. Because of their ability to store and provide large quantities of energy, they are considered to be the most commercially attractive source of energy (X. Wang & Economides, 2009). The various functions that fossil fuels offer from the production of value-added products to the supply of electricity and power has led to a drastic increase in the industries' dependence on this source of energy. The industrial sector's energy consumption is forecast to grow by 32% by the year 2050 (T. Wang, 2019). This trend raises major environmental concerns due to the high CO_2 emissions associated with fossil fuel utilization. Recent studies have shown that 40% of the carbon emissions result from the combustion of coal, 31% from the combustion of oil and 18% from the combustion of natural gas (Olivier & Peters, 2018). Therefore, to meet the Paris Agreement global targets, several works have focused on developing carbon reduction strategies that could be implemented in industrial clusters.

2.1. The integration of biomass and renewable sources

One method that has gained a lot of attention in the past years involves the use of cleaner energy sources. Biomass consists of any animal or plant material that can be used to either produce energy or value-added products in various industrial processes (Irmak, 2017). Because several types of biomass take in CO_2 during their harvesting, they have the potential to yield a carbon-neutral source of energy (Ren et al., 2017). Over the years, some researchers sought ways to potentially incorporate the latter in the

industrial sector by either co-firing it with fossil fuels or even replacing them completely to reduce the overall emissions. Others proposed the integration of renewable sources into clusters as a mitigation strategy and assessed its economic feasibility. Table 1 presents an overview of the aforementioned existing works highlighting the approaches used as well as the main results and conclusions.

2.2. The integration of carbon capture and storage technologies

Another method that has gained a lot of attention in the past years consists of capturing the CO_2 emitted in a given plant and either feeding it to a different process or storing it in underground reservoirs for sequestration. This technique is known as carbon capture, utilization and storage (CCUS) and results in a reduction of the carbon footprint (Hasan et al., 2015). Several works focused on assessing the application of the CCUS technology to already existing clusters as a means to significantly diminish the emissions. Others analyzed the economic feasibility of developing a CCUS-integrated cluster. Some also incorporated the technology with renewable co-fired plants. Table 2 presents an overview of the carbon reduction strategies that involve CCUS.

Table 1 Literature on the integration of renewable sources to fossil-fuel dependent industrial clusters with a focus on fuel allocation

Reference	Method of Analysis	Aim	Plant Type	Fuel Type	Results
(Tan & Foo, 2007)	Pinch analysis technique	Graphical procedure for a carbon-constrained energy sector planning with the allocation of energy sources to meet the imposed limits.	N/A	Coal, oil, natural gas	Successful application of the graphical procedure on cases focused on the energy planning of one type of GHG emissions. Limitations include the implementation of such an analysis for more detailed planning.
(Lee, Sum Ng, Yee Foo, & Tan, 2009)	Graphical pinch analysis with mathematical optimization	Targeting the reduction of CO_2 emissions through the optimal allocation and segregated planning of low-carbon emitting energy sources to different subsectors of geographic regions.	N/A	Coal, oil, natural gas, biodiesel, biogas, and zero-emission renewable sources	The successful development of an energy planning and allocation tool

(X. Jia, 2010)	Graphical pinch analysis	The energy integration across an industrial park to reduce its overall emissions.	Chemical plants	Coal, Oil, natural gas, biomass gasoline, zero-emission renewable sources	29.7% reduction in CO2 emissions
(Peng, Wang, Lei, & Cheng, 2012)	Experimental study	The assessment of the gasification of a blended biomass feedstock	Wastewater and power plants	Blended biomass consisting of sewage sludge and forestry waste	The reduction of sewage sludge through gasification and the production of a dry gas yield of 0.7Nm3/kg and H2 yield of 11.67 mol/kg
(Al-Mayyahi, Hoadley, & Rangaiah, 2013)	Composite-curve analysis with a bi-objective mathematical linear optimization	Finding a trade-off solution between the minimum utility cost and the minimum CO_2 emissions	N/A	Coal, natural gas, oil, and biodiesel	The successful implementation of the composite curve analysis on the case study
(McIlveen-Wright et al., 2013)	Process simulation approach using ECLIPSE	A comparison of the techno-economic assessment of three large-scale plants using coal as fuel vs biomass as fuel with the introduction of	Power plants	Coal and biomass	For low wood feedstock costs without ROCs or for high wood feedstock costs with ROCs, the biomass plant can compete with the coal-fired plant and constitute a greener

		Renewables Obligation Certificates (ROCs)			substitution for large scale applications.
(Andersson, Broberg Viklund, Hackl, Karlsson, & Berntsson, 2014)	Case study on an industrial cluster	The investigation of the integration of an algae-based biorefinery to an existing industrial cluster for carbon footprint reduction coupled with the assessment of the potential synergies.	Power plants and refineries	Natural gas, coal, nutrient-rich wastewater, and sewage sludge, and algae biomass.	The introduction of the algae-based biorefinery resulted in a reduction of the cluster's carbon footprint. Limitations include low maturity of the technology and algae's seasonal fluctuating growth rate.
(Holmgren, Andersson, Berntsson, & Rydberg, 2014)	Pinch analysis process integration	The assessment of the integration of biomass-fired gasification into a chemical cluster on the economic and environmental aspects.	Power and production plants	Wood biomass	Clusters that include methanol synthesis and biomass gasification systems have more potential to reduce the overall CO_2 emissions than standalone clusters.

(Yu, Han, & Cui, 2015)	Case study on an industrial enterprise	The assessment of the effect of the industrial symbiosis on carbon reduction for a case study on a large industrial enterprise Xinfa group.	Power and production plants	Coal, diesel, and natural gas	The reduction in the carbon emitted from the Xinfa group due to the application of industrial symbiosis.
(AlNouss, McKay, & Al-Ansari, 2018)	Aspen Plus simulation	Modeling a gasification system for the state of Qatar that utilizes the waste biomass for the production of biogas	Power plant	Biomass waste consisting of date pits, manure, and sludge	The possibility of utilizing waste as gasification feedstock under optimal conditions.
(AlNouss, McKay, & Al-Ansari, 2019)	Superstructure optimization using Aspen Plus simulation	The development of the optimal biomass-utilization superstructure for the poly-generation of products in a petro-chemical industry coupled with the environmental and economic assessment of the network.	Power and production plants.	Natural gas (for reference) and biomass (manure, waste date pits and sewage sludge)	The optimized superstructure resulted in a reduction of the carbon footprint of the industry.
(AlNouss,	Aspen Plus	The	Power and	Blended	The

McKay, & Al-Ansari, 2020)	model simulation	optimization of a blended biomass feedstock to four technologies for the production of high value-added products.	production plants	biomass (dried sewage sludge, waste date pits, and manure)	production of a quality syngas from an optimized biomass-blended gasification process resulted in lower operating energy as well as required gasifying agent quantity.

Table 2 Literature on the carbon reduction strategies that involve CCUS

Reference	Method of Analysis	Aim	Plant Type	Fuel Type	Results
(Turk, Cobb, Jankowski, A.M., & F.T., 1987)	Modified knapsack assignment problem	The selection of power plants, mainlines, and oil fields that yield the maximum return for the CO_2 transport and geological storage.	Power plants	N/A	The approach yielded logical results. However, in terms of its applicability, With the unstable oil prices, mainline utilizations, and acid rain legislation that were imposed during the time of the study, the approach could not be implemented.

(Middleton & Bielicki, 2009)	Geospatial and economic optimization model	The development of a scalable infrastructure model *simCCUS* for the estimation of the optimal CCUS cost and infrastructure arrangement of an integrated CCUS system.	N/A	N/A	Successful implementation of the developed model on 37 CO_2 sources and 14 reservoirs.
(Pękala, Tan, Foo, & Jeżowski, 2010)	Source-sink superstructure network analysis with resource conservation	Formulating a mathematical model for the optimization of energy systems under carbon constraints for CCUS		Biofuels, gasoline, and diesel	Successful and flexible implementation of the source-sink framework on the extended applications
(Fimbres Weihs & Wiley, 2012)	Mathematical optimization approach	The design of an optimal CCUS CO_2 pipeline network with minimal avoided CO_2 costs.	Power plants and refineries	Natural gas and coal	Successful implantation of the approach for a steady-state CCUS network with minimal avoided CO_2 costs.
(Munir, Abdul Manan, & Wan Alwi, 2012)	Pinch analysis-based waste-to-resource carbon Integration approach	Designing a carbon planning approach for a minimum emission-industrial cluster through the use of source-	Production plants with carbon sinks and sources and cogeneration plant with renewable energy	N/A	Successful allocation of point sources into the carbon distribution network

		sink mapping and energy integration.			
(Ooi, Foo, Tan, Ng, & Smith, 2013)	Linear optimization-based automated targeting model (ATM) for energy Planning under carbon constraints	Minimizing the energy loss for retrofitted CCUS power plants while still meeting the carbon emission limit	Existing power plants retrofitted with CCUS and new CCUS power plants	Coal, natural gas, and oil	The successful development of a revised ATM for the integration of CCUS in the power sector (linear formulation)
(Hasan, Boukouvala, First, & Floudas, 2014)	Mixed-integer-nonlinear programming	The design and optimization of a CCUS supply-chain network that targets the selection of stationary co_2 sources, capture technologies, and co_2 utilization, sequestration in geological storage sinks in the United States.	Power plants and production plants.	Coal, natural gas, oil, and biomass	The successful implementation of the optimization problem resulting in a cost-effective CCUS supply-chain network for CO_2 management in the United States
(Al-Sobhi & Elkamel, 2015)	Integrated simulation and optimization network	The optimal allocation of natural gas in an industrial cluster with maximum return	Production and power plants	Natural gas	Successful monetization of natural gas. In this work, the carbon footprint reduction and CO_2 utilization were not considered in

					the optimization model
(Yu et al., 2015)	Case study on an industrial enterprise	The assessment of the effect of the industrial symbiosis on carbon reduction for a case study on a large industrial enterprise Xinfa group.	Power and production plants	Coal, diesel, and natural gas	The reduction in the carbon emitted from the Xinfa group due to the application of industrial symbiosis.
(D. M. Al-Mohannadi & Linke, 2016)	Optimization based approach and systematic analysis	The design of a low emission carbon integrated system	Production and power plants.	Natural gas	Successful design of a carbon integration network that gives the minimum cost, considering CO_2 sources, utilization and storage alternatives.
(von der Assen, Müller, Steingrube, Voll, & Bardow, 2016)	Merit-order curve	The development of an environmental-merit-order (EMO) curve for the identification of the highest ranked CO_2 sources and their	Production and power plants	Natural gas, coal, and biomass	Successful development of the EMO with potential CO_2 footprint reduction

		utilization to reduce the overall CO_2 emissions.			
(Ali et al., 2017)	Comparative approach with modelling using Aspen Plus	The comparison of the performance of natural gas, coal and biomass power plants with CCUS and carbon compression	Power plants with CCUS	Natural gas, coal, and biomass	The natural gas-fired plant with exhaust gas recirculation showed a lower efficiency penalty and carbon dioxide emissions than the biomass-fired and coal-fired. This is due to the lower flow rate of flue gas into the system
(D. M. Al-Mohannadi, Abdulaziz, Alnouri, & Linke, 2017)	Superstructure - based modelling and optimization using What"s Best	The development of a systematic approach for the identification of gas utilization strategies that yield maximum profits for an industrial cluster under carbon constraints	Power and production plants with carbon capture and storage	Natural gas and renewable energy	Successful monetization of the natural gas following the carbon constraints applied to the cluster

(Manan, Mohd Nawi, Wan Alwi, & Klemeš, 2017)	Comprehensive review of existing work on process integration analyses for carbon dioxide emissions reduction	Providing an understanding of the existing graphical, algebraic, and numerical process integration tools for carbon reduction and mitigation.	N/A	N/A	N/A
(Zhang & Huisingh, 2017)	A qualitative assessment	The assessment of the techno-economic aspect of various CO_2 storage and transportation options.	N/A	N/A	N/A
(Yang, Wei, Hou, Li, & Wang, 2019)	LCA approach	The assessment of integrating a CCUS unit to a biomass and coal co-fired plant to reduce the overall emissions	Power plant	Pulverized coal and biomass	The co-firing of biomass with coal in a carbon capture integrated plant provides a feasible and promising alternative for the mitigation of the carbon footprint as well as the fossil fuel dependency

2.3. The novelty of this work

The relative literature discussed in sections 2.1 and 2.2 covered the feasibility of several carbon reduction techniques that can be divided into two main topics; the integration of biomass or renewable energy to a fossil-fuel based cluster and the incorporation of CCUS technology with some papers involving the possibility of adding a renewable plant. Few to no studies targeted the incorporation of more than one type of fossil fuel with biomass and/or renewable energy for both the production of value-added products and the generation of electricity in a carbon constrained industrial cluster. Furthermore, most of the existing works assessed the environmental feasibility of their approaches, while others focused on the economic aspect. However, very few targeted both evaluations. Therefore, the aim of this study is to combine both approaches by optimizing the allocation of multiple types of fuels, including blended fossil fuel and biomass, to a carbon constraint industrial cluster by maximizing the latter's profit and investigating its environmental and economic feasibilities.

CHAPTER 3

METHODOLOGY

3.1.Design problem

The purpose of this study is to maximize the profit of a carbon-constrained industrial cluster through the optimal allocation of multiple types of fuel. The cluster consists of a number of different production plants and a power plant for the processing of value-added products as well as the generation of electricity. The power plant is connected to the electric grid and constitutes the main source of electricity for the cluster. It also has the ability to produce more power and export it to the grid. The integration of additional plants that could generate new products, convert, or store carbon dioxide through CCUS technologies, and produce cleaner power through the use of renewable and/or multiple and blended fuels is assessed.

In the initial analysis, the cluster contains several production plants and a power plant restricted to one type of fossil fuel or blended fuel. Each production plant contributes to the total CO_2 emissions of the cluster based on the number of products it produces, the quantity of fuel, and the amount of electricity it requires to meet the set production. The power plant, in turn, contributes based on the amount of electricity the cluster requires and the quantity exported to the grid as an additional revenue source.

The integration of the additional plants, the option of utilizing several types of fuels as well as renewable power within the cluster serve the following functions:

- The reduced dependence of the cluster on one type of fossil fuel.
- The reduction of the total CO_2 footprint of the cluster through the use of carbon utilization technology with the possibility of monetizing the captured carbon.

- The production of a clean source of power to satisfy the cluster's requirement and reduce the fossil fuel requirement for power production.

To achieve the aforementioned, this research introduces a superstructure optimization-based approach that aims at developing sustainable fuel and carbon utilization strategies to meet the environmental restrictions at a maximum end-profit.

The optimization model will be able to determine:

- The selection the production plants and the type of power plant.
- The integration of renewable energy as a replacement to the fuel-derived energy with regard to the economic and environmental aspects.
- The optimal allocation of the fuel options to the production and power plants.
- The integration of carbon capture technologies onto the cluster.
- The capturing, treating, and monetizing the captured carbon.

To achieve the model formulation's objective, the following factors are assumed to be known:

- The existing production plants, their capacities, and their locations in the cluster.
- The products that are produced in every production plant in the cluster.
- The characteristics and costs of the fuels to be allocated.
- The power requirements of the production plants in the cluster.
- The maximum renewable percentage that can replace the fuel-derived power.
- The product-to-fuel and power-to-fuel requirements.
- The parameter that describes the carbon emitted per ton of product, kWh of power produced, during the transport of solid fuels, and in the carbon integration network.
- The revenue/cost parameter of every revenue/cost stream.

- The capital and operating costs of every plant.
- The cost of the carbon integration network (transportation, capture, treatment, compression, and pumping parameters).
- The cluster's carbon capture limit.

3.2.Generic application

The generic plant in this model can have several active sinks and sources. The sink options include: a fuel sink, a power sink, and a CO_2 sink, while the source options include: a product source, a CO_2 source, and a power source. A general setup of the production and power plant options is represented in Figure 1. As can be seen in the latter, a plant can be of two types: a production plant or a power plant with one source of fuel allocated to it. In terms of inputs, the plant requires a fuel input either to produce a value-added product or to generate power, a power input to satisfy its electricity requirements, and/or a carbon input, as in the case of a carbon utilization plant. In terms of outputs, a plant can produce products to be exported out of the industrial cluster, generate power to either satisfy the cluster's need or to be exported as revenue to the electricity grid, and emit carbon dioxide, which in turn is either released into the Atmosphere or captured, stored, or utilized by the carbon capture and utilization technologies.

Not all the plants will have all the available sinks and sources activated. The different plant options that can be included in the cluster are summarized in Table 3 and are classified based on the active sinks and sources. An illustration of the cluster's plant types is also depicted in Figure 2.

Figure 1 A generic illustration of sinks and sources within an industrial cluster

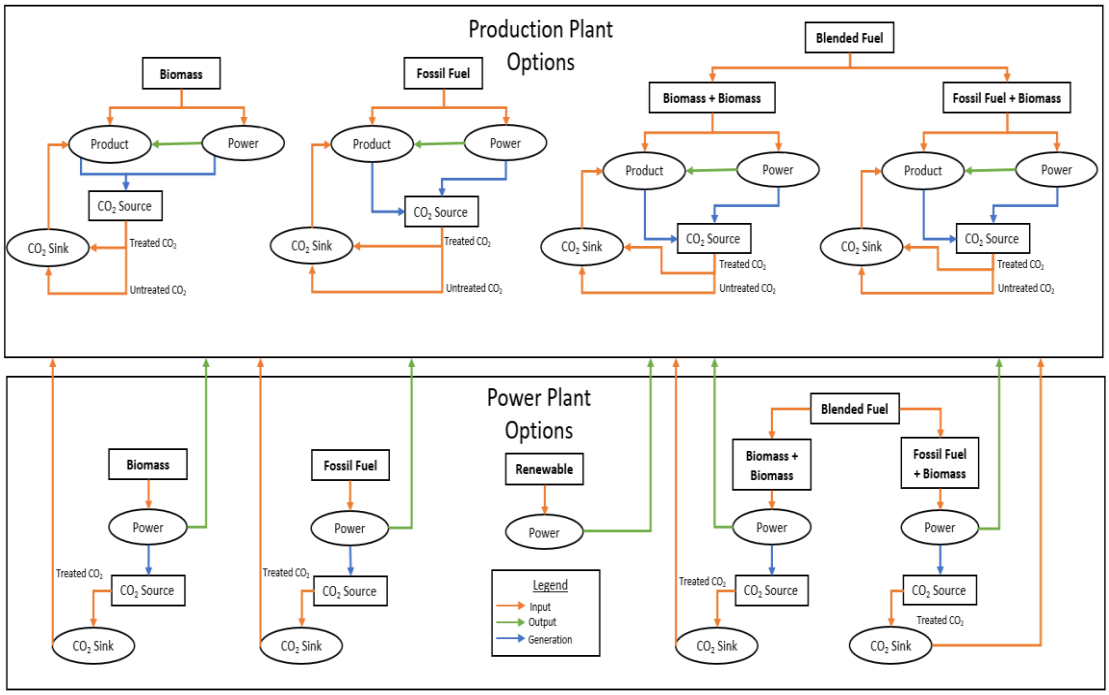

Table 3 Available plant options for the industrial cluster.

Plant Type	Active Sink(s)	Active Source(s)	Brief Description
Production Plant A	Fuel and power	Product and CO_2	Typical production plant that requires a fuel intake and power supplied from the grid, produces a product ($), and generates CO_2 emissions
Production Plant B	Fuel and power	Product, power, and CO_2	Typical production plant that requires a fuel intake, generates power to be either used by the plant itself or exported to the grid ($), produces a product ($), and emits CO_2.
Production Plant C	Fuel, power, and CO_2	Product and CO_2	Typical production plant that requires a fuel intake and power, takes in CO_2, produces a product ($), and emits CO_2.
Production Plant D	Fuel, power, and CO_2	CO_2, product, and power	Typical production plant that requires a fuel intake, generates power to be either used by the plant itself or exported to the grid ($), takes in CO_2, produces a product ($), and emits CO_2.

Carbon Utilization Plant	Fuel, power, and CO_2	Power and CO_2	Typical carbon utilization plant that requires fuel, power, and CO_2, and could potentially emit CO_2.
Power Plant A	Fuel	Power and CO_2	Typical power plant that requires a fuel intake, generates power to be exported to the grid ($), and emits CO_2.
Renewable Power Plant	No sinks	Power	Renewable power plant that produces power.
Carbon-Capture Plant	Fuel and CO_2	Potential CO_2	CCUS plant that captures CO_2 and could potentially generate CO_2 emissions

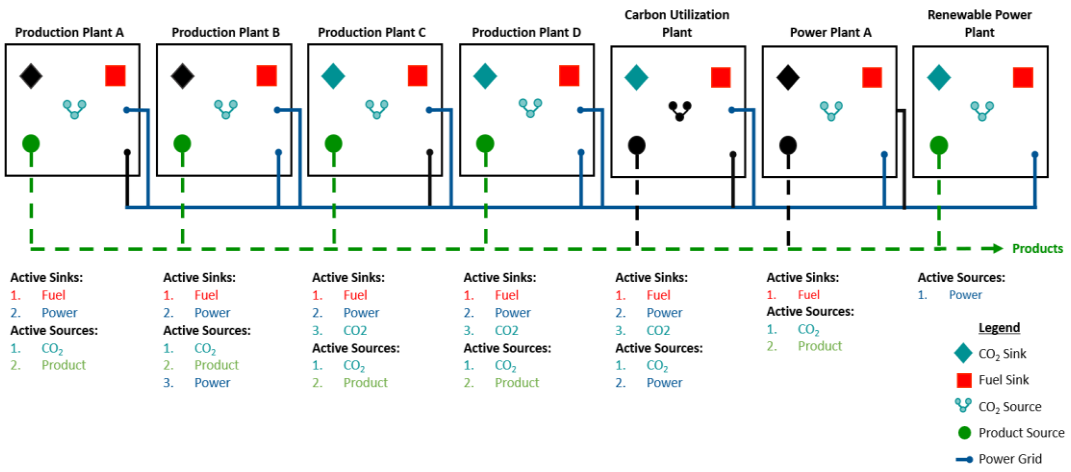

Figure 2 Summary of all possible plant types in the industrial cluster with the active sinks and sources.

An application of the superstructure optimization network on a random industrial cluster is visualized in Figure 3. The cluster in the example has the following production plants: a Liquified Natural Gas (LNG) plant (production plant

type A), which takes in fuel and power and processes products and releases CO_2, an algae plant (production type C), whereby the active sinks comprise a CO_2 sink and a fuel sink and the sources include CO_2 and products, a methanol (B) plant (production plant type D) with active power, CO_2, and fuel sinks and active power, CO_2, and product sources. A carbon utilization plant is also present, with a CO_2 active sink, a power sink, and a CO_2 active source. The whole cluster's power requirement is satisfied by the power plant which has an active fuel sink and active CO_2 and power sources.

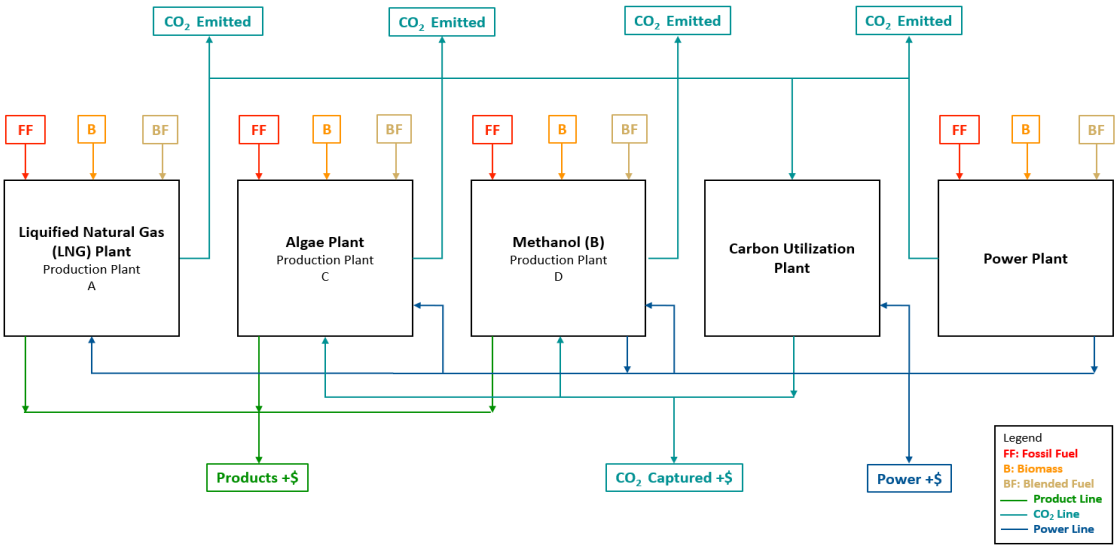

Figure 3 An example of an industrial cluster involving a set of production/power plants

3.3.The network superstructure

Because of the large number of variables involved in the optimization problem, from fuel allocation to CO_2 utilization, and power generation, a superstructure network approached is used to capture all the available configurations and determine the optimal

selection. The cluster has an infrastructure suitable for the allocation and transportation of the different types of fuels that are introduced, from natural gas, to coal, to biomass, and blended fuel. All the product streams as well as the power exported to the grid are considered as revenue streams that serve the end profit of the cluster. All active power sources are connected to the cluster's electricity grid which is supplied by the existing power plant. The CO_2 streams, treated and untreated, are connected to the CO_2 active sinks of all plants and the uncaptured CO_2 sources are emitted into the atmosphere. Taking all the aforesaid connections and networks into account, the optimization model will determine the optimal scenario that respects all constraints and results in the maximum profit for the cluster.

3.4.Model formulation

In this section, the superstructure optimization model is formulated and presented. It consists of three main parts: the sets used, the balances and constraints, and the objective function.

3.4.1. The sets

The sets used are described as follows:

P is a set of plants $\{p \mid p = 1,2,3,\ldots,N_{plants}\}$;

E is a subset of existing plants that belongs to set P $\{p \mid p = 1,2,3,...,N_{existingplants}\}$;

O is a subset of optional plants that belongs to set P $\{p \mid p = 1,2,3,...,N_{optionalplants}\}$;

C_{pr} is a set of chemical products produced in plant p $\{c \mid c = 1,2,3,...,N_{chemicalproducts}\}$;

K is a set of carbon sinks in a plant p $\{k \mid k = 1,2,3,...,N_{sinks}\}$;

S is a set of carbon sources in a plant p $\{s \mid s = 1,2,3,...,N_{sources}\}$;

PW is a set of available power types, including renewable, used to satisfy the cluster's power demand {pw | pw = 1,2,3,...,N_{power}};

$PW_{renewable}$ is a subset of the set PW, which consists of the different types of available renewable energies that can be used in the cluster {pw | pw = 1,2,3,...,$N_{renewable}$};

PW_{fuel} is a subset of the set PW, which comprises the available types of fuel derived power (whether fossil fuel, biomass or blended fuel) {pw | pw = 1,2,3,...,N_{fuel}};

FF is a set of fossil fuel options {ff | ff = 1,2,3,...,$N_{fossilfuels}$};

SF_{ff} is a subset of solid fossil fuels that belongs to set FF {ff | ff = 1,2,3,...,$N_{sfossilfuels}$};

LF_{ff} is a subset of liquid/gaseous fossil fuels that belongs to set FF {ff | ff = 1,2,3,...,$N_{lfossilfuels}$};

B is a set of biomass options {b | b = 1,2,3,...,$N_{biomass}$};

SF_b is a subset of solid biomass that belongs to set B {b | b = 1,2,3,...,$N_{sbiomass}$};

LF_b is a subset of liquid/gaseous biomass that belongs to set B {b | b = 1,2,3,...,$N_{lbiomass}$};

BF is a set of blended fuel options {bf | bf = 1,2,3,...,$N_{blendedfuel}$};

SF_{bf} is a subset of solid blended fuel that belongs to set BF {bf | bf = 1,2,3,...,$N_{sblendedfuel}$};

LF_{bf} is a subset of liquid/gaseous blended fuel that belongs to set BF {bf | bf = 1,2,3,..., $N_{lblendedfuel}$};

3.4.2. The balances and constraints

In this section, the equality and inequality constraints for the plant and integrated network superstructure are presented.

3.4.2.1.The plant balances and constraints

The chemical product flow requirement in an existing plant is given by Equations 1, 2 and 3.

$$L^{c}_{c,p} \leq F^{c}_{c,ff,p} \leq U^{c}_{c,p} \qquad \forall\ ff \in FF,\ c \in C_{pr},\ p \in E \qquad (1)$$

$$L^{c}_{c,p} \leq F^{c}_{c,b,p} \leq U^{c}_{c,p} \qquad \forall\ b \in B,\ c \in C_{pr},\ p \in E \qquad (2)$$

$$L^{c}_{c,p} \leq F^{c}_{c,bf,p} \leq U^{c}_{c,p} \qquad \forall\ bf \in BF,\ c \in C_{pr},\ p \in E \qquad (3)$$

Where, $F^{c}_{c,ff,p}$, $F^{c}_{c,b,p}$ and $F^{c}_{c,bf,p}$ (t product /d) are variables with lower bounds $L^{c}_{c,p}$ and an upper bounds $U^{c}_{c,p}$ (t product /d) that represent the flow of chemical product c associated with fossil fuel ff, biomass b and blended fuel bf, respectively, in an existing plant p.

The chemical product flow requirements in an optional plant are given by Equations 4, 5, and 6.

$$L^{c}_{c,p} I_o \leq F^{c}_{ff,c,p} \leq U^{c}_{c,p} I_o \qquad \forall\ ff \in FF,\ c \in C_{pr},\ p \in O \qquad (4)$$

$$L^{c}_{c,p} I_o \leq F^{c}_{b,c,p} \leq U^{c}_{c,p} I_o \qquad \forall\ b \in B,\ c \in C_{pr},\ p \in O \qquad (5)$$

$$L^{c}_{c,p} I_o \leq F^{c}_{bf,c,p} \leq U^{c}_{c,p} I_o \qquad \forall\ bf \in BF,\ c \in C_{pr},\ p \in O \qquad (6)$$

Where, $F^{c}_{c,ff,p}$, $F^{c}_{c,b,p}$ and $F^{c}_{c,bf,p}$ (t product /d) are variables with lower bounds $L^{c}_{c,p}$ and an upper bounds $U^{c}_{c,p}$ (t product /d) that represent the flow of chemical product c associated with fossil fuel ff, biomass b and blended fuel bf, respectively, in an optional plant p. I_p is a binary variable (0,1) used to determine the activation/deactivation of an optional plant.

The total flow of chemical product c in plant p is presented in Equation 7.

$$F^{c}_{c,p} = \sum_{ff \in FF} I_{ff,c,p} F^{c}_{c,ff,p} + \sum_{b \in B} I_{b,c,p} F^{c}_{c,b,p} + \sum_{bf \in BF} I_{bf,c,p} F^{c}_{c,bf,p} \qquad \forall\ c \in C_{pr},\ p \in P \qquad (7)$$

Where, $F^{c}_{c,p}$ (t product /d) is the total flow of the chemical product c. $I_{ff,c,p}$, $I_{b,c,p}$, and $I_{bf,c,p}$ are the binary variables (0,1) associated to each fossil fuel ff, biomass b, and blended fuel bf for each product c in plant p. Only one type of fuel will be allocated to each production plant p, as shown in Equation 8

$$\sum_{ff \in FF} I_{ff,c,p} + \sum_{b \in B} I_{b,c,p} + \sum_{bf \in BF} I_{bf,c,p} = 1 \qquad \forall\ c \in C_{pr},\ p \in P \qquad (8)$$

The chemical product c to fossil fuel ff , biomass b, and blended fuel bf intakes are described in Equations 9, 10, and 11.

$$F^{c}_{ff,p} = \sum_{c \in C_{pr}} I_{ff,c,p} F^{c}_{c,ff,p} \alpha^{c}_{ff,c,p} \qquad \forall\ ff \in FF,\ p \in P \qquad (9)$$

$$F^{c}_{b,p} = \sum_{c \in C_{pr}} I_{b,c,p} F^{c}_{c,b,p} \alpha^{c}_{b,c,p} \qquad \forall\ b \in B,\ p \in P \qquad (10)$$

$$F^{c}_{bf,p} = \sum_{c \in C_{pr}} I_{bf,c,p} F^{c}_{c,bf,p} \alpha^{c}_{bf,c,p} \qquad \forall\ bf \in BF,\ p \in P \qquad (11)$$

Where, $F^{c}_{ff,p}$ (t fossil fuel/d), $F^{c}_{b,p}$ (t biomass/d), and $F^{c}_{bf,p}$ (t blended fuel/d) represent the fossil fuel ff, biomass b and blended fuel bf flows to a plant p. $\alpha^{c}_{ff,c,p}$ (t fossil fuel/t product), $\alpha^{c}_{ff,c,p}$ (t biomass/t product), and $\alpha^{c}_{ff,c,p}$ (t blended fuel/t product) are parameters that represent the amount of fossil fuel ff, biomass b and blended fuel bf required for the production of chemical product c in plant p.

The maximum CO_2 emitted from chemical products in the industrial cluster depends on the type of fuel used and is determined by Equation 12.

$$M^{c}_{s,c,p} = \sum_{ff \in FF} I_{ff,c,p} F^{c}_{ff,c,p} \beta^{c}_{ff,s,c,p} + \sum_{b \in B} I_{b,c,p} F^{c}_{b,c,p} \beta^{c}_{b,s,c,p} + \sum_{bf \in BF} I_{bf,c,p} F^{c}_{bf,c,p} \beta^{c}_{bf,s,c,p} \quad \forall\, s \in S, c \in C_{pr}, p \in P \qquad (12)$$

Where, $M^{c}_{s,c,p}$ (t CO_2/d) is the maximum CO_2 emitted. $\beta^{c}_{ff,s,c,p}$ (t CO_2/t product), $\beta^{c}_{b,s,c,p}$ (t CO_2/t product), and $\beta^{c}_{bf,s,c,p}$ (t CO_2/t product) are parameters, associated with the fuel type, representing the CO_2 emissions from a source s through the production of product c in plant p.

The total carbon emitted during the production of the products in the cluster is shown in Equation 13.

$$M_{production} = \sum_{p \in P} \sum_{c \in C_{pr}} \sum_{s \in S} M^{c}_{s,c,p} \qquad (13)$$

Where, $M_{production}$(t CO_2/d) is the total amount of carbon emitted during the production of products c in the industrial cluster.

The electricity requirements of a product c in a plant p is calculated as represented in Equation 14.

$$PW_{pw,c,p} = \sum_{ff \in FF} I_{pw,ff} F^{c}_{c,ff,p} \varphi^{pw}_{pw,ff,c,p} + \sum_{b \in B} I_{pw,b} F^{c}_{c,b,p} \varphi^{pw}_{pw,b,c,p} + \sum_{bf \in BF} I_{bf,pw} F^{c}_{c,bf,p} \varphi^{pw}_{pw,bf,c,p} \quad \forall\, pw \in PW_{fuel},\ c \in C_{pr}, p \in P \qquad (14)$$

Where, $PW_{pw,c,p}$ (kWh/d) is the electricity requirement of a product c in a plant p, derived from power type pw. $\varphi^{pw}_{pw,ff,c,p}$, $\varphi^{pw}_{pw,b,c,p}$, and $\varphi^{pw}_{pw,bf,c,p}$ (kWh/t product) are the power requirements per product c. $I_{pw,ff}$, $I_{pw,b}$, and $I_{pw,bf}$ are the binary variables (0,1) associated to the type of fuel used in the power generation of the cluster. Only one type of fuel derived power plant will be included, requiring the sum of the binaries to be equal to 1, as shown in Equation 15.

$$\sum_{ff\in FF} I_{ff,pw} + \sum_{b\in B} I_{b,pw} + \sum_{bf\in BF} I_{bf,pw} = 1 \tag{15}$$

The total electricity required in the cluster $PW^{required}_{cluster}$ (kWh/d) is described in Equation 16.

$$PW^{required}_{cluster} = \sum_{p\in P} \sum_{c\in C_{pr}} \sum_{pw\in PW_{fuel}} PW_{pw,c,p} \tag{16}$$

The total power exported to the grid is given by Equation 17. In this model, the power exported is assumed to be derived from the fuel-based power plants, therefore belonging to the set PW_{fuel}.

$$PW^{exp} = \sum_{ff\in FF} \sum_{pw\in PW_{fuel}} I_{pw,ff} PW^{exp} + \sum_{b\in B} \sum_{pw\in PW_{fuel}} I_{pw,b} PW^{exp} + \sum_{bf\in FF} \sum_{pw\in PW_{fuel}} I_{pw,bf} PW^{exp} \tag{17}$$

Where, PW^{exp} (kWh/d) is the power exported to the grid. It is bounded by a lower bound L^{exp}_{power} (kWh/d) and an upper bound U^{exp}_{power} (kWh/d), as shown in Equation 18.

$$L^{exp}_{power} \leq PW^{exp} \leq U^{exp}_{power} \quad (18)$$

The option of replacing part of the fuel-derived required power by renewable power is also integrated, as represented in Equations 19 and 20.

$$PW_{renewable,pw} = \%_{renewable} \sum_{pw \in PW_{renewable}} I_{pw,renewable} \; PW^{required}_{cluster} \qquad \forall\, pw \in PW_{renewable} \quad (19)$$

Where, $PW_{renewable,pw}$ (kWh/d) is the renewable power that will replace a fraction of the fuel-derived power, $\%_{renewable}$ is the percentage of the required power that can be replaced by a renewable source, and $I_{pw,renewable}$ is the binary variable (0,1) associated to the type of renewable energy that is integrated into the cluster. The integration of one type of renewable energy is considered in this formulation as shown in Equation 20.

$$\sum_{pw \in PW_{renewable}} I_{pw,renewable} = 1 \quad (20)$$

The total available power in the cluster is represented in Equation 21.

$$PW_{cluster} = PW^{required}_{cluster}(1 - \%_{renewable}) + PW^{exp} + PW^{renewable} \quad (21)$$

Where, $PW_{cluster}$ (kWh/d) is the total power available in the industrial cluster and can consist of a combination of renewable energy and fuel derived energy.

The fossil fuel, biomass, or blended fuel required for the total power generation in the cluster are given by Equations 22, 23, and 24.

$$F_{ff}^{pw} = \sum_{ff \in FF} \sum_{pw \in PW_{fuel}} I_{pw,ff}(PW_{cluster}^{required} + PW_{exp})\alpha_{pw,ff}^{pw} \quad (22)$$

$$F_{b}^{pw} = \sum_{b \in B} \sum_{pw \in PW_{fuel}} I_{pw,b}(PW_{cluster}^{required} + PW_{exp})\alpha_{pw,b}^{pw} \quad (23)$$

$$F_{bf}^{pw} = \sum_{bf \in BF} \sum_{pw \in PW_{fuel}} I_{pw,bf}(PW_{cluster}^{required} + PW_{exp})\alpha_{pw,bf}^{pw} \quad (24)$$

Where, F_{ff}^{pw} (t fossil fuel/d), F_{bf}^{pw}(t biomass/d), and F_{bf}^{pw} (t blended fuel/d) are the fuel required for the power production. $\alpha_{pw,ff}^{pw}$ (kWh/t fossil fuel), $\alpha_{pw,b}^{pw}$ (kWh/t biomass), and $\alpha_{pw,bf}^{pw}$ (kWh/t blended fuel) are the fuel to power parameters used to determine the amount of fuel required for the total power generation of the cluster.

The carbon emitted during the power generated to satisfy the cluster's demand is described in Equation 25.

$$M_{required}^{pw} = \sum_{s \in S} \sum_{ff \in FF} \sum_{pw \in PW_{fuel}} I_{pw,ff}\, \beta_{pw,ff,s}^{pw}\, PW_{cluster}^{required} + \sum_{s \in S} \sum_{b \in B} \sum_{pw \in PW_{fuel}} I_{pw,b}\, \beta_{pw,b,s}^{pw}\, PW_{cluster}^{required} + \sum_{s \in S} \sum_{bf \in BF} \sum_{pw \in PW_{fuel}} I_{pw,bf}\, \beta_{pw,bf,s}^{pw}\, PW_{cluster}^{required} \quad (25)$$

Where, $M_{required}^{pw}$ (tCO_2/d) is the carbon emitted during the generation of the required power. $\beta_{pw,ff,s}^{pw}$, $\beta_{pw,b,s}^{pw}$, and $\beta_{pw,bf,s}^{pw}$(t CO_2/ kWh) are, respectively, the fossil fuel

ff, biomass b, and blended fuel bf parameters associated with the amount of carbon emitted during the generation of power.

The carbon emitted after the integration of renewable energy is represented in Equation 26.

$$M_{required}^{pw,renewable} =$$

$$\sum_{s\in S}\sum_{ff\in FF}\sum_{pw\in PW_{fuel}} I_{pw,ff}\,\beta_{pw,ff,s}^{pw}\,PW_{cluster}^{required}\,(1-\%_{renewable})$$

$$+\sum_{s\in S}\sum_{b\in B}\sum_{pw\in PW_{fuel}} I_{pw,b}\,\beta_{pw,b,s}^{pw}\,PW_{cluster}^{required}\,(1-\%_{renewable}) \quad (26)$$

$$+\sum_{s\in S}\sum_{bf\in BF}\sum_{pw\in PW_{fuel}} I_{pw,bf}\,\beta_{pw,bf,s}^{pw}\,PW_{cluster}^{required}\,(1-\%_{renewable})$$

Where, $M_{required}^{pw,renewable}$ (t CO_2/d) is the carbon emitted after the integration of a renewable source of energy into the cluster.

The carbon emitted during the generation of the power to be exported is represented in Equation 27.

$$M_{exp}^{pw} = \sum_{s\in S}\sum_{ff\in FF}\sum_{pw\in PW_{fuel}} I_{pw,ff}\,\beta_{pw,ff,s}^{pw}PW_{ff}^{exp} +$$

$$\sum_{s\in S}\sum_{b\in B}\sum_{pw\in PW_{fuel}} I_{pw,b}\,\beta_{pw,b,s}^{pw}PW_{b}^{exp} + \quad (27)$$

$$\sum_{s\in S}\sum_{bf\in BF}\sum_{pw\in PW_{fuel}} I_{pw,bf}\,\beta_{pw,bf,s}^{pw}PW_{bf}^{exp}$$

Where, M_{exp}^{pw} (tCO_2/d) represents the carbon emitted during the generation of the power to be exported.

The total carbon emitted for all power generation in the cluster before the integration of renewable energy is given by Equation 28.

$$M_{power}=M_{production}+ M_{exp}^{pw}+ M_{required}^{pw} \tag{28}$$

Where, M_{power} (tCO_2/d) is the total carbon emitted during the whole power generation of the cluster before the integration of renewable energy.

The total carbon emitted for all power generation in the cluster after the possible integration of renewable energy is given by Equation 29.

$$M_{power}^{pw,renewable}=M_{production}+ M_{exp}^{pw}+ M_{required}^{pw,renewable} \tag{29}$$

Where, $M_{power}^{pw,renewable}$ (tCO_2/d) is the total carbon emitted during the whole power generation of the cluster after the integration of renewable energy.

The carbon emitted during the transportation of solid fuels to a plant p in the industrial cluster is represented in Equation 30.

$$F_{transport}^{CO_2}= \sum_{ff\in SF_{ff}} I_{ff,pw}F_{ff}^{pw}\beta_{ff,transport} + \sum_{p\in P}\sum_{c\in C_{pr}} I_{ff,c,p}F_{ff,p}^{c}\beta_{ff,transport} + \sum_{b\in SF_b} I_{b,pw}F_{b}^{pw}\beta_{b,transport} + \sum_{p\in P}\sum_{c\in C_{pr}} I_{b,c,p}F_{b,p}^{c}\beta_{b,transport} \tag{30}$$

$$+\sum_{bf\in SF_{bf}} I_{bf,pw} F_{bf}^{pw} \beta_{bf,transport} +$$

$$\sum_{p\in P}\sum_{c\in C_{pr}} I_{bf,c,p} F_{bf,p}^{c} \beta_{bf,transport}$$

Where, $F_{transport}^{CO_2}$ (t CO_2/d) is the carbon emitted during the transportation of a solid fossil fuel into the cluster. $\beta_{ff,transport}$, $\beta_{b,transport}$, and $\beta_{bf,transport}$ (t CO_2/t solid fuel) are the parameters associated with the amount of carbon emitted during the transport of solid fuel into the industrial cluster.

The total carbon emitted throughout the cluster before the integration of carbon capture and utilization technologies, and before the possibility of introducing renewable energy, consists of the sum of the carbon emitted during production, power generation and transport of solid fuels. It is summarized in Equation 31.

$$CE_{pre\text{-}capture} = M_{production} + MW_{exp}^{pw} + MW_{required}^{pw} + F_{transport}^{CO_2} \quad (31)$$

Where, $CE_{pre\text{-}capture}$ (t CO_2/d) is the total amount of carbon emitted in the cluster before the renewable integration.

The total carbon emitted throughout the cluster before the integration of carbon capture and utilization technologies, but after the possibility of introducing renewable energy, consists of the sum of the carbon emitted during production, power generation and transport of solid fuels. It is summarized in Equation 32.

$$CE_{pre\text{-}capture}^{renewable} = M_{production} + MW_{exp}^{pw} + MW_{required}^{pw,renewable} + F_{transport}^{CO_2} \quad (32)$$

Where, $CE^{renewable}_{pre\text{-}capture}$ (t CO_2/d) is the total amount of carbon emitted in the cluster, post renewable integration.

3.4.2.2.The network superstructure

The CO_2 captured from a source s emitted either during the production of product c in plant p or during the generation of power depends on the type of fuel used and is represented accordingly in Equations 33.

$$R_{s,p} = \sum_{ff\in FF} R_{ff,s,c,p} + \sum_{b\in B} R_{b,s,c,p} + \sum_{bf\in BF} R_{bf,s,c,p} + \sum_{ff\in FF} \sum_{pw\in PW_{fuel}} R_{pw,ff,s} + \sum_{b\in B} \sum_{pw\in PW_{fuel}} R_{pw,b,s} + \sum_{bf\in BF} \sum_{pw\in PW_{fuel}} R_{pw,bf,s} \quad \forall\, s\in S,\ c\in C,\ p\in P \qquad (33)$$

Where, $R_{s,p}$ (tCO_2/d) is the CO_2 captured from a source s. $R_{ff,s,c,p}$, $R_{b,s,c,p}$, $R_{bf,s,c,p}$, $R_{pw,ff,s}$, $R_{pw,b,s}$, and $R_{pw,bf,s}$ (t CO2/d) are variables that represent the captured CO_2 from the use of fossil fuel ff, biomass b, and blended fuel bf respectively, for either the production of products c or the power generation in the cluster.

The upper and lower bounds $L^{carbon}_{ff,s,c,p}$, $L^{carbon}_{b,s,c,p}$, $L^{carbon}_{bf,s,c,p}$, $L^{carbon}_{pw,ff}$, $L^{carbon}_{pw,b}$, $L^{carbon}_{pw,bf}$ (t CO_2/d) of the fuel dependent captured carbon are shown in Equations 34, 35, 36, 37, 38, and 39 respectively. The upper bound is the summation of all emissions generated during the production of products and the generation of power.

$$L^{carbon}_{ff,s,c,p} \le R_{ff,s,c,p} \le F^{c}_{ff,c,p}\beta^{c}_{ff,s,c,p} + F^{p}_{ff,c,p}\beta^{p}_{ff,s,c,p} \quad \forall\, ff\in FF,\ s\in S,\ c\in C,\ p\epsilon \qquad (34)$$

$$L^{carbon}_{b,s,c,p} \leq R_{b,s,c,p} \leq F^{c}_{b,c,p}\beta^{c}_{b,s,c,p} + F^{p}_{b,c,p}\beta^{p}_{b,s,c,p} \quad \forall\ b\in B,\ s\in S,\ c\in C,\ p\in P \tag{35}$$

$$L^{carbon}_{bf,s,c,p} \leq R_{bf,s,c,p} \leq F^{c}_{bf,c,p}\beta^{c}_{bf,s,c,p} + F^{p}_{bf,c,p}\beta^{p}_{bf,s,c,p} \quad \forall\ bf\in BF,\ s\in S,\ c\in C,\ p\in P \tag{36}$$

$$L^{carbon}_{pw,ff} \leq R_{pw,ff,s} \leq I_{pw,ff}\beta^{pw}_{pw,ff,s}PW^{required}_{cluster} \quad \forall\ pw\in PW_{fuel},\ ff\in FF,\ s\in S, \tag{37}$$

$$L^{carbon}_{pw,b} \leq R_{pw,b,s} \leq I_{pw,b}\beta^{pw}_{pw,b,s}PW^{required}_{cluster} \quad \forall\ pw\in PW_{fuel},\ b\in B,\ s\in S, \tag{38}$$

$$L^{carbon}_{pw,bf} \leq R_{pw,bf,s} \leq I_{pw,bf}\beta^{pw}_{pw,bf,s}PW^{required}_{cluster} \quad \forall\ pw\in PW_{fuel},\ bf\in BF,\ s\in S, \tag{39}$$

The captured carbon mass balance is shown in Equation 40.

$$R_{s,p} = \sum_{k\in K}\left(T_{s,k,p} + \sum_{ff\in FF} G_{ff,k,c,s,p} + \sum_{b\in B} G_{b,k,s,c,p} + \sum_{bf\in BF} G_{bf,k,s,c,p} + \sum_{ff\in FF} G_{ff,k,s,pw} + \sum_{b\in B} G_{b,k,s,pw} + \sum_{bf\in BF} G_{bf,k,s,pw}\right) \quad \forall\ c\in C,\ pw\in PW,\ s\in S,\ p\in P \tag{40}$$

Where, $T_{s,k,p}$ (t CO_2/d) represents the treated CO_2 flow from source s (either from the production of product c or the generation of power pw) that is allocated to sink k. $G_{ff,k,s,c,p}$, $G_{b,k,s,c,p}$ and $G_{bf,k,s,c,p}$ (t CO_2/d) represent the untreated CO_2 flows associated with the type of fuel and product c in a production plant p, and $G_{ff,k,s,pw}$, $G_{b,k,s,pw}$, and

$G_{bf,k,s,pw}$ (t CO_2/d) represent the untreated CO_2 flows associated with the power production pw in the cluster.

The total carbon that is treated in the cluster is represented in the mass balance shown in Equation 41.

$$T_{cluster} = \sum_{p \in P} \sum_{k \in K} \sum_{s \in S} T_{s,k,p} \tag{41}$$

Where, $T_{cluster}$ (tCO_2/d) represents the total amount of carbon treated in the cluster and sent to sink k.

The carbon emitted during the treatment of flows in the cluster is represented in Equation 42.

$$M_{treatment} = T_{cluster} \gamma_{treatment} \tag{42}$$

Where, $M_{treatment}$ (t CO_2/d) is the amount of carbon emitted during the treatment process. $\gamma_{treatment}$ (t CO_2 emitted/ t CO_2 treated) is the treatment efficiency.

Each source s is being sent to a sink k. The flow and concentration requirements of each sink k should be respected. The sink flow requirement and the concentration requirement are depicted in Equations 43 and 44 respectively.

$$F_{k,p} \leq \frac{F_{k,p}^{max}}{z_{k,p}} \qquad \forall\, k \in K,\ p \in P \tag{43}$$

Where, $F_{k,p}$ (t CO_2 mix/d) is the flow into sink k from plant p. $F_{k,p}^{max}$ (t CO_2 /d) is the CO_2 flow into sink k and $z_{k,p}$ (t CO_2/ t CO_2 stream) is the minimum required CO_2 concentration of a sink k. The CO_2 flow into the sink should meet the minimum requirement for each sink.

$$T_{s,k,p}+\sum_{s\in S}\sum_{k\in K}\Big(\sum_{ff\in FF}G_{ff,k,s,c,p}+\sum_{b\in B}G_{b,k,s,c,p}+\sum_{bf\in BF}G_{bf,k,s,c,p}$$

$$+\sum_{ff\in FF}G_{ff,k,s,pw}+\sum_{b\in B}G_{b,k,s,pw}+\sum_{bf\in BF}G_{bf,k,s,pw}\Big)\ \geq\ F_{k,p}^{max} \qquad \forall\ k\in K,\ p\in P \qquad (44)$$

The sink balance is represented in Equation 45.

$$\frac{T_{s,k,p}}{y_{s,k,p}}+\sum_{s\in S}\sum_{k\in K}\Big(\sum_{ff\in FF}\frac{G_{ff,k,s,c,p}}{y_{ff,s,c,p}}+\sum_{b\in B}\frac{G_{b,k,s,c,p}}{y_{b,s,c,p}}+\sum_{bf\in BF}\frac{G_{bf,k,s,c,p}}{y_{bf,s,c,p}}$$

$$+\sum_{ff\in FF}\frac{G_{ff,k,s,pw}}{y_{ff,s,pw}}+\sum_{b\in B}\frac{G_{b,k,s,pw}}{y_{b,s,pw}}+\sum_{bf\in BF}\frac{G_{bf,k,s,pw}}{y_{bf,s,pw}}\Big)=F_{k,p} \qquad \forall\ k\in K,\ p\in P \qquad (45)$$

Where, $y_{s,k,p}$, $y_{ff,s,c,p}$, $y_{b,s,c,p}$, $y_{bf,s,c,p}$, $y_{ff,s,pw}$, $y_{b,s,pw}$, and $y_{bf,s,pw}$ are the CO_2 concentrations of the treated and untreated streams respectively.

The carbon emitted from the sinks is calculated in Equation 46.

$$M_{sinks}=\sum_{p\in P}\sum_{k\in K}F_{k,p}\eta_{k,p} \qquad (46)$$

Where, M_{sinks} (t CO_2/d) is the total amount of carbon emitted from the sinks. $\eta_{k,p}$ (t CO_2 out/ t CO_2 into sink) is a parameter that represents the ratio of emitted carbon per carbon into the sink.

The mass balance around the fossil fuel biomass flow, and blended fuel flow F_{bf} into the industrial cluster are presented in Equations 47, 48 and 49, respectively.

$$F_{ff}=\ I_{ff,pw}F_{pw}^{ff}+\sum_{p\in P}\sum_{c\in C_{pr}}I_{ff,c,p}F_{ff,p}^{c} \qquad \forall\ ff\in FF \qquad (47)$$

$$F_b = I_{b,pw}F^b_{pw} + \sum_{p\in P}\sum_{c\in C_{pr}} I_{b,c,p}F^c_{b,p} \qquad \forall\ b\in B \qquad (48)$$

$$F_{bf} = I_{bf,pw}F^{bf}_{pw} + \sum_{p\in P}\sum_{c\in C_{pr}} I_{bf,c,p}F^c_{bf,p} \qquad \forall\ bf\in BF \qquad (49)$$

Where, F_{ff} (t fossil fuel/d), F_b (t biomass/d), F_{bf} (t blended fuel/d) are the total fuel flows into the city.

The maximum fossil fuel, biomass and blended fuel available are shown in Equations 50, 51, and 52 respectively.

$$0 \le F_{ff} \le MF_{ff} \qquad \forall\ ff\in FF \qquad (50)$$

$$0 \le F_b \le MF_b \qquad \forall\ b\in B \qquad (51)$$

$$0 \le F_{bf} \le MF_{bf} \qquad \forall\ bf\in BF \qquad (52)$$

The total carbon emitted into the atmosphere post capture CE (t CO_2/d) is represented in Equation 53. It consists of the carbon captured pre-capture, the carbon released during the sink processing, treatment, and transport of fuel into the city subtracted by the amount of carbon captured.

$$CE_{\text{post capture}} = CE^{\text{renewable}}_{\text{pre capture}} - \sum_{p\in P}\sum_{s\in S} R_{s,p} + M_{\text{treatment}} + M_{\text{sinks}} \qquad (53)$$

The carbon captured should respect the set carbon constraint in the cluster as represented in Equation 54.

$$\sum_{p\in P}\sum_{s\in S} R_{s,p} \geq NCCR\ CE^{renewable}_{pre\ capture} \quad (54)$$

Where, NCCR is the net carbon capture rate (%) imposed onto the cluster to meet the set CO_2 emission limit.

3.4.2.3.The objective function

The objective of this optimization model is to find the optimal allocation of different fuel types to maximize the profit of the carbon-constrained industrial cluster. The revenue streams considered are the revenues generated from the products, the power exported, and any sink products associated to the captured CO_2. The cost streams consist of the costs of the fuels, the capital and operating costs of the existing and optional plants, the CO_2 transportation, capture, treatment and compression and pumping.

The objective function is described in Equation 55.

$$\text{Profit (\$/y)} = REV^{c} + REV^{pw} + REV^{CO_2} \quad (55)$$

$$- (Cost^{ff}+Cost^{b}+Cost^{bf})$$

$$- (Cost^{E}+Cost^{O})$$

$$- (Cost^{transport,CO_2} + Cost^{capture,untreated}$$

$$+ Cost^{capture,\ treated} + Cost^{compression,\ pumping})$$

Where, REV^{c} (\$/y) is the revenue from the products produced in the industrial cluster, as depicted in Equation 56. dy is the conversion from days to year, assuming the

cluster is operating 24/7. C^c ($/t product) is a parameter that represents the price of the products generated in the industrial city.

$$REV^c = dy \sum_{p \in P} \sum_{c \in C_{pr}} F^c_{c,p} C^c \quad (56)$$

$$dy = 1 \text{ day} \times \frac{365 \text{ days}}{\text{year}} \quad (57)$$

REV^{pw} ($/y) is the revenue from the power exported to the grid, as shown in Equation 58. C^{pw} ($/kWh) is a parameter that represents the price of the power generated in the industrial city.

$$REV^{pw} = dy\ (PW^{exp} C^{pw}) \quad (58)$$

REV^{CO_2} ($/y) is the revenue from the captured carbon in the cluster. $C^{CO_2}_{k,p}$ ($/t CO_2) is a parameter representing the revenue/cost of the carbon utilization method, as represented in Equation 59.

$$REV^{CO_2} = dy \left(\sum_{p \in P} \sum_{k \in K} F_{k,p} C^{CO_2}_{k,p} \right) \quad (59)$$

$Cost^{ff}$ ($/y), $Cost^b$($/y), and $Cost^{bf}$($/y) are the costs of fossil fuel, biomass, and blended fuel used in the industrial city and are presented in Equations 60, 61, and 62. C^{ff} ($/t fossil fuel), C^b ($/t biomass), and C^{bf} ($/t blended fuel) are parameters that represent the fuels' respective costs.

$$Cost^{ff} = \sum_{ff \in FF} F_{ff} C^{ff} dy \quad (60)$$

$$\text{Cost}^{b} = \sum_{b \in B} F_b C^b dy \tag{61}$$

$$\text{Cost}^{bf} = \sum_{bf \in BF} F_{bf} C^{bf} dy \tag{62}$$

Cost^{E} and Cost^{O} ($/y) are the respective costs of existing and optional plants in the industrial cluster and are shown in Equations 63 and 64. CRF is the capital recovery factor, represented in Equation 65 (D. Al-Mohannadi, 2014). $C_{c,p}^{capex}$($/t product) and $C_{c,p}^{opex}$ ($/t product) are the capital cost and operating cost associated with production of product c. hy is the conversion from hours to years. $C_{ff,pw}^{capex}$ ($/kWh), $C_{b,pw}^{capex}$ ($/kWh), and $C_{bf,pw}^{capex}$ ($/kWh) and $C_{ff,pw}^{opex}$ ($/kWh), $C_{b,pw}^{opex}$($/kWh), and $C_{bf,pw}^{opex}$($/kWh) are the respective capital and operating costs associated with the power generation in the cluster. C_{pw}^{capex} ($/kWh) and C_{pw}^{opex} ($/kWh) are the capital and operating costs associated to the renewable plant in the cluster.

$$\begin{aligned}\text{Cost}^{E} = \text{CRF} * dy * \sum_{p \in E} \sum_{c \in C_{pr}} C_{c,p}^{capex} F_{c,p}^{c} + hy \sum_{p \in E} \sum_{c \in C_{pr}} C_{c,p}^{opex} F_{c,p}^{c} \\ +\text{CRF}*dy \left(\sum_{ff \in FF} C_{ff,pw}^{capex} I_{pw,ff} \left(PW_{cluster}^{required} + PW_{exp} \right) \right. \\ \left. + \sum_{b \in B} C_{b,pw}^{capex} I_{pw,b} \left(PW_{cluster}^{required} + PW_{exp} \right) + \sum_{bf \in FF} C_{bf,pw}^{capex} I_{pw,bf} \left(PW_{cluster}^{required} + PW_{exp} \right) \right. \\ +hy \left(\sum_{ff \in FF} C_{ff,pw}^{opex} I_{pw,ff} \left(PW_{cluster}^{required} + PW_{exp} \right) \right.\end{aligned} \tag{63}$$

$$+\sum_{b\in B} C_{b,pw}^{opex} I_{pw,b}\left(PW_{cluster}^{required}+PW_{exp}\right)+\sum_{bf\in FF} C_{bf,pw}^{opex} I_{pw,bf}(PW_{cluster}^{required}+PW_{exp}))$$

$$+CRF*dy*\sum_{pw\in PW_{renewable}} I_{pw,renewable}\, C_{pw}^{capex} PW_{renewable}$$

$$+hy*\sum_{pw\in PW_{renewable}} I_{pw,renewable} C_{pw}^{opex}\, PW_{renewable}$$

$$Cost^{O} = CRF * dy * \sum_{p\in O}\sum_{c\in C_{pr}} C_{c,p}^{capex,pr} F_{c,p}^{c} + hy \sum_{p\in O}\sum_{c\in C_{pr}} C_{c,p}^{opex}\ F_{c,p}^{c}$$

$$+CRF*dy\ (\sum_{ff\in FF} C_{ff,pw}^{capex} I_{pw,ff}\left(PW_{cluster}^{required}+PW_{exp}\right)$$

$$+\sum_{b\in B} C_{b,pw}^{capex} I_{pw,b}\left(PW_{cluster}^{required}+PW_{exp}\right)+\sum_{bf\in FF} C_{bf,pw}^{capex} I_{pw,bf}\left(PW_{cluster}^{required}+PW_{exp}\right) \quad (64)$$

$$+hy(\sum_{ff\in FF} C_{ff,pw}^{opex} I_{pw,ff}\left(PW_{cluster}^{required}+PW_{exp}\right)$$

$$+\sum_{b\in B} C_{b,pw}^{opex} I_{pw,b}\left(PW_{cluster}^{required}+PW_{exp}\right)+\sum_{bf\in FF} C_{bf,pw}^{opex} I_{pw,bf}(PW_{cluster}^{required}+PW_{exp}))$$

$$CRF=\frac{i(1+i)^{n}}{(1+i)^{n}-1} \quad (65)$$

Where, CRF will be fixed for a discount rate i (%) of 20% and a production plant lifetime n (y) of 20 y and a power plant lifetime of 40y (AlNouss et al., 2019).

$Cost^{transport,CO_2}$ ($/y) is the cost associated with the transport of both treated and untreated CO_2, as shown in Equation 66. It is calculated based on the distance between

each sink k and source s. $C_{s,k}^{CO_2\ transport}$ (\$/t CO_2 transported) is a variable that represents the cost per ton of CO_2 transported, depending on the distance $d_{s,k,p}$ (km) and the transport cost $C_{transport}$ (\$/t CO_2). It is calculated as seen in Equation 67.

$$Cost^{transport,CO_2} = \sum_{p\in P}\sum_{k\in K}\sum_{s\in S} C_{s,k}^{CO_2\ transport} F_{k,p} \quad (66)$$

$$C_{s,k}^{CO_2\ transport} = d_{s,k,p} C_{transport} \qquad \forall\ s\in S,\ k\in K,\ p\in P \quad (67)$$

$Cost^{capture,untreated}$ (\$/y) is the cost of capturing the untreated emitted CO_2 from plant p during the production of product c as represented in Equation 68. $C_{c,p}^{capture}$ (\$/t CO_2) is a parameter associated with the cost of capturing the emitted CO_2.

$$Cost^{capture,untreated} = dy \sum_{p\in P}\sum_{c\in C}\sum_{k\in K}\sum_{s\in S}\Big(\sum_{ff\in FF} G_{ff,s,k,c,p} C_{c,p}^{capture} + \sum_{b\in B} G_{b,s,k,c,p} C_{c,p}^{capture} + \sum_{bf\in BF} G_{bf,s,k,c,p} C_{c,p}^{capture}\Big) + \sum_{k\in K}\sum_{s\in S}\Big(\sum_{ff\in FF} C_{pw}^{capture} G_{ff,s,k,pw} + \sum_{b\in B} C_{pw}^{capture} G_{b,s,k,pw} + \sum_{bf\in BF} C_{pw}^{capture} G_{bf,s,k,pw}\Big) \quad (68)$$

$Cost^{capture,treated}$ (\$/y) is the cost of capturing and treating the emitted CO_2 as shown in Equation 69. $C_{c,p}^{treatment,capex}$ is the capital cost and $C_{c,p}^{treatment,opex}$ is the operating cost of treating the captured CO_2 during the production of product c in plant p.

$$Cost^{capture,treated} = dy\ CRF\Big(\sum_{p\in P}\sum_{k\in K}\sum_{c\in C}\sum_{s\in S} T_{s,c,k,p}\ C_{c,p}^{treatment,capex} \quad (69)$$

$$+\sum_{p\in P}\sum_{c\in C}\sum_{s\in S} T_{s,c,p} C_{c,p}^{treatment,capex}) + hy(\sum_{p\in P}\sum_{k\in K}\sum_{c\in C}\sum_{s\in S} T_{s,c,k,p}\, C_{c,p}^{treatmen}$$

$$+\sum_{p\in P}\sum_{c\in C}\sum_{s\in S} T_{s,c,p} C_{c,p}^{treatment,opex})$$

$Cost^{compression,\ pumping}$ of the CO_2 stream is calculated in Equation 70. It consists of the sum of $Cost_{treated}^{compression,pumping}$, the cost of compressing and pumping the treated flows, and $Cost_{untreated}^{compression,pumping}$, the cost of compressing and pumping the untreated flows, as shown in Equations 71 and 74 respectively. The cost of compressing and pumping carbon depends on two cost factors, the capex $Cost_{treated,\ capex}^{compression,pumping}$, and $Cost_{untreated,\ capex}^{compression,pumping}$and the opex $Cost_{treated,\ opex}^{compression,pumping}$, $Cost_{untreated,\ opex}^{compression,pumping}$ (respectively, 72,75, 73, and 76). The correlation is obtained from (D. M. Al-Mohannadi et al., 2017) and is dependent on the amount of flow, the sink type, and the flow type (treated or untreated). $a_{s,k,p}^{capex}$, $b_{s,k,p}^{capex}$, $a_{s,k,p}^{opex}$, and $b_{s,k,p}^{opex}$ are cost parameters associated with the capital costs and operational costs of the compression and pumping processes.

$$Cost^{compression,pumping} = C_{treated}^{compression,\ pumping} + C_{untreated}^{compression,\ pumping} \quad (70)$$

$$Cost_{treated}^{compression,pumping} = C_{treated,capex}^{compression,\ pumping} + C_{treated,opex}^{compression,\ pumping} \quad (71)$$

$$Cost_{treated,\ capex}^{compression,pumping} = \sum_{p\in P}\sum_{k\in K}\sum_{s\in S} a_{s,k,p}^{capex} T_{s,k,p} + b_{s,k,p}^{capex} \quad (72)$$

$$Cost_{treated,opex}^{compression,pumping} = \sum_{p\in P}\sum_{k\in K}\sum_{s\in S} a_{s,k,p}^{opex} T_{s,k,p} + b_{s,k,p}^{opex} \quad (73)$$

$$Cost^{compression,pumping}_{untreated} = C^{compression,\ pumping}_{untreated,capex} + C^{compression,\ pumping}_{untreated,opex} \quad (74)$$

$$Cost^{compression,pumping}_{untreated,\ capex} = \sum_{p\in P}\sum_{k\in K}\sum_{s\in S} a^{capex}_{s,k,p} \sum_{c\in C}\Big(\sum_{ff\in FF} G_{ff,s,k,c,p} + \sum_{b\in B} G_{b,s,k,c,p} + \sum_{bf\in BF} G_{bf,s,k,c,p}\Big) + b^{capex}_{s,k,p} \quad (75)$$

$$+ \sum_{k\in K}\sum_{s\in S} a^{capex}_{s,k,p}\Big(\sum_{ff\in FF} G_{ff,s,k,pw} + \sum_{b\in B} G_{b,s,k,pw} + \sum_{bf\in BF} G_{bf,s,k,pw}\Big) + b^{capex}_{s,k,p}$$

$$Cost^{compression,pumping}_{untreated,\ opex} = \sum_{p\in P}\sum_{k\in K}\sum_{s\in S} a^{opex}_{s,k,p} \sum_{c\in C}\Big(\sum_{ff\in FF} G_{ff,s,k,c,p} + \sum_{b\in B} G_{b,s,k,c,p} + \sum_{bf\in BF} G_{bf,s,k,c,p}\Big) + b^{opex}_{s,k,p} \quad (76)$$

$$+ \sum_{k\in K}\sum_{s\in S} a^{opex}_{s,k,p}\Big(\sum_{ff\in FF} G_{ff,s,k,pw} + \sum_{b\in B} G_{b,s,k,pw} + \sum_{bf\in BF} G_{bf,s,k,pw}\Big) + b^{opex}_{s,k,p}$$

3.5.Software Used

The Mixed Integer Non-Linear Program (MINLP) presented in Section 3.4 was implemented using “What’sBest 17.0” Lindo Global solver for MS-Excel 2021 on a Windows laptop with the following specifications: Intel(R) Core(USDepartmentofEnergy) i7-7820HQ CPU @ 2.90GHz 2.90 GHz, installed RAM 16.0 GB, and a 64-bit operating System.

3.6.Case Studies

This section described all case studies that were investigated in this work, in addition to the different scenarios that were considered. It is worth noting that the analysis presented is very case sensitive and any modifications in the parameters could lead to a completely different optimal allocation. Hence, this study was based on a built-up scenario obtained from different sources from within literature. As such, all associated parameters are described in the following section and can be found in detail in Appendix B.

For each case study, the model will determine (1) the optimal plant selection for the industrial cluster, (2) the optimal capture and allocation of the different types of fuel, and (3) the optimal source-sink CO_2 allocation that will yield the maximum profit that can be attained for the set carbon limit.

The proposed methodology is illustrated in the form of five case studies that differ in terms of the type and the number of fuels used in the analysis. They consist of a natural gas case study, a coal case study, a biomass case study, a blended fuel case study, and finally a multiple fuel case study. The general assumptions that are taken in all case studies are as follows:

- The capacities for every production plant are bounded based on the industrial cluster's product portfolio.
- The power requirement of each plant is considered to be known.
- Only one type of fuel per plant is considered in the analysis, except for the final case study where a mix of different fuels is used.
- Some plants have the option of producing their own power and/or exporting it to the electricity grid.

- Only one type of power plant is used in the cluster. Power to be exported to the grid is also considered an optional variable that the formulation will select.
- Renewable energy is bounded and set to replace a maximum of 5% of the fossil fuel-derived power and is considered an optional plant in the cluster.
- There are two types of methanol plants: a standard conventional methanol synthesis plant, and a CO_2 receiving plant that constitutes both a carbon utilization plant and a production plant.
- Two types of cement plants can be operated: a Portland cement plant and a Fly Ash cement plant. In the fly ash cement process, fly ash from coal power plants is used to partially replace cement and yield a blended product that can be used in industrial practice. This process relies on the fly ash obtained from the combustion of coal (CFA), resulting in a large quantity of CO_2 emitted into the atmosphere. With the newly imposed stricter environmental regulations, the cost of processing cement-blended-CFA is expected to surge and result in a decrease in the end profit. This pushed the concrete industry to look for techniques that mitigate its excessive carbon footprint and reduce the amounts of emissions released into the atmosphere (Fořt et al., 2021). In fact, various emerging technologies are focusing on the introduction of biomass fly ash (BFA) as a replacement to CFA in the aforementioned process. The attractiveness of biomass as a coal replacement in several sectors has been growing intensively in the past decades, as it can be considered a greener alternative to coal. Because biomass in a lot of cases can be considered a zero carbon fuel, it serves as a way to address both the environmental and economic aspects (Rajamma, 2011). Therefore, because the latter also serves the purpose of this study, the

introduction of the fly ash cement plant is assessed in this work. The methodology consists of allowing the formulation to choose between the cement plants following all the imposed constraints.

- The carbon emissions from the production plants, power plants, carbon integration network (capture, compression and pumping, treatment, and processing in the sinks), and transportation of solid fossil fuel are all considered to be known and make up the industrial cluster's carbon footprint.
- All CO_2 sources are considered to have known concentrations.
- All CO_2 sink requirements are considered to be known.
- In the analysis, the carbon capture rate (NCCR) value is set at a minimum of 20% of the total carbon emissions of the cluster and represents the carbon limit imposed on the cluster.
- The yearly operating hours in the cluster are 7,884 hours, assuming a 10% margin that accounts for sudden shutdowns of operations, maintenance, or any other disruptions of work.
- The lifetime of power plants is assumed to be 40 years, whereas that of production plants is assumed to be 20 years (EIA, 2020a).
- The discount rate is taken as 20% and the CRF is calculated to be 0.2 for power plants and 0.205 for production plants.
- The operating costs considered in the analysis consist of labor, material, and utilities.

3.6.1. General overview

3.6.1.1.Methanol (A) plant

Methanol (A) consists of a conventional methanol plant with the following main processes: steam reforming, methanol synthesis, and product refining and water degasification (Pellegrini, Soave, Gamba, & Langè, 2011). The plant characteristics were derived from different sources in the literature. The maximum product capacity was obtained from (D. M. Al-Mohannadi et al., 2017), the plant fuel requirement, the electricity requirement, and cost components (CAPEX and OPEX) were all obtained from (Pellegrini et al., 2011). The methanol (A) parameters are described in Appendix B.

3.6.1.2.Methanol B plant

Methanol (B) synthesis is made out of different main stages; the gaseous inlet is first compressed to reach the reactor's final feed pressure, then heated up and fed to the reactor, where the main methanol synthesis takes place, and finally the outlet stream which consists of methanol and water is sent to a distillation column where separation takes place. The governing reactions are shown in Equations 77 and 78 (Pérez-Fortes, Schöneberger, Boulamanti, & Tzimas, 2016).

$$CO_2 + 3H_2 \rightleftharpoons CH_3OH + H_2O \quad (77)$$

$$CO_2 + H_2 \rightleftharpoons CO + H_2O \quad (78)$$

The hydrogen (H_2) needed for the methanol (B) production can be supplied from a water electrolysis process described in Equation 79.

$$H_2O + electricity \rightleftharpoons H_2 + O_2 \quad (79)$$

The MeOH (B) parameters used in the analysis were obtained from (Pérez-Fortes et al., 2016) and (D. M. Al-Mohannadi & Linke, 2016) and are described in Appendix B.

3.6.1.3.Cement plant

There are two options for the cement plant in the cluster: Portland cement and fly ash cement. The Portland cement plant and the fly ash cement plant parameters are described in Appendix B. The maximum product capacity was obtained from (D. M. Al-Mohannadi & Linke, 2016), the process fuel requirement, electricity requirement, the cost components (CAPEX and OPEX) were all obtained for both types of plants from (Worrell, 2007).

3.6.1.4.Aluminum plant

The primary aluminum production consists of a combination of different processes, namely bauxite mining, aluminum oxide (Al_2O_3) production, carbon electrode product, aluminum electrolysis, etc (Gao et al., 2009). The aluminum plant general parameters are described in Appendix B. The maximum product capacity was determined from (D. M. Al-Mohannadi & Linke, 2016), the process fuel requirement and electricity requirement were obtained from (Worrell, 2007), and the cost components (CAPEX and OPEX) were determined from (Rosenberg, 2012). It is worth noting that in this analysis, the operating cost of the aluminum plant was taken as €1225/tAluminum.

3.6.1.5.The power plant

Only one type of power plant can be used in the cluster. The available types of power plants consist of natural gas, coal, biomass, and blended fuel power plants. All power plant characteristics are taken from (EIA, 2020a) and summarized in Appendix B. It is worth noting that the capital cost for the blended fuel power plant consists of the cost of retrofitting an existing coal power plant for the combustion of a blended fuel.

3.6.1.6.Solar photovoltaic plant

The solar photovoltaic plant characteristics are also taken from (EIA, 2020a) and are summarized in Appendix B.

3.6.1.7.Carbon integration network

3.6.1.7.1. Capture

The carbon capture plant included in this study consists of a monoethanolamine (MEA) based carbon capture plant that follows the second-generation model based on the eNRLTRK thermodynamic property package. Its design specifications are described in Appendix B and are obtained from (Agbonghae, 2014).

3.6.1.7.2. Sources

The sources considered in the analysis are namely, methanol (A), cement (Portland or fly ash), aluminum, methanol (B), and the power plant. The CO_2 concentrations of the sources are considered to be the same for all the case studies and are summarized in Table Appendix B.

3.6.1.7.3. Sinks

The CO_2 sinks considered in this analysis consist of a methanol plant which takes in CO_2 as raw material, an enhanced oil recovery (EOR) technology, whereby CO_2 is injected into an oil field to increase the latter's overall pressure and to improve the oil's mobility (Alagorni, Yaacob, & Nour, 2015), a geological sequestration consisting of a saline aquifer, and a greenhouse. Each sink has its own capacity, concentration requirement, efficiency, cost/revenue of processing, and distance from the sources. All parameters are summarized in Appendix B and obtained from (D. M. Al-Mohannadi & Linke, 2016) and (D. M. Al-Mohannadi et al., 2017).

3.6.1.7.4. Treatment

The sinks considered in this analysis receive CO_2 from different sources. Because every sink has a specific concentration requirement that must be respected, some source streams allocated to it must undergo treatment and separation processes to ensure safe operations (D. M. Al-Mohannadi & Linke, 2016). The treatment technology in this work is assumed to be a chemical absorption unit with amine solvents. The amine-based chemical absorption process has been used as gas-treatment technologies since the 1950s and are in fact considered to be the most mature and developed carbon treatment technique (F. C. Vega, M.; Camino, S.; et al. , 2017). Amine solvents are widely used in the chemical absorption units due to their significant absorption-stripping kinetic rates at low CO_2 concentrations and high water solubility (F. S. Vega, A.; Navarrete, B., 2014). The treatment costs exclude the compression and pumping costs, as those will be calculated independently for the untreated and treated source streams. The treatment capital cost and operating cost components were obtained from (D. Al-Mohannadi, 2014) and (Bergen, 2004), the CO_2 treatment efficiency is taken

from (D. Al-Mohannadi, 2014), and the treatment removal parameter is estimated from (D. Chapel, 1999) as summarized in Table Appendix B.

3.6.1.7.5. Compression and pumping

When a sink's pressure surpasses the critical pressure, compression is needed to pressurize the steam up to the critical pressure and pump it (D. M. Al-Mohannadi et al., 2017). The specific costs for the compression and pumping technologies are calculated are linearized using a correlation obtained from (Kwak, 2016). The methodology consists of first identifying the source-sink mapping, then determining the pipeline unit, compression and pumping units. For every flow rate, the minimum and optimum costs were derived and plotted as a function of CO_2 treated and untreated flow rates (D. M. Al-Mohannadi et al., 2017). The costs are determined for both treated and untreated sources and depend on the sink-source allocation, as described in Equations 70 to 76. The parameters used in the analysis are summarized in Appendix B. It is worth noting that in this study, the carbon emitted during the compression and pumping phenomenon is not considered in the cluster's footprint.

3.6.1.8.Revenues from products and power exported

The industrial cluster's revenue portfolio consists of products produced from the standard methanol (A) plant and the CO_2 receiving methanol (B) plant, the cement plant, the aluminum plant, and the power exported into the grid. The revenue parameters for the mentioned streams are summarized in Appendix B.

3.6.1.9. Cost of fuels

The costs of the natural gas, coal, biomass, and blended fuel used in the analysis are summarized in Appendix B.

3.6.1.10. Fuel characteristics

In this analysis, the natural gas, the coal and the biomass used in the cluster have the characteristics summarized in Appendix B, all obtained from (Ali et al., 2017). The coal used is of bituminous type and the biomass consists of dried pelletized forestry residue. The blended fuel used consists of a 15% biomass to coal blend, with the characteristics calculated based on the weight fraction.

3.6.1.11. Carbon emission parameters

As mentioned in section 2 of the general parameters, the CO_2 sources in this study consist mainly of the carbon emitted during the production, the power, the treatment, the CO_2 network processes, as well as the emissions from the transportation of solid fuels in the cluster. The parameters used in the analysis, obtained from ("Default CO2 Emission Factors and High Heat Values for Various Types of Fuel," 2016), depend mainly on the type of fuel and are calculated based on the quantity of fuel required for each source listed. All parameters can be found in Appendix B.

A general overview of the cluster and the available plant options for each case study are presented in Table 4. The green color refers to an existing or optional plant, while the red color represents a plant that is not included in the case study.

Table 4 Industrial cluster overview

Plant	Type	Existing/ Optional	Case Study 1	Case Study 2	Case Study 3	Case Study 4	Case Study 5
Methanol (A)	Production	Existing	Included	Included	Included	Included	Included
Portland Cement	Production	Optional	Included	Included	Included	Included	Included
Fly Ash Cement	Production	Optional	Included	Included	Included	Included	Included
Aluminum	Production	Optional	Included	Included	Included	Included	Included
Methanol (B)	Production/ Carbon Utilization	Optional	Included	Included	Included	Included	Included
Natural Gas Power Plant	Power	Existing	Included	Not Included	Not Included	Not Included	Included
Coal Power Plant	Power	Existing	Not Included	Included	Not Included	Not Included	Included
Biomass Power Plant	Power	Existing	Not Included	Not Included	Included	Not Included	Included
Blended Fuel Power Plant	Power	Existing	Not Included	Not Included	Not Included	Included	Included
Solar Photovoltaic Plant	Power	Optional	Included	Included	Included	Included	Included
Enhanced Oil Recovery	Carbon Utilization	Existing	Included	Included	Included	Included	Included
Saline Storage	Carbon Utilization	Existing	Included	Included	Included	Included	Included
Greenhouse	Carbon Utilization	Existing	Included	Included	Included	Included	Included

3.6.2. Case 1: natural gas case study

The first case study consists of a natural gas industrial cluster. The latter includes a set of existing and optional production plants, a renewable power plant, a natural gas power plant, and carbon utilization technologies, as described in Table 3 of section 3.6.1. The assumptions specific to case study 1 are as follows:

- Natural gas is the only type of fuel available in the city.

- The power plant consists of a natural gas power plant.
- The net carbon capture rate is set to a minimum of 20%. The optimization model will select the optimal carbon capture percentage based on the set constraints.

3.6.3. Case 2: coal case study

The second case study consists of a coal industrial cluster. The latter includes a set of existing and optional production plants, a renewable power plant, a coal power plant, and carbon utilization technologies, as described in Table 3 of section 3.6.1. The assumptions specific to case study 2 are as follows:

- Coal is the only type of fuel available in the city.
- The power plant consists of a coal power plant.
- The net carbon capture rate is set to a minimum of 20%. The optimization model will select the optimal carbon capture percentage based on the set constraints.

3.6.4. Case 3: biomass case study

In this third case study, the effects of using biomass as the only source of fuel on the economic and environmental profiles of the industrial cluster are assessed. Similar to the first two case studies, the cluster includes a set of existing and optional production plants, a renewable power plant, a biomass power plant, and carbon utilization technologies, as described in Table 3 of section 3.6.1. The assumptions specific to case study 3 are as follows:

- Biomass is the only type of fuel available in the city.
- The power plant consists of a biomass power plant.

- The net carbon capture rate is set to a minimum of 20%. The optimization model will select the optimal carbon capture percentage based on the set constraints.

3.6.5. Case 4: blended fuel case study

In this fourth case study, a blend of biomass with coal is used as fuel and its effect will be assessed regarding the amount of fuel required and its effect on the economic and environmental profiles of the cluster. As with the previous case studies, the latter includes a set of existing and optional production plants, a renewable power plant, a natural gas power plant, and carbon utilization technologies, as described in Table 3 of section 3.6.1. The assumptions specific to case study 4 are as follows:

- The fuel consists of a 15% biomass to coal blend.
- Blended fuel is the only type of fuel available in the city.
- The power plant consists of a blended fuel power plant.
- The net carbon capture rate is set to a minimum of 20%. The optimization model will select the optimal carbon capture percentage based on the set constraints.

3.6.6. Case 5: multiple fuel case study

In this last case study, the integration of different types of fuels is assessed based on both the economic and environmental feasibilities. Similar to the other case studies, the cluster includes a set of existing and optional production plants, a renewable power plant, and has the option of choosing between a natural gas, coal, biomass, and blended fuel power plants, and carbon utilization technologies. The assumptions specific to case study 5 are as follows:

- Natural gas, coal, biomass, and blended fuel are all integrated in the cluster.

- Only one type of fuel-derived power plant exists.
- Each production plant can have one type of fuel allocated to it.
- The net carbon capture rate is set to a minimum of 20%. The optimization model will select the optimal carbon capture percentage based on the set constraints. A sensitivity analysis is then carried out on the carbon capture rate and is presented in Chapter 4.

The main objective of this case study is to investigate the effect of integrating different types of fuel into the cluster with a set capture rate on the profit and the total carbon emissions. A comparison of case study 5 with prior case studies, which in turn only included one type of fuel, was also conducted. Moreover, a sensitivity analysis that studies the effect of varying the net capture rate, as well as the set renewable percentage, was also performed. The findings of the aforementioned are discussed in Chapter 4.

CHAPTER 4

RESULTS AND DISCUSSIONS

In this chapter, the results obtained from the case studies described in Chapter 3 are discussed in detail. Sensitivity analyses on the carbon capture rate and the renewable energy percentage for case study 5 are also presented with their respective findings. It is worth noting that all the results and discussions in the following sections are case sensitive and based on the parameters collected from different sources in the literature. The purpose of the analysis is not focused on the values obtained but rather on the overall observed trends, since a change in the parameter could lead to slightly different end results and assessment. The detailed results obtained are included in Appendix C.

4.1. Case Studies

4.1.1. Case 1: natural gas case study

For the first case study, it was found that with a natural gas total flow of 559 t natural gas/d and a carbon capture rate constraint set to a minimum of 20%, the cluster produced 5000 tMeOH(A), 10000 t Portland-cement, 1047.05 tAluminum, and 2600 tMeOH(B) and generated a profit of $920.76 million/y. The allocation of natural gas to each product is provided in Appendix C. The power plant satisfied all the power requirements of the production plants. The power allocation to each product can be found in Appendix C. The optimization did not choose to generate any exported power and did not activate the renewable energy option, as both result in a higher cost.

To better understand the economics of the cluster, its cost distribution is visualized in Figure 4. As can be seen, the highest cost is attributed to the cluster's

production sector requiring a total of $984.7 million/y, which is expected with the high product flow rates.

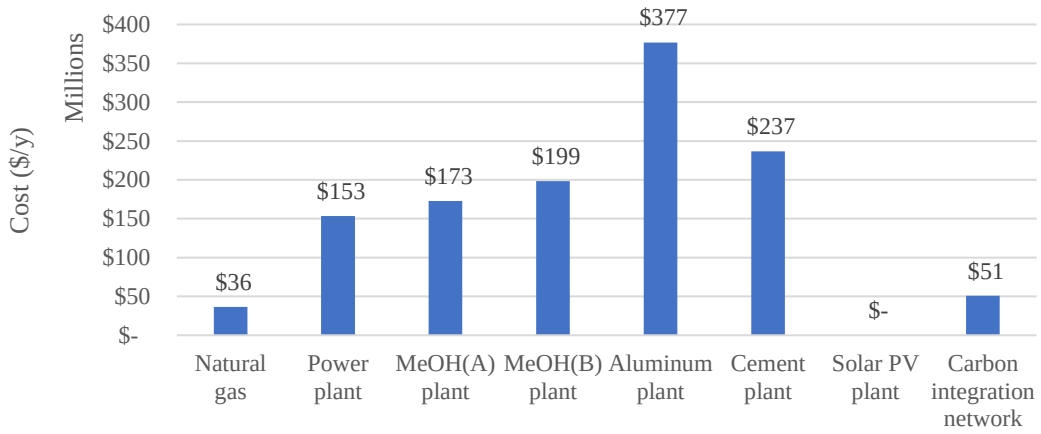

Figure 4 Case study 1: cost distribution

Analysing the carbon integration network's cost distribution, displayed in Figure 5, it can be seen that the highest cost is attributed to the treatment of the CO_2 streams, accounting for 74.59% of the total carbon integration costs. This high number is associated with the fact that 99.9% of the carbon streams are being treated. This can also be seen in the second highest cost attributed to the compression and pumping of the treated flow rates, taking up ~23% of the total.

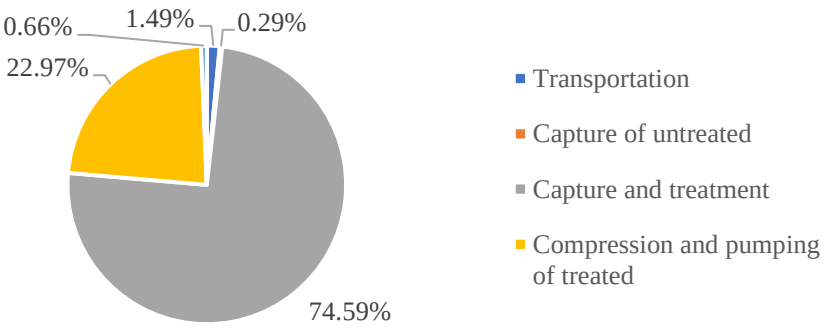

Figure 5 Case study 1: carbon integration network's cost distribution

Regarding the carbon footprint, the total emissions of the cluster without capture was found to be 21234 t CO_2/d, with 8055.19 t emitted from the products t CO_2/d and 13269 t CO_2/d from the power. The high emissions from the power sector are expected, given that only one power plant exists to meet all the power requirements. After applying carbon capture and utilization technologies and selecting the optimal source to sink mapping (refer to Figure 6) the carbon captured amounted to 13796 t CO_2/d reducing the cluster's emissions by 39% resulting in a final footprint of 13034 t CO_2/d, including the carbon network's emissions from the sinks and treatment unit. As can be seen in Figure 6, the optimization allocated treated CO_2 from methanol (A) and aluminum to methanol (B), treated CO_2 from methanol (A) and untreated CO_2 from the power plant to the enhanced oil recovery, treated CO_2 from methanol (A) and methanol (B) to the greenhouse, and treated CO_2 from cement, aluminum, and the natural gas power plant to the saline storage. The flow rates of the source to sink optimal allocation are summarized in Table 5, where T represents the treated carbon streams and U represents the untreated carbon streams. The most profitable sink turned out to be the enhanced oil recovery, generating a total revenue of $31.9 million/y and operating at maximum capacity with 2913.83 t CO_2/d., and the least profitable was the saline storage with a cost of $30.9 million/y. However, due to the saline storage's high capacity and given the carbon restrictions imposed onto the cluster, the optimization allocated 8486.73 t CO_2/d to it.

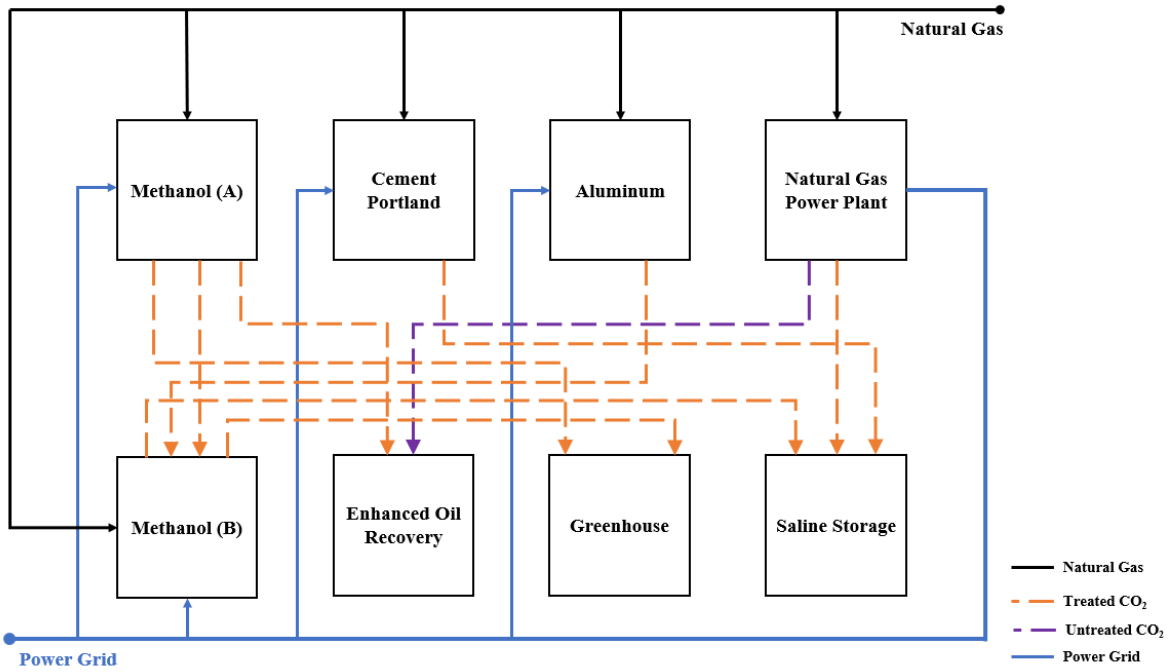

Figure 6 Case study 1: natural gas CO_2 network attained, with optimal allocations illustrated

Table 5 Case 1: Source-sink mapping

Sink	Methanol (B)		Enhanced Oil Recovery		Saline Storage		Greenhouse	
Source	T (tCO_2/d)	U (tCO_2/d)	T (tCO_2/d)	U (tCO_2/d)	T (tCO_2/d)	U (tCO_2/d)	T (tCO_2/d)	U (tCO_2/d)
Methanol (A)	676.58	0.00	2730.03	0.00	0.00	0.00	747.73	0.00
Cement - Portland	0.00	0.00	0.00	0.00	1361.87	0.00	0.00	0.00
Aluminum	1033.42	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Methanol (B)	0.00	0.00	0.00	0.00	329.69	0.00	282.27	0.00
Natural Gas Power	0.00	0.00	0.00	8.97	6625.44	0.00	0.00	0.00

Looking at the carbon emissions distribution in the cluster (illustrated in Figure 7) it can be seen that the source with the highest emissions consists of the power generation emitting a total of 13269 t CO_2/d followed by the production sector with 8055 t CO_2/d. This can be attributed to the fact that the optimization chose not to activate the renewable option and replace part of the total power requirement with renewable energy. Given that only one source of power exists in the cluster to satisfy its electricity demand, the emission from this sector is expected to be this high with such a low percentage of green energy used. It is worth noting that the emissions from the carbon integration network consist of the sink emissions with 681 tCO_2/d and the treatment emissions with 4825 tCO_2/d.

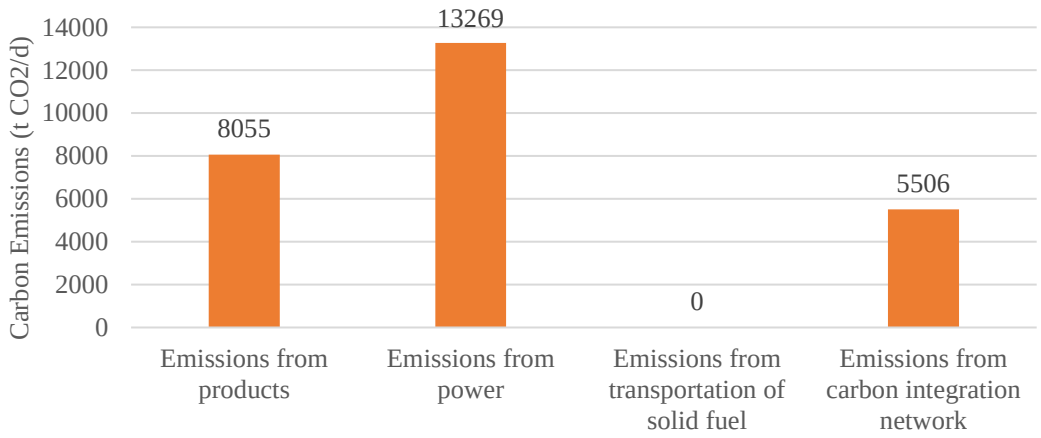

Figure 7 Case study 1: carbon emissions distribution in the cluster

Although the natural gas cluster was able to generate a high profit, with the world's shift towards the use of green and renewable energy sources, the result obtained regarding the solar plant highlights the need to integrate different types of energy sources and meet the targets imposed by governments worldwide in regard to the emissions as well as the fossil fuel reliance.

4.1.2. Case 2: coal case study

For the second case study, it was found that with a coal total flow of 5461.9 t coal/d and a carbon capture rate constraint set to a minimum of 20%, the cluster produced 5000 tMeOH(A),10000 t Portland-cement, 1337 tAluminum, but no tMeOH(B). The latter can be attributed to the higher cost associated with the production and CO_2 processing of the MeOH(B) plant from coal. The allocation of coal to each product is provided in Appendix C. The power plant satisfied all the power requirements of the production plants. The optimization did not activate the option of exporting power into the grid nor the option of using renewable energy due to the higher costs. The cluster's profit turned out much lower than the first case study, yielding a final value of $280.37 million /y with the optimal allocation selected. This shows that coal alone could not generate a high-end profit for the cluster with all the available carbon mitigation techniques. In fact, given the carbon restrictions on the cluster and the aforementioned constraints imposed by governments, this result is expected and shows the need to switch to a more profitable and greener source of energy. Furthermore, a high quantity of coal is required to fulfil the cluster's requirement, thus integrating different types of fuel, especially green fuels, would also reduce the industry's high dependency.

To better understand the economics of the cluster a cost distribution is visualized in Figure 8. The highest cost is attributed to the production sector with a total of $633.44 million/y, followed by the cost of coal with $99.68 million/y. The latter further shows the need to expand the cluster's fuel portfolio and reduce the dependency of the industry on this type of fossil fuel.

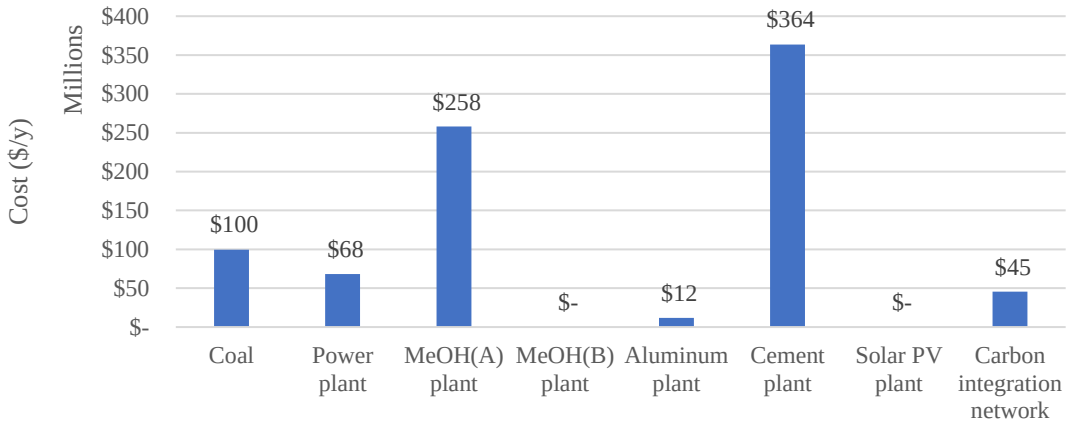

Figure 8 Case study 2: cost distribution

Analysing the carbon integration network's cost distribution, displayed in Figure 9, it can be seen that the highest cost is attributed to the treatment unit, similarly to the natural gas case study, accounting for 72.6% of the total carbon integration costs. This high number is also associated with the fact that the optimization model selected the treatment of 99.93% of the carbon streams to allocate to the sinks with only 0.07% left untreated. This trend can also be seen in the compression and pumping costs.

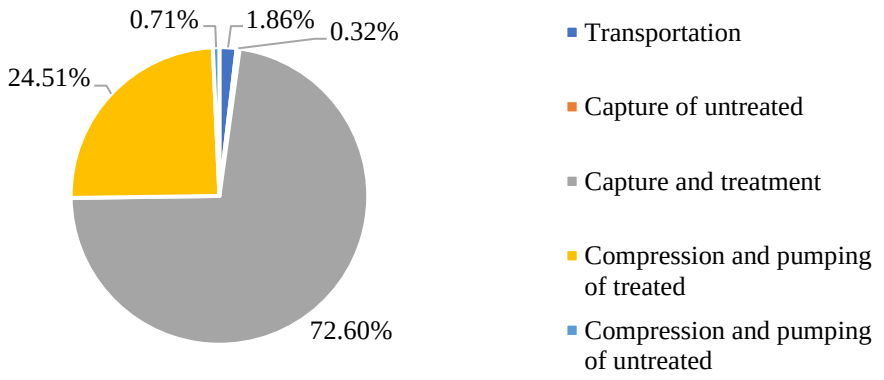

Figure 9 Case study 2: carbon network cost distribution

Regarding the carbon footprint, the total emissions of the cluster without capture was found to be 16115 t CO_2/d, less than the one for the natural gas case, due to the lower production of the coal cluster. After applying carbon capture and utilization

technologies and selecting the optimal source to sink mapping (refer to Figure 10) the carbon captured amounted to 12086 t CO_2/d reducing the cluster's emissions by 41% resulting in a final footprint of 9535 t CO_2/d, and a capture rate of 75%. As can be seen in Figure 10, the optimization allocated treated and untreated CO_2 from the coal power plant to the enhanced oil recovery, treated CO_2 from methanol (A) to the greenhouse, treated CO_2 from methanol (A) and cement to the saline storage and chose not to operate the methanol (B) plant. The flow rate of the source to sink optimal allocation are summarized in Table 6, where T represents the treated carbon streams and U represents the untreated carbon streams.. The most profitable sink turned out to be the enhanced oil recovery, generating a total revenue of $31.9 million/y and operating at maximum capacity with 2913.83 t/d, and the least profitable was the saline storage with a cost of $30.9 million/y. However, due to the saline storage's high capacity and given the carbon restrictions imposed onto the cluster, the optimization allocated 8486.73 t/d to it.

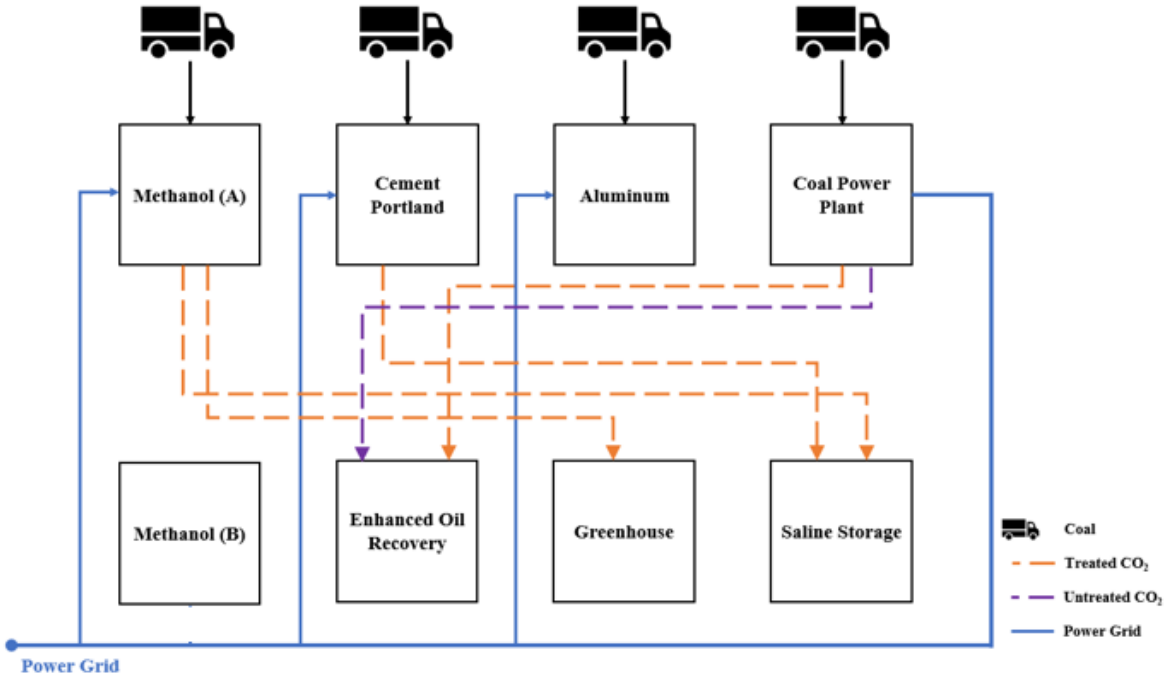

Figure 10 Case study 2: coal CO_2 network attained, with optimal allocations illustrated

Table 6 Case 2: Source-sink mapping

Sink	Methanol (B)		Enhanced Oil Recovery		Saline Storage		Greenhouse	
Source	T (tCO_2/d)	U (tCO_2/d)	T (tCO_2/d)	U (tCO_2/d)	T (tCO_2/d)	U (tCO_2/d)	T (tCO_2/d)	U (tCO_2/d)
Methanol (A)	0.00	0.00	0.00	0.00	5917.93	0.00	1030.00	0.00
Cement - Portland	0.00	0.00	0.00	0.00	2399.07	0.00	0.00	0.00
Aluminum	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Methanol (B)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Coal Power	0.00	0.00	2730.03	8.97	0.00	0.00	0.00	0.00

Looking at the carbon emissions distribution in the cluster (illustrated in Figure 11) it can be seen that the power generation and the production sectors both generated

the highest emissions with 3435.55 t CO_2/d and 11314.79 t CO_2/d emitted. Given that the optimization chose not to activate the renewable energy plant, the carbon footprint of the cluster is expected to be this high with such no green energy used. The carbon network emissions consist of the sink emissions with 680.97 tCO_2/d and the treatment emissions with 4825.31 t CO_2/d.

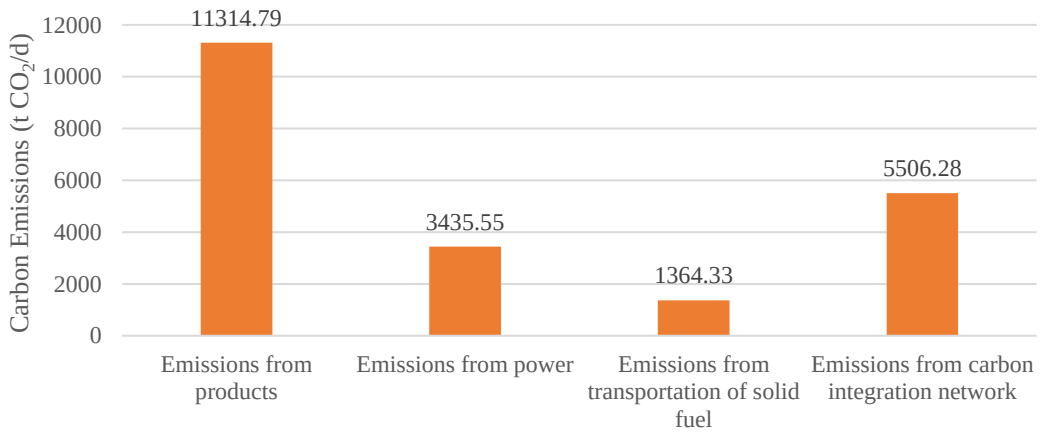

Figure 11 Case study 2: carbon emissions distribution in the cluster

Similar to the natural gas case study, with the world's shift towards the use of greener sources of energy, the result obtained from the coal cluster shows the need to integrate different sources of fuel to mitigate the emissions resulting from the production sector.

4.1.3. Case 3: biomass case study

For the third case study, it was found that with a biomass total flow of 8762.69 t biomass/d and a carbon capture rate constraint set to a minimum of 20%, the cluster produced 5000 tMeOH(A), 10000 t Portland-cement, 25.21 tAluminum, and 2600

tMeOH(B). The allocation of biomass to each product is provided in Appendix C. The power plant satisfied all the power requirements of the production plants. The power allocation to each plant can be found in Appendix C. The optimization selected the option of exporting power into the grid, generating 100,000 kWh/d and chose not to activate the option of using renewable energy due to the higher costs associated with it. The cluster's profit turned out to be higher than the coal case study, but lower than the natural gas case study, with a final value of $498.3 million /y. The cost distribution of the cluster is summarized in Figure 12. As can be seen, the highest cost is attributed to the cost of biomass as well as the production sector requiring $313.44 million/y and $616.7 million/y respectively. In this case study, the biomass is considered to be bought dried and pelletized, and as a standalone fuel, a high quantity is required to fulfil the cluster's product and power demands resulting in a high cost. Therefore, the need to integrate more than one type to operate a cluster with a large product portfolio is further highlighted.

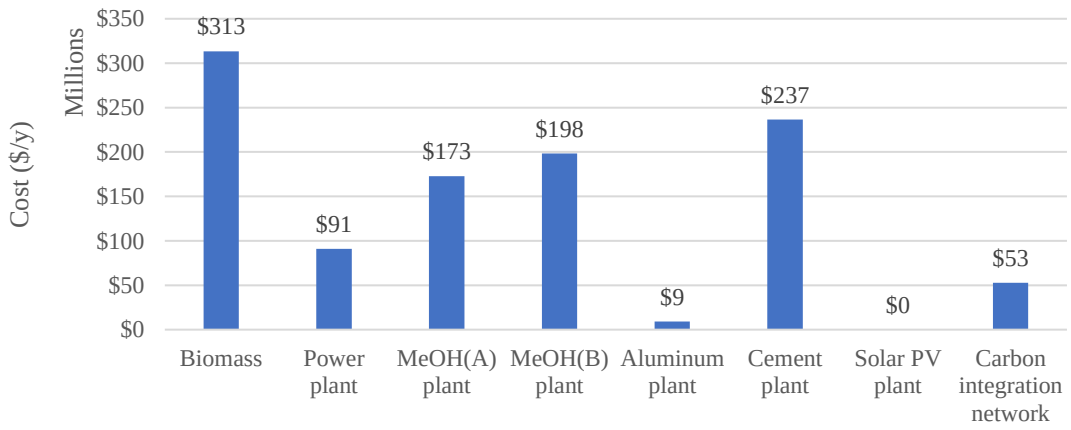

Figure 12 Case study 3: cost distribution

Analysing the carbon integration network's cost distribution, displayed in Figure 13, it can be seen that the highest cost is attributed to the treatment unit, similarly to the

first two case studies, accounting for 71.76% of the total carbon integration costs. This high number is also associated with the fact that the optimization model selected the treatment of 99.71% streams leaving only 0.29% untreated. This can also be seen from the compression and pumping costs.

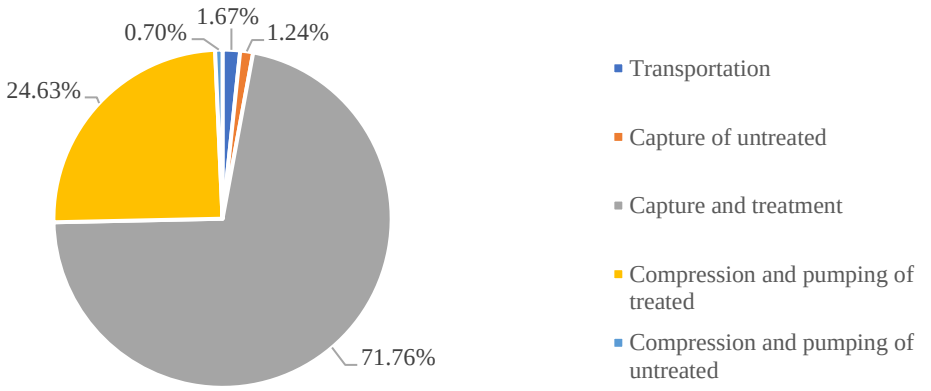

Figure 13 Case study 3: carbon network cost distribution

Regarding the carbon footprint, the total emissions of the cluster without capture was found to be 18394.67 t CO_2/d, less than the natural gas case but higher than the coal case. The latter is due to the higher production capacity that this cluster is operating. After applying carbon capture and utilization technologies and selecting the optimal source to sink mapping (refer to Figure 14) the carbon captured amounted to 13796 t CO_2/d reducing the cluster's emissions by 45% resulting in a final footprint of 10116.75 t CO_2/d, and a capture rate of 75%. As can be seen in Figure 14, the optimization allocated treated carbon from the biomass power plant to methanol (B), treated carbon from methanol (A) and untreated carbon from the biomass power plant to the enhanced oil recovery, treated carbon from methanol (B) and untreated carbon from biomass power plant to the greenhouse, and treated carbon from methanol (A) and cement, with

a mixture of untreated and treated carbon from the biomass power plant to the saline storage. The flow rate of the source to sink optimal allocation are summarized in Table 7, where T represents the treated carbon streams and U represents the untreated carbon streams. The sink yielding the highest revenues is the enhanced oil recovery generating $31.9 million/y from a maximum flow of 2913.83 t/d and the least profitable sink was found to be the saline storage with a cost of $30.38 million/y. However, due to the saline storage's high capacity and given the carbon restrictions imposed onto the cluster, the optimization allocated 8317 t/d to it.

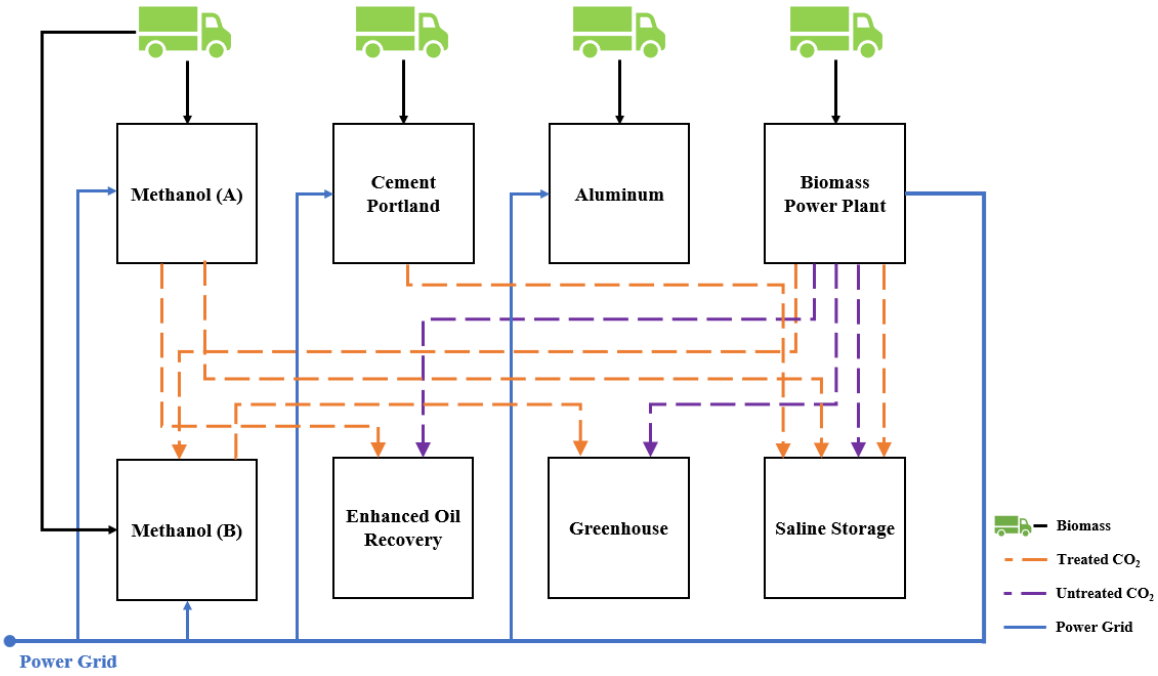

Figure 14 Case study 3: biomass CO_2 network attained, with optimal allocations illustrated

Table 7 Case 3: Source-sink mapping

Sink	Methanol (B)		Enhanced Oil Recovery		Saline Storage		Greenhouse	
Source	T (tCO_2/d)	U (tCO_2/d)	T (tCO_2/d)	U (tCO_2/d)	T (tCO_2/d)	U (tCO_2/d)	T (tCO_2/d)	U (tCO_2/d)
Methanol (A)	0.00	0.00	2730.03	0.00	3890.72	0.00	0.00	0.00
Cement - Portland	0.00	0.00	0.00	0.00	2409.34	0.00	0.00	0.00
Aluminum	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Methanol (B)	0.00	0.00	0.00	0.00	0.00	0.00	1026.63	0.00
Biomass Power	1710.00	0.00	0.00	8.97	1989.72	27.22	0.00	3.37

Looking at the carbon emissions distribution in the cluster (illustrated in Figure 15) it can be seen that the production sector generated the highest emissions with 12466,55 t CO_2/d emitted. Given that the optimization chose not to activate the renewable energy plant and that biomass in general has a lower energy capacity than coal, requiring a larger amount of fuel, the carbon footprint of the cluster is expected to be this high.

However, it is worth noting that biomass is considered a greener alternative to natural gas and coal when looking at a life cycle analysis of the whole cluster. Given that this case study does not cover the cradle to grave assessment, the full potential of biomass as a green source of energy is not highlighted. Thus, performing an LCA on the cluster could result in significantly lower emissions highlighting the growing attractiveness of biomass as an alternative to fossil fuels.

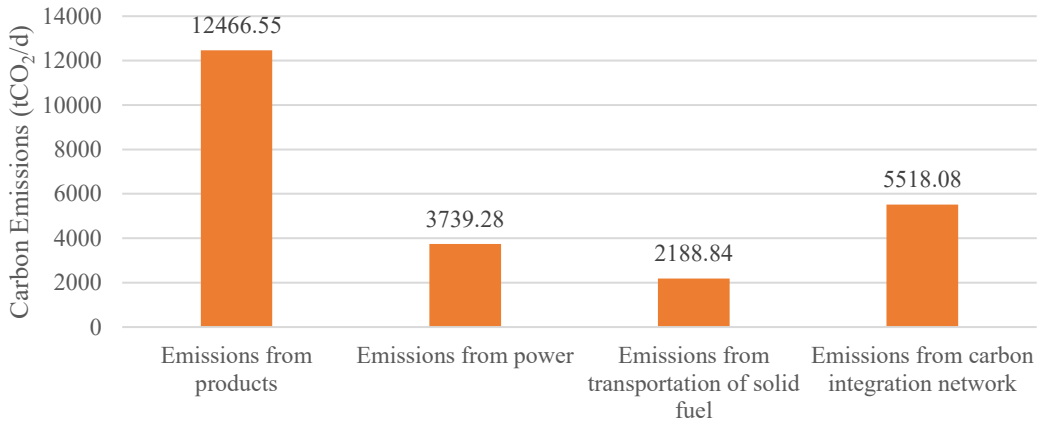

Figure 15 Case study 3: carbon emissions distribution in the cluster

4.1.4. Case 4: blended fuel case study

For the fourth case study, it was found that with a blended fuel total flow of 6515.61 t blended fuel/d and a carbon capture rate constraint set to a minimum of 20%, the cluster produced 5000 tMeOH(A), 10000 t Portland-cement, 74.23 tAluminum, and 2600 tMeOH(B). The allocation of blended fuel to each product is provided in Appendix C. The power plant satisfied all the power requirements of the production plants. The optimization selected the option of exporting 100000 kWh/d of power into the grid but chose not to activate the option of using renewable energy due to the higher costs. The cluster's profit also turned out to be $684.07 million /y, lower than that of the natural gas cluster, but higher than those of the coal and the biomass clusters. Thus, the integration of biomass into the cluster resulted in a positive effect on its end profit. Furthermore, because the blended fuel consists of a 15% biomass to coal weight ratio, the reliance on one type of fuel is reduced. This shows the potential of utilizing a blend of both fossil fuel and biomass as a greener alternative to a fossil fuel industrial cluster.

To better understand the cluster's economics, a cost distribution is introduced in Figure 16. As can be seen, the highest costs are attributed to the production sector and

the fuel requiring $634.35 million/y and $136 million/y respectively. The resulting cost of fuel is much lower than that of biomass in case study 3 and slightly higher than that of the coal in case study 2. Given that the blended fuel cluster's product portfolio is much higher than the previous two, blending two types of fuel as a means to mitigate both the carbon emissions as well as the reliance on one type of fuel shows great potential.

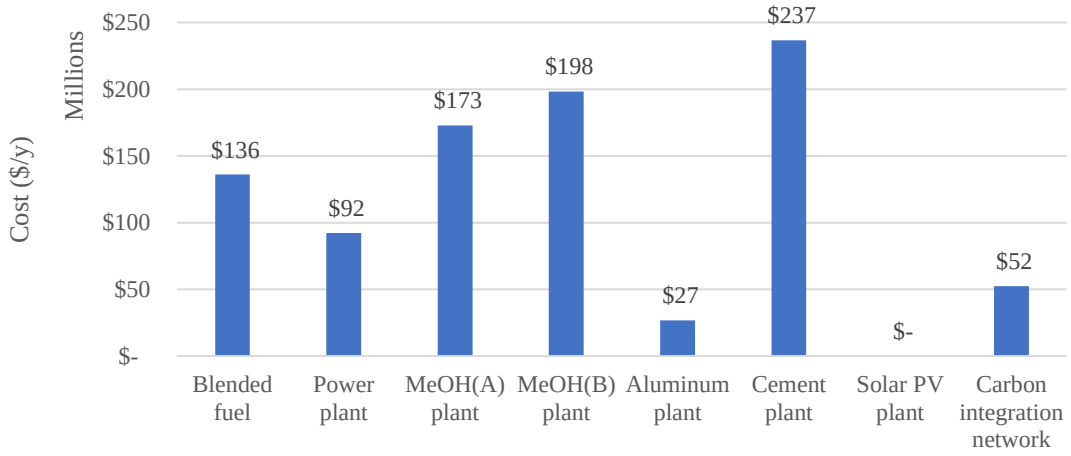

Figure 16 Case study 4: cost distribution

Analysing the carbon integration network's cost distribution, displayed in Figure 17, it can be seen that the highest cost is attributed to the treatment unit, similarly to the other case studies, accounting for 72.12% of the total carbon integration costs. This high number is also associated with the fact that the optimization model selected to treat 99.91% of the carbon streams and to keep 0.09% untreated. This can also be seen from the difference in the compression and pumping costs of the treated and untreated flows.

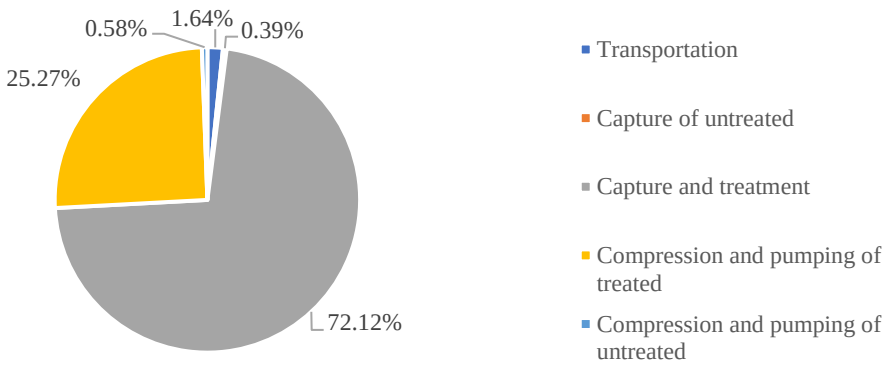

Figure 17 Case study 4: carbon network cost distribution

Regarding the carbon footprint, the total emissions of the cluster without capture was found to be 18395 t CO_2/d. After applying carbon capture and utilization technologies and selecting the optimal source to sink mapping (refer to Figure 18) the carbon captured amounted to 13796 t CO_2/d reducing the cluster's emissions by 45% resulting in a final footprint of 10105 t CO_2/d, and a capture rate of 75%. Comparing it to the coal and biomass standalone case studies, whereby the CO_2 emissions pre-capture were 16115 t CO_2/d and 18394.6 t CO_2/d respectively and post-capture were 9535 t CO_2/d and 10116.75 t CO_2/d respectively, it can be seen that the emissions post capture in this case study were slightly higher than the second, due to this cluster's higher production, and slightly lower than the third. Moreover, as discussed in the biomass case study, performing an LCA analysis on this cluster could result in even lower emissions further highlighting the advantages of using a blend of both fuels

As can be seen in Figure 18, the optimization allocated treated carbon from cement, aluminum, and methanol (B) to methanol (B), treated carbon from methanol (A) and untreated carbon from the blended fuel power plant to the enhanced oil recovery, treated carbon from methanol (A) and the blended fuel power plant to the greenhouse, and treated carbon from methanol (A), cement, and the blended fuel power

plant to the to the saline storage. The flow rate of the source to sink optimal allocation are summarized in Table 8, where T represents the treated carbon streams and U represents the untreated carbon streams. The sink generating the highest revenue was found to be the enhanced oil recovery with $31.9 million/y operating at full capacity with 2913.83 tCO_2/d and the sink generating the lowest was found to be the saline storage yielding a negative value of $30.97 million/y. However, due to the latter's high capacity and the carbon restrictions applied to the cluster, the optimization allocated 8486.73 tCO_2/d to it.

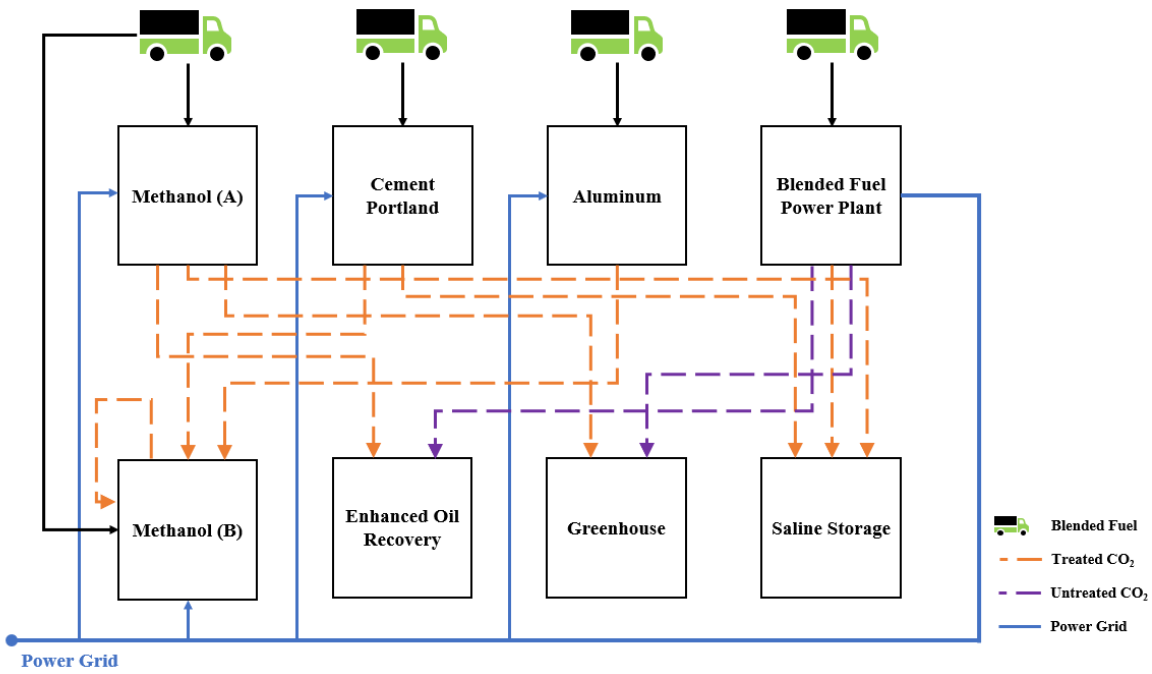

Figure 18 Case study 4: blended fuel CO_2 network attained, with optimal allocations illustrated

Table 8 Case 4: Source-sink mapping

Sink	Methanol (B)		Enhanced Oil Recovery		Saline Storage		Greenhouse	
Source	T	U	T	U	T	U	T	U

	(tCO_2/d)	(tCO_2/d)	(tCO_2/d)	(tCO_2/d)	(tCO_2/d)	(tCO_2/d)	(tCO_2/d)	(tCO_2/d)
Methanol (A)	0.00	0.00	2730.03	0.00	2170.40	0.00	1026.63	0.00
Cement - Portland	502.14	0.00	0.00	0.00	1898.46	0.00	0.00	0.00
Aluminum	129.15	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Methanol (B)	1078.71	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Biomass Power	0.00	0.00	0.00	8.97	4248.14	0.00	0.00	3.37

Looking at the carbon emissions distribution in the cluster (illustrated in Figure 19) it can be seen that the production sector generated the highest emissions with 12406.65 t CO_2/d, followed by the emissions from the carbon integration network, namely the sinks emissions with 680.6 t CO_2 emitted/d and the treatment emissions with 4825 tCO_2 emitted/d. This can be attributed to the lower energy capacity of biomass, requiring more fuel to generate the same amount of power, thereby highlighting the effect of blending biomass with coal. However, as mentioned previously, an LCA approach of the cluster could potentially result in a reduced carbon footprint, increasing the attractiveness of using a blend of fossil fuel with a greener source of energy as a carbon mitigation technique in industrial clusters.

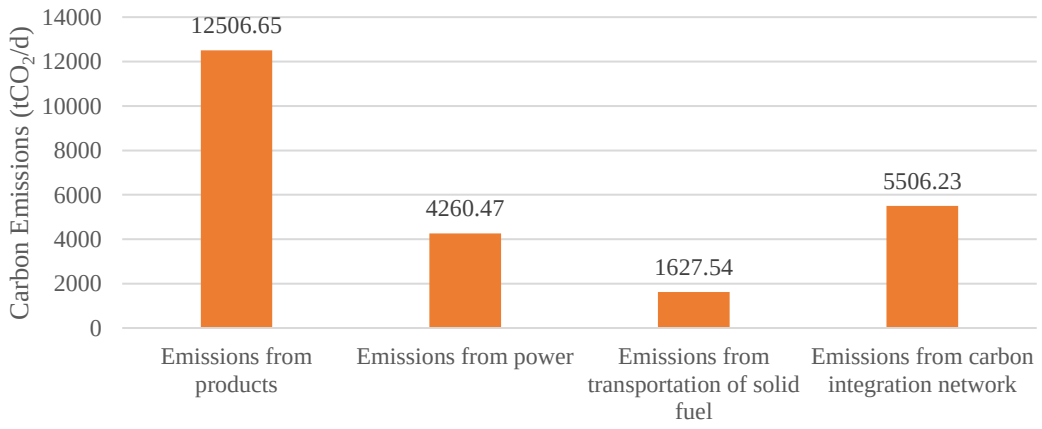

Figure 19 Case study 4: carbon emissions distribution in the cluster

4.1.5. Case 5: multiple fuel case study

For the fifth and last case study, it was found that with a natural gas flow of 444.25 t natural gas/d, a coal flow of 888.35 t coal/d, a biomass flow of 585.39 t biomass/d, and a blended fuel flow of 756.14 t blended fuel/d and a carbon capture rate constraint set to a minimum of 20%, the cluster produced 5000 tMeOH(A), 10000 t Portland-cement, 1118.44 tAluminum, and 2600 tMeOH(B). The fuel to product allocation is included in Appendix C. The optimization selected the natural gas plant as the operating power plant, which satisfied the cluster's power requirements (the power allocation to every plant is summarized in Appendix C). The optimization did not activate the option of exporting power to the grid but activated the option of operating the renewable energy plant at the highest capacity to replace 5% (1010526.32 kWh/d) of the power supplied by the fossil fuel plant. The cluster's profit turned out to be $907.16 million/y, slightly lower than that for the natural gas case study, but higher than the remaining case studies. However, the different fuel requirements are much lower, reducing the dependency on one type and showing the advantage of integrating more than one fuel into an industrial cluster. The activation of the renewable solar plant further shows the opportunity of gradually integrating more sources of green energy, such as green hydrogen, without being limited by capacity or by efficiency. To better understand the cluster's economics, a cost distribution is presented in Figure 20. As can be seen, with the cluster's large product requirements, the highest costs resulted from the production sector, requiring $1010.12 million/y, followed by the power sector,

consisting of the natural gas power plant and the solar photovoltaic plant costs with $151.53 million/y.

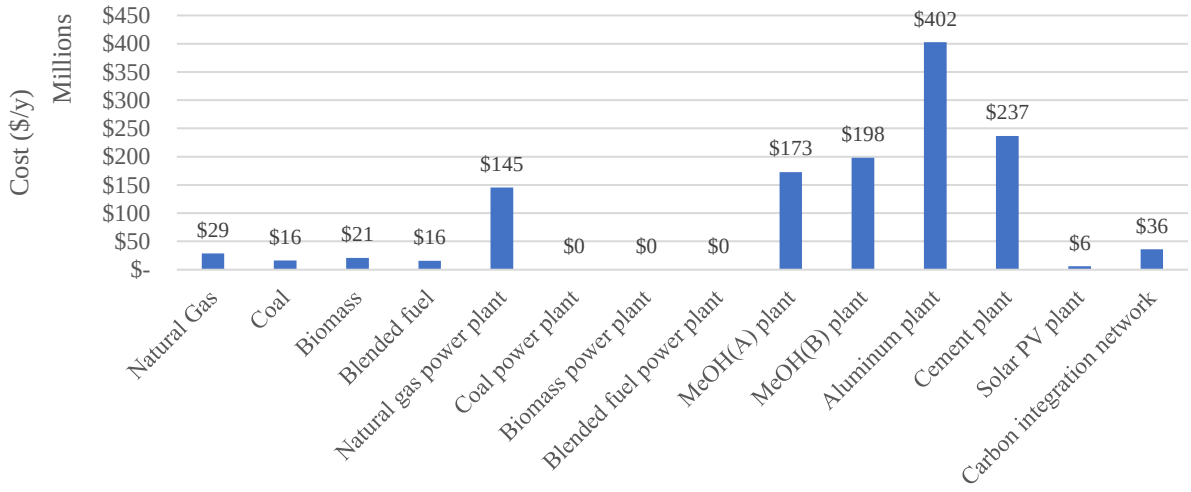

Figure 20 Case study 5: cost distribution

Analysing the carbon integration network's cost distribution, displayed in Figure 21, it can be seen that the highest cost is attributed to the treatment unit, similarly to the four other case studies, accounting for 65.28% of the total carbon integration costs. This high number is also associated with the fact that the optimization model selected to treat 99.91% of the carbon streams. This trend can also be seen from the difference in the compression and pumping costs of treated and untreated carbon streams.

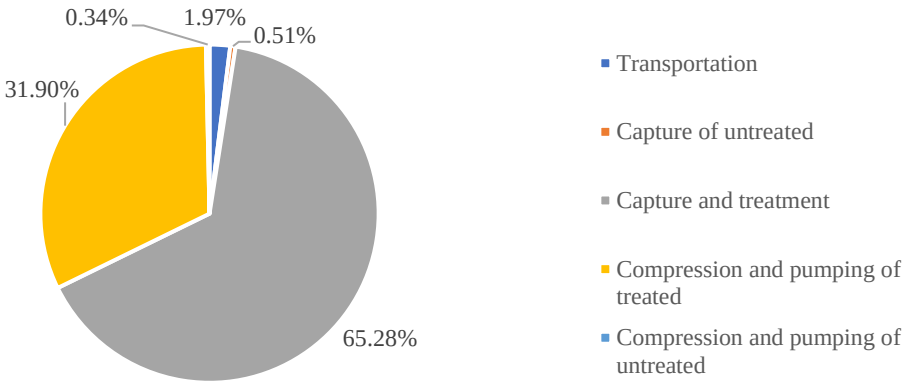

Figure 21 Case study 5: carbon network cost distribution

To assess the revenues of this case study, each revenue stream is compared with those of the other case studies. Revenues from the sinks, from the products, and from the exported power are all depicted in Figures 22, 23, and 24 respectively. As can be seen, the revenues from the sinks for the multiple fuel case study is close to those for the natural gas, biomass, and blended fuel, and greater than those of the coal case study. Given that the amount of carbon captured in each case is close to constant, this trend is expected.

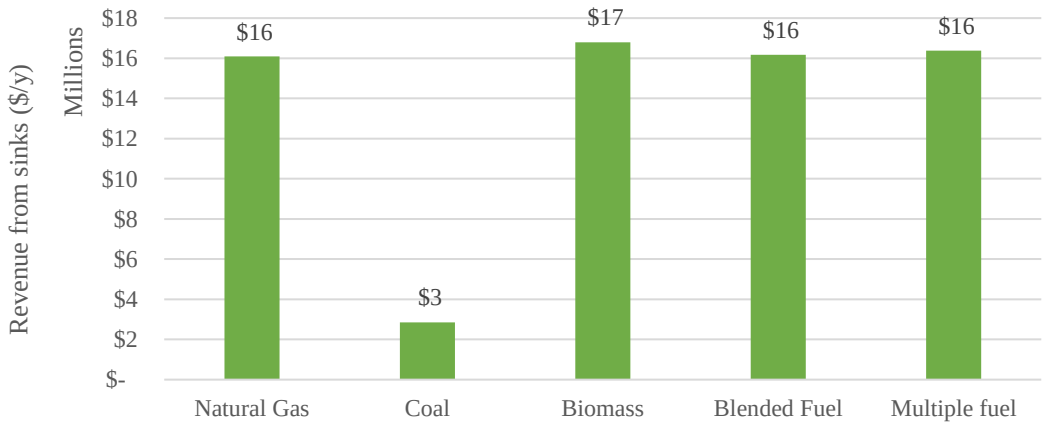

Figure 22 Revenues from sinks for case studies 1 to 5

As for the revenues from the products, the multiple fuel case generated the highest revenues with $2170 million/y. Because this cluster's capacity is higher than the other case studies, the revenues from the value-added products will concurrently be higher. Regarding the exported power, the optimization chose to activate this revenue stream for the biomass and blended fuel cases only. Given that the same amount of power is exported in both cases (100000kWh/d), equal revenues are expected.

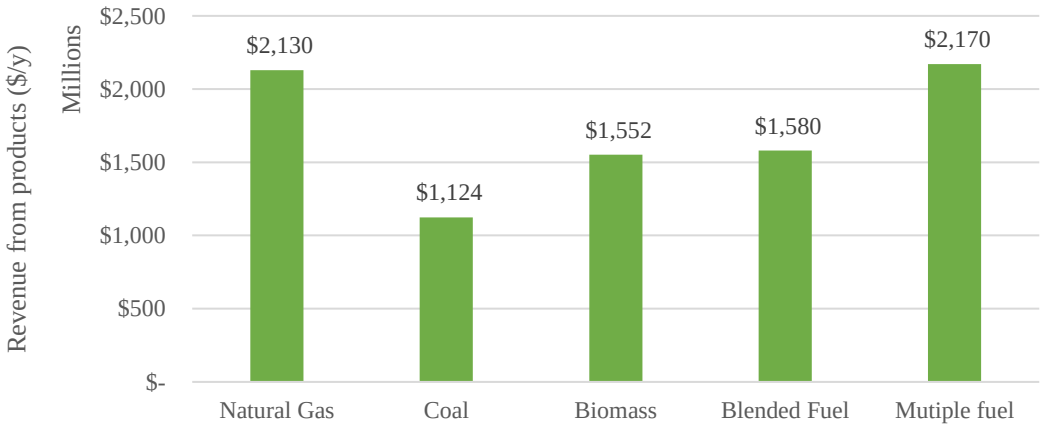

Figure 23 Revenues from products for case studies 1 to 5

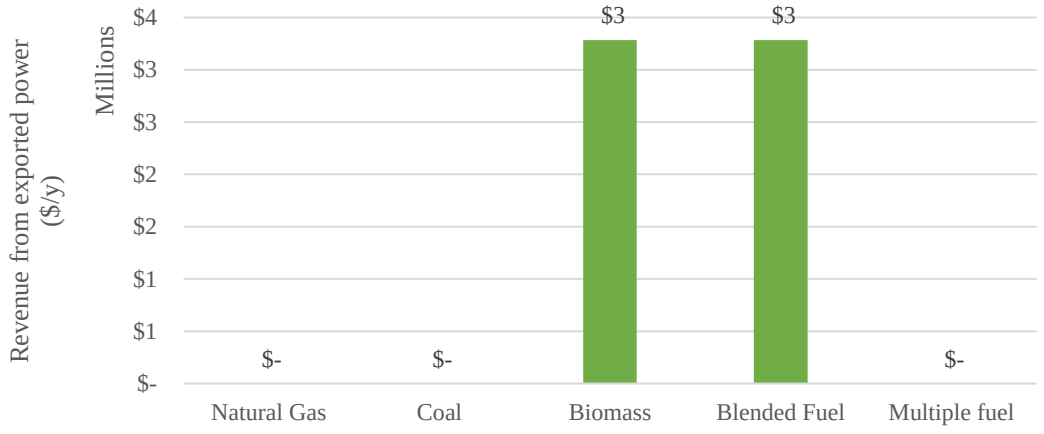

Figure 24 Revenues from exported power for case studies 1 to 5

Regarding the carbon footprint, the total emissions of the cluster without capture was found to be 17640 t CO_2/d, lower than those for the natural gas, biomass, and blended fuel cases, but slightly higher than that for the coal case study. The latter can be attributed to the higher production capacity of this cluster in comparison to the coal cluster. After applying carbon capture and utilization technologies and selecting the optimal source to sink mapping (refer to Figure 25) the carbon captured amounted to 13796 t CO_2/d reducing the cluster's emissions by 47% resulting in a final footprint of 9345 t CO_2/d, and a capture rate of 79%. Compared to the standalone and blended fuel case studies, the resulting emissions post capture of the multiple fuel case study turned out to be the lowest showing the great economic and environmental potentials of integrating multiple fuels into a cluster to mitigate its carbon footprint. Furthermore, the optimization chose to operate the solar photovoltaic plant at full capacity. Therefore, adding more capacity or integrating more than one type of renewable energy could result in a higher replacement of the fossil-fuel derived energy.

Figure 25 summarizes the optimal source to sink mapping obtained. The optimization chose to allocate treated carbon from aluminum to methanol (B), treated carbon from cement and a mixture of treated and untreated carbon from the natural gas power plant to the enhanced oil recovery, treated carbon from methanol (B) to the greenhouse, and treated carbon from methanol (A) and the natural gas power plant to the saline storage. The flow rate of the source to sink optimal allocation are summarized in Table 9, where T represents the treated carbon streams and U represents the untreated carbon streams.

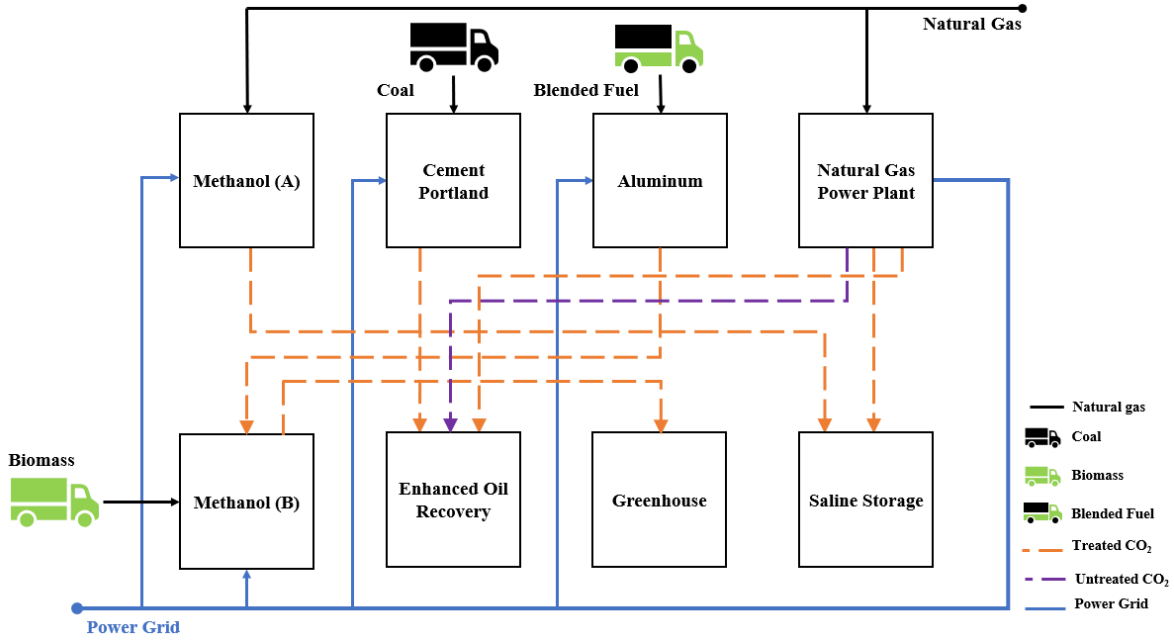

Figure 25 Case study 5: multiple fuel CO2 network superstructure

Table 9 Case 5: Source-sink mapping

Sink	Methanol (B)		Enhanced Oil Recovery		Saline Storage		Greenhouse	
Source	T (tCO_2/d)	U (tCO_2/d)	T (tCO_2/d)	U (tCO_2/d)	T (tCO_2/d)	U (tCO_2/d)	T (tCO_2/d)	U (tCO_2/d)
Methanol (A)	0.00	0.00	0.00	0.00	5047.96	0.00	0.00	0.00
Cement - Portland	0.00	0.00	2399.07	0.00	0.00	0.00	0.00	0.00
Aluminum	1710.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Methanol (B)	0.00	0.00	0.00	0.00	0.00	0.00	1030.00	0.00
Power	0.00	0.00	328.85	11.09	3269.04	0.00	0.00	0.00

Looking at the carbon emissions distribution in the cluster (illustrated in Figure 26) it can be seen that the production and power sector generated the highest emissions with 10780.58 t CO_2/d and 6302.69 t CO_2/d. Comparing the power emissions in every

case study, natural gas resulted in 0.000691 tCO2/kWh, coal in 0.00077 tCO2/kWh, biomass in 0.000773 tCO2/kWh, blended fuel in 0.00077 tCO2/kWh, and finally multiple fuels in 0.000328 tCO2/kWh. The values were obtained by dividing the carbon emissions by the fuel derived power. As can be observed, the multiple fuel case yielded the lowest emissions per kWh, proving the advantage of adding renewable sources of energies into the power portfolio of a cluster.

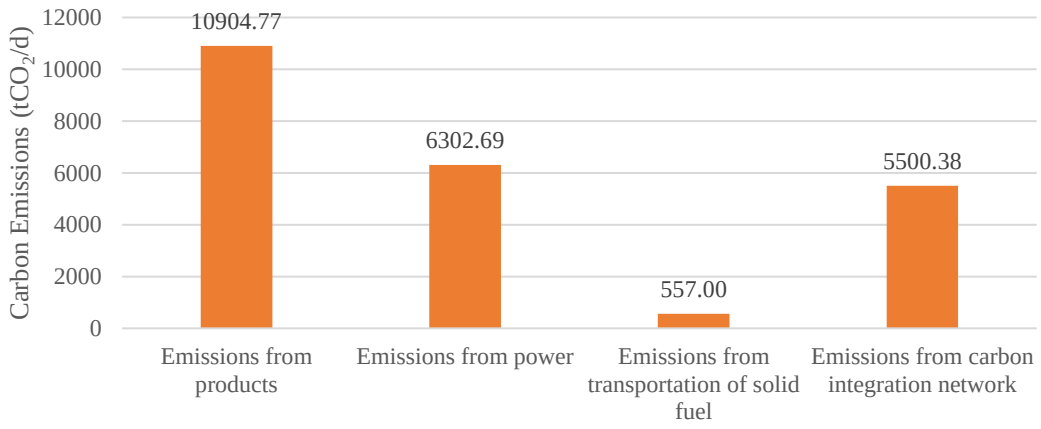

Figure 26 Case study 5: carbon emissions distribution in the cluster

The flow rates of the different types of fuel are represented in Figure 27, showing the lower flow requirements needed in this analysis compared to those of the standalone and blended fuels. This further proves that integrating different types of fuel results in a reduction in the reliance of the industry on one type.

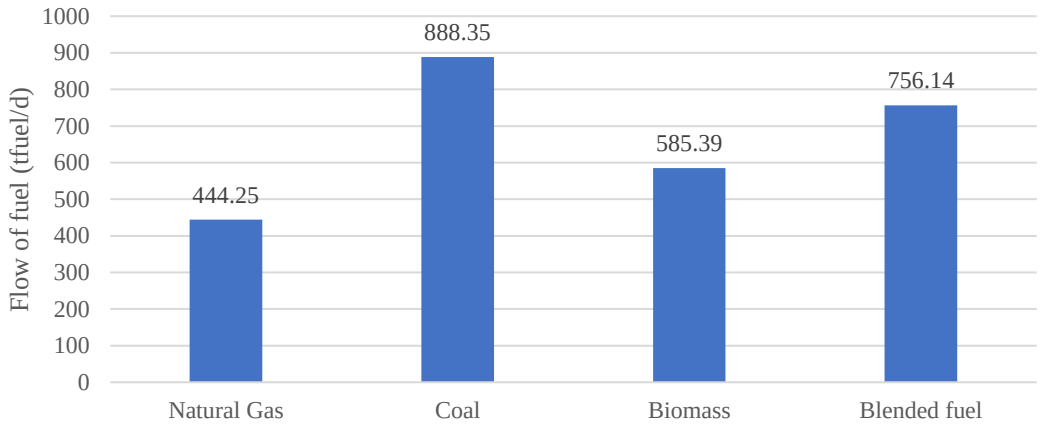

Figure 27 Case study 5: Total fuel flows fuel into the multiple fuel industrial cluster

4.2. Sensitivity analysis

Sensitivity analyses on case study 5 were carried out in terms of the net carbon capture rate and the renewable energy % to study the effect of their variation on the cluster's profit, carbon reduction %, fuel flow rates, and product flow rates. The findings are presented and interpreted in this section and all the respective results are included in Appendix C.

4.2.1. Case 5: Carbon capture rate

In this sensitivity analysis, the carbon capture rate described in Equations 80 and 81, was varied from a value of 40% to a value of 70% and its effects on the cluster's profit, its product portfolio, its carbon footprint, and its fuel requirements are assessed. The renewable percentage was fixed to 5% and the amount of carbon captured (numerator in Equation 80) was also fixed as a basis for comparison. The findings of the different scenarios are summarized in Appendix C.

$$\text{NCCR}(\%)=\frac{\text{CO}_2\text{ captured}}{\text{Pre-capture emissions}} \tag{80}$$

$$\text{Pre-capture emissions}=\text{Emissions from products} + \text{Emissions from power} + \text{Emissions from transport of solid fuels} \tag{81}$$

From Equations 80 and 81, it can be expected that increasing the NCCR value while fixing the amount of carbon captured should result in a decrease of the pre-capture emissions to meet the restrictions. This trend was in fact observed, as depicted in Figure 28. At an NCCR of 40%, the pre-capture emissions are much higher than those for the 70% scenario. The fixed carbon captured can also be seen from the constant difference between the two distributions.

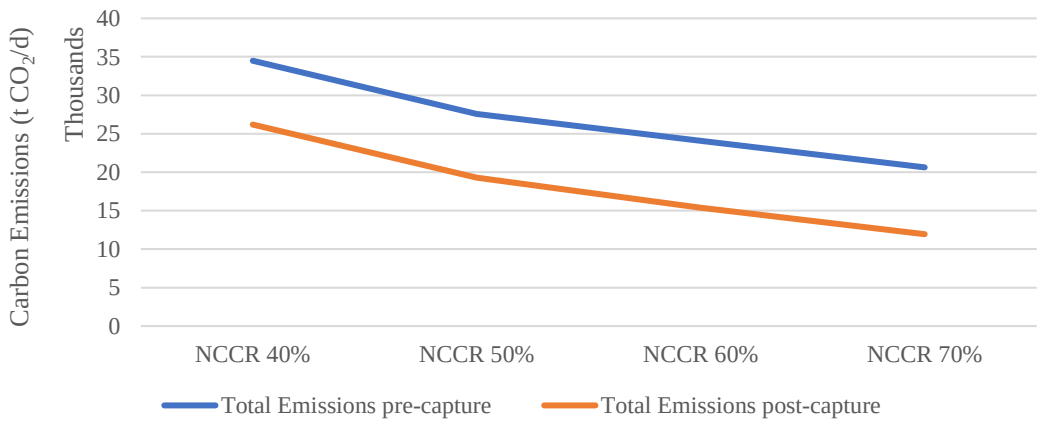

Figure 28 The variation of the pre-capture emissions and post-capture emissions as a function of NCCR

From the results, the reason for the difference in carbon emissions can be attributed to the changes in the flow rates of the fuel and the exported power. As can be seen in Table 10, at lower NCCR values, meaning at higher pre-capture emissions, the optimization selected the export of power to the grid as an additional revenue stream. However, at lower pre-capture emissions, the optimization was restricted in the utilization options of the carbon sources, and, in turn, decided not to activate the exported emissions and to allocate the power generation purely to the product requirement of the cluster.

Table 10 NCCR sensitivity analysis: power flow rates

Carbon capture %	NCCR 40%	NCCR 50%	NCCR 60%	NCCR 70%
Type	Coal	Coal	Natural Gas	Natural Gas
Power Supplied to products (kWh/d)	19150184.76	16307239.42	18665362.30	18766332.22
Exported power (kWh/d)	49815.24	49815.24	0.00	0.00
Renewable %	0.05	0.05	0.05	0.05

The discrepancy in the power is related to the fuel utilization for both power and products. As visualized in Figure 29, the flow of fuel decreased as the NCCR increased. Table 11 shows the difference in fuel allocations between the different NCCR values. The power plant shifted from a coal plant for the 40% and 50% cases to a natural gas plant from the 60% to the 70% case.

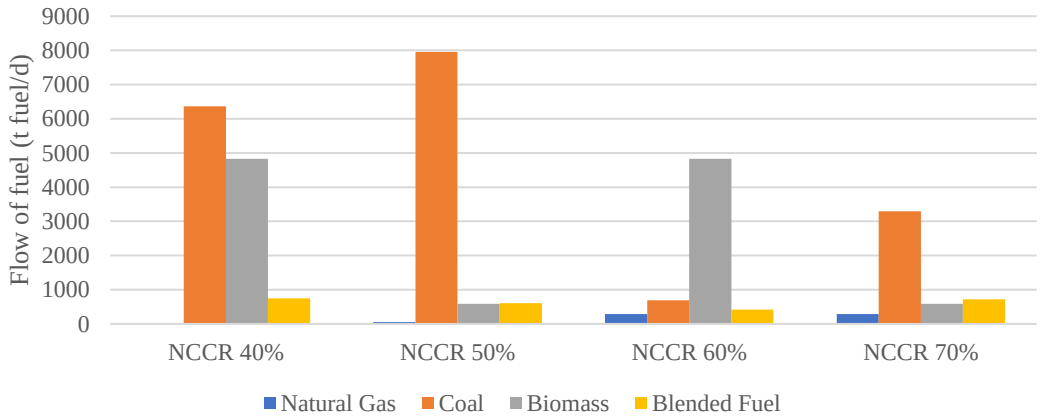

Figure 29 The variation of the flow of fuel as a function of the NCCR

Table 11 NCCR sensitivity analysis: fuel flow rates

Carbon capture %	NCCR 40%		
Utilization	Production (t fuel/d)	Product type	Power (t fuel/d)
Natural gas	23.27	Methanol (B)	0.00
Coal	888.35	Cement - Portland	5474.70
Biomass	4828.86	Methanol (A)	0.00
Blended Fuel	750.54	Aluminum	0.00
Carbon capture %	NCCR 50%		
Utilization	Production (t fuel/d)	Product type	Power (t fuel/d)
Natural gas	51.79	Cement	0.00
Coal	3292.79	Methanol (A)	4664.06
Biomass	585.39	Methanol (B)	0.00
Blended Fuel	610.71	Aluminum	0.00
Carbon capture %	NCCR 60%		
Utilization	Production (t fuel/d)	Product type	Power (t fuel/d)
Natural gas	39.75	Aluminum	245.26
Coal	688.39	Cement	0.00
Biomass	4828.86	Methanol (A)	0.00
Blended Fuel	419.18	Methanol (B)	0.00
Carbon capture %	NCCR 70%		
Utilization	Production (t fuel/d)	Product type	Power (t fuel/d)
Natural gas	40.03	Aluminum	246.59
Coal	3292.79	Methanol (A)	0.00
Biomass	585.39	Methanol (B)	0.00
Blended Fuel	722.88	Cement	0.00

Regarding the product portfolio of the cluster, represented in Figure 29, and as previously stated, the optimization kept the product flow rates constant and shifted between the fuel allocation to satisfy their requirements (refer to Table 11).

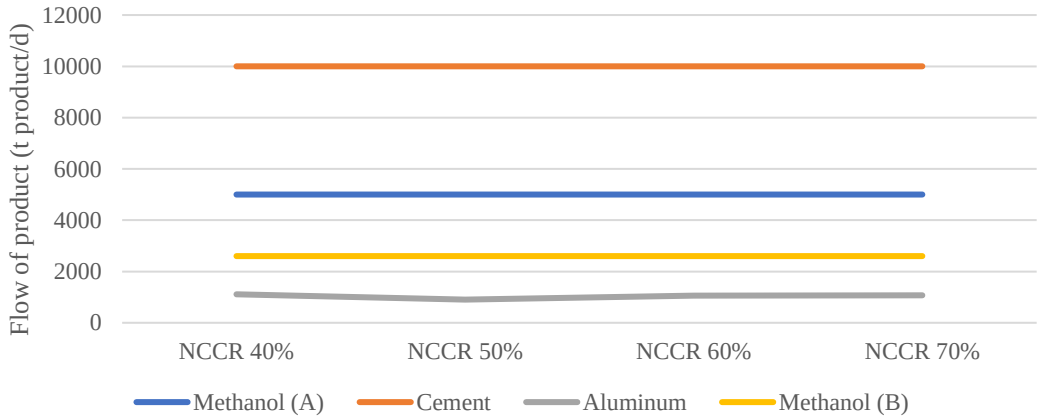

Figure 30 The variation of the product flow with respect to the NCCR

Given that the objective of the optimization is to maximize the cluster's profit, a profit distribution of the cluster is represented in Figure 31. As can be seen, the profit increased concurrently with the variation of the NCCR value.

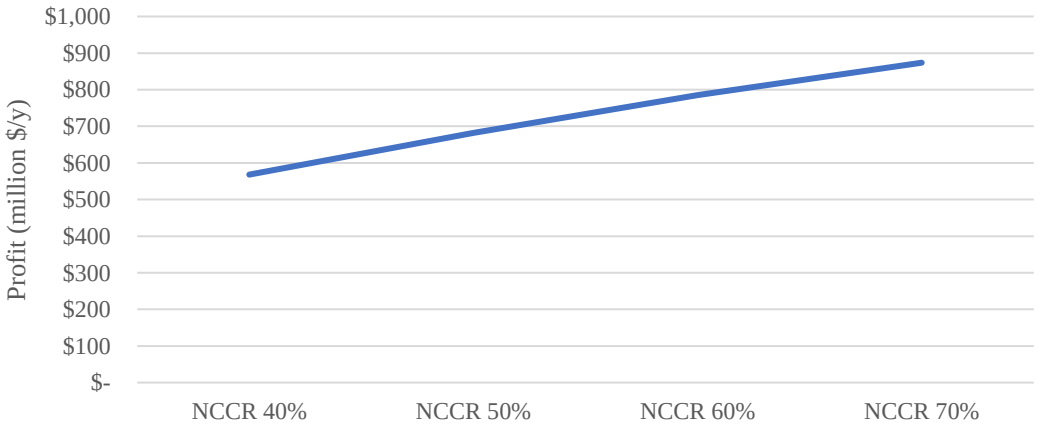

Figure 31 The variation of the cluster's profit as a function of the NCCR

This increase in profit can be attributed to the decrease in the total costs of the fuels due to the reduction in their respective flow rates. The fuel cost distribution, represented in Figure 32, shows the aforementioned decrease as the NCCR is increased.

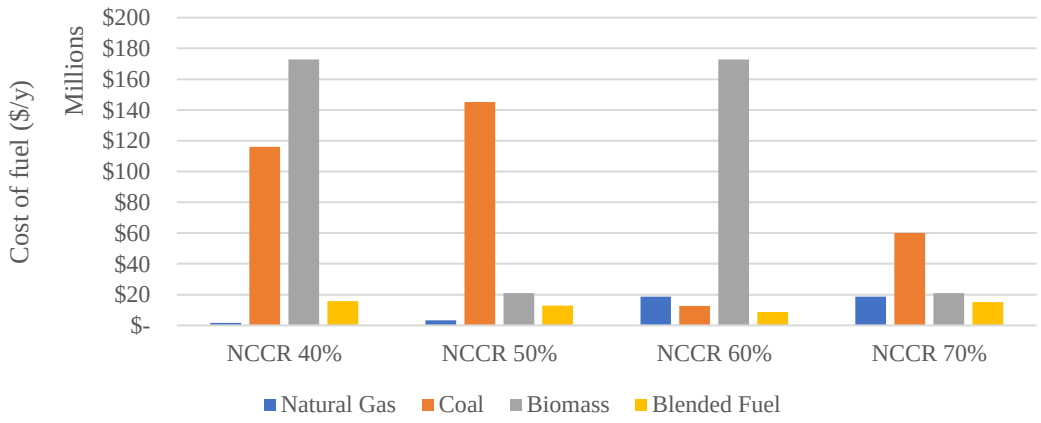

Figure 32 Cost breakdown of the fuels at every NCCR %

Therefore, from the aforementioned, it can be concluded that when the NCCR % is increased, the ratio of carbon captured over pre-capture emissions is concurrently increased. By fixing the amount of carbon captured, the optimization is being forced to reduce the total emissions while maintaining a maximum profit. Given that the model shifted from the activation to the deactivation of exporting power and decreased the flow of fuel into the city, it can be concluded that the revenue from exporting power onto the grid is lower than the significant costs of fuel, forcing the optimization to shift all the fuel used to generate exported power towards the power required to maintain the cluster's product portfolio.

4.2.2. Case 5: Renewable %

In the carbon capture sensitivity analysis, a maximum of 5% of the fuel-derived power could be replaced by renewable energy. This imposed constraint is due to the capacity restriction of the solar PV plant used in the analysis. From the results, it was shown that all scenarios operated at full renewable capacity. Therefore, in this analysis a higher capacity of renewable energy is integrated by relaxing the constraint and setting it to a range of 0% to 100%. The purpose of this scenario is to assess the effect of integrating a higher capacity of renewable energy at different NCCR values, either by increasing the plant's capacity or by adding more renewable energy options, on the cluster's product portfolio, fuel requirements, carbon footprint, and profit. It is worth noting that a 100% power replacement is assumed to be available for the purpose of the analysis.

From the results obtained, and the relaxation of the renewable constraint, it was shown that at higher carbon capture rate, the optimization shifted towards renewable energy. At an NCCR of 40% the renewable % was 11%. As the NCCR was increased to 70%, the renewable % increased to a maximum of 100% renewable. The integrated renewable energy serves to replace the fuel-derived energy as a means to reduce the carbon emissions from the power sector. This trend is observed in Figure 33, where the carbon emissions from the power sector decreased with the increase in the renewable percent. This successfully proves the proportional relationship between NCCR and the integration of renewable energy; at higher NCCR values, renewable energy is expected to be favoured over the fuel-derived power given the imposed environmental constraints.

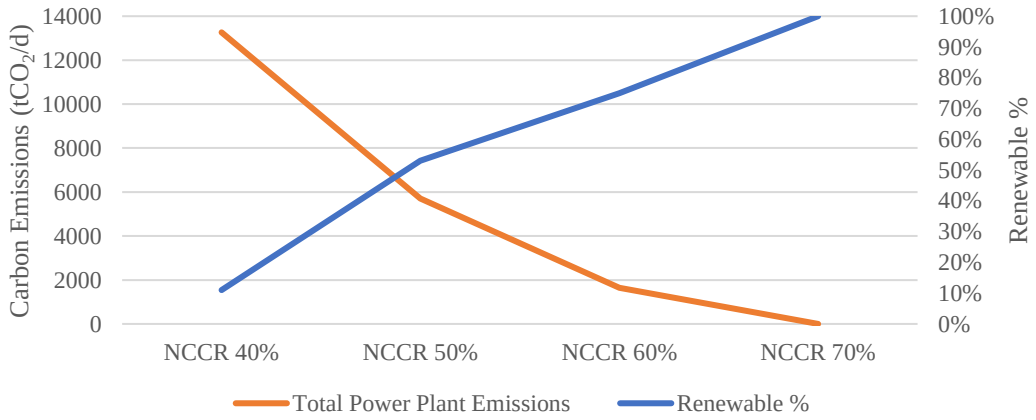

Figure 33 The variations of the power sector's carbon emissions and renewable % as a function of NCCR

However, in practice, a 100% renewable replacement is close to impossible. As mentioned, the purpose of setting this high upper bound is to show the favorable switch towards renewable. Further, the switch to renewable results in a higher cost. Assuming that the solar PV plant is able to achieve the aforementioned maximum replacement %, its cost upsurges. This trend is visualized in Figure 34.

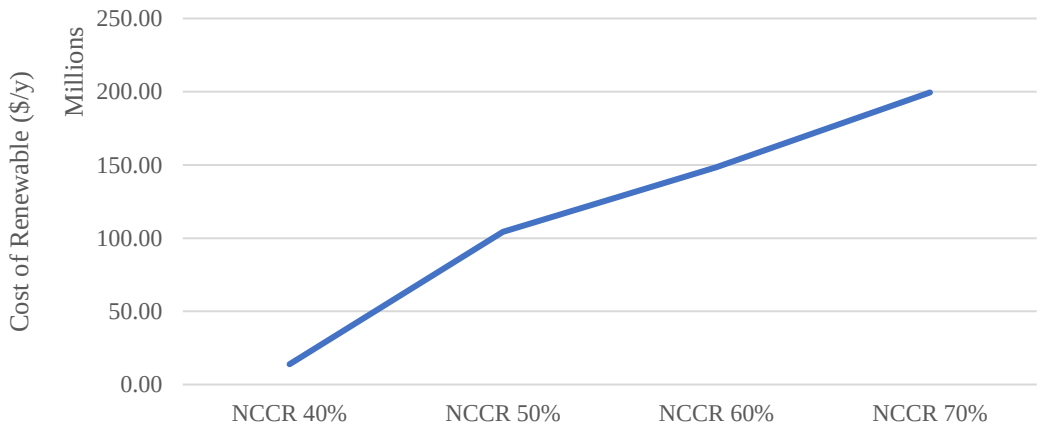

Figure 34 The variation of the cost of renewable as a function of NCCR

Furthermore, as shown in Table 12, when integrating a higher capacity of renewable energy, the power plant shifted from fossil fuel to blended fuel and biomass, which are considered to be greener alternatives. This further highlights the potential that renewable energy offers to mitigate the stricter restrictions imposed onto the cluster. However, it is expected that the cost of renewable energy increases when shifting towards the greener alternative.

Table 12 The variation of the type of fuel used for power, the power supplied and exported, the renewable power and the renewable % as a function of NCCR

Carbon capture %	NCCR 40%	NCCR 50%	NCCR 60%	NCCR 70%
Type	Biomass	Blended Fuel	Blended Fuel	Blended Fuel
Fuel-derived power (kWh/d)	19200000	15546500.34	8261797.59	0.45
Renewable power (kWh/d)	2292195.22	17243022.97	24527725.72	32967301.31
Renewable %	11%	53%	75%	100%

Limitations and recommendations

In the analysis, certain limitations were identified and are listed below:

- The cluster analysed consisted of a collection of different sources. Therefore, for more accurate results, it is advisable to use data from an existing industrial cluster.
- The emissions from the transportation of fuel through pipelines and from the compression and pumping of CO_2 were not included. To obtain an overall overview of the cluster's carbon footprint, all emission sources should be included in the analysis.

- The analysis in regard to biomass was limited to the cluster's boundaries. For future works, it is recommended to perform an LCA on the integration of biomass into the cluster to be able to properly assess its green potential as a replacement to fossil fuels.
- The biomass included in the analysis is assumed to be bought. Further works could assess the integration of forestry wastes and the cost of treatment as a potential cheaper alternative.
- The renewable energy used consists of a solar photovoltaic plant with limited capacity. As shown in the second sensitivity analysis, integrating more than one source of renewable energy could ultimately lead to a better footprint and end profit. The integration of green hydrogen onto the existing natural gas pipeline could be evaluated given its growing attractiveness in the EU (EuropeanCommission, 2020).

However, despite the aforementioned limitations, the optimization model was able to determine mitigation strategies to guide the industrial sectors and reduce their footprint while also shifting towards more sustainable sources of energy. No previous study has covered both the economic and environmental aspects of their proposed methodology as well as the integration of more than one type of fuel.

CHAPTER 5

CONCLUSION AND RECOMMENDATIONS

With the world's shift towards green sources of energy and the newly imposed environmental restrictions, industrial clusters are facing major challenges in overcoming their dependence on fossil fuels. Therefore, the main purpose of the presented model is to guide decision-makers to screen through all the potential configurations and determine the optimal strategies to reduce a cluster's carbon footprint as well as its reliance on fossil fuel. To do so, this work introduced a systematic approach that integrates multiple types of fuels into a cluster and determines the optimal product and power portfolios, the optimal allocation of the different fuels, the optimal renewable energy % that will replace the fuel-derived power and the optimal source to sink mapping and carbon utilization strategies.

The analysed industrial cluster consisted of a combination of production plants with one fuel-derived power plant, one renewable power plant, and different carbon utilization technologies. Five case studies were presented: a natural gas cluster, a biomass cluster, a blended fuel cluster, and a multiple fuel cluster to assess the potential of a multiple fuel-integrated clusters in comparison to the standalone cases. From the analysis, the multiple fuel case study showed the greatest potential in yielding the highest profit, generating \$907.16 million/y at the lowest carbon footprint of 9469 t CO_2 emitted /d with a 78% optimal carbon capture. The study successfully proved that the integration of multiple types of fuel can be used as a mitigation technique to significantly reduce the carbon footprint while maintaining a high-end profit.

Sensitivity analyses on the net carbon capture rate and the renewable energy % were also conducted to assess their effect on the model. From the first sensitivity analysis it was concluded that increasing the NCCR led to a lower fuel requirement and a higher end profit. The latter can be attributed to the lower pre-carbon emissions imposed that resulted in different fuel allocations and utilizations that the optimization selected for each case. The purpose of the second sensitivity analysis was to show the optimization's shift towards renewable energy at high carbon capture rates. The latter was successfully proven from the increase of the renewable % from 11% to 100% with the variation of the NCCR from 40% to 70%. However, further analysis with the integration of higher capacity of renewable energy and its full economic assessment.

In summary, with the obtained results, and if the limitations mentioned in section 4 are addressed, the model presented in this work could ultimately lead to a greener more sustainable future for the industrial sector by proposing a tool that allows decision makers to make the optimal selection of variables that favour both the economic as well as environmental targets.

APPENDIX A

NOMENCLATURE

Sets

P	is a set of plants
E	is a subset of existing plants belonging to P
O	is a subset of optional plants belonging to P
C_{pr}	is a set of chemical products produced in the cluster
K	is a set of carbon sinks in a plant p
S	is a set of carbon sources in a plant p
PW	is a set of available power types, including renewable power, used to satisfy the cluster's power demand
PW_{fuel}	is a subset of the set PW, which comprises the available types of fuel derived power (whether fossil fuel, biomass or blended fuel)
$PW_{renewable}$	is a subset of the set PW, which consists of the different types of available renewable energies that can be used in the cluster
FF	is a set of fossil fuel options
SF_{ff}	is a subset of solid fossil fuels that belongs to set FF
LF_{ff}	is a subset of liquid/gaseous fossil fuels that belongs to set FF
B	is a set of biomass options
SF_b	is a subset of solid biomass that belongs to set B
LF_b	is a subset of liquid/gaseous biomass that belongs to set B
BF	is a set of blended fuel options
SF_{bf}	is a subset of solid blended fuel that belongs to set BF
LF_{bf}	is a subset of liquid/gaseous blended fuel that belongs to set BF

Indices

p	plant
c	product
k	sink
s	source
pw	power
ff	fossil fuel
b	biomass
bf	blended fuel

Variables

$F^c_{c,ff,p}$	Flow of product c in a plant p associated with fossil fuel ff (t product/d)
$F^c_{c,b,p}$	Flow of product c in a plant p associated with biomass b (t product/d)
$F^c_{c,bf,p}$	Flow of product c in a plant p associated with blended fuel bf (t

	product/d)
$F^{c}_{c,p}$	Total flow of product c in a plant p (t product/d)
I_o	binary (0,1) that determines the activation/deactivation of an optional plant
$I_{ff,c,p}$	Binary (0,1) that determines the usage of fossil fuel ff
$I_{b,c,p}$	Binary (0,1) that determines the usage of biomass b
$I_{bf,c,p}$	Binary (0,1) that determines the usage of blended fuel bf
$F^{c}_{ff,p}$	Flow of fossil fuel ff in a plant p (t fossil fuel/d)
$F^{c}_{b,p}$	Flow of biomass b in a plant p (t biomass/d)
$F^{c}_{bf,p}$	Flow of blended fuel bf in a plant p (t blended fuel/d)
$M^{c}_{s,c,p}$	The maximum carbon emitted in a plant p from source s during the production of product c (t CO_2/d)
$M_{production}$	The total amount of carbon emitted during the production processes in the industrial cluster (t CO_2/d)
$PW_{pw,c,p}$	The electricity requirement of a product c in a plant p derived from power type pw (kWh/d)
$I_{pw,ff}$	Binary (0,1) associated with the type of fossil fuel used for the power generation
$I_{pw,b}$	Binary (0,1) associated with the type of biomass used for the power generation
$I_{pw,bf}$	Binary (0,1) associated with the type of blended fuel used for the power generation
$PW^{required}_{cluster}$	The total power requirement of the cluster (kWh/d)
PW^{exp}	The power to be exported to the electricity grid (kWh/d)
$PW_{renewable,pw}$	The renewable power that will replace part of the fuel-derived power (kWh/d)
$\%_{renewable}$	The percent of the fuel-derived power that can be replaced by renewable power
$I_{pw,renewable}$	The binary (0,1) that determines the type of renewable power used
$PW_{cluster}$	The total available power in the cluster (kWh/d)
F^{pw}_{ff}	The fossil fuel required for the total power generation in the cluster (t fossil fuel/d)
F^{pw}_{b}	The biomass required for the total power generation in the cluster (t biomass/d)
F^{pw}_{bf}	The blended fuel required for the total power generation in the cluster (t blended fuel/d)
$M^{pw}_{required}$	The amount of carbon emitted from the power generation used to satisfy the cluster's requirement before the integration of renewable energy (t CO_2/d)
$M^{pw,renewable}_{required}$	The amount of carbon emitted from the power generation used to satisfy the cluster's requirement after the integration of renewable energy (t CO_2/d)
M^{pw}_{exp}	The amount of carbon emitted from the power to be exported to the electricity grid (t CO_2/d)
M_{power}	The total power emitted during the power generation before the integration of renewable energy (t CO_2/d)

$M_{power}^{pw,renewable}$	The total power emitted during the power generation after the integration of renewable energy (t CO_2/d)
$F_{transport}^{CO_2}$	The carbon emitted during the transport of solid fuel into the city (t CO_2/d)
$CE_{pre\text{-}capture}$	The total amount of carbon emitted in the cluster pre-renewable energy integration and pre-capture (t CO_2/d)
$CE_{pre\text{-}capture}^{renewable}$	The total amount of carbon emitted in the cluster post-renewable energy integration and pre-capture (t CO_2/d)
$R_{s,p}$	The amount of carbon captured from a source s in a plant p (t CO_2/d)
$R_{ff,s,c,p}$	The amount of carbon captured from the use of fossil fuel ff from a source s in a plant p (t CO_2/d)
$R_{b,s,c,p}$	The amount of carbon captured from the use of biomass b from a source s in a plant p (t CO_2/d)
$R_{bf,s,c,p}$	The amount of carbon captured from the use of blended fuel bf from a source s in a plant p (t CO_2/d)
$R_{pw,ff,s}$	The amount of carbon captured from the use of fossil fuel ff from a source s in a plant p (t CO_2/d)
$R_{pw,b,s}$	The amount of carbon captured from the use of biomass b from a source s in a plant p (t CO_2/d)
$R_{pw,bf,s}$	The amount of carbon captured from the use of blended fuel bf from a source s in a plant p (t CO_2/d)
$T_{s,k,p}$	is the treated carbon emitted from source s during the production of product c or power generation pw in plant p that is sent to a sink k (t CO_2/d)
$G_{ff,k,c,s,p}$	Is the untreated carbon emitted from a source s associated with fossil fuel ff during the production of product c that is sent to a sink k (t CO_2/d)
$G_{b,k,c,s,p}$	Is the untreated carbon emitted from a source s associated with biomass b during the production of product c that is sent to a sink k (t CO_2/d)
$G_{bf,k,c,s,p}$	Is the untreated carbon emitted from a source s associated with blended fuel bf during the production of product c that is sent to a sink k (t CO_2/d)
$G_{ff,k,s,pw}$	Is the untreated carbon emitted from a source s associated with fossil fuel ff during the power generation that is sent to a sink k (t CO_2/d)
$G_{b,k,s,pw}$	Is the untreated carbon emitted from a source s associated with biomass b during the power generation that is sent to a sink k (t CO_2/d)
$G_{bf,k,s,pw}$	Is the untreated carbon emitted from a source s associated with blended fuel bf during the power generation that is sent to a sink k (t CO_2/d)
$T_{cluster}$	The total carbon treated in the cluster (t CO_2/d)
$M_{treatment}$	The carbon emitted during the treatment process in the cluster (t CO_2/d)
$F_{k,p}$	The flow of carbon into a sink k from a plant p (t CO_2/d)
M_{sinks}	The carbon emitted from the sinks in the cluster (t CO_2/d)

F_{ff}	The flow of fossil fuel ff into the industrial cluster (t fossil fuel/d)
F_{b}	The flow of biomass b into the industrial cluster (t fossil fuel/d)
F_{bf}	The flow of blended fuel bf into the industrial cluster (t fossil fuel/d)
NCCR	The net carbon capture rate imposed on the industrial cluster (%)
Profit	The industrial cluster's profit ($/y)
REV^{c}	The revenue from the products in the industrial cluster ($/y)
REV^{pw}	The revenue from the exported power ($/y)
REV^{CO_2}	The revenue from the processing of CO_2 in the sinks ($/y)
$Cost^{ff}$	The cost of fossil fuel ff in the industrial cluster ($/y)
$Cost^{b}$	The cost of biomass b in the industrial cluster ($/y)
$Cost^{bf}$	The cost of blended fuel bf in the industrial cluster ($/y)
$Cost^{E}$	The cost of the existing plant in the industrial cluster ($/y)
$Cost^{O}$	The cost of the optional plant in the industrial cluster ($/y)
$Cost^{transport,CO2}$	The cost of transporting carbon in the industrial cluster ($/y)
$Cost^{capture,untreated}$	The cost of capturing untreated carbon in the industrial cluster ($/y)
$Cost^{capture,treated}$	The cost of treating and capturing treated carbon in the industrial cluster ($/y)
$Cost^{compression,pumping}$	The cost of compressing and pumping the CO_2 streams in the cluster ($/y)
$C_{s,k}^{CO_2\ transport}$	The cost of transporting CO_2 from source to sink ($/t CO_2 transported)
$Cost_{treated}^{compression,pumping}$	The cost compressing and pumping the treated CO_2 ($/y)
$Cost_{untreated}^{compression,pumping}$	The cost compressing and pumping the untreated CO_2 ($/y)
$Cost_{treated,capex}^{compression,pumping}$	The capital cost compressing and pumping the treated CO_2 ($/y)
$Cost_{treated,opex}^{compression,pumping}$	The operating cost compressing and pumping the treated CO_2 ($/y)
$Cost_{treated,opex}^{compression,pumping}$	The capital cost compressing and pumping the untreated CO_2 ($/y)
$Cost_{untreated,opex}^{compression,pumping}$	The operating cost compressing and pumping the untreated CO_2 ($/y)

Parameters

$L_{c,p}^{c}$	the minimum production capacity of product c in a plant p (t product/d)
$U_{c,p}^{c}$	the maximum production capacity of product c in a plant p (t product/d)
$\alpha_{ff,c,p}^{c}$	the amount of fossil fuel ff required for the production of product c in a plant p (t fossil fuel/t product)
$\alpha_{b,c,p}^{c}$	the amount of biomass b required for the production of product c in a plant p (t biomass/t product)
$\alpha_{bf,c,p}^{c}$	the amount of blended fuel bf required for the production of product c in a plant p (t blended fuel/t product)
$\beta_{ff,s,c,p}^{c}$	the amount of carbon dioxide emitted per product associated with fossil fuel ff (t CO_2/t product)
$\beta_{b,s,c,p}^{c}$	the amount of carbon dioxide emitted per product associated with biomass b (t CO_2/t product)

$\beta^{c}_{bf,s,c,p}$	the amount of carbon dioxide emitted per product associated with blended fuel bf (t CO_2/t product)
$\varphi^{pw}_{pw,ff,c,p}$	power requirement per product c associated with fossil fuel ff (kWh/t product)
$\varphi^{pw}_{pw,b,c,p}$	power requirement per product c associated with biomass b (kWh/t product)
$\varphi^{pw}_{pw,bf,c,p}$	power requirement per product c associated with blended fuel bf (kWh/t product)
L^{exp}_{power}	the minimum power to be exported out of the industrial cluster (kWh/d)
U^{exp}_{power}	the maximum power to be exported out of the industrial cluster (kWh/d)
$\alpha^{pw}_{pw,ff}$	the amount of fossil fuel required for the total power generation of the cluster (kWh/t fossil fuel)
$\alpha^{pw}_{pw,b}$	the amount of biomass required for the total power generation of the cluster (kWh/t biomass)
$\alpha^{pw}_{pw,bf}$	the amount of blended fuel required for the total power generation of the cluster (kWh/t blended fuel)
$\beta^{pw}_{pw,ff,s}$	the amount of carbon emitted from the power generation associated with fossil fuel ff (tCO_2/kWh)
$\beta^{pw}_{pw,b,s}$	the amount of carbon emitted from the power generation associated with biomass b (tCO_2/kWh)
$\beta^{pw}_{pw,bf,s}$	the amount of carbon emitted from the power generation associated with blended fuel bf (tCO_2/kWh)
$\beta_{ff,transport}$	the amount of carbon emitted during the transport of fossil fuel ff (t CO_2/t fossil fuel)
$\beta_{b,transport}$	the amount of carbon emitted during the transport of biomass b (t CO_2/t biomass)
$\beta_{bf,transport}$	the amount of carbon emitted during the transport of blended fuel bf (t CO_2/t blended fuel)
$L^{carbon}_{ff,s,c,p}$	the lower bound of the carbon captured from fossil fuel ff, source s, during the production of product c in plant p (tCO_2/d)
$L^{carbon}_{b,s,c,p}$	the lower bound of the carbon captured from biomass b, source s, during the production of product c in plant p (tCO_2/d)
$L^{carbon}_{bf,s,c,p}$	the lower bound of the carbon captured from blended fuel bf, source s, during the production of product c in plant p (tCO_2/d)
$L^{carbon}_{pw,ff}$	the lower bound of the carbon captured from fossil fuel ff, source s, during the power generation of pw in plant p (tCO_2/d)
$L^{carbon}_{pw,b}$	the lower bound of the carbon captured from biomass b, source s, during the power generation of pw in plant p (tCO_2/d)
$L^{carbon}_{pw,bf}$	the lower bound of the carbon captured from blended fuel bf, source s, during the power generation of pw in plant p (tCO_2/d)
$\gamma_{treatment}$	the carbon treatment efficiency (t CO_2 emitted/ t CO_2 treated)
$z_{k,p}$	the concentration requirement of a sink k
$F^{max}_{k,p}$	the maximum allowable concentration for sink k in a plant p (t CO_2/d)
$y_{s,k,p}$	the CO_2 concentration in the treated stream
$y_{ff,s,c,p}$	the CO_2 concentration in the untreated stream associated with fossil fuel ff and product c
$y_{b,s,c,p}$	the CO_2 concentration in the untreated stream associated with biomass b

	and product c
$y_{bf,s,c,p}$	the CO_2 concentration in the untreated stream associated with blended fuel bf and product c
$y_{ff,s,pw}$	the CO_2 concentration in the untreated stream associated with fossil fuel ff and power pw
$y_{b,s,pw}$	the CO_2 concentration in the untreated stream associated with biomass b and power pw
$y_{bf,s,pw}$	the CO_2 concentration in the untreated stream associated with blended fuel bf and power pw
$\eta_{k,p}$	the CO_2 efficiency of a sink k (t CO_2 out/ t CO_2 into the sink)
MF_{ff}	the upper bound for fossil fuel ff (t fossil fuel/d)
MF_{b}	the upper bound for biomass b (t biomass/d)
MF_{bf}	the upper bound for blended fuel bf (t blended fuel/d)
$CE_{post\ capture}$	the carbon emissions of the industrial cluster after the integration of carbon capture technology (t CO_2/d)
dy	The conversion from day to year
hy	The number of operating hours in a year
C^{c}	the revenue parameter of product c ($/ t product)
C^{pw}	The revenue parameter of the exported power pw ($/kWh)
$C_{k,p}^{CO_2}$	The revenue/cost parameter from the processing of CO_2 in sink k ($/t CO_2)
C^{ff}	The cost of fossil fuel ff ($/t fossil fuel)
C^{b}	The cost of biomass b ($/t biomass)
C^{b}	The cost of blended fuel bf ($/t blended fuel)
CRF	The annualization factor
i	Discount rate (%)
n	Lifetime of a plant (y)
$C_{c,p}^{capex}$	The capex parameter associated with production plant p ($/t product)
$C_{c,p}^{opex}$	The opex parameter associated with production plant p ($/h.t product)
$C_{ff,pw}^{capex}$	The capex parameter associated with fossil fuel power plant p ($/kWh)
$C_{ff,pw}^{opex}$	The opex parameter associated with fossil fuel power plant p ($/h. kWh)
$C_{b,pw}^{capex}$	The capex parameter associated with biomass power plant p ($/kWh)
$C_{b,pw}^{opex}$	The opex parameter associated with biomass power plant p ($/h. kWh)
$C_{bf,pw}^{capex}$	The capex parameter associated with blended fuel power plant p ($/kWh)
$C_{bf,pw}^{opex}$	The opex parameter associated with blended fuel power plant p ($/h. kWh)
C_{pw}^{capex}	The capex parameter associated with renewable power plant p ($/kWh)
C_{pw}^{opex}	The opex parameter associated with renewable power plant p ($/h. kWh)
$d_{s,k,p}$	The distance from source s to sink k (km)
$C_{c,p}^{capture}$	The cost of capturing untreated carbon associated with product c ($/t CO_2)
$C_{pw}^{capture}$	The cost of capturing untreated carbon associated with power pw ($/t CO_2)
$C_{c,p}^{treatment,capex}$	The capital cost of treating carbon

$C_{c,p}^{treatment,opex}$	The operating cost of treating carbon
$a_{s,k,p}^{capex}$	The parameter associated with the capital cost of compressing and pumping CO_2 ($/t CO_2)
$b_{s,k,p}^{capex}$	The parameter associated with the capital cost of compressing and pumping CO_2 ($/y)
$a_{s,k,p}^{opex}$	The parameter associated with the operating cost of compressing and pumping CO_2 ($/t CO_2)
$b_{s,k,p}^{opex}$	The parameter associated with the operating cost of compressing and pumping CO_2 ($/y)

APPENDIX B

PARAMETERS

Methanol (A) plant

Table 13 Methanol (A) plant general parameters

Parameter	Value	Reference
Maximum production capacity	5000 tMeOH(A)/d	(D. M. Al-Mohannadi & Linke, 2016)
Process fuel requirement in the form of energy	20,090 kJ/kg	(Pellegrini et al., 2011)
Electricity requirement	0.71 kWh/kg MeOH(A)	(Pellegrini et al., 2011)
CAPEX	$0.46/kg MeOH(A)	(Pellegrini et al., 2011)
OPEX	$0.047/kg MeOH(A)	(Pellegrini et al., 2011)

Methanol (B) plant

Table 14 Methanol (B) plant general parameters

Parameter	Value	Reference
Maximum product capacity	2,600 tMeOH(B) /d	(D. M. Al-Mohannadi & Linke, 2016)
Cooling requirements	0.439 MWh/tMeOH(B)	(Pérez-Fortes et al., 2016)
Heating requirements	0.862 MWh/tMeOH(B)	(Pérez-Fortes et al., 2016)
Electricity requirement	0.147 MWh/t MeOH(B)	(Pérez-Fortes et al., 2016)
CO_2 input	1.46 tCO_2/MeOH(B)	(Pérez-Fortes et al., 2016)
CAPEX	€846.73/tMeOH(B)	(Pérez-Fortes et al., 2016)
Fixed OPEX	€42.84/tMeOH(B).y	(Pérez-Fortes et al., 2016)
Variable OPEX	€358.08/tMeOH(B).y	(Pérez-Fortes et al., 2016)

Cement plant

Table 15 Cement plant general parameters

Type	Parameters	Value	Reference
Portland Cement	Maximum product capacity	10000 tCement/d	(D. M. Al-Mohannadi & Linke, 2016)
	Process fuel requirement	2.71 GJ/tCement	(Worrell, 2007)
	Electricity requirement	0.26 GJ/tCement	(Worrell, 2007)
	CAPEX	€263/tCement	(Worrell, 2007)
	OPEX	€29/tCement	(Worrell, 2007)
Fly Ash Cement with 25% Fly Ash	Maximum product capacity	2000 tCement/d	(D. M. Al-Mohannadi & Linke, 2016)
	Process fuel requirement	2.1 GJ/tCement	(Worrell, 2007)
	Electricity requirement	0.36 GJ/tCement	(Worrell, 2007)
	CAPEX	€263/tCement	(Worrell, 2007)
	OPEX	€29/tCement	(Worrell, 2007)

Aluminum plant

Table 16 Aluminum plant general parameters

Parameters	Value	Reference
Maximum product capacity	10000 tAluminumt/d	(D. M. Al-Mohannadi & Linke, 2016)
Process fuel requirement	19.64 GJ/tPrimary Aluminum	(Worrell, 2007)
Electricity requirement	50.96 GJ/tPrimary Aluminum	(Worrell, 2007)
CAPEX	€4000/tAluminum	(Rosenberg, 2012)
OPEX	€950-1500/tAluminum	(Rosenberg, 2012)

Power plants

Natural gas power

Table 17 Natural gas power plant characteristics

Parameter	Value	Reference
Fuel Heat input, HHV (MW_{th})	1528	(EIA, 2020a)
Natural Gas inlet (kg/s)	29.2	(EIA, 2020a)
HHV (kJ/kg)	52,329	(EIA, 2020a)
Total Power without steam extraction (MW_e)	800	(EIA, 2020a)
Total Power with steam extraction (MW_e)	714	(EIA, 2020a)
Specific CO_2 emissions from power plant (g/kWh)	431	(EIA, 2020a)
Flue Gas CO_2 composition (mol %)	4.16	(EIA, 2020a)
CAPEX Engines ($)	11974000	(EIA, 2020a)
Mechanical BOP	5521000	(EIA, 2020a)
Total CAPEX ($/kWnet)	782	(EIA, 2020a)
OPEX Fixed ($/kW-year)	35.16	(EIA, 2020a)

Coal

Table 18 Coal power plant characteristics

Parameter	Value	Reference
Fuel Heat input, HHV (MW_{th})	1933	(EIA, 2020a)
Total Power without steam extraction (MW_e)	800	(EIA, 2020a)
Total Power with steam extraction (MW_e)	664	(EIA, 2020a)
Specific CO_2 emissions from power plant (g/kWh)	1092	(EIA, 2020a)
Flue Gas CO2 composition (mol%)	13.28	(EIA, 2020a)
CAPEX ($) – Boilet plant	905,100,000	(EIA, 2020a)
Turbine Plant	155,200,000	(EIA, 2020a)
BOP	19,300,000	(EIA, 2020a)
Total CC ($)	1,079,600,000	(EIA, 2020a)
Net capacity (MW net)	650	(EIA, 2020a)
Total CC ($/ kWnet)	1660.92	(EIA, 2020a)
OPEX Fixed ($/kW-year)	40.58	(EIA, 2020a)

Biomass

Table 19 Biomass power plant characteristics

Parameter	Value	(EIA, 2020a)
Fuel Heat input, HHV (MW_{th})	1933	(EIA, 2020a)
Total Power without steam extraction (MW_e)	800	(EIA, 2020a)
Total Power with steam extraction (MW_e)	656	(EIA, 2020a)
Specific CO_2 emissions from power plant (g/kWh)	1142	(EIA, 2020a)
Flue Gas CO2 composition (mol%)	14.35	(EIA, 2020a)
CAPEX Boiler Plant ($)	60477000	(EIA, 2020a)
Turbine Plant	8230000	(EIA, 2020a)
Balance of the Plant	20111000	(EIA, 2020a)
Total ($)	88818000	(EIA, 2020a)
Net Capacity (MW)	50	(EIA, 2020a)
CAPEX ($/kWnet)	1776.36	(EIA, 2020a)
OPEX Fixed ($/kW-year)	95.2	(EIA, 2020a)

Blended fuel

Table 20 Co-fired power plant characteristics

Parameter	Value	Reference
CAPEX retrofit ($/kW net)	329	(EIA, 2020a)
Total CAPEX (coal + retrofit) ($/kW net)	1693.92	(EIA, 2020a)
OPEX Fixed retrofit ($/kW-year)	20.57	(EIA, 2020a)
OPEX Fixed total ($/kW-y)	61.05	(EIA, 2020a)

Solar PV

Table 21 Solar photovoltaic plant characteristics

Parameter	Value	Reference
CAPEX ($/kW net)	637.5	(EIA, 2020a)
OPEX ($/kW-y)	14.3	(EIA, 2020a)
Capacity (MW_{AC})	150	(EIA, 2020a)
Capacity (MW_{DC})	195	(EIA, 2020a)
DC/AC ratio	1.3	(EIA, 2020a)
Annual average Efficiency	1327 /kWp	(EIA, 2020a)

Carbon integration network

Carbon capture plant

Table 22 Carbon capture plant general specifications

Unit	Parameter	Value	Reference
General	Flue Gas Flow Rate (kg/s)	821.26	(Agbonghae, 2014)
	Optimal Lean CO_2 loading (mol/mol)	0.2	(Agbonghae, 2014)
	Optimal Liquid/Gas ratio (kg/kg)	2.93	(Agbonghae, 2014)
Absorber	Number of Absorbers	2	(Agbonghae, 2014)
	Absorber Packing	Mellapack 250Y	(Agbonghae, 2014)
	Diameter (m)	16.13	(Agbonghae, 2014)
	Optimum height (m)	23.04	(Agbonghae, 2014)
Stripper	Number of strippers	1	(Agbonghae, 2014)
	Packing	Mellapack 250Y	(Agbonghae, 2014)
	Diameter (m)	14.61	(Agbonghae, 2014)
	Optimum height (m)	25.62	(Agbonghae, 2014)
	Specific reboiler duty (MJ/kg CO_2)	3.69	(Agbonghae, 2014)

Sources

Table 23 Sources CO_2 concentrations

Source	Concentration	Reference
Methanol (A)	7 wt%	(D. M. Al-Mohannadi & Linke, 2016)
Cement	27 wt%	(D. M. Al-Mohannadi & Linke, 2016)
Aluminum	7 wt%	(D. M. Al-Mohannadi & Linke, 2016)
Methanol (B)	7 wt%	(D. M. Al-Mohannadi & Linke, 2016)
Power plant	7 wt%	(D. M. Al-Mohannadi & Linke, 2016)

Sinks

Table 24 Sink data and parameters

Sink	Maximum Flow Requirement	Concentration Requirement	Revenue/Cost	Reference
Methanol (B)	1710 tCO_2/d	99 wt%	\$21/tCO_2	(D. M. Al-Mohannadi & Linke, 2016), (D. M. Al-Mohannadi et al., 2017)
EOR	2739 tCO_2/d	94 wt%	\$30/tCO_2	(D. M. Al-Mohannadi & Linke, 2016), (D. M. Al-Mohannadi et al., 2017)
Saline Storage	8317 tCO_2/d	94 wt%	-\$10/tCO_2	(D. M. Al-Mohannadi & Linke, 2016), (D. M. Al-Mohannadi et al., 2017)
Greenhouse	1030 tCO_2/d	94 wt%	\$5/tCO_2	(D. M. Al-Mohannadi & Linke, 2016), (D. M. Al-Mohannadi et al., 2017)

Table 25 Distances between the sinks and the sources in the industrial cluster

Sink/Source	Methanol (B)	EOR	Saline Storage	Greenhouse	Reference
Methanol (A)	10 km	12 km	12 km	20 km	(D. M. Al-Mohannadi & Linke, 2016), (D. M. Al-Mohannadi et al., 2017)
Cement – Portland	10 km	6 km	6 km	25 km	(D. M. Al-Mohannadi & Linke, 2016),
Cement – Fly Ash	10 km	6 km	6 km	25 km	(D. M. Al-Mohannadi & Linke, 2016), (D. M. Al-Mohannadi et al., 2017)
Aluminum	3 km	8 km	8 km	24 km	(D. M. Al-Mohannadi & Linke, 2016), (D. M. Al-Mohannadi et al., 2017)
Power plant	11 km	7 km	7 km	26 km	(D. M. Al-Mohannadi & Linke, 2016), (D. M. Al-Mohannadi et al., 2017)

Treatment

Table 26 Treatment general parameters

Sources	Treatment CAPEX	Treatment OPEX	CO2 treatment efficiency	Treatment removal
Methanol (A)	38 $/tCO$_2$	10 $/tCO$_2$	35%	90%
Cement – Portland	30 $/tCO$_2$	8 $/tCO$_2$	35%	90%
Cement – Fly ash	30 $/tCO$_2$	8 $/tCO$_2$	35%	90%
Aluminum	38 $/tCO$_2$	10 $/tCO$_2$	35%	90%
Methanol (B)	38 $/tCO$_2$	10 $/tCO$_2$	35%	90%
Power plant	38 $/tCO$_2$	10 $/tCO$_2$	35%	90%
Reference	(D. Al-Mohannadi, 2014) and (Bergen, 2004)	(D. Al-Mohannadi, 2014) and (Bergen, 2004)	(D. Al-Mohannadi, 2014)	(D. Chapel, 1999)

Compression and pumping

Reference: (D. M. Al-Mohannadi et al., 2017; Kwak, 2016)

Table 27 Compression and pumping cost parameters for treated flow rates

Source/Sink		Methanol (A)	Cement - Portland	Cement – Fly Ash	Aluminum	Methanol (B)	Power Plant
Greenhouse	a^{capex}	300	300	300	300	300	300
	b^{capex}	67950	76740	76740	74780	67950	78700
	a^{opex}	570	570	570	570	570	570
	b^{opex}	32980	41220	41220	39570	32980	42800
EOR	a^{capex}	220	220	220	220	220	217
	b^{capex}	144000	126300	126300	131500	144000	129300
	a^{opex}	560	550	550	560	560	550
	b^{opex}	31000	13000	13000	17360	31000	18110
Storage	a^{capex}	220	220	220	220	220	217
	b^{capex}	144000	126300	126300	131500	144000	129300
	a^{opex}	560	550	550	560	560	550
	b^{opex}	31000	13000	13000	17360	31000	18110
Methanol (B)	a^{capex}	230	225	225	214	-	230
	b^{capex}	61400	61400	61400	51400	-	78700
	a^{opex}	530	530	530	520	-	530

	b^{opex}	12100	12100	12100	3600	-	13300

Where, a^{capex} is in $/ t product and b^{capex} is in $.

Table 28 Compression and pumping parameters for untreated flow rates

Source/Sink		Methanol (A)	Cement - Portland	Cement - Fly Ash	Aluminum	Methanol (B)	Power Plant
Greenhouse	a^{capex}	700	740	740	700	700	706
	b^{capex}	16500	17150	17150	16500	16500	16500
	a^{opex}	270	270	270	280	270	290
	b^{opex}	74000	78180	78180	86200	74000	92300
EOR	a^{capex}	640	670	670	640	640	640
	b^{capex}	95200	99000	99000	95200	95200	95200
	a^{opex}	200	180	180	200	200	200
	b^{opex}	117000	54000	54000	82400	117000	18110
Storage	a^{capex}	640	670	670	640	640	640
	b^{capex}	95200	99000	99000	95200	95200	95200
	a^{opex}	200	180	180	200	200	200
	b^{opex}	117000	54000	54000	82400	117000	18110
Methanol (B)	a^{capex}	690	720	720	690	-	690
	b^{capex}	25000	26130	26130	25130	-	25130
	a^{opex}	120	70	70	87	-	120
	b^{opex}	43300	21020	21020	22310	-	46330

Where, a^{capex} is in $/ t product and b^{capex} is in $

Revenues from products

Table 29 Revenue from products and exported power

Product	Value	Referemce
Methanol (A)	$442/tMeOH(A)	(D. Al-Mohannadi, 2014)
Cement	$85/tCement	(D. Al-Mohannadi, 2014)
Aluminum	$1550/tAluminum	(D. Al-Mohannadi, 2014)
Methanol (B)	$442/tMeOH(B)	(D. Al-Mohannadi, 2014)
Natural gas power	$0.02/kWh	(D. Al-Mohannadi, 2014)
Coal power	$0.07644/kWh	(EIA, 2020b)
Biomass power	$0.09/kWh	(Cuellar & Herzog, 2015)
Blended fuel power	$0.0983/kWh	(EIA, 2020b)

Costs of fuel

Table 30 Cost of fuels used in the industrial cluster

Cost of fuel	Value	Reference
Natural gas	$178.734/t natural gas	(EIA, 2020)
Coal	$50/t coal	(EIA, 2020)
Biomass (forestry wood)	$98/t biomass	(Cuellar & Herzog, 2015)
Coal and forestry wood (15%)	$57.2/t blended fuel	(EIA, 2020), (Cuellar & Herzog, 2015)

Fuel characteristics

Natural gas

Table 31 Natural gas characteristics

Natural Gas	Molar Composition (%)	Reference
CH_4	93.1	(Ali et al., 2017)
C_2H_6	3.2	(Ali et al., 2017)
C_3H_8	0.7	(Ali et al., 2017)
Iso-C_4H_{10}	0.4	(Ali et al., 2017)
CO_2	1	(Ali et al., 2017)
N_2	1.6	(Ali et al., 2017)
HHV	52,329 (kJ/kg)	(Ali et al., 2017)

Coal, biomass, and blended fuel

Table 32 Coal and biomass characteristics

Fuel	Coal	Biomass	Blended fuel	Reference
Type	Dried bituminous type Illinois No. 6	Dried pelletized forestry residue	15% forestry residue 85% bituminous coal	(Ali et al., 2017)
Ash (wt. %)	10.91	0.75	9.38	(Ali et al., 2017)
HHV (kJ/kg)	30506	20802	29050	(Ali et al., 2017)

LHV (kJ/kg)	29444	19398	27937	(Ali et al., 2017)

Carbon emissions factor

Table 33 Carbon emissions factor

Type of fuel	Default CO_2 factor	Reference
Natural Gas	53.02 kg CO_2/mmBtu	("Default CO2 Emission Factors and High Heat Values for Various Types of Fuel," 2016)
Coal	93.4 kg CO_2/mmBtu	("Default CO2 Emission Factors and High Heat Values for Various Types of Fuel," 2016)
Biomass	93.8 kg CO_2/mmBtu	("Default CO2 Emission Factors and High Heat Values for Various Types of Fuel," 2016)
Co-fired	93.46 kg CO_2/mmBtu	("Default CO2 Emission Factors and High Heat Values for Various Types of Fuel," 2016)

APPENDIX C

CASE STUDIES

Case study 1

Table 34 Case study 1: products, fuel, carbon, and power

Natural Gas Case Study	Flow of product (t product/d)	Flow of fuel (t natural gas/d)	Carbon Emissions (tCO_2/d)	Power Required (kWh/d)
Methanol (A)	5000.00	191.96	5047.96	3550000.00
Cement - Portland	10000.00	51.79	1361.87	722222.80
Aluminum	1047.05	39.30	1033.42	14821610.45
Methanol (B)	2600.00	23.27	611.95	106166.75
Total	-	306.31	8055.19	19200000

Table 35 Case study 1: fuel, carbon, and power

Natural Gas Case Study	Flow of power (kWh/d)	Flow of fuel (t natural gas/d)	Carbon Emissions (tCO2/d)
Exported	0.00	0.00	0.00
Power	19200000.00	252.29	13268.82
Renewable	0.00	0.00	0.00
Total	19200000.00	252.29	13268.82

Table 36 Case study 1: carbon emissions

Source	Value (t CO_2/d)
Emissions from products	8055
Emissions from power	13269
Emissions from transportation of fuel	0
Emissions from carbon integration network	5506
Emissions from sink	681
Emissions from treatment	4825
Total Emissions pre-capture (t CO2/d)	21324
Carbon captured (t CO2/d)	13796
Total Emissions post-capture (t CO2/d)	13034
% Carbon capture (t CO2/d)	65%
% Carbon reduction (t CO2/d)	-39%

Table 37 Case study 1: revenue/cost of sinks

Revenues/Cost of sinks	$	16,087,512
Methanol (B)	$	13,239,545
Enhanced Oil Recovery	$	31,906,436
Saline Storage	$	-30,976,582
Greenhouse	$	1,918,112

Table 38 Case study 1: revenues from products

Revenues from products	$	2,129,876,703
Methanol (A)	$	806,650,000
Cement - Portland	$	310,250,000
Aluminum	$	592,369,503
Methanol (B)	$	420,607,200

Table 39 Case study 1: revenue from exported power

Revenue from exported power	$	-

Table 40 Case study 1: cost of fuel

Cost of fuel		
Natural Gas	$	36,441,991

Table 41 Case study 1: cost of plants

Cost of plants	$	1,138,035,857
Power plant	$	153,333,187
MeOH(A) plant	$	172,799,836
MeOH(B) plant	$	198,543,940
Aluminum plant	$	376,784,381
Cement plant	$	236,574,513
Solar PV plant	$	-

Table 42 Case study 1: cost of carbon integration network

Cost of carbon integration network	**$**	50,729,487
Carbon transportation	$	756,954.28
Capture of untreated	$	147,260.47
Capture and treatment	$	37,839,392.83
Compression and pumping of treated	$	11,652,838.53
Compression and pumping of untreated	$	333,041.13

Case study 2

Table 43 Case study 2: products, fuel, carbon, and power

Coal Case Study	Flow of product (t product/d)	Flow of fuel (t natural gas/d)	Carbon Emissions (tCO_2/d)	Power Required (kWh/d)
Methanol (A)	5000.00	3292.79	8892.48	3550000.00
Cement - Portland	10000.00	888.35	2399.07	722222.80
Aluminum	13.37	8.61	23.25	189257.62
Methanol (B)	0.00	0.00	0.00	0.00
Total	-	4189.75	11314.79	4461480.42

Table 44 Case study 2: fuel, carbon, and power

Coal Case Study	Flow of power (kWh/d)	Flow of fuel (t natural gas/d)	Carbon Emissions (tCO2/d)
Exported	0.00	1272.15	0.00
Power	4461480.42		3435.55
Renewable	0.00	0.00	0.00
Total	4461480.42	1272.15	3435.55

Table 45 Case study 2: carbon emissions

Source	Value (t CO_2/d)
Emissions from products	11315
Emissions from power	3436
Emissions from transportation of fuel	1364
Emissions from carbon integration network	5506
Emissions from sink	681
Emissions from treatment	4825

Total Emissions pre-capture (t CO2/d)	16115
Carbon captured (t CO2/d)	12086
Total Emissions post-capture (t CO2/d)	9535
% Carbon capture (t CO2/d)	75%
% Carbon reduction (t CO2/d)	-41%

Table 46 Case study 2: revenue/cost of sinks

Revenues/Cost of sinks	$	2,847,967
Methanol (B)	$	-
Enhanced Oil Recovery	$	31,906,436.17
Saline Storage	$	(30,976,581.63)
Greenhouse	$	1,918,112.24

Table 47 Case study 2: revenues from products

Revenues from products	$	1,124,463,985
Methanol (A)	$	806,650,000.00
Cement - Portland	$	310,250,000.00
Aluminum	$	7,563,985.19
Methanol (B)	$	-

Table 48 Case study 2: revenue from exported power

Revenue from exported power	$	-

Table 49 Case study 2: cost of fuel

Cost of fuel		
Coal	$	99,679,686.11

Table 50 Case study 2: cost of plants

Cost of plants	$	701,856,900.87
Power plant	$	68,413,372.38
MeOH(A) plant	$	257,881,278.62
MeOH(B) plant	$	-
Aluminum plant	$	11,983,847.91
Cement plant	$	363,578,401.97

Solar PV plant	$	-

Table 51 Case study 2: cost of carbon integration network

Cost of carbon integration network	$	45,407,040
Carbon transportation	$	844,704.11
Capture of untreated	$	147,260.47
Capture and treatment	$	32,965,748.70
Compression and pumping of treated	$	11,129,185.71
Compression and pumping of untreated	$	320,141.13

Case study 3

Table 52 Case study 3: products, fuel, carbon, and power

Biomass Case Study	Flow of product (t product/d)	Flow of fuel (t natural gas/d)	Carbon Emissions (tCO_2/d)	Power Required (kWh/d)
Methanol (A)	5000.00	4828.86	8930.56	3550000.00
Cement - Portland	10000.00	1302.76	2409.34	722222.80
Aluminum	25.21	23.80	44.01	356817.03
Methanol (B)	2600.00	585.39	1082.63	106166.75
Total	-	6740.81	12466.55	4735206.58

Table 53 Case study 3: fuel, carbon, and power

Biomass Case Study	Flow of power (kWh/d)	Flow of fuel (t natural gas/d)	Carbon Emissions (tCO2/d)
Exported	100000.00	2021.87	77.33
Power	4735206.58		3661.94
Renewable	0.00	0.00	0.00
Total	4835206.58	2021.87	3739.28

Table 54 Case study 3: carbon emissions

Source	Value (t CO_2/d)
Emissions from products	12466.55

Emissions from power	3739.28
Emissions from transportation of fuel	2188.84
Emissions from carbon integration network	5518.08
Emissions from sink	703.33
Emissions from treatment	4814.75
Total Emissions pre-capture (t CO2/d)	18394.67
Carbon captured (t CO2/d)	13796.00
Total Emissions post-capture (t CO2/d)	10116.75
% Carbon capture (t CO2/d)	75%
% Carbon reduction (t CO2/d)	-45%

Table 55 Case study 3: revenue/cost of sinks

Revenues/Cost of sinks	$	16,788,665.67
Methanol (B)	$	13,239,545.45
Enhanced Oil Recovery	$	31,906,436.17
Saline Storage	$	(30,357,050.00)
Greenhouse	$	1,999,734.04

Table 56 Case study 3: revenues from products

Revenues from products	$	1,551,767,966
Methanol (A)	$	806,650,000
Cement - Portland	$	310,250,000
Aluminum	$	14,260,766
Methanol (B)	$	420,607,200

Table 57 Case study 3: revenue from exported power

Revenue from exported power	$	3,285,000

Table 58 Case study 3: cost of fuel

Cost of fuel		
Biomass	$	313,441,345

Table 59 Case study 3: cost of plants

Cost of plants	$	707,501,084
Power plant	$	90,803,947.31

MeOH(A) plant	$	172,799,836.35
MeOH(B) plant	$	198,252,040.49
Aluminum plant	$	9,070,747.25
Cement plant	$	236,574,513.08
Solar PV plant	$	-

Table 60 Case study 3: cost of carbon integration network

Cost of carbon integration network	$	52,599,601
Carbon transportation	$	879,756.13
Capture of untreated	$	649,795.58
Capture and treatment	$	37,743,803.19
Compression and pumping of treated	$	12,957,068.98
Compression and pumping of untreated	$	369,177.51

Case study 4

Table 61 Case study 4: products, fuel, carbon, and power

Blended Fuel Case Study	Flow of product (t product/d)	Flow of fuel (t natural gas/d)	Carbon Emissions (tCO_2/d)	Power Required (kWh/d)
Methanol (A)	5000.00	3457.78	8898.19	3550000.00
Cement - Portland	10000.00	932.86	2400.61	722222.80
Aluminum	74.23	50.19	129.15	1050808.15
Methanol (B)	2600.00	419.18	1078.71	106166.75
Total	-	4860.01	12506.65	5429197.70

Table 62 Case study 4: fuel, carbon, and power

Blended Fuel Case Study	Flow of power (kWh/d)	Flow of fuel (t natural gas/d)	Carbon Emissions (tCO2/d)
Exported	100000.00	1655.59	77.05
Power	5429197.70		4183.42
Renewable	0.00	0.00	0.00
Total	5529197.70	1655.59	4260.47

Table 63 Case study 4: carbon emissions

Source	Value (t CO_2/d)
Emissions from products	12506.65
Emissions from power	4260.47
Emissions from transportation of fuel	1627.54
Emissions from carbon integration network	5506.23
Emissions from sink	680.96
Emissions from treatment	4825.27
Total Emissions pre-capture (t CO2/d)	18394.67
Carbon captured (t CO2/d)	13796.00
Total Emissions post-capture (t CO2/d)	10104.90
% Carbon capture (t CO2/d)	75%
% Carbon reduction (t CO2/d)	-45%

Table 64 Case study 4: revenue/cost of sinks

Revenues/Cost of sinks	$	16,169,134
Methanol (B)	$	13,239,545
Enhanced Oil Recovery	$	31,906,436
Saline Storage	$	(30,976,582)
Greenhouse	$	1,999,734

Table 65 Case study 4: revenues from products

Revenues from products	$	1,579,504,438
Methanol (A)	$	806,650,000
Cement - Portland	$	310,250,000
Aluminum	$	41,997,238
Methanol (B)	$	420,607,200

Table 66 Case study 4: revenue from exported power

Revenue from exported power	$	3,285,000

Table 67 Case study 4: cost of fuel

Cost of fuel		
Blended fuel	$	136,032,837

Table 68 Case study 4: cost of plants

Cost of plants	$	726,518,647
Power plant	$	92,168,191
MeOH(A) plant	$	172,799,836
MeOH(B) plant	$	198,263,213
Aluminum plant	$	26,712,893
Cement plant	$	236,574,513
Solar PV plant	$	-

Table 69 Case study 4: cost of carbon integration network

Cost of carbon integration network	$	52,339,147
Carbon transportation	$	857,624
Capture of untreated	$	202,638
Capture and treatment	$	37,749,141
Compression and pumping of treated	$	13,225,285
Compression and pumping of untreated	$	304,459

Case study 5

Table 70 Case study 5: products, fuel, carbon, and power

Multiple Fuel Case	Flow of product (t product/d)	Type of fuel	Flow of fuel (t fuel/d)	Carbon Emissions (tCO_2/d)	Power Required (kWh/d)
Methanol (A)	5000.00	Natural Gas	191.96	5047.96	3550000.00
Cement - Portland	10000.00	Coal	888.35	2399.07	722222.80
Aluminum	1118.44	Blended fuel	756.14	1945.83	15832136.76
Methanol (B)	2600.00	Biomass	585.39	1511.92	106166.75
Total	-	-	-	10904.77	20210526.32

Table 71 Case study 5: fuel, carbon, and power

Multiple Fuel Case	Flow of power (kWh/d)	Type of fuel	Flow of fuel (t fuel/d)	Carbon Emissions (tCO2/d)
Exported	0.00	Natural Gas	0.00	0.00
Power	19200000.00	Natural Gas	252.29	6302.69
Renewable	1010526.32		0.00	0.00
Total	20210526.32	-	252.29	6302.69

Table 72 Case study 5: carbon emissions

Source	Value (t CO_2/d)
Emissions from products	10904.77
Emissions from power	6302.69
Emissions from transportation of fuel	557.00
Emissions from carbon integration network	5500.38
Emissions from sink	675.66
Emissions from treatment	4824.72
Total Emissions pre-capture (t CO2/d)	17764
Carbon captured (t CO2/d)	13796
Total Emissions post-capture (t CO2/d)	9469
% Carbon capture (t CO2/d)	78%
% Carbon reduction (t CO2/d)	-47%

Table 73 Case study 5: revenue/cost of sinks

Revenues/Cost of sinks	$	16,169,134
Methanol (B)	$	13,239,545
Enhanced Oil Recovery	$	31,906,436
Saline Storage	$	(30,976,582)
Greenhouse	$	1,999,734

Table 74 Case study 5: revenues from products

Revenues from products	$	2,170,264,012
Methanol (A)	$	806,650,000
Cement - Portland	$	310,250,000
Aluminum	$	632,756,812
Methanol (B)	$	420,607,200

Table 75 Case study 5: revenue from exported power

Revenue from exported power	$	-

Table 76 Case study 5: cost of fuel

Cost of fuel	$	81,920,219
Natural Gas	$	28,981,631.33
Coal	$	16,212,384.45
Biomass	$	20,939,533.08
Blended fuel	$	15,786,669.86

Table 77 Case study 5: cost of plants

Cost of plants	$	1,161,644,611
Natural gas power plant	$	145,414,701
Coal power plant	$	-
Biomass power plant	$	-
Blended fuel power plant	$	-
MeOH(A) plant	$	172,799,836
MeOH(B) plant	$	198,267,995
Aluminum plant	$	402,473,258
Cement plant	$	236,574,513
Solar PV plant	$	6,114,307

Table 78 Case study 5: cost of carbon integration network

Cost of carbon integration network	$	35,921,93
Carbon transportation	$	705,993.31
Capture of untreated	$	182,074.77
Capture and treatment	$	23,450,682.41
Compression and pumping of treated	$	11,460,560.25
Compression and pumping of untreated	$	122,621.59

Sensitivity analysis

NCCR sensitivity analysis

Table 79 NCCR sensitivity analysis: product flow rates

Carbon capture %	NCCR 40%	NCCR 50%	NCCR 60%	NCCR 70%
Methanol (A)	5000.00	5000.00	5000	5000
Cement	10000.00	10000.00	10000	10000
Aluminum	1110.16	903.33	1059.059123	1066.567414
Methanol (B)	2600.00	2600.00	2600	2600

Table 80 NCCR sensitivity analysis: emissions breakdown

Carbon capture %	NCCR 40%	NCCR 50%	NCCR 60%	NCCR 70%
Emissions from products	17414.14	13337.85	16454.73	13317.32
Emissions from power	14092.74	11967.82	6127.19	6160.33
Emissions from transportation of solid fuel	2983.12	2286.33	1482.87	1149.31
Emissions from carbon integration network	5500.38	5500.38	5756.93	5756.93
Emissions from sink	675.66	675.66	703.33	703.33
Emissions from treatment	4824.72	4824.72	5053.61	5053.61
Total Emissions pre-capture (t CO2/d)	34490.00	27592.00	24064.79	20626.96
Total Emissions post-capture (t CO2/d)	26194.38	19296.38	15382.85	11945.02
% Carbon reduction (t CO2/d)	-24%	-30%	-36%	-42%

Table 81 NCCR sensitivity analysis: profit

Carbon capture %	NCCR 40%	NCCR 50%	NCCR 60%	NCCR 70%
Profit ($ million/y)	568.05	681.97	785.17	873.74

Table 82 NCCR sensitivity analysis: revenue breakdown

Carbon capture %	NCCR 40%	NCCR 50%	NCCR 60%	NCCR 70%
Sinks ($/y)	16.38	16.38	14.85	14.85
Products ($/y)	2165.58	2048.57	2136.67	2140.92
Exported Power ($/y)	0.73	0.73	0.00	0.00
Total ($/y)	2182.69	2065.68	172.73	2155.77

Table 83 NCCR sensitivity analysis: cost breakdown

Carbon capture %	NCCR 40%	NCCR 50%	NCCR 60%	NCCR 70%
Plants ($/y)	1292.80	1175.56	1139.06	1136.56
Natural Gas ($/y)	1.52	3.38	18.8	18.70
Coal ($/y)	116.13	145.21	12.56	60.09
Biomass ($/y)	172.73	20.94	172.73	20.94
Blended Fuel ($/y)	15.67	12.75	8.75	15.09
Carbon transport ($/y)	1.08	0.86	1.10	0.88
Carbon capture and treatment ($/y)	2.95	13.12	4.49	14.68
Carbon capture of untreated carbon ($/y)	0.18	0.18	0.00	0.00
Compression and pumping of treated carbon ($/y)	11.46	11.58	12.07	12.08
Compression and pumping of untreated carbon ($/y)	0.12	0.12	0.00	0.00
Costs ($/y)	1614.64	1383.71	1366.35	1282.03

REFERENCES

Agbonghae, E. O., Hughes, K.J., Ingham, D.B., Ma, L., Pourkashanian, M. (2014). Optimal process design of commercial-scale amine-based CO2 capture plants. *Ind. Eng. Chem. Res.*

Al-Mayyahi, M. A., Hoadley, A. F. A., & Rangaiah, G. P. (2013). A novel graphical approach to target CO2 emissions for energy resource planning and utility system optimization. *Applied Energy, 104*, 783-790. doi:10.1016/j.apenergy.2012.11.077

Al-Mohannadi, D. (2014). *A systematic approach to carbon footprint reduction strategies in industrial parks.* (Masters of Science). Texas A&M University,

Al-Mohannadi, D. M., Abdulaziz, K., Alnouri, S. Y., & Linke, P. (2017). On the synthesis of carbon constrained natural gas monetization networks. *Journal of Cleaner Production, 168*, 735-745. doi:10.1016/j.jclepro.2017.09.012

Al-Mohannadi, D. M., & Linke, P. (2016). On the systematic carbon integration of industrial parks for climate footprint reduction. *Journal of Cleaner Production, 112*, 4053-4064. doi:10.1016/j.jclepro.2015.05.094

Al-Sobhi, S. A., & Elkamel, A. (2015). Simulation and optimization of natural gas processing and production network consisting of LNG, GTL, and methanol facilities. *Journal of Natural Gas Science and Engineering, 23*, 500-508. doi:10.1016/j.jngse.2015.02.023

Alagorni, A. H., Yaacob, Z. B., & Nour, A. H. (2015). An Overview of Oil Production Stages: Enhanced Oil Recovery Techniques and Nitrogen Injection. *International Journal of Environmental Science and Development, 6*(9), 693-701. doi:10.7763/ijesd.2015.V6.682

Ali, U., Font-Palma, C., Akram, M., Agbonghae, E. O., Ingham, D. B., & Pourkashanian, M. (2017). Comparative potential of natural gas, coal and biomass fired power plant with post - combustion CO 2 capture and compression. *International Journal of Greenhouse Gas Control, 63,* 184-193. doi:10.1016/j.ijggc.2017.05.022

AlNouss, A., McKay, G., & Al-Ansari, T. (2018). Optimum Utilization of Biomass for the Production of Power and Fuels using Gasification. In *28th European Symposium on Computer Aided Process Engineering* (pp. 1481-1486).

AlNouss, A., McKay, G., & Al-Ansari, T. (2019). Superstructure Optimization for the Production of Fuels, Fertilizers and Power using Biomass Gasification. In *29th European Symposium on Computer Aided Process Engineering* (pp. 301-306).

AlNouss, A., McKay, G., & Al-Ansari, T. (2020). Production of syngas via gasification using optimum blends of biomass. *Journal of Cleaner Production, 242*. doi:10.1016/j.jclepro.2019.118499

Andersson, V., Broberg Viklund, S., Hackl, R., Karlsson, M., & Berntsson, T. (2014). Algae-based biofuel production as part of an industrial cluster. *Biomass and Bioenergy, 71,* 113-124. doi:10.1016/j.biombioe.2014.10.019

Bergen, C. H. W. G. F. V. (2004). Global carbon dioxide storage potential and costs.

Chalvatzis, K. J., & Ioannidis, A. (2017). Energy supply security in the EU: Benchmarking diversity and dependence of primary energy. *Applied Energy, 207,* 465-476. doi:10.1016/j.apenergy.2017.07.010

Cuellar, A., & Herzog, H. (2015). A Path Forward for Low Carbon Power from Biomass. *Energies, 8*(3), 1701-1715. doi:10.3390/en8031701

D. Chapel, C. M., J. Ernest. (1999). *Recovery of CO2 from flue gases: commercial trends*. Paper presented at the Canadian Society of Chemical Engineers Annual Meeting.

de Pee, A., Pinner, D., Roelofsen, O., Somers, K., Speelman, E., & Witteveen, M. (2018). *Decarbonization of industrial sectors: the next frontier*. Retrieved from

Default CO2 Emission Factors and High Heat Values for Various Types of Fuel, § 98 (2016).

EIA. (2020a). *Capital Cost Estimates for Utility Scale Electricity Generating Plants*. Retrieved from

EIA. (2020b). *Levelized Cost and Levelized Avoided Cost of New Generation Resources in the Annual Energy Outlook 2020*. Retrieved from

EuropeanCommission. (2020). *A hydrogen strategy for climate neutral Europe*. Retrieved from

Fimbres Weihs, G. A., & Wiley, D. E. (2012). Steady-state design of CO2 pipeline networks for minimal cost per tonne of CO2 avoided. *International Journal of Greenhouse Gas Control, 8*, 150-168. doi:10.1016/j.ijggc.2012.02.008

Fořt, J., Šál, J., Ševčík, R., Doleželová, M., Keppert, M., Jerman, M., . . . Černý, R. (2021). Biomass fly ash as an alternative to coal fly ash in blended cements: Functional aspects. *Construction and Building Materials, 271*. doi:10.1016/j.conbuildmat.2020.121544

Gao, F., Nie, Z., Wang, Z., Li, H., Gong, X., & Zuo, T. (2009). Greenhouse gas emissions and reduction potential of primary aluminum production in China. *Science in China Series E: Technological Sciences, 52*(8), 2161-2166. doi:10.1007/s11431-009-0165-6

Hasan, M. M. F., Boukouvala, F., First, E. L., & Floudas, C. A. (2014). Nationwide, Regional, and Statewide CO2 Capture, Utilization, and Sequestration Supply Chain Network Optimization. *Industrial & Engineering Chemistry Research, 53*(18), 7489-7506. doi:10.1021/ie402931c

Hasan, M. M. F., First, E. L., Boukouvala, F., & Floudas, C. A. (2015). A multi-scale framework for CO2 capture, utilization, and sequestration: CCUS and CCU. *Computers & Chemical Engineering, 81*, 2-21. doi:10.1016/j.compchemeng.2015.04.034

Holmgren, K. M., Andersson, E., Berntsson, T., & Rydberg, T. (2014). Gasification-based methanol production from biomass in industrial clusters: Characterisation of energy balances and greenhouse gas emissions. *Energy, 69*, 622-637. doi:10.1016/j.energy.2014.03.058

IPPC. (2018). *Global Warming of 1.5°C*. Retrieved from https://www.ipcc.ch/sr15/

Irmak, S. (2017). Biomass as Raw Material for Production of High-Value Products. In *Biomass Volume Estimation and Valorization for Energy*.

Kwak, G. (2016). *A Systematic approach to optimize the cost of carbon integration network.* (Masters). Texas A&M University,

Lee, S. C., Sum Ng, D. K., Yee Foo, D. C., & Tan, R. R. (2009). Extended pinch targeting techniques for carbon-constrained energy sector planning. *Applied Energy, 86*(1), 60-67. doi:10.1016/j.apenergy.2008.04.002

Liu, Z., Geng, Y., Zhang, P., Dong, H., & Liu, Z. (2014). Emergy-based comparative analysis on industrial clusters: economic and technological development zone of Shenyang area, China. *Environ Sci Pollut Res, 21*.

Manan, Z. A., Mohd Nawi, W. N. R., Wan Alwi, S. R., & Klemeš, J. J. (2017). Advances in Process Integration research for CO2 emission reduction – A review. *Journal of Cleaner Production, 167*, 1-13. doi:10.1016/j.jclepro.2017.08.138

McIlveen-Wright, D. R., Huang, Y., Rezvani, S., Redpath, D., Anderson, M., Dave, A., & Hewitt, N. J. (2013). A technical and economic analysis of three large scale biomass combustion plants in the UK. *Applied Energy, 112*, 396-404. doi:10.1016/j.apenergy.2012.12.051

Middleton, R. S., & Bielicki, J. M. (2009). A scalable infrastructure model for carbon capture and storage: SimCCS. *Energy Policy, 37*(3), 1052-1060. doi:10.1016/j.enpol.2008.09.049

Munir, S. M., Abdul Manan, Z., & Wan Alwi, S. R. (2012). Holistic carbon planning for industrial parks: a waste-to-resources process integration approach. *Journal of Cleaner Production, 33*, 74-85. doi:10.1016/j.jclepro.2012.05.026

Olivier, J. G. J., & Peters, J. A. H. W. (2018). *Trends in Global CO2 and Total Greenhouse Gas Emissions*. Retrieved from The Hague: www.pbl.nl/en

Ooi, R. E. H., Foo, D. C. Y., Tan, R. R., Ng, D. K. S., & Smith, R. (2013). Carbon Constrained Energy Planning (CCEP) for Sustainable Power Generation Sector with Automated Targeting Model. *Industrial & Engineering Chemistry Research, 52*(29), 9889-9896. doi:10.1021/ie4005018

Pękala, Ł. M., Tan, R. R., Foo, D. C. Y., & Jeżowski, J. M. (2010). Optimal energy planning models with carbon footprint constraints. *Applied Energy, 87*(6), 1903-1910. doi:10.1016/j.apenergy.2009.12.012

Pellegrini, L. A., Soave, G., Gamba, S., & Langè, S. (2011). Economic analysis of a combined energy–methanol production plant. *Applied Energy, 88*(12), 4891-4897. doi:10.1016/j.apenergy.2011.06.028

Peng, L., Wang, Y., Lei, Z., & Cheng, G. (2012). Co-gasification of wet sewage sludge and forestry waste in situ steam agent. *Bioresour Technol, 114*, 698-702. doi:10.1016/j.biortech.2012.03.079

Pérez-Fortes, M., Schöneberger, J. C., Boulamanti, A., & Tzimas, E. (2016). Methanol synthesis using captured CO2 as raw material: Techno-economic and environmental assessment. *Applied Energy, 161*, 718-732. doi:10.1016/j.apenergy.2015.07.067

Porter, M. (1998). Clusters and the New Economics of Competition. *Harvard Business Review*.

Rajamma, R. (2011). *Biomass fly ash incorporation in cement based materials.* University of Aveiro,

Ren, X., Sun, R., Meng, X., Vorobiev, N., Schiemann, M., & Levendis, Y. A. (2017). Carbon, sulfur and nitrogen oxide emissions from combustion of pulverized raw and torrefied biomass. *Fuel, 188*, 310-323. doi:10.1016/j.fuel.2016.10.017

Rosenberg, E. S., G. (2012). *Aluminium Production*. Retrieved from

Tan, R. R., & Foo, D. C. Y. (2007). Pinch analysis approach to carbon-constrained energy sector planning. *Energy, 32*(8), 1422-1429. doi:10.1016/j.energy.2006.09.018

Turk, G., Cobb, T. B., Jankowski, D. J., A.M., W., & F.T., S. (1987). CO2 Transport: A new application of the assignment problem. *Energy, 12*(2), 123-130.

USDepartmentofEnergy. (2016). *Biomass For Electricity Generation* Retrieved from https://www.wbdg.org/resources/biomass-electricity-generation

Valkila, N., & Saari, A. (2010). Urgent need for new approach to energy policy: The case of Finland. *Renewable and Sustainable Energy Reviews, 14*(7), 2068-2076. doi:10.1016/j.rser.2010.03.039

Vega, F. C., M.; Camino, S.; et al. . (2017). *Solvents for Carbon Dioxide Capture*. Retrieved from

Vega, F. S., A.; Navarrete, B. (2014). Degradation of amine-based solvents in CO2 capture process by chemical absorption. *Greenhouse Gas Sci Technol, 4*.

von der Assen, N., Müller, L. J., Steingrube, A., Voll, P., & Bardow, A. (2016). Selecting CO2 Sources for CO2 Utilization by Environmental-Merit-Order Curves. *Environmental Science & Technology, 50*(3), 1093-1101. doi:10.1021/acs.est.5b03474

Vora, B., Senetar, J. (2012). Monetization of Natural Gas. Retrieved from www.oilgasmonitor.com/monetization-natural-gas/2453/

Wang, T. (2019). Forecast for worldwide industrial energy consumption from 2018 to 2050, by fuel. In. Statistia 2020.

Wang, X., & Economides, M. (2009). Natural Gas Supply, Alternative Energy Sources, and the Environment. *Advanced Natural Gas Engineering*, 303–331. doi:10.1016/b978-1-933762-38-8.50016-2

Worrell, E. P., L.; Neelis, M.; et al. (2007). *World Best Practice Energy Intensity Valzues for Selected Industrial Sectors*. Retrieved from

X. Jia, C. L. a. Y. Q. (2010). Carbon Emission Reduction using Pinch Analysis. *2010 4th International Conference on Bioinformatics and Biomedical Engineering*, 1-4.

Yang, B., Wei, Y.-M., Hou, Y., Li, H., & Wang, P. (2019). Life cycle environmental impact assessment of fuel mix-based biomass co-firing plants with CO2 capture and storage. *Applied Energy, 252*. doi:10.1016/j.apenergy.2019.113483

Yu, F., Han, F., & Cui, Z. (2015). Reducing carbon emissions through industrial symbiosis: a case study of a large enterprise group in China. *Journal of Cleaner Production, 103*, 811-818. doi:10.1016/j.jclepro.2014.05.038

Zhang, Z., & Huisingh, D. (2017). Carbon dioxide storage schemes: Technology, assessment and deployment. *Journal of Cleaner Production, 142*, 1055-1064. doi:10.1016/j.jclepro.2016.06.199