MULTI-OBJECTIVE RESOURCE INTEGRATION FOR SUSTAINABLE INDUSTRIAL CLUSTERS

A Thesis

by

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ABSTRACT

With the current global climate change and resource depletion concerns, industrial clusters are challenged to focus on implementing sustainability designs and policies. These policies target the decrease of greenhouse gas (GHG) emissions, primarily CO_2, and the reduction of the usage of water and non-renewable energy sources. A useful element in the area of process design is material and energy integration. Numerous tools for resource integration (material and energy) have been developed to achieve sustainability goals. The design of sustainable integration networks of clusters includes economic and environmental consideration, which often conflict. A trade-off normally exist between profit and reducing environmental impact due to the addition of emission capture and water treatment units, sequestration, or the usage of cleaner energy sources which are more expensive. The existence of this trade-off between objectives led to the development of multi-objective optimization (MOO) tools, which attempt to simultaneously optimize more than one objective function. A prominent MOO tool is the ε-constraint method, and a recent improvement of it is the augmented ε-constraint method. MOO tools are applied to resource integration tools for simultaneous targeting of economic as well as environmental performance. When applied to integration networks, MOO tools generate pareto-optimal set of solutions which illustrate the trade-off between the objective functions, where each solution correspond to a specific cluster design and an integration network. However, recent integration tools (as well as MOO application to those tools) allow the interaction of only specific species; hence limit the possibility of obtaining an optimal solution. A recent resource integration tool was developed that allows the integration of multiple material and energy resources in a cluster. This work introduces a holistic multi-objective resource integration tool, which applies the augmented

ε-constraint multi-objective tool to the holistic resource integration approach. The tool generates pareto surfaces that captures the trade-offs and propose different integration networks. The tool is illustrated through two case studies, where the profit, emission impact, and water consumption of industrial clusters are optimized simultaneously.

DEDICATION

I dedicate this work to my family and friends. A special feeling of gratitude to my loving parents who have showed continuous support throughout my academic journey. Many thanks to my friends for being there for me throughout the entire process.

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CONTRIBUTORS AND FUNDING SOURCES

Contributors

This research work was supervised by a thesis committee consisting of Dr. Patrick Linke, head if the Chemical Engineering Department, chair of committee, Dr. Dhabia Al-Mohannadi, from the Chemical Engineering Department, co-chair of committee, and Dr. Eyad Msaad, from the Chemical Engineering Department, committee member.

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NOMENCLATURE

CE	Circular Economy
RE	Renewable Energy
PI	Process Integration
EIP	Eco-Industrial Park
CCUS	Carbon Capture Utilization and Storage
MOO	Multi-Objective Optimization
r	Resource
P	Process
IF_{α}	input flow to the cluster of resource α
$F_{\alpha\beta}$	the flow exchanged through the infrastructure line from/to plant β
OF_{α}	exported flow from the cluster of resource α
$a_{\alpha\beta}$	parameter of resource α in plant β
C_{β}	capacity of plant β
EF_{γ}	the total output flow of that component γ
$x_{\alpha\gamma}$	composition of component γ of the exported resource flows
TR	total revenue
$CAPEX$	capital cost of the cluster
$OPEX$	operating cost of the cluster
P_{α}	price of resource α
cc_{β}^{CAPEX}	annualized capital cost parameter for process β
$ao_{\beta}^{variable}$	variable cost for process β

ao_{β}^{fixed}	fixed cost of process β
z_1	optimum value of the first objective function
z_2	optimum value of the second objective function
z_3	optimum value of the third objective function
GHG	greenhouse gas
ASU	Air Separation Unit
FTS	Fischer Tropsch Synthesis

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1. INTRODUCTION

1.1 Motivation

Current models of human production and consumption cause major challenges to the planet. Two main issues caused by the human activity are climate change and resource depletion. The average global temperature increased by 0.85°C from 1880 to 2012 and is likely to continue increasing due to greenhouse gas emissions and fossil fuel use (IPCC, 2019). The increase in the concentration of greenhouse gases (such as CO_2, water vapor, and nitrous oxides) is caused by human activity mainly in the production process of power and chemical products. In the past 150 years, the industrial activity caused the concentration level of carbon dioxide to increase from 280 parts per million to 414 parts per million (IPCC Report, 2014). At the same time, the world population is expected to reach 9.6 billion people by 2050, which means there will be an increase in demand for energy and water (UN, 2019). According to the International Water Management Institute, it is expected that by 2025 countries south of the 35N latitude will experience either economic or water scarcity (PwC, 2016).

To address these challenges, the United Nations have introduced the Sustainable Development Goals (SDGs) (UN, 2015). The 17 sustainable development goals are designed to ensure better future for humanity, and at their core, they aim at efficient use of resources, reduction of emissions, environment conservation and enabling economic growth. The Paris agreement (adopted in 2015) aims to keep the average global temperature rise below 2 ºC above pre-industrial levels, which would significantly limit the impact of climate change (UN, 2019).

The industrial sector, which significantly contributes to greenhouse gas emissions and the depletion of natural resources, is thus encouraged to adopt these sustainability policies in process design and operation, and to incorporate circular economy (CE) policies. CE call for better resource allocation and reduction of wastes and emissions (World Economic Forum, 2014). Efforts to reduce emissions were directed towards exploring cleaner alternatives for power production (since power production is a huge contributor to greenhouse gas emission). Examples of such renewable energy (RE) sources are solar and wind power. The use of renewable energy sources contributes significantly to sustainable developments, mainly through 1) decreasing environmental impact caused by emission, and 2) energy security, since shifting to renewable energy sources allows reserving resources such as oil and natural gas (IPCC, 2014). However, RE resources are also accompanied with drawbacks. The main drawback is the variability constraint of RE sources that is a result of weather changes and diurnal changes. This can be tackled through energy storage or through integrating renewable and non-renewable energy supply systems (IPCC, 2014). These solutions influence either come with additional cost or influence the environmental impact of the energy supply system, and therefore should be considered when assessing the sustainability performance.

Goals to minimize the use of natural resources and reduction of waste streams emphasized the need to use Process Integration (PI). PI includes approaches that allows the interaction of processing units by integrating mass and energy resources. The purpose of these PI networks is to optimize the economic performance of and industrial process while decreasing waste streams, emissions, as well as the use of natural resources such as water and other nonrenewable energy sources. An example of a PI network designed by Al-Mohannadi and Linke (2015) is shown in Figure 1. As shown in the figure, integration networks often include sinks and sources of a specific material/energy resource, and treatment units to meet the specification requirement of the sink.

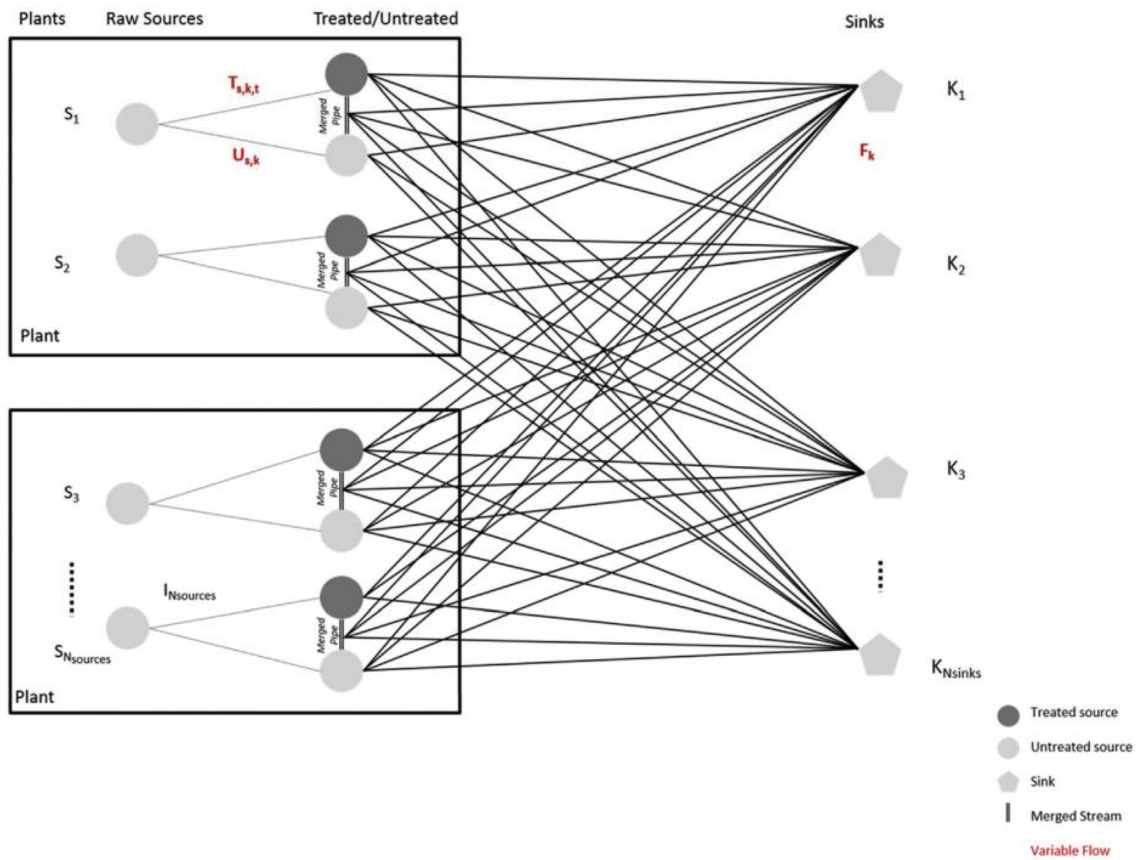


Figure 1: Illustration of a Process Integration Technique (reprinted from Al-Mohannadi and Linke, 2015)

Recent enhancement to the concept of PI networks is the development of eco-industrial parks (EIPs) (Somoza-Tornos et al., 2021). EIPs target the reduction of wastes through heat and mass integrations between industrial plants to enhance the overall economic and environmental performance (Saikku, 2006). Examples of EIPs that integrate materials, water and energy have been recently reviewed by Duhbaci et al. (2020). EIP methods can also be used for emission reduction to create Carbon Capture Utilization and Storage (CCUS) networks such as the work of Al-Mohannadi and Linke (2016). Integrating resources comes with addition cost of treatment units, transportation, or use of more expensive alternatives to meet environmental constraints.

Therefore, integration methods involve a trade-off between economic and environmental performance, where the improvement of one performance worsens the other. Hence, optimizing process performance becomes a complex issue, and industrial sectors face a challenge when designing optimum integration networks (Leong et al., 2017). Conflict between different sustainability goals can be studied using multi-objective optimization (MOO) tools. MOO tools allow the simultaneous optimization of more than one objective. These objectives often conflict and the trade-off between them is explored. Recent Implementation of multi-objective optimization tools in integration network design allows capturing solutions that cannot be captured using single-objective optimization, and results in integration networks that optimize economic and environmental goals simultaneously.

The purpose of this work is to apply multi-objective optimization to process integration in EIPs. The goal is to simultaneously optimize the economic performance, the greenhouse gas emission, and the water consumption of industrial clusters through exploring different integration network designs. The next section summarizes development in the area of resource integration and multi-objective optimization.

1.2 Literature Review

Multiple integration approaches have been explored to optimize economic performance under environmental footprint constraints. Al-Mohanndi and Linke (2016) explored CO_2 conversion processes to reduce the overall process emissions. Hassiba et al (2017) expanded the representation to include waste heat exchange. Al-Mohannadi et al. (2017) studied the allocation of resources in industrial processes focusing on natural gas and CO_2 material exchange. Other works included the integration methods that consider the allocation of both water and energy resources (Gabriel et al., 2016). Another water-energy network optimization method use an analytic hierarchy process is introduced by Leong et al. (2017). An integration approach to C-H-O symbiosis has been proposed with a focus on enabling the balancing of Carbon, Hydrogen, and Oxygen atoms in process integration (Noureldin and El-Halwagi, 2015). Panu et al. (2019) expanding on the representation to include the reduction of carbon dioxide emissions. Recent work by Ahmed et al. (2020) addressed the limitations in the aforementioned approaches in their ability to include all relevant material and energy resources in the integration networks. The work introduces a linear resource integration model that allows the exchange of all possible raw materials, intermediates, waste streams, as well as energy resources between processing units in a cluster (Ahmed et al. 2020).

Regarding multi-objective optimization, various mathematical models have been developed that allow simultaneous optimization of objective functions. The tools generate a Pareto set, which is a set of multiple optimal solutions that represent different trade-offs between conflicting objectives. Examples of MOO mathematical tools are the ε-constraint method, the weighted average method, and genetic algorithm (Hwang, 1979). These methods are applied in multiple process optimization applications to target sustainability objectives.

The ε-constraint method converts the multi-objective optimization problem to a single-objective problem through optimizing one objective, while setting constraints on the remaining objectives. The constraint values of the objectives are varied to generate a Pareto set of solutions that capture the trade-offs. Increasing the number of constraints increases the number of optimal solutions captured by the model. Mavrotas (2009) improved the ε-constraint method to an augmented ε-constraint one, which guarantees the generation of a stronger Pareto optimal set. Figure 2 illustrates an example of a pareto curve generated by the original ε-constraint MOO tool (Mavrotas, 2009). In this example, 5 constraints of objective function X1 are set to optimize the main objective function X2. The bold region represents the actual pareto optimal region, and the dotted lines illustrate the pareto solutions obtained from the tool. Figure 3 shows the pareto surface to the same example when the augmented ε-constraint MOO tool is applied. The enhanced method captures 5 solutions within the optimum region (as opposed to 1 from the original tool) and therefore results in a stronger Pareto set.

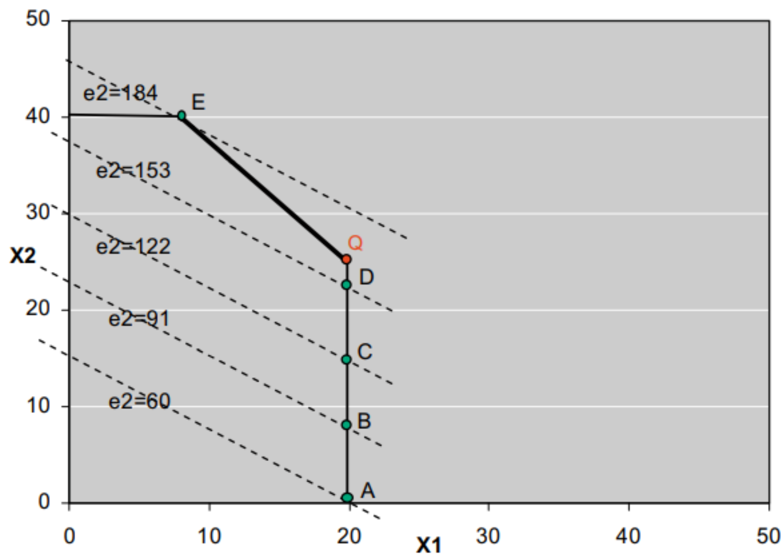


Figure 2: Illustration of a Pareto curve of a conventional ε-constraint MOO model (reprinted from Mavrotas, 2009)

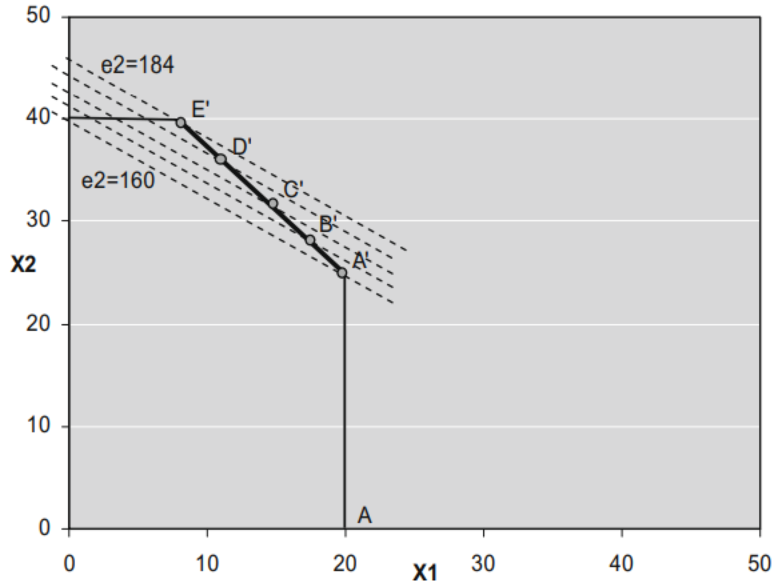


Figure 3: Illustration of a Pareto curve of the augmented ε-constraint MOO model (reprinted from Mavrotas, 2009)

To achieve the multi-objective optimization of industrial clusters, MOO models are applied to process integration networks to explore different resource allocations that meet sustainability goals. Different studies explored models that simultaneously optimize economic and environmental performance through developing exchange heat and/or material networks. Bolliger et al. (2005) proposed an approach that combines energy integration network design and genetic algorithm multi-objective optimization. Pelet et al. (2005) illustrated a holistic approach for the design of optimum complex integrated energy systems, considering economic and environmental objectives. Fazlollahi and Maréchal (2011) developed a multi-objective optimization model for the optimization of energy systems. The approach uses an evolutionary algorithm for the integration of biomass resources into energy systems. García et al. (2013) applied the ε-constraint method to integrate waste streams to targets the minimization of utility consumption under environmental and economic objectives. To reduce the problem of complexity in the previous work, the MILP characterizes waste through treatment unit models prior to MOO. Harkin et al. (2012) used an Excel based genetic algorithm to optimize the design of a CO_2 capture system in coal fired power station unit. Valencia et al. (2014) proposed a heat integration model for eco-industrial parks, including shared Organic Ranking Cycles for waste heat recovery. The superstructure allows the minimization of the capital and operating cost simultaneously. Čuček et al. (2012) also develop a multi-criteria optimization tool for biomass supply chains considering carbon, water, and energy footprints. Türkay et al. (2016) revised the standard mathematical optimization model for supply chain management to add environmental and social factors. Onishi et al. (2017) applied the ε-constraint method in a work and heat exchange network. The MOO method was applied to simultaneously decrease the emissions of CO_2 and the total annual cost of processes, therefore optimize both economic and environmental performance in a Pareto frontier. Li et al. (2018) introduced a systematic approach to decompose the MOO model solution into user-defined regions of interest. Yang et al. (2019) proposed a nonlinear thermos-economic MOO model to optimize the thermodynamic and economic performance of a heat exchange network that include pressure changing streams. Leon et al. (2019) used a weighted average method to optimize water supply systems for mining industries. The MOO tool is used to minimize the total operating cost while minimizing the emissions of greenhouse gases. Shi et al. (2020) used a genetic multi-objective algorithm to optimize the side-stream extractive distillation in terms of economic and environmental performance through creating heat integration networks. Liu et al. (2020) also optimized heat exchange networks across plants, where different steam levels are generated and utilized considering both economic and environmental objectives. Rajakal et al. (2020) applied a fuzzy based MOO approach for sustainable land allocation accounting for CO_2 and water use.

Most of the applications to MOO models involve the integration of heat resources, or the application of multi-objective optimization on the integration of only specific material or energy resources. Integrating a single or two resources does not guarantee optimum cost minimization or maximum resource reuse. Also, the improvement of environmental objective, does not necessarily mean the improvement of resource conservation (Laurent et al. 2012). Therefore, an optimum integration network must integrate all possible resources within an industrial cluster. The work by Ahmed et al. (2020) proposed a linear model that allow the integration of material and/or energy resources to optimize the economic performance of a cluster. In this work, a new superstructure is presented that combines the recently introduced integration model by Ahmed et al. (2020) and the augmented ε-constraint multi-objective optimization model to optimize industrial clusters. The model explores the trade-off between economic, environmental, and natural resource conservation objectives and presents those trade-offs in Pareto optimal sets.

2. OVERVIEW

In this work, the integration model proposed by Ahmed et al. (2020) is combined with a multi-objective integration model. This section summarizes the resource integration model, where an integration network is created to allow the exchange of all material and energy resources in a cluster.

The integration model explores different resource allocation networks to optimize the performance of an industrial cluster. Figure 5 shows the representation introduced by Ahmed et al. (2020). The cluster is composed of multiple processes that can receive or produce resources. Resources can be fresh raw materials, products, any required intermediates, energy streams, or waste streams. The plants within the cluster can exchange material or energy through an infrastructure line. Each line has specified conditions (temperature, pressure, and composition). Plants can be of any scale and type (production plant, treatment unit, power generation...etc.).

The integration model allows the exchange of resources between plants through the infrastructure line. The conditions of each line (temperature, pressure, composition) must be met to allow the exchange of resources. The inputs and outputs of each plant are represented as constant parameters. This results in a linear integration network as the parameters and compositions are fixed. The inlet and outlet flow to/from the cluster are considered control variables. Plant capacities are the main output variables of the model, and integration of material and power is achieved through balances around the cluster and plants.

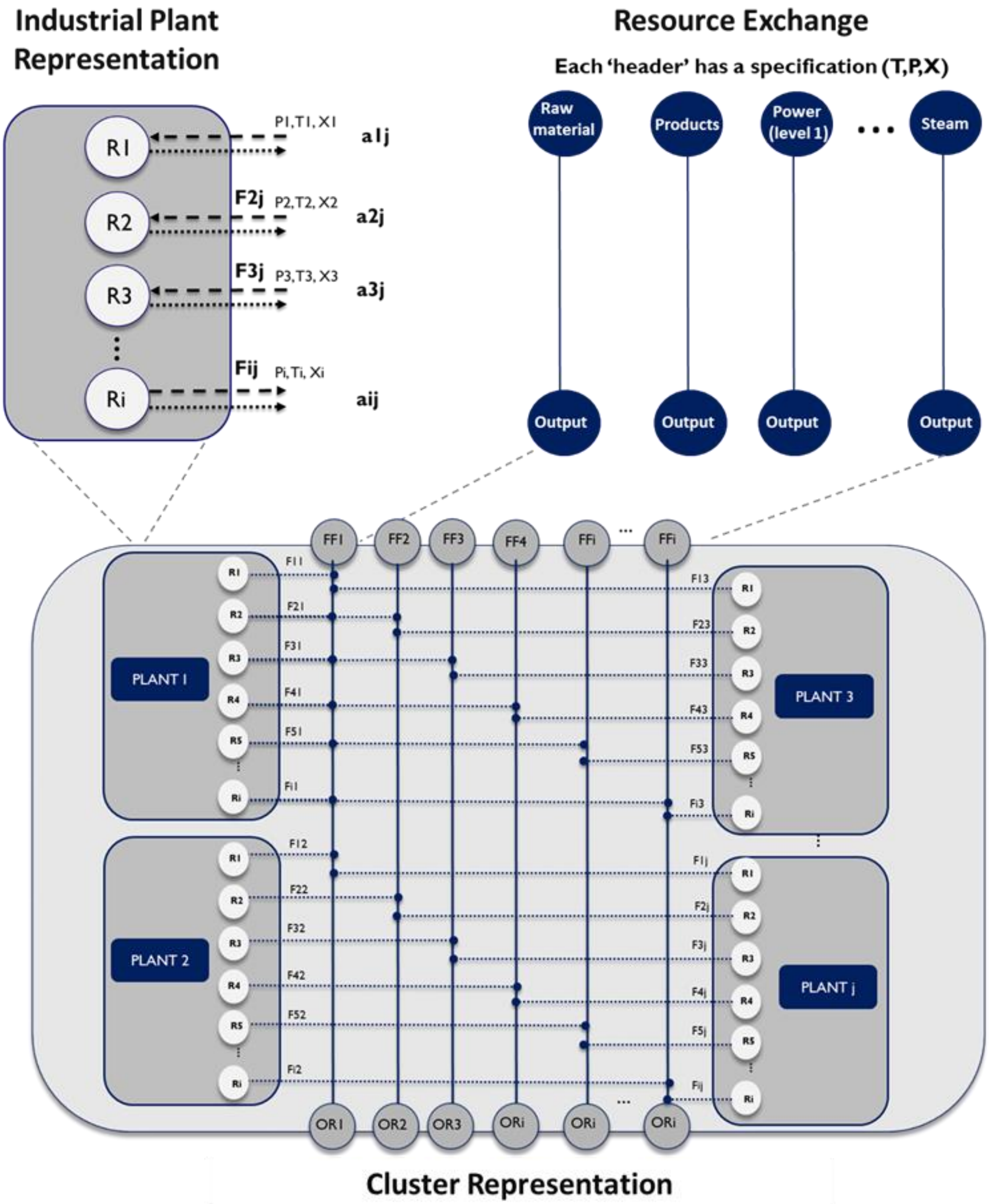


Figure 4: Cluster representation introduced by Ahmed et al. (2020)

The resource balance around the cluster is represented with the following equation:

$$IF_\alpha + \sum_{\beta=1}^{\beta} F_{\alpha\beta} = OF_\alpha \tag{1}$$

IF_α is the input flow to the cluster of resource α. This applies to both material and energy resources. $F_{\alpha\beta}$ represents the flow exchanged through the infrastructure line from/to plant β. and OF_α is the exported flow from the cluster. IF_α and OF_α are variables that are subjected to user-defined constraints. $F_{\alpha\beta}$ is the flow of resource α from or to plant β, and therefore is a function of the capacity of plant β and parameters $a_{\alpha\beta}$. This relation is shown in the following equation:

$$F_{\alpha\beta} = a_{\alpha\beta}\, C_\beta \tag{2}$$

For material resources, equation 2 ensures mass balance within the individual plants. Plant capacities C_β are the main model variables and are subject to user defined boundary values. Resources are integrated by allowing shared flows (flows that have the same specifications) to be exchanged between plants. However, resources are only allowed to be exchanged if pressure, temperature, as well as composition match.

In cases where the total flow of a certain component is of interest, a component balance can be achieved. It can be used to set limitations on the output, or input of a certain component. If the component of interest is denoted by γ, the total output flow of that resource EF_γ is

$$EF_\gamma = \sum x_{\alpha\gamma} OF_\alpha \tag{3}$$

$x_{\alpha\gamma}$ is the user defined composition of component γ of the exported resource flows. Equation 3 is useful when assessing the emission footprint of the cluster. Since greenhouse gas emissions are typically a part of a flue gas stream, accounting for the total emission of those gases from the whole cluster requires adding the amount of the gas in each resource exiting the cluster.

The economic performance of the cluster is assessed by calculating the overall profit, which is calculated as follows:

$$Profit = TR - CAPEX - OPEX \tag{4}$$

Where TR is the total revenue, and the CAPEX and OPEX are the capital and operating costs of the entire cluster. The three terms are dependent on the model variables since they are functions of the inputs and outputs of the cluster, and are calculated with the following equations:

$$TR = \sum_{\alpha} OF_{\alpha} P_{\alpha} \tag{5}$$

$$CAPEX = \sum_{\beta} cc_{\beta}^{CAPEX} C_{\beta} \tag{6}$$

$$OPEX = \sum_{\alpha} IF_{\alpha}\, P_{\alpha} + \sum_{\beta} \left(ao_{\beta}^{variable} C_{\beta} + ao_{\beta}^{fixed} \right) \tag{7}$$

P_{α} is the price of resource α, cc_{β}^{CAPEX} is the annualized capital cost parameter for process β. $ao_{\beta}^{variable}$ is the variable cost and ao_{β}^{fixed} is any fixed cost of process β that compose the operating costs. It must be noted that P_{α} can either be the purchase or the selling price of a resource, and in cases where these two prices differ for the same resource, different infrastructure lines must be generated for the resource.

In a single objective optimization study, the resource integration model is used to optimize the profit. However, as previously mentioned, the purpose of this work is to optimize three objectives simultaneously. The next section illustrates the MOO model and the utilization of the resource integration tool to achieve sustainability goals of a cluster.

3. MULTI-OBJECTIVE RESOURCE INTEGRATION MODEL

3.1 Proposed Superstructure

In this work, a multi-objective optimization of resource integration approach is proposed which combines the resource integration network introduced by Ahmed et al. (2020) and the enhanced multi-objective optimized proposed by Mavrotas (2009). The purpose is to optimize the economic performance, emission footprint, as well as the resource conservation simultaneously through integrating resources in an industrial cluster. The problem statement is stated as: Given an existing cluster with multiple resources ($r \in R$), where r can be material, energy or wastes that are produced or consumed by a number of processing plants ($p \in P$) within the cluster. The resources can be imported to the cluster or exported at a fixed price. Each resource can be exchanged through an existing infrastructure with a specified temperature, composition, and pressure. Inputs and outputs to/from each plant are related through fixed parameters, which can be negative, indicating imports or positive, indicating exports. The problem is divided into two sections: the first section of the problem deals with the construction of the resource integration network summarized in the previous section, and the second is the multi-objective optimization of the network.

The objective is to develop a sustainable cluster that maximizes profit, minimizes carbon dioxide emissions, and minimizes fresh resource depletion. Given specific sustainability objectives, the model determines the optimized capacity of each plant in the cluster, as well as imports and exports of the cluster. The following sub-sections provide an overview of resource integration and the multi-objective model. Figure 4 shows the superstructure of the proposed work. Inputs to the model are resource parameters to/from plants, resource specifications, input/output constraints, as well as cost parameters. These inputs are used to generate integration networks through the holistic resource integration model. Sustainability performance indicators are then calculated to be optimized through the augmented ε-constraint method. The number of constraints intervals are selected, and Pareto optimal solutions are obtained. The solution set can be represented graphically in a curve or a surface depending on the number of objectives. The following sections present both the resource integration and the multi-objective optimization models.

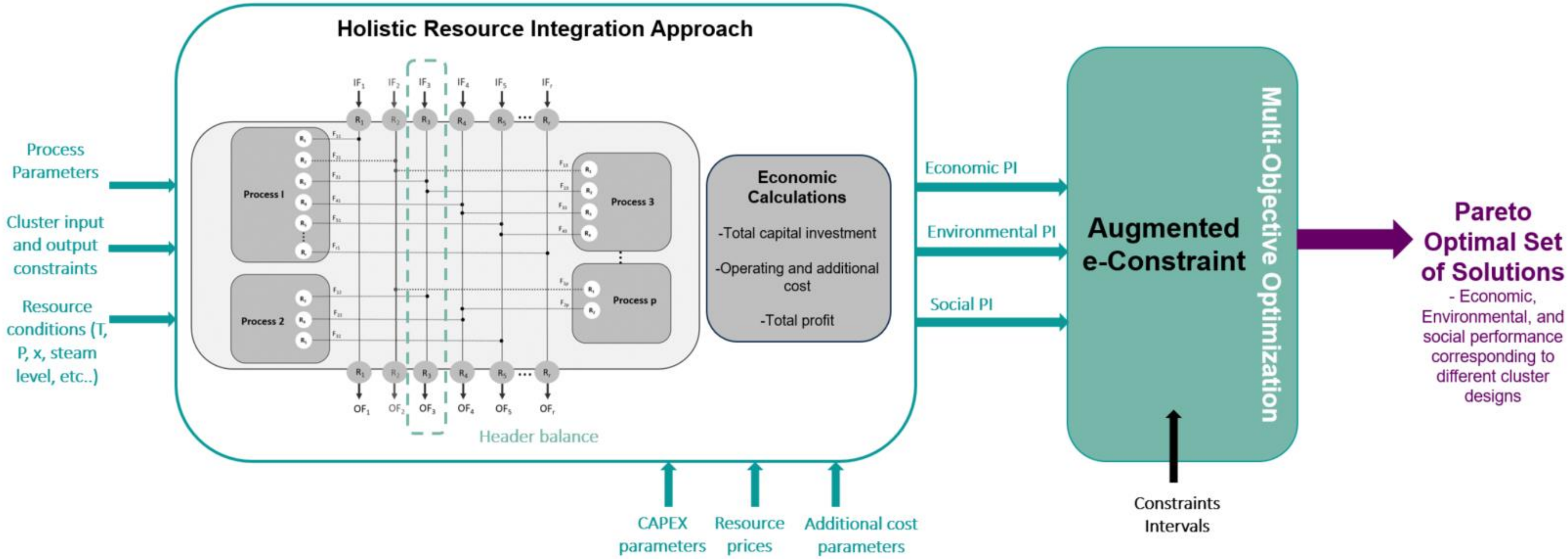


Figure 5: Multi-objective Resource Integration Model Superstructure

3.2 Multi-Objective Optimization Model

Once the resource exchange formulation is achieved, the multi-objective model is constructed. As illustrated in the superstructure in Figure 4, the first step towards the multi-objective optimization process is the identification of objective functions and performance indicators to those functions. For economic indicators, this is typically set as the total cost or the total profit. For environmental /resource depletion indicators, this involves calculating the total amount of material of interest (emission or resource e.g., water) from all output streams as in Equation 3, and thus requires knowledge of the composition of the material of interest in each stream. Other indicators such as social indicators can be considered only if a trade-off exists, and mostly, environmental indicators account for social factors and can be quantified through impact assessment tools. In this work, the focus is on material based quantifiable indicators (economic, environmental and resource depletion).

Once performance indicators are specified, they are used as inputs to the multi-objective model. The model used in this approach is the augmented ε-constraint method, which is an improvement of the original ε-constraint method (Mavrotas, 2009). This improved method aims at the production of stronger and more efficient Pareto optimal solutions compared to the original method. Both the original and the ε-constraint methods are applied through the following steps:

1) The identification of the main objective function (assume a number of f objective functions) to be optimized. The method achieves multi-objective optimization by converting the problem to a single-objective problem, where one objective is optimized (the main objective function) and the remaining f-1 objectives are set as constraints. The main objective function in this study is assumed to be the economic performance (cluster

total profit), while the emission footprint and the resource conservation are the secondary objectives set as constraints.

2) The second step is the generation of the pay-off table. This step ensures that even though the MOO problem is converted to a single-objective one, optimum performance of the second and third objective functions are still captured and represented in the Pareto optimal set. The pay-off table represents extreme points of the Pareto set of solutions, which are the points where each objective function is optimized individually. One objective function is optimized at a time and the remaining functions are observed. In a multi-objective optimization problem, the pay-off table must show the conflict between objective functions (i.e. when optimizing one objective function, at least one of the other objective functions will be at its worse value).

   The main difference between the augmented ε-constraint method and the original ε-constraint method is in this second step. In the original method, the pay-off table is created simply by optimizing one objective function while recording the corresponding output to the other objective functions. Then, the second objective function is optimized, and the other values are recorded. The augmented ε-constraint method guarantees a denser and more efficient pay-off table. This is achieved through implementing lexicographic optimization when creating the pay-off table (Mavrotas, 2009). The first row of the pay-off table represents the objective values when the first objective function is optimized. Similarly, the second and third rows represent the values when the second and thirds objectives are optimized, respectively. The following section illustrates the lexicographic optimization approach.

The first objective function (of highest priority) is optimized as follows:

$$Max\ (Objective\ function\ 1) = z_1 \tag{8}$$

Where z_1 is the optimum value of the first objective function when no constraints are set on the 2nd and 3rd objectives. The second objective function is then optimized while setting a constraint on the first objective function to be the optimum value z_1

$$Max\ (Objective\ function\ 2) = z_2, \quad \text{while} \quad Objective\ function\ 1 = z_1 \tag{9}$$

The original ε-constraint method does not include the step in Equation 9. This step guarantees that while the first objective function is at an optimum value, an improved value of the second objective function is obtained. This narrows down the range of the intervals set for the second objective function and allows exploring a denser Pareto optimal region. For a third objective function, a similar trend follows where the objective function is optimized while setting constraints on objective functions 1 and 2,

$$Max\ (Objective\ function\ 3) = z_3 \tag{10}$$

While

$$Objective\ function\ 1 = z_1 \text{ and } Objective\ function\ 2 = z_2 \tag{11}$$

At this point, first row of the payoff table is complete. The second and third rows are generated by repeating the same procedure. However, the objective function aimed to be optimized is prioritized in each run. Thus, when generating the 2nd row, the 2nd objective function is optimized first and is optimum value is set as constraint. Similarly, the 3rd objective function is optimized first when generating the 3rd row.

3) Once the pay-off table is generated, the range of the f-1 objective function to be set as constraints are divided into q_i equal intervals, forming a total of q_{i+1} grid points for each of the f-1 objective functions. The larger number of grid points considered, the higher the accuracy of the Pareto curve/surface. However, choosing many grid points increases the time consumed for the calculations. Once grid points are selected for each objective function (other than the main objective function being optimized), each grid point for one objective is combined with all the grid points for the other objective, forming a total of (q2+1)*(q3+1)…*(qf+1) number of runs. For example, for a three-objective study, two objectives are set as constraints. If 15 grid points are selected for each objective, a total of 225 (15*15) runs are generated.
4) Finally, the three sustainability objectives are optimized by optimizing the main objective function is for the runs generated in step 3. In this step, the resource integration tool is combined with the MOO tool, where the sustainability objectives are optimized by varying the capacities of the plants and the input/output flows of the cluster. In each run, a unique set of plant capacities and an integration network is generated.

Each cluster design (plant capacities and flows) obtained from the model formulation indicates a distinct sustainability cluster performance and represents a Pareto optimal solution. Therefore, a Pareto optimal set of solutions is generated, where each optimal solution represents a trade-off between the different objective functions. The set can be represented in a graph in case of a two-objective problem, or a surface in case of a three-objective problem. The next sections apply the model to two cluster integration networks.

4.CASE STUDY I: APPLYING THE TOOL TO A CARBON DIOXIDE CONVERTING CLUSTER

CO_2 is a primary GHG that affect the climate of the earth. Many research areas target technologies that mitigate or convert emitted CO_2. Multiple routes exist that consume or convert CO_2 in the chemical industry. These routes involve hydrogenating CO_2 to produce value added products such as methanol and urea (Fernández et al. 2020). However, hydrogen production comes with a large CO_2 footprint if produced from fossil resources. Thus, there has been a move towards the use of electrolysis using renewable energy to produce low carbon hydrogen. Therefore, in this study, the conversion of CO_2 to value added products only using green technologies is evaluated.

A CO_2 converting cluster is explored. The cluster consumes only air, CO_2, and water as fresh resources. The cluster utilizes the raw materials to produce ammonia, urea, and methanol through three individual production plants. These plants produce secondary GHG emissions, but only urea and methanol plants emission streams include CO_2. Air separation converts air to oxygen and nitrogen production, while water splitting electrolysis is available for hydrogen production. Energy (heat and power) is imported at a fixed cost from external renewable energy sources that sit beyond the cluster boundary. The cluster is required to utilize 120,000 metric tons per year of CO_2. The 120,000 t/y CO_2 are fed to the cluster without charge (0 $/t).

CO_2 capture units are available for both the urea and methanol production plants for treatment and separation of the plant emissions. CO_2 sequestration option is also considered that stores a pure CO_2. The set-up allows CO_2 to leave the cluster as pure stream or as emissions from methanol or urea production plants, and from carbon capture units. However, \$20/t flat tax is imposed on any CO_2 that exits the cluster. Figure 6 shows the representation of the plant adopted from Ahmed et al. (2020) with the possible resource interactions. The complete data is provided in section 3.1. The purpose is to maximize the economic performance of the cluster while adhering to CO_2 emission limits and freshwater use.

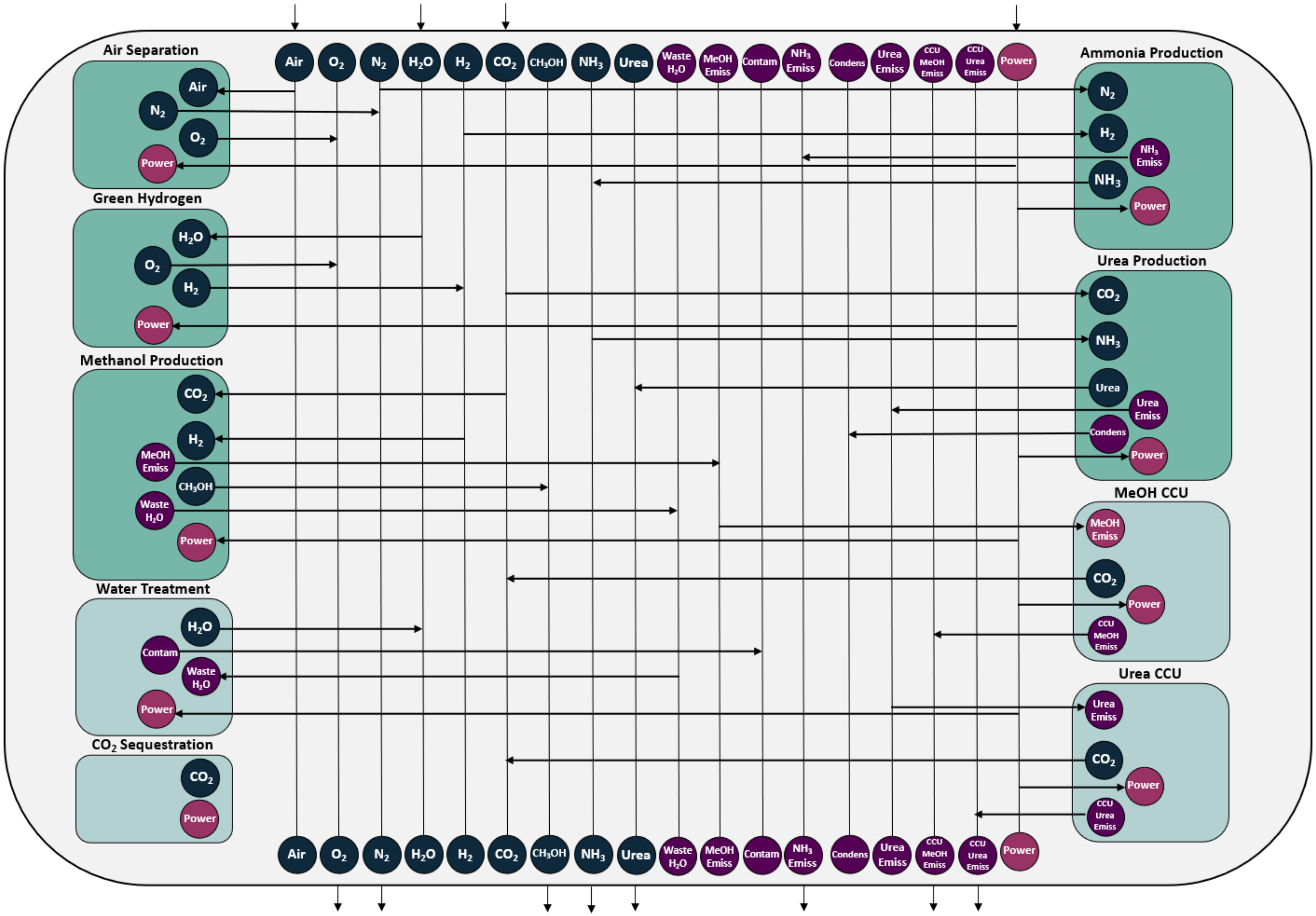


Figure 6: Cluster representation showing possible resource interactions

4.1 Case Study Data

This section provides the data used for implementing the multi-objective integration model. As illustrated earlier, the main input data are the process resource parameters (for both material and energy resources), any resource specifications necessary for resource exchange, as well as capital and operating cost parameters. Table 1 provides the CAPEX parameters, power consumption parameters, as well as the main product prices for each processing plant. Table 2 provides the parameters of all raw materials, intermediates, and product resources fed to, exported from, and within the cluster. The positive parameters represent the output from the process, while negative parameters represent the input. Table 3 illustrates the parameters of all energy and waste stream resources. Each production plant is assumed to have a minimum capacity of 0 t/y and a maximum capacity of 100,000 t/y. CO_2 sequestration has a maximum capacity of 120,000 t/y, which means that all the CO_2 forced into the cluster can be sequestered. All data shown in Table 1, 2 and 3 are adopted from Ahmed et al. (2020).

In order to quantify emission footprint, the composition of CO_2 in streams exiting the cluster must be determined. Methanol production plant emission contained 30 % CO_2, while the urea production plant had 26 % CO_2 (Shehab et al., 2019). The carbon capture treatment units use an amine-based solvent and are assumed to have an efficiency of 90% (Lameh et al. 2020). Component mass balance was performed to calculate the amount of CO_2 leaving the treatment units. The operating cost of the cluster was assumed to be the cost required to purchase the fresh feed resources entering the cluster, primarily water and electricity, and the additional tax associated with the untreated CO_2. The cluster was optimized for a water price of \$0.05/ton and two electricity price. The case study was solved using "What'sBest!16.0" optimization tool in Microsoft Excel 2016 (Lindo Systems, 2019).

Table 1: Industrial cluster plants CAPEX parameters and product prices

Plant	**Capex ($/t)**	**Primary Product**	**Product Price ($/t)**	**Power demand (kWh/t Product)**
Air Separation (ASU)	18.2	O_2	79.0	245
Water Splitting	779	H_2	1200	5,400
Methanol Production	21.5	CH_3OH	320	169
Ammonia Production	29.2	NH_3	415	785
Urea Production	16.1	Urea	305	20
Carbon Capture unit	1.70	CO_2	40.0	27.3
CO_2 Sequestration	9.0	-	-	1.4
H_2O treatment	0.26	H_2O	5.00	5

Table 2: Parameters of raw materials and products

Resource	ASU	Green H_2	CH_3OH Production	NH_3 Production	Urea Production	Carbon Capture	CO_2 Sequestration	H_2O treatment
Air	-4.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00
O_2	1.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00
N_2	3.27	0.00	0.00	-0.85	0.00	0.00	0.00	0.00
H_2O	0.00	-9.00	0.00	0.00	0.00	0.00	0.00	1.00
H_2	0.00	1.00	-0.20	-0.18	0.00	0.00	0.00	0.00
CO_2	0.00	0.00	-1.76	0.00	-0.73	1.00	-1.00	0.00
NH_3	0.00	0.00	0.00	1.00	-0.57	0.00	0.00	0.00
CH_3OH	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00

Table 3: Parameters of waste streams and energy resources

Resource	ASU	Green H_2	CH_3OH Production	NH_3 Production	Urea Production	Carbon Capture	CO_2 Sequestration	H_2O treatment
Methanol Emission	0.00	0.00	0.40	0.00	0.00	-2.45	0.00	0.00
Ammonia Emission	0.00	0.00	0.00	0.03	0.00	0.00	0.00	0.00
Waste H_2O	0.00	0.00	0.56	0.00	0.00	0.00	0.00	-1.11
Urea Emission	0.00	0.00	0.00	0.00	0.30	-4.27	0.00	0.00
Carbon Capture Unit Emissions	0.00	0.00	0.00	0.00	0.00	6.72	0.00	0.00
Urea	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
Contaminant	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.11
Cooling water	0.00	0.00	-26.5	0.00	-75	0.00	0.00	0.00
Low pressure Steam	0.00	0.00	0.00	0.00	-1.2	-2.26	0.00	0.00

4.2 Multi-Objective Analysis

The goal of the study was to optimize multiple sustainability goals simultaneously. The performance indicators were set as follows:

1) the economic performance determined by the total profit of the cluster
2) the environmental performance indicated by the emission footprint of CO_2. This was quantified by determining the total flow of CO_2 leaving the cluster (using equation 3)
3) water conservation, which is quantified by the total water fed to the cluster.

Table 4 summarizes the three objectives optimized in this case study as well as the performance indicators used to quantify the objectives. The economic performance is optimized through maximizing the total profit of the cluster, which increases by increasing the production of methanol, urea, and ammonia, and decreasing the treatment of CO_2 through carbon capture units and sequestration. The environmental performance is optimized through minimizing the emissions leaving the cluster. These emissions are decreased by decreasing the production of methanol and urea (hence ammonia) or by increasing the treatment of CO_2 through capture and sequestration. It can be seen at this point that the environmental and the economic objective conflict, and an optimum solution would result in a trade-off between the two performances. The third objective function is the resource conservation, where the targeted material is water fed to the cluster. Water is consumed to produce both urea and methanol, optimizing this objective is achieved by minimizing the production of both plants. Therefore, water conservation conflicts with the economic performance of the cluster.

Table 4: Illustration of case study I objectives

Plant	Performance Indicator (PI)	PI quantification in the case study
Economic performance	Total profit	Revenue from selling methanol, urea, ammonia, and oxygen
Environmental performance	Total CO_2 emissions	CO_2 content in emission streams from: - Methanol production - Urea production - Carbon capture units - Pure CO_2 leaving cluster (untreated)
Resource conservation	Total water consumption	Total freshwater inlet as: - Fresh water to the cluster - Steam to carbon capture units and urea production plant - Cooling water to methanol and urea production plants

The cluster was optimized in terms of the three objectives at two electricity prices to explore variations in the network design. The two prices considered are \$0.02/kWh and \$0.03/kWh. The following section illustrates the result for each optimization runs.

4.3 Results and Discussion

The multi-objective integration tool was applied to the cluster presented in the previous section. First, the cluster was optimized for an electricity price of $0.02/kWh. The total profit was set as the primary objective to be optimized, while CO_2 emissions and water consumption were set as constraints. 18 constraints were selected for each constraint objective and therefore, a total of 324 runs was performed. Table 5 shows the pay-off table obtained for the cluster, while Table 6 shows the cluster design network corresponding to each pay-off point. It can be observed that a maximum economic performance involves the activation of all production plants. Partial production of methanol is a result of the limitation put on the CO_2 entering the cluster. Figure 3 shows the cluster networks for the maximum profit design. On the contrary, minimizing CO_2 emissions results in deactivating both methanol and urea production plants. Since energy and hydrogen are obtained only from renewable resources, ammonia plant is activated as no CO_2 is produced in the process. Profit for this network design is mainly obtained from oxygen and ammonia production. For a cluster with minimum water consumption, all production plants are deactivated since water consumption is essential to produce both methanol and ammonia (hence urea).

Table 5: Pay-off table for the cluster for an electricity price of $0.02/kWh

Pay-off Table	Profit ($/y)	CO_2 Emissions (t/y)	Water Consumption (t/y)
Maximum Profit	17,421,532	1,333	8,695,746
Minimum CO_2 Emissions	5,754,702	0	163,736
Minimum water consumption	4,283,000	0	0

Table 6: Network designs at the three pay-off points for an electricity price of $0.02/kWh

Plant	Capacity at maximum profit (t/y)	Capacity at minimum CO_2 emissions (t/y)	Capacity at minimum water consumption (t/y)
Air Separation	100,000	100,000	100,000
H_2O Splitting	24,672	18,193	0
Methanol Production	32,429	0	0
Ammonia Production	100,000	100,000	0

Table 6 Continued

Plant	**Capacity at maximum profit (t/y)**	**Capacity at minimum CO_2 emissions (t/y)**	**Capacity at minimum water consumption (t/y)**
Urea Production	100,000	0	0
Methanol CO_2 treatment Unit	3,288	0	0
Urea CO_2 treatment Unit	7,032	0	0
CO_2 sequestration	0	120,000	120,000

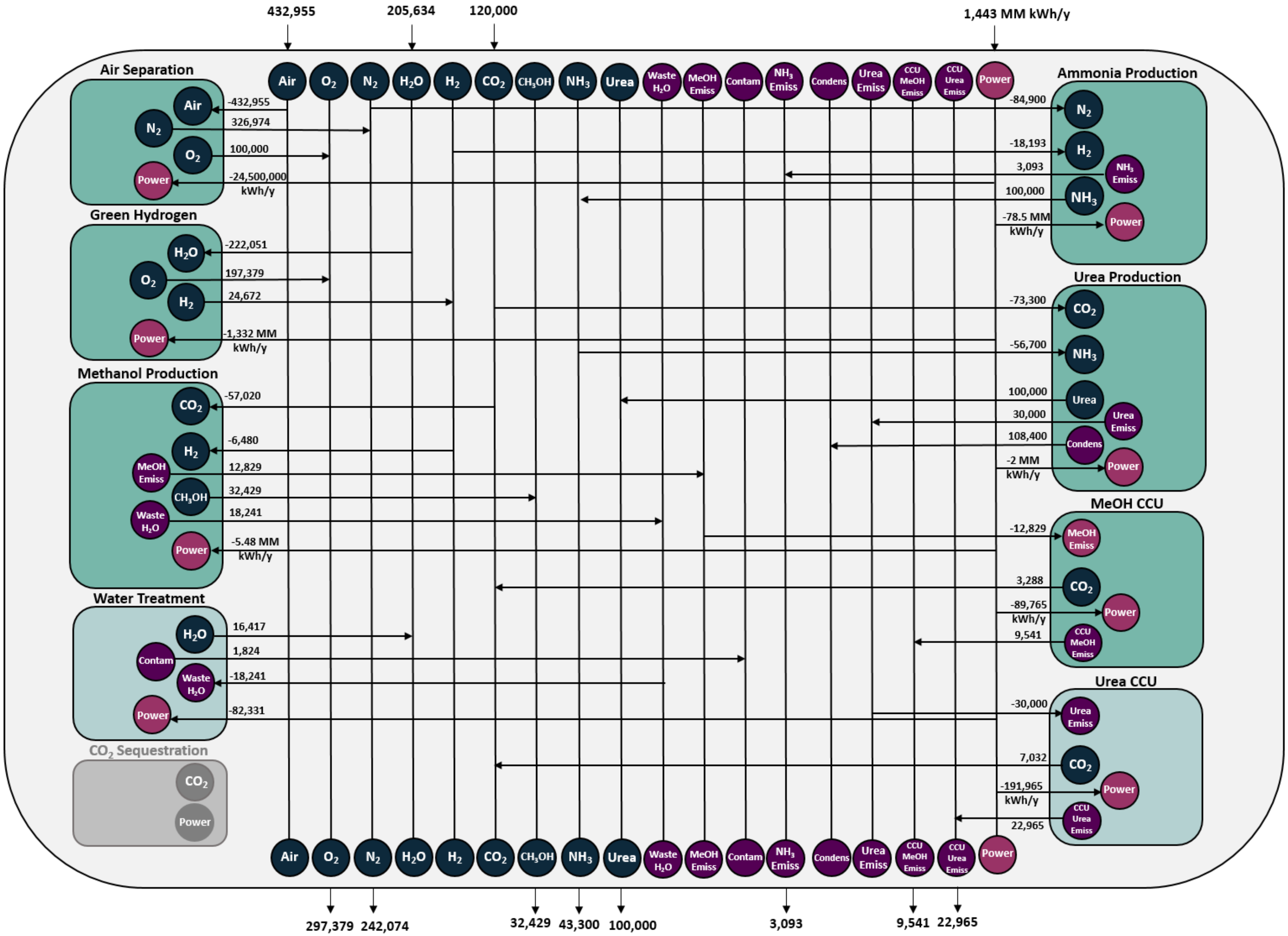


Figure 7: Cluster design for maximum profit (Case study I)

The trade-off between the three objective functions were then explored. Figure 8 shows the Pareto surface obtained when optimizing the cluster integration network using the augmented ε-constraint method. The figure shows a continuous surface where each point in the cluster represents distinct profit, CO_2 emissions, and total water consumption values, and is a result of a specific cluster network defined by the plant capacities. The continuity of the surface is a result of allowing a minimum capacity of 0 t/y for each processing unit (as noted in section 3.1). The pay-off points, which illustrate the designs where the three objective functions are optimized individually are marked in Figure 8. It can be seen from the figure that there is a trade-off between profit and CO_2. This is a result of the treatment costs of secondary CO_2 emissions, which are activated when the CO_2 emission constraint is set. A trade-off also exists between profit and water consumption as increasing the production (i.e., revenue) increases the water demand.

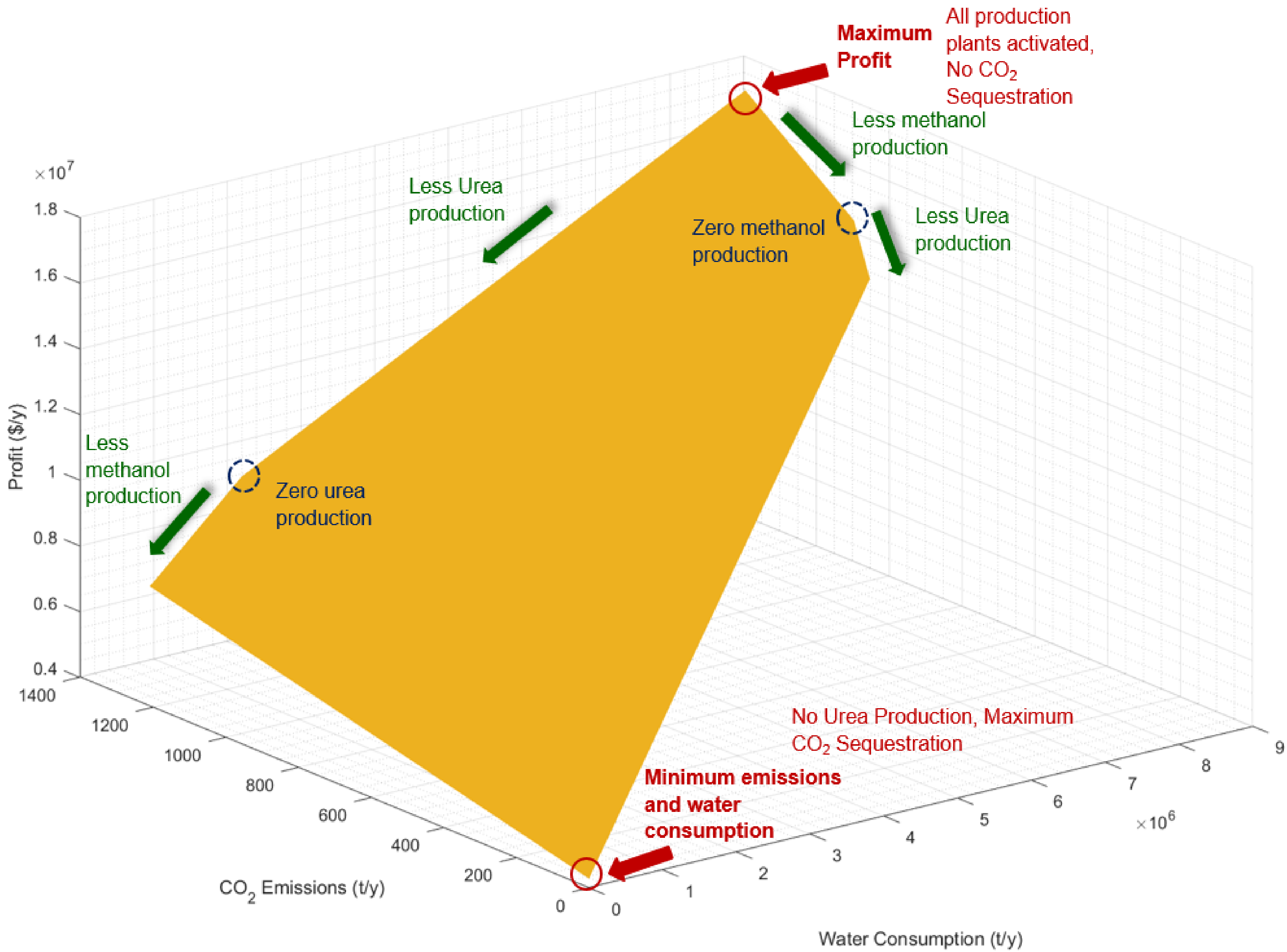
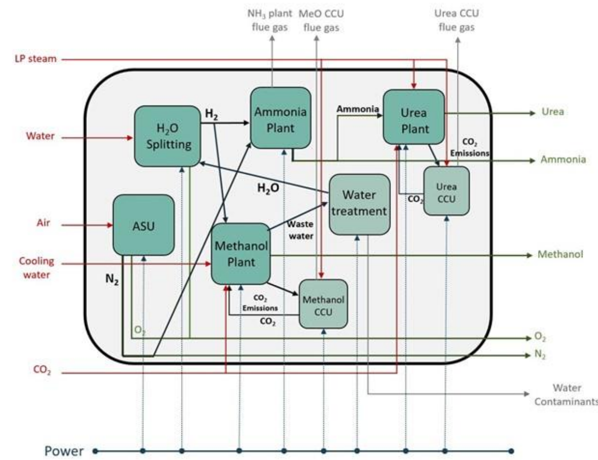


Figure 8: Pareto surface representing the trade-off between the three objectives (at electricity price $0.02/kWh)

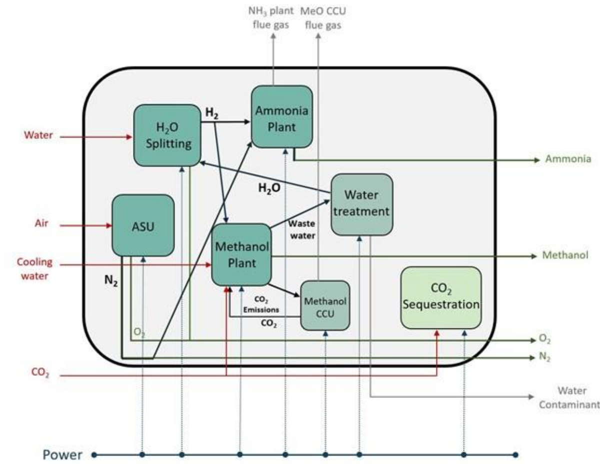
Figure 9 presents the 5 different design configurations offered by the Pareto surface. The 5 designs have varying capacities as illustrated in the Pareto surface (Figure 8). The optimum design in terms of economic performance (Figure 5-Design A) achieves an annual profit of $17.4 million. The design produces the highest emissions and highest water consumption. This network (shown in Table 6) involves the maximum production of ammonia and urea, as well as the production of 32,429 t/y of methanol. The production of methanol is limited since all the CO_2 available is consumed. CO_2 sequestration is deactivated since there are no emission limitations at this point.

As water consumption is forced to decrease, profit decreases. This decrease in profit is due to the decrease in urea production as urea requires cooling water. In this region, methanol production increases to make up for the profit loss and converts the available CO_2. However, as water consumption is forced to decrease further, a new design configuration forms where urea production is deactivated completely, and water consumption is decreased by decreasing the production of methanol (Figure 9- Design B). This happens as methanol requires hydrogen that consumes fresh water in addition to cooling water. A further decrease in water consumption leads to the decrease and deactivation of methanol production and a decrease in ammonia production (Figure 9- Design C). As the water consumption limitation reaches zero, ammonia production deactivates, and all production plans are deactivated (Figure 9- Design D). While production plants are decreasing at this point, CO_2 sequestration is increasing to allow the conversion of CO_2.

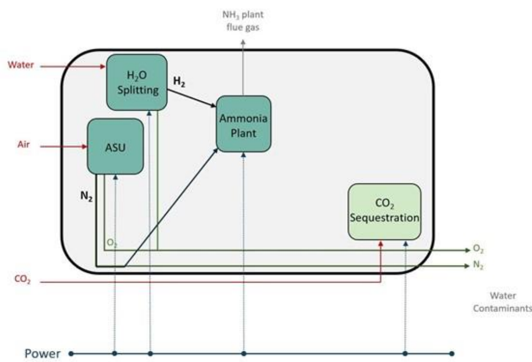
A change in the network also occurs when forcing a decrease in the CO_2 emissions. As emissions decrease, the production of methanol decreases (as methanol production comes with a higher cost). A further decrease leads to a new network design where methanol is deactivated (Figure 9- Design E). As emissions decrease more, urea production decreases until it is deactivated. Throughout the three design networks, the less the production of value-added products, the more CO_2 is sequestered, and the lower the profit.



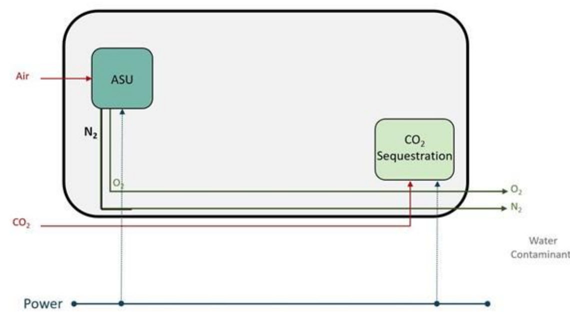
Design (A): Activation of all production plants



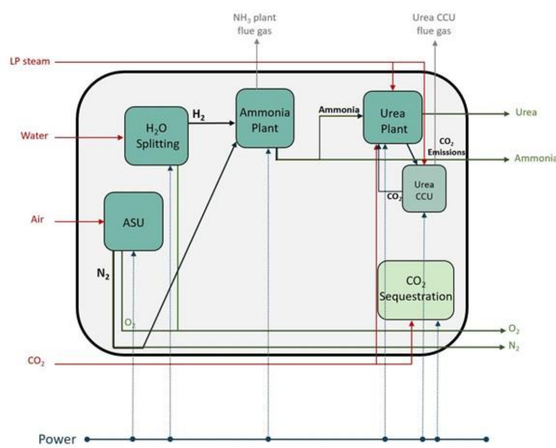
Design (B) Deactivation of urea production



Design (C): Deactivation of methanol and urea production



Design (D): Deactivation of all production plants



Design (E): Deactivation of methanol production

Figure 9: Cluster network designs of Pareto optimal set (at electricity price \$0.02/kWh)

The trade-off between the three objective functions was also explored at a higher electricity price of $0.03/t. New pay-off points were generated and are shown in Table 7, and the cluster designs corresponding to those points are shown in Table 8. It can be observed that the maximum profit is lower than the maximum profit in the previous electricity price (due to the higher energy consumption cost). Also, the maximum profit network includes CO_2 sequestration. This is due to the high energy demand for water splitting and methanol production (at this electricity price, the cost of sequestration is less than the cost of producing methanol from CO_2). The optimum designs for CO_2 emissions and water consumption are identical. In this design range, methanol production is always deactivated and there is no trade-off between emissions and water consumption. Figure 10 shows the cluster network the maximum profit design.

Table 7: Pay-off table for the cluster for an electricity price of $0.03/kWh

Pay-off Table	**Profit ($/y)**	**CO_2 Emissions (t/y)**	**Water Consumption (t/y)**
Maximum Profit	8,516,643	774	7,720,826
Minimum CO_2 Emissions	3,923,700	0	0
Minimum water consumption	3,923,700	0	0

Table 8: Network designs at the three pay-off points for an electricity price at \$0.03/kWh

Plant	Capacity at maximum profit (t/y)	Capacity at minimum CO_2 emissions (t/y)	Capacity at minimum water consumption (t/y)
Air Separation	100,000	100,000	100,000
H_2O Splitting	10,315	0	0
Methanol Production	0	0	0
Ammonia Production	56,700	0	0
Urea Production	100,000	0	0
Methanol CO_2 treatment Unit	0	0	0
Urea CO_2 treatment Unit	7,032	0	0
CO_2 sequestration	53,732	120,000	120,000

Figure 10 shows the Pareto surface obtained when optimizing the cluster at an electricity price of \$0.03/kWh. As can be seen from the network designs, methanol production is deactivated at all conditions because of the increased electricity price. The production of ammonia is limited and is produced just enough to produce urea; therefore no ammonia is exported from the cluster. This gives the same network of Design E shown in Figure 9. The increase in the electricity price highly affected the production of hydrogen from the water splitting plant, which in return affected the production cost of methanol and ammonia. Therefore, only two design options are available: the activation and deactivation of urea (and ammonia).

The capacities follow a similar trend to the network at the lower electricity price. As less water consumption and emissions are allowed, the production of urea and ammonia decreases until both are deactivated (Figure 9- Design D). The sequestration of CO_2 increases since it still requires less cost than taxation.

Observing the two Pareto surfaces at the different electricity prices (Figure 8 and Figure 10), the two surfaces following a similar trend. This is expected as the model is linear and continuous. The regions that exist only at the lower electricity price surface correspond to points that cannot be achieved by the higher electricity surface design. Therefore, it can be noticed that the electricity price highly influences the range of Pareto optimal solutions that can be obtained from the multi-objective integration tool.

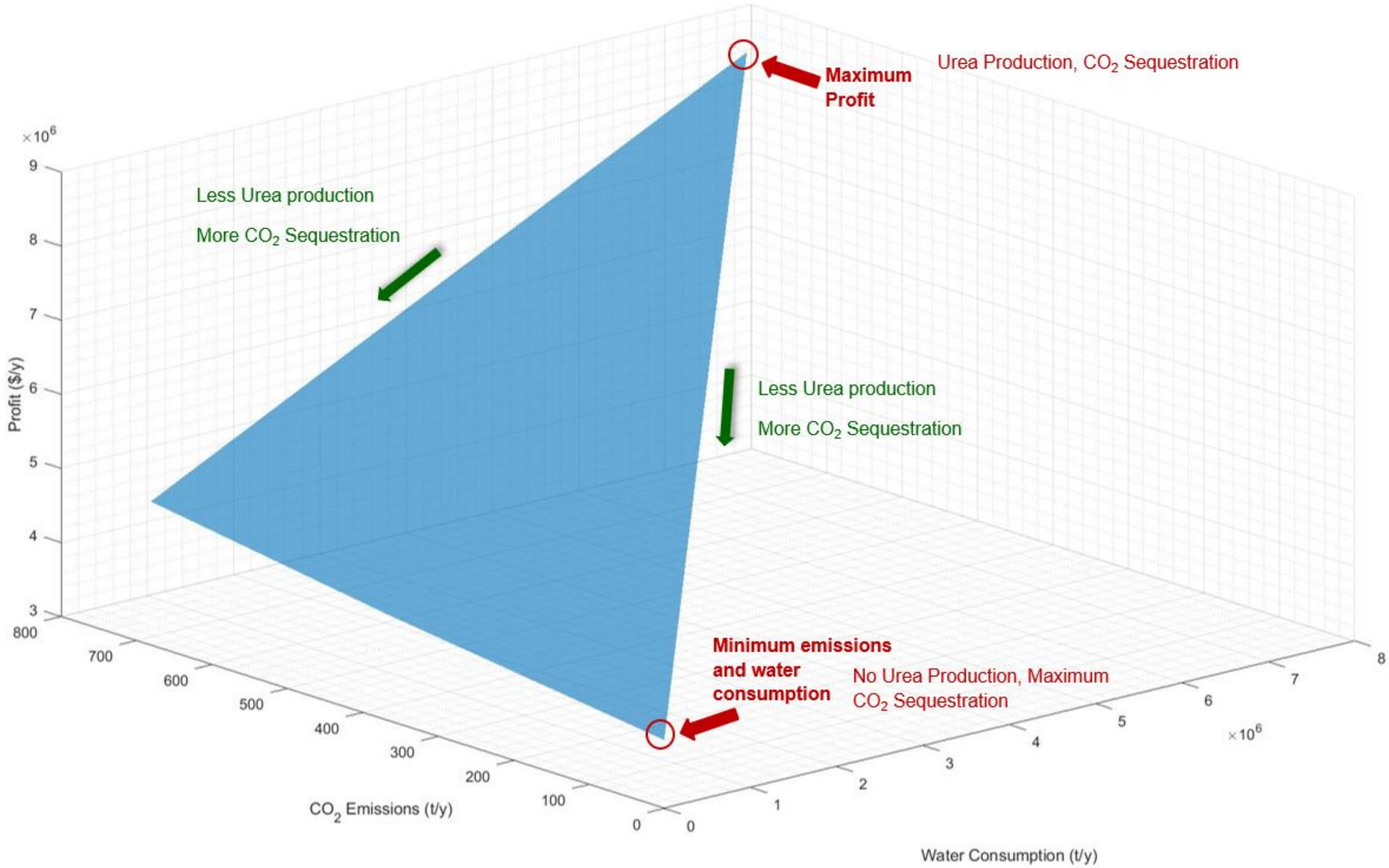


Figure 10: Pareto surface representing the trade-off of the three objectives (at electricity price \$0.03/kWh)

4.4 Case Study I Summary

In this case study, a carbon dioxide converting cluster was explored. The multi-objective resource integration tool was used to optimize the integration network of a cluster in terms of the economic, emission footprint, and resource conservation. that utilizes water, are, and carbon dioxide to produce value added products. The cluster only used renewable energy sources for power production. Methanol, ammonia, and urea are produced from the cluster. The economic performance was quantified by the total profit, the emission footprint by the total amount of carbon dioxide emitted from the cluster, and the resource conservation was optimized by minimizing the total water consumption. The cluster was optimized twice for two different electricity prices: \$0.02/kWh and \$0.03/kWh. For both electricity prices, there was a trade-off between the economic performance and both the emissions and water consumptions. As increasing production increases the profit but also increases the emissions and the water consumed. Two distinct Pareto surfaces were generated that illustrate the optimum solutions. For the lower electricity price, 5 different design alternatives were obtained that include the production of the three value added products (methanol, ammonia, and urea). For the higher electricity price, only ammonia and urea were produced, and two design alternatives were included in the Pareto surface.

5. CASE STUDY II: APPLYING THE TOOL TO A CARBON DIOXIDE EMITTING CLUSTER

In the recent years, natural gas became one of the primary energy sources in the world. Its abundance aids in meeting the global industrial demand for energy. Natural gas is primarily used to produce electricity and heat but is also utilized to produce value-added products such as synthetic crude, ammonia, methanol. Natural gas is also used as raw material to produce hydrogen which is used as an intermediate for production as seen in the previous case study. Even though it is considered a cleaner burning-hydrocarbon compared to fossil fuels, carbon emissions released from the combustion of natural gas are still significant. In this case study, the performance of a natural gas utilizing cluster is explored.

The cluster investigated consists of only natural gas, water, and air as feed. The three resources are utilized to produce Fischer Tropsch (F-T) synthetic crude, methanol, ammonia, and urea. Intermediates required for the productions are nitrogen, synthetic gas (a mixture of carbon monoxide and hydrogen), and pure hydrogen. The different plants required to produce these intermediates are added to the cluster design. Nitrogen is produced through an air separation unit. Synthetic gas (syngas) is produced through a two parallel reactor system of steam methane reforming and dry methane reforming. The syngas production unit uses water and CO_2 as feed to produce the syngas mixture. The process makes a syngas stream consisting of hydrogen and carbon monoxide with an H_2/CO ratio of 2. Two routes are available for the production of hydrogen: 1) steam reforming of methane, which uses natural gas and water as feed, and 2) water electrolysis, which is considered a cleaner (but a more expensive) path. The air separation and water electrolysis units both produce oxygen is a byproduct which can also be sold. Two options are also available for the production of power: 1) a combined cycle natural gas fired power plant, which is be used to generate electricity, and 2) a solar power plant which is considered a source of power production with zero emissions. Power is delivered to production plants from a power grid. Due to the efficiency limitation of solar panels, it is assumed that solar power is only consumed during the daylight (8 hours per day) where the remaining operation hours are covered by the natural gas power plant. This is included in the integration model by setting a minimum capacity of the natural gas power plant as follows:

$$2 \times C_{Solar} \leq C_{NG} \tag{12}$$

Where C_{NG} is the capacity of the natural gas power plant and C_{Solar} is the capacity of the solar power plant. Also, the space limitation of solar panels is accounted for by setting a maximum annual capacity of 100 MWh for the solar power plant. Figure 11 shows the possible connections of the cluster in a process flow diagram, and Figure 12 shows the connection in the representation suggested in Ahmed et al. (2020).

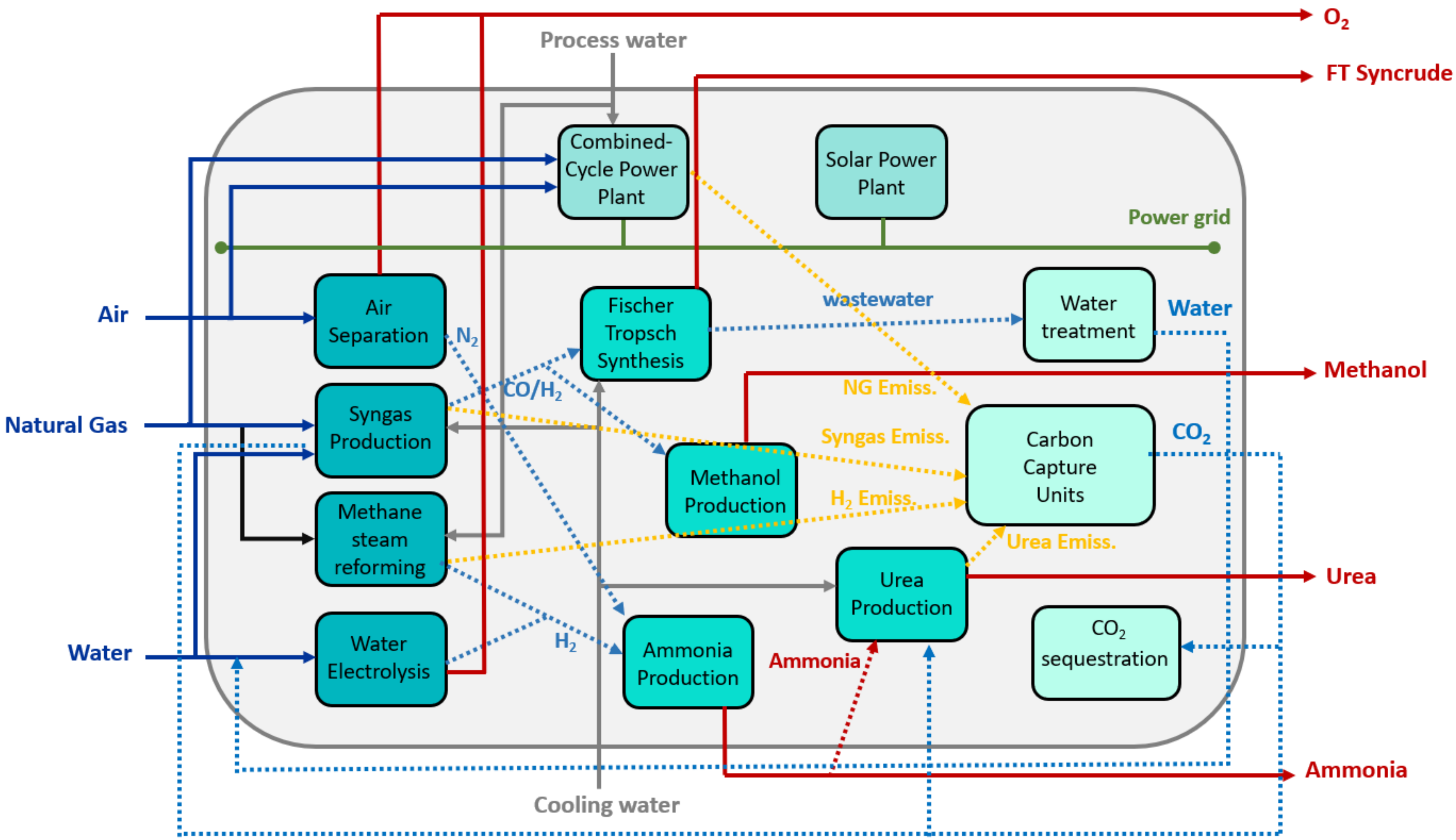


Figure 11: Process flow diagram of cluster showing possible interactions (Case Study II)

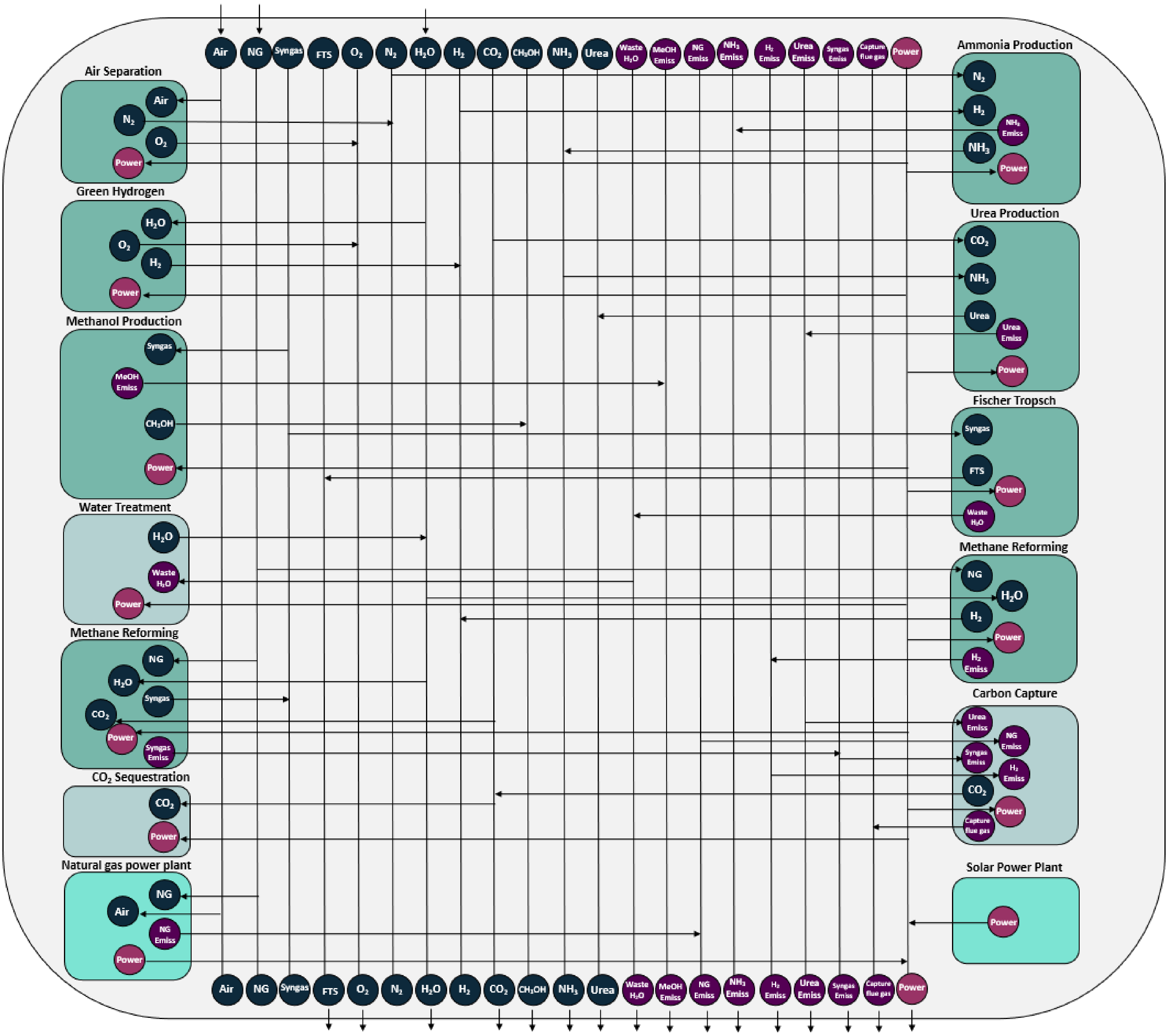


Figure 12: Integration network representation showing possible interactions (Case Study II)

The main source of greenhouse gas (GHG) emissions is the combustion of natural gas for power production. Emissions are also produced from the syngas production unit, the hydrogen production plant through methane reforming, as well as the urea production plant. Since the primary chemical emitted in those streams is CO_2, emission treatment units for each carbon emitting plant is introduced to the cluster design. The capture units are assumed to have efficiencies of 90%. When CO_2 is purified, it is allowed to be recycled to the urea and the syngas production units. CO_2 sequestration is also available as an emission minimization option. The Fischer Tropsch plant produces a significant amount of wastewater. Therefore, a water treatment plant is also present that allows the wastewater to be treated and recycled to the cluster production plants.

The goal of this study is to optimize the economic performance, the climate change impact, and the resource depletion impact of the cluster simultaneously. The economic performance is measured with the total profit of the cluster, the climate change impact is measured with the total greenhouse gas emissions from the cluster, while the water fed to the cluster is considered for resource depletion. The next section illustrates the data used to apply the multi-objective integration model.

5.1 Case Study Data

This section provides the data used for implementing the multi-objective integration model. Similar to the first case study data, Table 9 provides the CAPEX parameters for the cluster plants in terms of reference products. power consumption parameters, as well as the main product prices for each processing plant. Table 10 to 13 provide the parameters of all resources imported, exported, and exchanged. Table 10 provides the parameters for all raw materials, intermediates, and product resources of the production plants. Table 11 shows the parameters for the waste streams and energy parameters of the production plants, and Table 12 illustrates the parameters of the emissions and energy resources from/to waste treatment units and power plants. Table 13 provides parameters of material resources of waste treatment and power plants. The flue gases leaving the carbon capture units are numbered 1 to 4. Flue gas 1 leaves the syngas emissions treatment unit; flue gas 2 leaves the urea plant treatment unit; while flue gas 3 and 4 leave the natural gas and the methane reforming plants, respectively.

Table 9: Capital cost parameters (case study II)

Plant	Reference Resource	Unit	CAPEX Parameter ($/unitProduct)
Air Separation	O_2	t	17.52
H2O Splitting	H_2	t	752.0
Methane reforming	H_2	t	91.00
Syngas Production	Syngas mixture	t	25.88
Fischer Tropsch Process	Syncrude	t	136.0
Methanol Production	CH_3OH	t	74.00
Ammonia Production	NH_3	t	28.14
Urea Production	Urea	t	15.54
NG Fired Power Plant	Electricity	kWh	0.011
Solar Power Plant	Electricity	kWh	0.008
Carbon capture units	CO_2	t	1.640
CO_2 sequestration	CO_2	t	9.040
Water treatment unit	H_2O	t	0.246

Table 10: Parameters of raw materials/ intermediates/ products of production plants

Resource	Air Separation	H_2O Splitting	Methane reforming	Syngas Production	F-T Process	Methanol Production	Ammonia Production	Urea Production
Natural gas	0.00	0.00	-2.00	-0.47	0.00	0.00	0.00	0.00
Syngas H_2/CO	0.00	0.00	0.00	1.00	-2.11	-1.01	0.00	0.00
Air	-4.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00
O_2	1.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00
N_2	3.27	0.00	0.00	0.00	0.00	0.00	-0.85	0.00
Process water	0.00	0.00	-4.50	0.00	0.00	0.00	0.00	0.00
H2O	0.00	-9.00	0.00	-0.71	0.00	0.00	0.00	0.00
H_2	0.00	1.00	1.00	0.00	0.00	0.00	-0.18	0.00

Table 10 Continued

Resource	Air Separation	H_2O Splitting	Methane reforming	Syngas Production	F-T Process	Methanol Production	Ammonia Production	Urea Production
CO_2	0.00	0.00	0.00	-0.50	0.00	0.00	0.00	-0.73
NH_3	0.00	0.00	0.00	0.00	0.00	0.00	1.00	-0.57
Methanol	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
Urea	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
FTS Product	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
Wastewater	0.00	0.00	0.00	0.00	1.09	0.00	0.00	0.00

Table 11: Parameters of emissions and energy resources of production plants

Resource	**Air Separation**	**H2O Splitting**	**Methane reforming**	**Syngas Production**	**F-T Process**	**Methanol Production**	**Ammonia Production**	**Urea Production**
NG Power Plant Emissions	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Urea Plant Emissions	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.30
Methane Emissions	0.00	0.00	11.00	0.00	0.00	0.00	0.00	0.00
Syngas Emissions	0.00	0.00	0.00	0.111	0.00	0.00	0.00	0.00
Water contaminants	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HP Steam	0.00	0.00	0.00	0.00	2.56	0.00	0.00	0.00
LP Steam	0.00	0.00	0.00	0.00	5.20	0.00	0.00	-1.2
Cooling Water	0.00	0.00	0.00	-22.62	-48.32	0.00	0.00	-75
Electricity	-245.00	-54000.00	-50880.00	-121.20	0.00	-319.00	-785.00	-20

Table 12: Parameters of raw materials/ intermediates/ products of power and treatment plants

Resource	**NG Fired Power Plant**	**Solar Power Plant**	**Syngas CO_2 treatment Unit**	**Urea CO_2 treatment Unit**	**Power Plant CO_2 treatment unit**	**Hydrogen CO_2 treatment unit**	**CO_2 sequestration**	**Water treatment**
Natural gas	-0.0003	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Syngas H_2/CO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Air	-0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.00
O_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Process water	-0.017	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H_2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
H2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO_2	0.00	0.00	1.00	1.00	1.00	1.00	-1.00	0.00

Table 12 Continued

Resource	NG Fired Power Plant	Solar Power Plant	Syngas CO_2 treatment Unit	Urea CO_2 treatment Unit	Power Plant CO_2 treatment unit	Hydrogen CO_2 treatment unit	CO_2 sequestration	Water treatment
NH_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Methanol	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Urea	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FTS Product	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Wastewater	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 13: Parameters of emissions and energy resources of power and treatment plants

Resource	NG Fired Power Plant	Solar Power Plant	Syngas CO_2 treatment Unit	Urea CO_2 treatment Unit	Power Plant CO_2 treatment unit	Hydrogen CO_2 treatment unit	CO_2 sequestration	Water treatment
NG Power Plant Emissions	0.008	0.00	0.00	0.00	-1.21	0.00	0.00	0.00
Urea Plant Emissions	0.00	0.00	0.00	-4.27	0.00	0.00	0.00	0.00
Methane Emissions	0.00	0.00	0.00	0.00	0.00	-1.40	0.00	0.00
Flue gas 1	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00
Flue gas 2	0.00	0.00	0.00	3.27	0.00	0.00	0.00	0.00
Flue gas 3	0.00	0.00	0.00	0.00	0.21	0.00	0.00	0.00
Flue gas 4	0.00	0.00	0.00	0.00	0.00	0.40	0.00	0.00

Table 13 Continued

Resource	**NG Fired Power Plant**	**Solar Power Plant**	**Syngas CO_2 treatment Unit**	**Urea CO_2 treatment Unit**	**Power Plant CO_2 treatment unit**	**Hydrogen CO_2 treatment unit**	**CO_2 sequestration**	**Water treatment**
Syngas Emissions	0.00	0.00	-1.11	0.00	0.00	0.00	0.00	0.00
Wastewater	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-1.111
Water contaminants	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.111
HP Steam	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LP Steam	0.00	0.00	-1.14	-1.14	-1.14	-1.14	0.00	0.00
Electricity	1.00	1.00	-27.30	-27.30	-27.30	-27.30	-95.25	0.00

Parameters of the air separation, water splitting, ammonia and urea production, CO_2 sequestration, as well as water treatment were adopted from Ahmed et al. (2020). Raw data for the capital cost and resource parameters for the syngas production plant was obtained from Baltrusaitis and Luyben (2015). Capital cost parameter for the Fischer Tropsch process was calculated from Wood et al. (2012), and the energy parameters were obtained from Bao et al. (2009). The methanol plant material parameters were obtained from Cui and Kaer (2020), and the power parameters and capital cost were obtained from Pellegrini et al. (2011). The solar power plant capital cost parameter was calculated from Al-Mohannadi et al. (2016). The capital cost raw data for the natural gas power plant were obtained from Bolland and Saether (1992). The natural gas power plant efficiency and parameters were calculated from Karimi et al. (2012), the emission parameters were obtained from Al-Mohannadi and Linke (2015), and the SOx and NOx emissions composition were obtained from Jaramillo et al. (2007). The methane reforming CAPEX and parameters were obtained from Sadeghia et al. (2020). The capital cost parameters were converted to 2020 values using the CEPCI indices.

Each production plant is assumed to have a minimum capacity of 0 t/y and a maximum capacity of 100,000 t/y. The solar power plant has a minimum annual capacity of 0 MWh and a maximum annual capacity of 100 MWh. The minimum annual capacity of the natural gas powerplant was constraint by Equation 12 as discussed in the previous section.

To quantify emission footprint, the composition of CO_2 in streams exiting the cluster must be determined. The compositions of CO_2, NO_X and SO_X of each emission stream leaving the cluster are summarized in Table 14. The carbon capture treatment units use an amine-based solvent and are assumed to have an efficiency of 90% (Lameh et al. 2020). Component mass balance was performed to calculate the amount of CO_2 leaving the treatment units.

The operating cost of the cluster was assumed to be the cost required to purchase the fresh feed resources entering the cluster, primarily water and natural gas. The prices of the resources purchased and sold are summarized in Table 15. The case study was solved using “What’sBest!16.0” optimization tool in Microsoft Excel 2016 (Lindo Systems, 2019).

Table 14: Composition of emission streams exiting the cluster (Case Study II)

Source	**CO_2 Composition**	**NO_x Composition**	**SO_x Composition**
Syngas Production	1.00	0.00	0.00
Urea Production	0.26	0.00	0.00
Hydrogen Production	0.79	0.09	0.07
NG Power Plant	0.92	0.00	0.00
Flue gas 1	0.95	0.00	0.00
Flue gas 2	0.03	0.00	0.00
Flue gas 3	0.52	0.01	0.01
Flue gas 4	0.27	0.32	0.24
Methanol Purge	0.00	0.00	0.00
FTS Purge	0.00	0.00	0.00

Table 15: Resource prices

Resource	Price
Natural gas	$16.20
Process water	$0.03
H_2O	$5.00
CO_2	$40.00
CO_2	$0.00
NH_3	$290.00
Methanol	$320.00
Urea	$280.00
FTS Product	$420.00
Oxygen	$79.00
Cooling Water	$0.03

5.2 Multi-Objective Analysis

This section provides the multi-objective analysis for the natural gas monetization cluster. The goal of the study was to optimize the same sustainability goals analyzed in Case Study I. The performance indicators were set as follows:

4) the economic performance determined by the total profit of the cluster.
5) the environmental performance indicated by the emission footprint of GHG gases, and since CO_2 is the dominant component in those emissions, the environmental footprint was quantified by the amount of CO_2 leaving the cluster.
6) water conservation, which is quantified by the total water fed to the cluster.

Table 16 summarizes the three objectives optimized in this case study as well as the performance indicators used to quantify the objectives. The economic performance is optimized through maximizing the total profit of the cluster, which increases by increasing the production of methanol, urea, ammonia, and syncrude and decreasing the treatment of CO_2 through carbon capture units and sequestration. When analyzing the two alternatives for hydrogen production, methane reforming is more profitable compared to water splitting. The environmental performance is optimized through minimizing the emissions leaving the cluster. These emissions are decreased by decreasing the production of the value-added products, by using water splitting for hydrogen production or by increasing the treatment of CO_2 through capture and sequestration. It can be seen at this point that the environmental and the economic objective conflict, and an optimum solution would result in a trade-off between the two performances. The third objective function is the minimization of water consumption where water is consumed as steam to produce urea and sygnas, and to treat CO_2 through the carbon capture units. Freshwater is also fed to the cluster to produce hydrogen through both methane reforming and water splitting. However, as shown in Table 10, the parameter of water consumption for water splitting is larger than that of methane reforming. Therefore, the total cost and water consumption for hydrogen production through water splitting are higher than methane reforming. However, the emission impact of methane reforming causes a trade-off between the two alternatives in terms of the sustainability performance.

Table 16: Illustration of case study II objectives

Plant	Performance Indicator (PI)	PI quantification in the case study
Economic performance	Total profit	Revenue from selling methanol, urea, ammonia, syncrude and oxygen
Environmental performance	Total CO_2 emissions	CO_2 content in emission streams from: - Natural gas power plant - Methane reforming plant - Syngas production - Carbon capture units - Pure CO_2 leaving cluster (untreated)
Resource conservation	Total water consumption	Total freshwater inlet as: - Fresh water to the cluster to produce hydrogen from methane reforming and water splitting - Steam to carbon capture units, urea and syngas production plants, as well methane reforming - Cooling water to urea production plants

5.3 Results and Discussion

The multi-objective integration tool was applied to optimize the three sustainability objectives. The total profit was set as the primary objective while water consumption and CO_2 emissions were set as constraints. The pay-off values are summarized in Table 17. As expected from section 4.2, maximizing the profit also maximizes the water consumption and the emissions, which means a trade-off exists between the sustainability objectives.

Table 17: Pay-off values for objectives optimized in Case Study II

Pay-off Table	**Profit ($/y)**	**CO_2 Emissions (t/y)**	**Water Consumption (t/y)**
Maximum Profit	72,055,431	12,348,108	46,441,735
Minimum CO_2 Emissions	0	0	0
Minimum water consumption	0	0	0

From the table, emissions range from 0 t/y to 12,348,108 t/y, while the water consumption ranges from 0 t/y to 46,441,735 t/y. Table 18 shows the network designs corresponding to the maximum profit pay-off point, and Figure 13 shows the cluster design corresponding to the network. All production plants are at maximum capacity, sequestration is deactivated, while the capture units are activated to recycle CO_2 for urea and syngas production and only methane reforming is activated for hydrogen production. The pay-off point for the optimum water consumption and emissions is the deactivation of the cluster.

Table 18: Network designs at the three pay-off points for Case Study II

Plant	Capacity at maximum profit (unit/y)	Capacity at minimum CO_2 emissions and water consumption (unit/y)	Unit
Air Separation	100,000	100,000	t
H2O Splitting	-	0	t
Methane reforming	28,508	0	t
Syngas Production	312,000	0	t
Fischer Tropsch Process	100,000	0	t
Methanol Production	100,000	0	t
Ammonia Production	156,700	0	t
Urea Production	100,000	0	t
NG Fired Power Plant	1,576,471	0	MWh
Solar Power Plant	100,000	24,500	MWh
Carbon Capture 1	31,200	0	t
Carbon Capture 2	7,032	0	t
Carbon Capture 3	100,000	0	t
Carbon Capture 4	91,068	0	t
CO2 sequestration	-	0	t
Water treatment unit	97,830	0	t

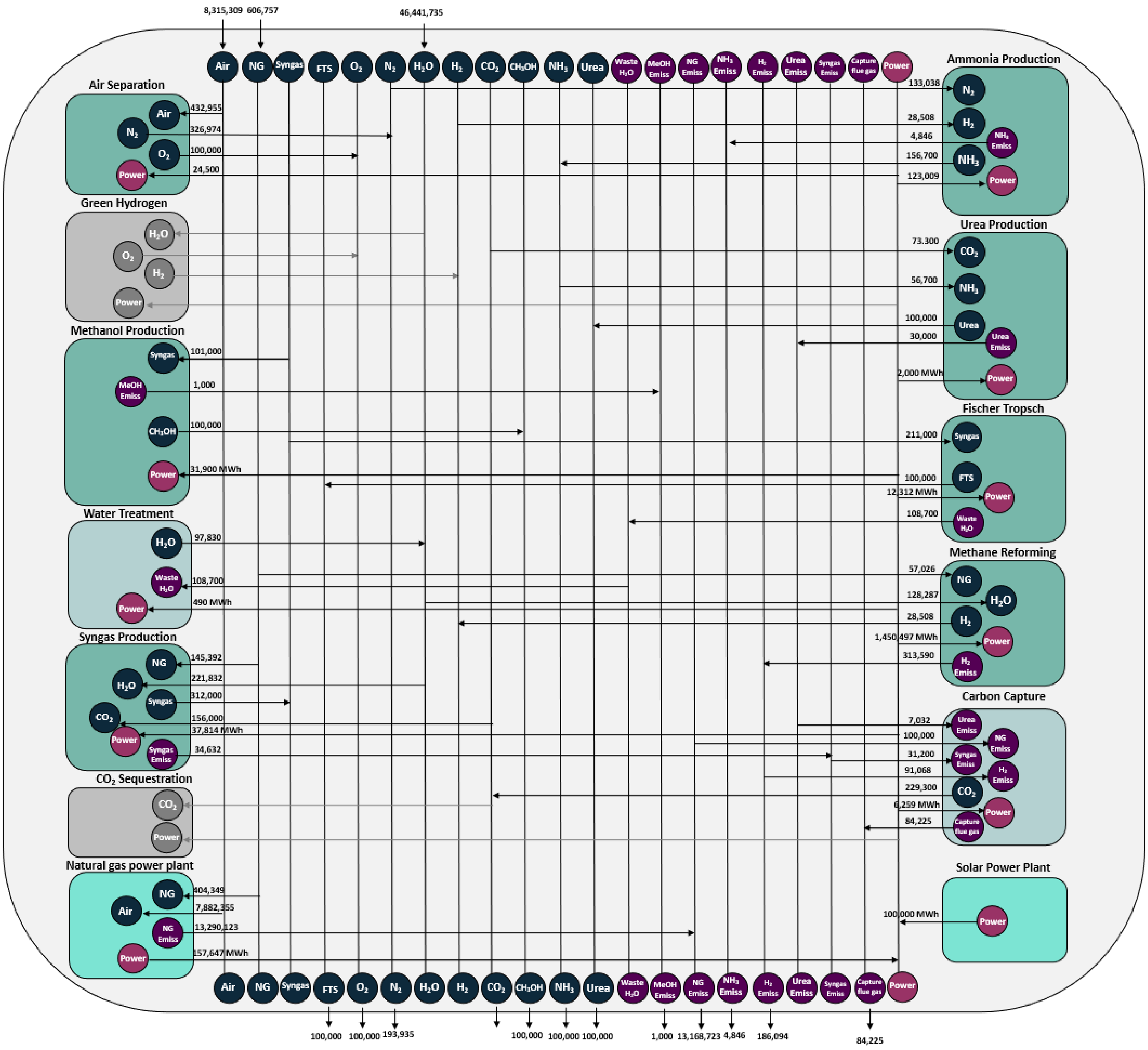


Figure 13: Cluster design for maximum profit (Case Study II)

To apply the multi-objective optimization model, 15 constraints were selected for each objective function within the minimum and maximum values in the pay-off table for the water consumption and emissions. Therefore, a total of 225 runs were performed. Figure 14 shows the pareto surface obtained when optimizing the cluster integration network using the model proposed. The figure also illustrates the trend of the production plants capacity as the constraints on both the water consumption and emissions are increased. As the constraint values on the water consumptions and emissions are altered, the design of the optimum solution changes. This change is reflected on the capacity of the plants and the integration network design. Figure 14 through 17 present the PFD of the different cluster designs obtained from the Pareto set.

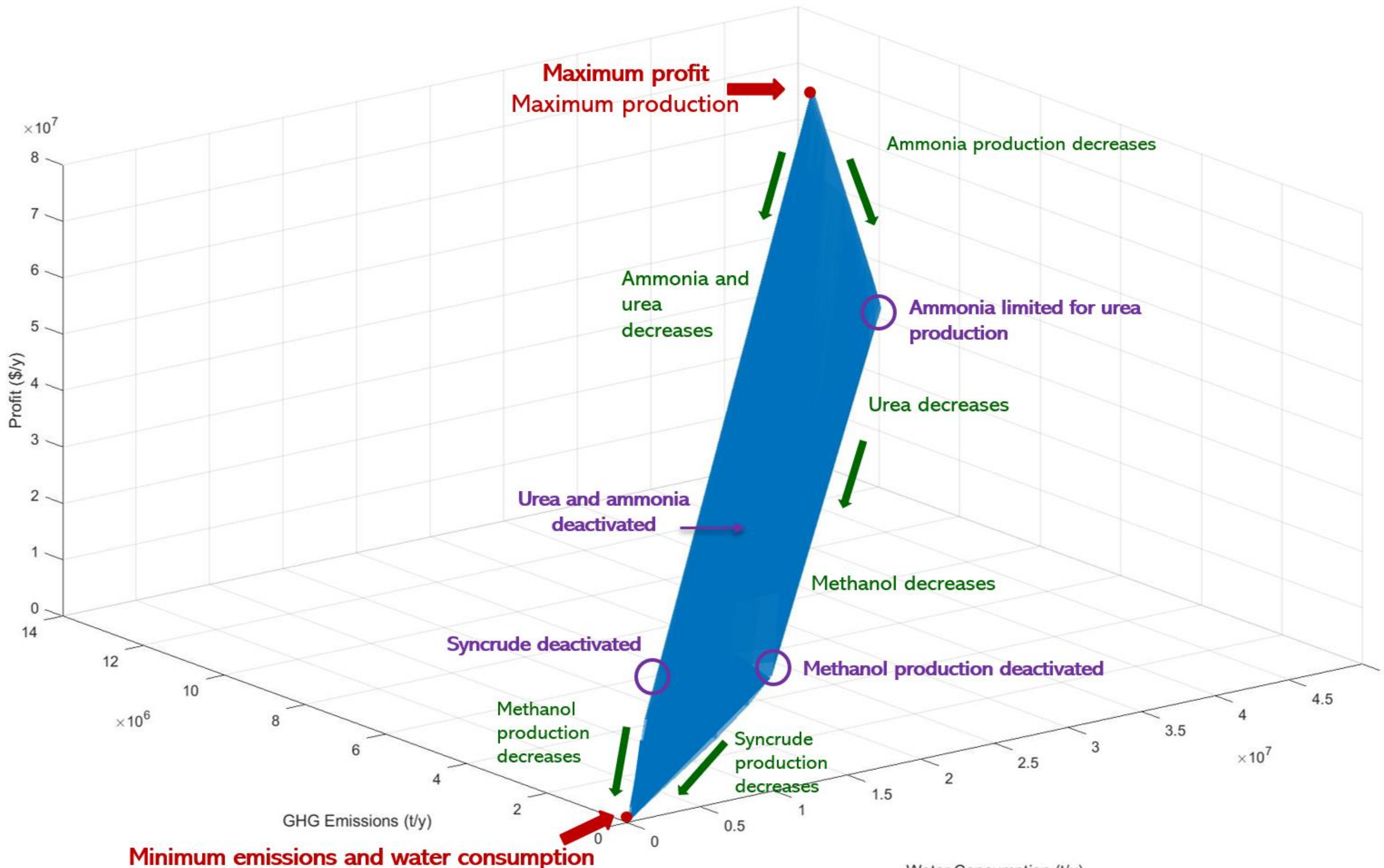


Figure 14: Pareto surface representing the trade-off between the three objectives (Case Study II)

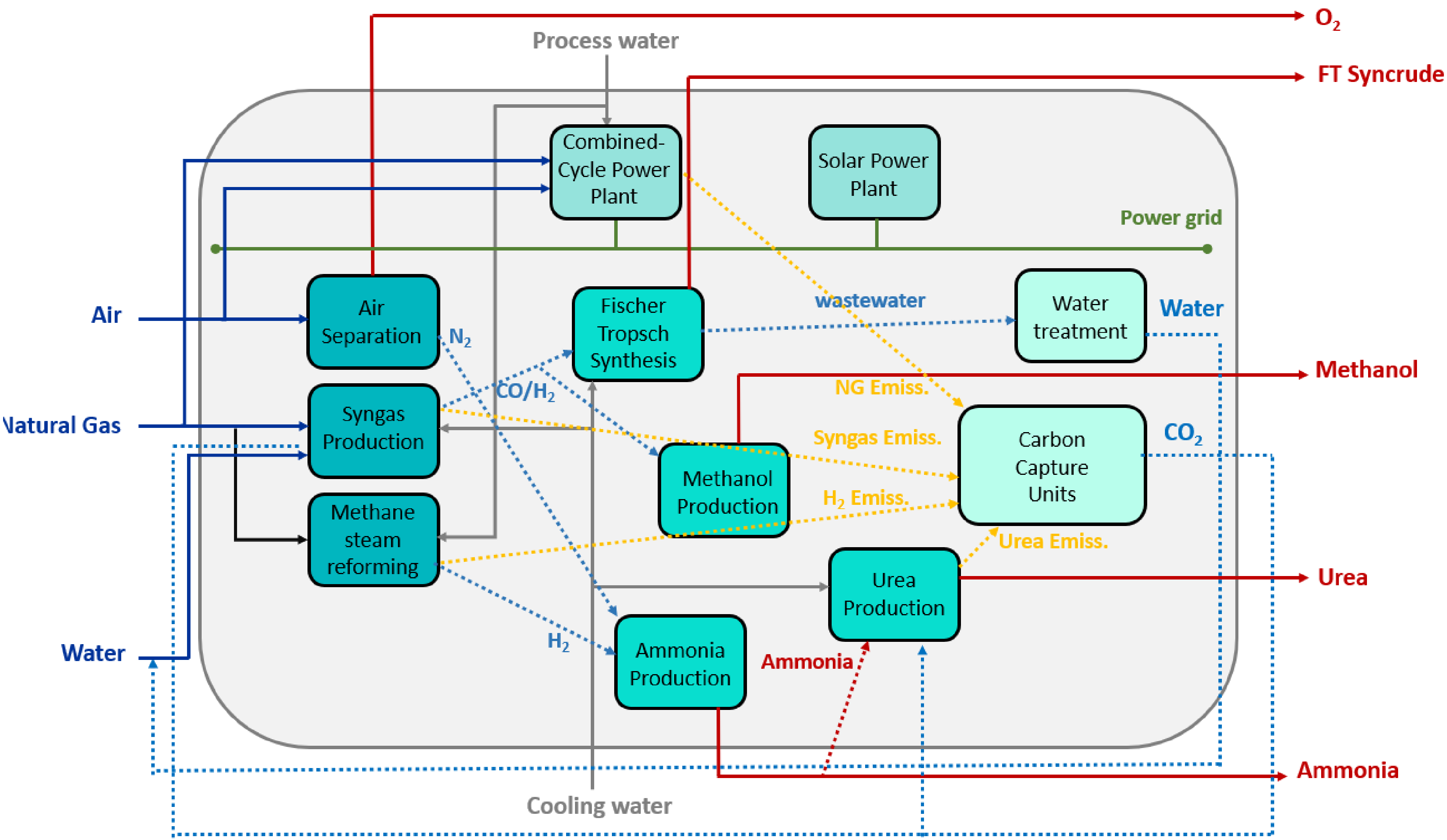


Figure 15: Cluster design corresponding to maximum profit (Case Study II)

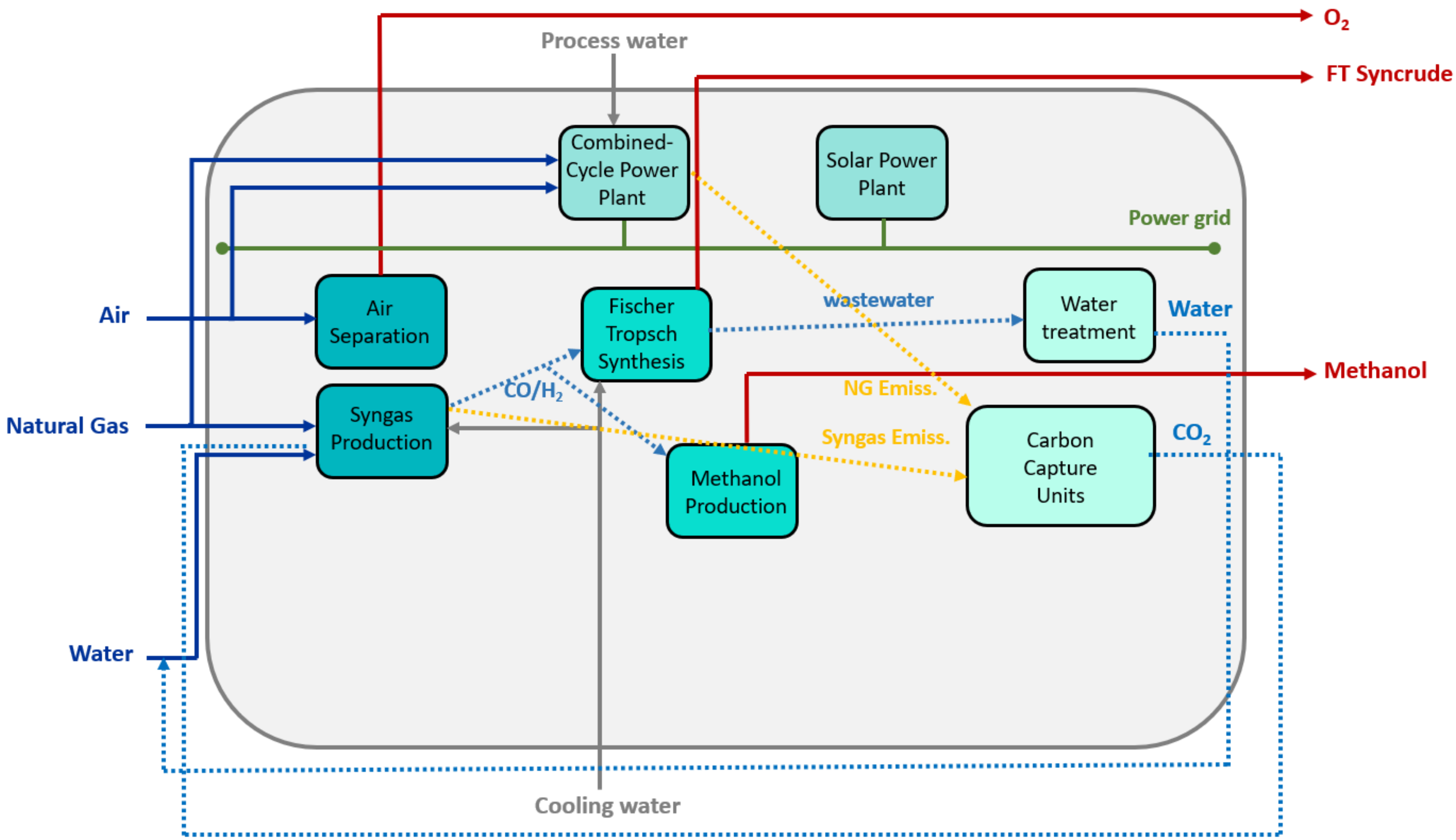


Figure 16: Cluster design where ammonia and urea productions are deactivated (Case Study II)

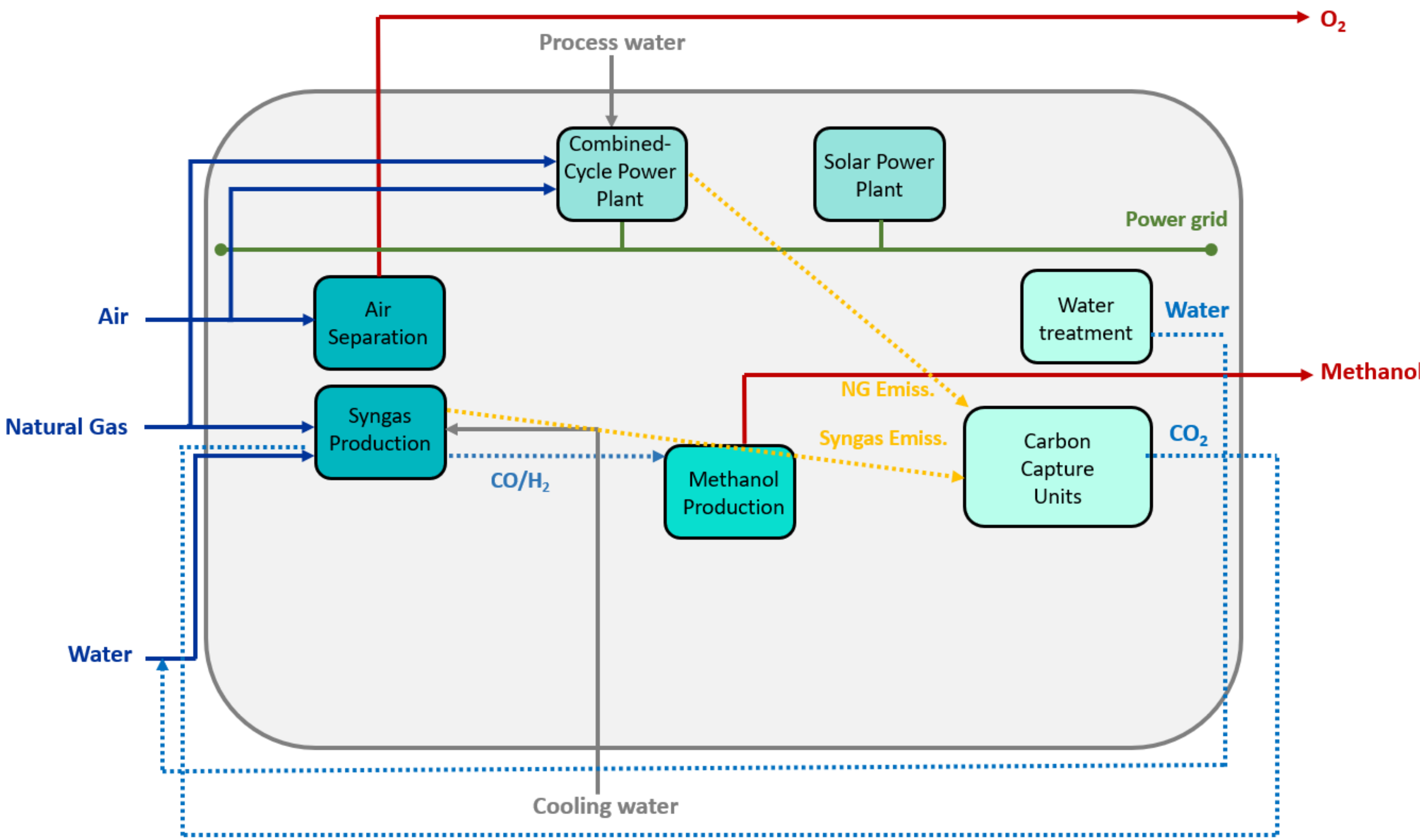


Figure 17: Cluster design where ammonia, urea, and syncrude productions are deactivated (Case Study II)

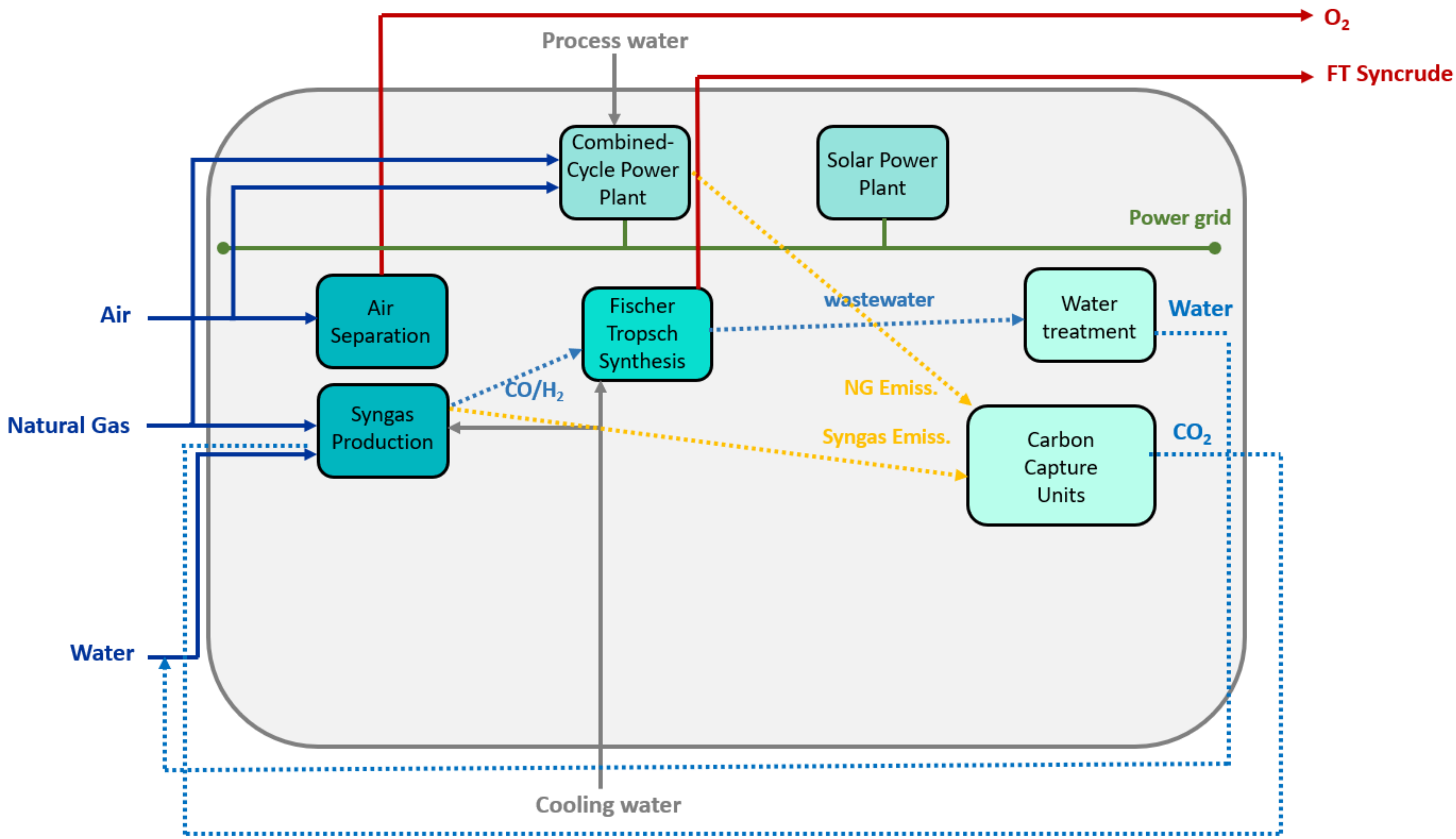


Figure 18: Cluster design where ammonia, urea, and methanol productions are deactivated (Case Study II)

As discussed previously, at maximum profit, all production plants are activated at maximum capacity and hydrogen is produced through methane reforming (Figure 14). As the constraints on water and emissions are introduced, the production of ammonia and urea decrease, since the two plants have the highest emission and water consumption impact on the cluster. The main influence of these two plants is the demand of hydrogen through methane reforming. Reducing the production of urea and ammonia reduces the demand of hydrogen, therefore, reduces the water consumption and GHG emissions caused by methane reforming. The production of both syncrude and methanol remain at maximum. As the emissions and water consumption are decreased more, the capacities of the two plants continue to decrease until a shift takes place where the production of ammonia is limited to urea production rather than exported from the cluster. Further reduction of the two objectives deactivates both the ammonia and urea plants and only syncrude and methanol are activated (Figure 15).

Once the emissions and water consumption and emissions are reduced further, two alternatives are possible: 1) the reduction and deactivation of syncrude production, or 2) the reduction and deactivation of methanol production. Observing the first option, reducing the emissions and water consumption reduces the capacity of the syncrude production. Since the production of syngas and syncrude requires power production through natural gas combustion and water consumption, decreasing the two objectives leads to the reduction of the FTS process capacity. The methanol plant remains at maximum production. Decreasing the constraints further leads to the deactivation of the syncrude production, this design is illustrated in Figure 16. Then, reducing the emission and water consumptions more decreases the methanol plant capacity until complete deactivation of the cluster.

The second path provides a comparative trade-off values but different design configurations. Starting with the design in Figure 15, the reduction of emissions and water consumption reduces the production of methanol rather than syncrude, while the FTS process remains at maximum. Production of methanol is affected by the two constraints since it syngas production and power. The production of methanol continue to decrease with the reduction of the two objective function until it is deactivated (design in Figure 17). Beyond this point, the FTS process starts to decrease. Comparing this production alternative to the first one, it can be seen that the deactivation of syncrude production results in a higher emission region but a lower water consumption one. Finally, at the minimum water consumption and emissions, all production plants are deactivated, and zero profit is reached.

5.4 Case Study II Summary

The optimization of a natural gas utilizing cluster was explored in this study. The multi-objective resource integration tool was used to optimize the integration network of the cluster in terms of the economic, emission footprint, and water consumption. The cluster utilizes natural gas, water, and air to produce syncrude, methanol, ammonia, and urea as value added products. The cluster included a power grid connected to a natural gas power plant and a solar power plant. Also, hydrogen is produced as in intermediate within the cluster and two alternatives were available for the production process: 1) methane reforming, which is accompanied by greenhouse gas emissions and water splitting, which is considered a cleaner alternative for the production. The multi-objective integration tool was used to optimize the three objectives. The economic performance was quantified by the total profit, the emission footprint by the total amount of carbon dioxide emitted from the cluster, and the resource conservation was optimized by minimizing the total water consumption. There was a trade-off between the economic performance and both the emissions and water consumptions, since increasing production increases the profit but also increases the emissions and the water consumed. A Pareto surfaces was generated that illustrate the optimum solutions, and three different design configurations were obtained. An economic optimum solution resulted in the activation of all production plants. As constraints were introduced, production was decreased, and 4 different design alternatives were introduced that involved the deactivation and activation of the different production plants.

6. CONCLUSION

A new superstructure was proposed which combines resource integration network and a multi-objective optimization tool to develop sustainable clusters. The model allows the integration of all material and energy integration resources in a cluster while simultaneously optimizing the economic, environmental, and material conservation performances. Pareto surfaces are generated, which capture the trade-off between the three objectives. Each point in the Pareto surface presents an optimum solution that corresponds to a distinct integration and cluster design (plant capacities and integration networks). The proposed superstructure was applied to optimize two cluster designs: a CO_2 converting cluster, and a natural gas utilizing cluster. The two clusters were optimized using the model in terms of profit, CO_2 emissions, and water consumption.

The CO_2 converting cluster uses air, water, and CO_2 to produce ammonia, urea, and methanol as value added products. Optimum solutions for the model were explored for two different electricity prices: \$0.02/kWh and \$0.03/kWh and Pareto surfaces were generated for the two prices. For an electricity price of \$0.02/kWh, the Pareto set of solutions included a different range of capacities between producing ammonia, urea, and methanol, and activating CO_2 sequestration. For the higher electricity price design, the production of methanol was eliminated from the optimum set of solutions due to the high energy demand of its production.

The same sustainability objectives were optimized for the natural gas converting cluster. The cluster only imports air, natural gas and water. Methanol, ammonia, urea, and syncrude were produces as the value-added products. Solar and natural gas power production were available. Hydrogen was produced as an intermediate through two alternatives: methane reforming and water splitting. A pareto surface was generated that shows the trade-off between the three objectives.

Three design alternatives were obtained from the Pareto set which included the activation of all production plants and deactivation of urea and syncrude production. The design alternatives included a range of capacities for the plants that correspond to different profit, water consumption, and emission values.

7. FUTURE WORK

The work can be used to generate scenarios to assess policy effects and tools to help inform decision-makers. The tool presented can have a wide range of applications for future work. The study of the Eco-industrial parks can be extended to include the assessment of indicators such as the Annual Sustainability Profit and TRACI metrics. Such indicators allow exploring the Pareto set of solutions in more depth for policy making. Future application of the proposed Multi-Objective Integration tool can explore more objective functions such as conservation of other depleting resources such as natural gas or consider social indicators (e.g. metrics that influence the human wellbeing, job creation and others). Other metrics that could be explored are toxicity of the resources emitted and waste streams. The multi-objective integration tool can also be extended to other MOO tools such as the weighted average method. The pareto set obtained from the different MOO tools can then be compared.

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