A SYSTEMATIC APPROACH FOR DESIGNING INDUSTRIAL PARK INTEGRATION NETWORKS ACROSS THE WATER-ENERGY NEXUS

A Thesis

by

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ABSTRACT

Nowadays, water-energy resource faces growing demands and constraints in many regions as a result of economic, population growth and climate change. The water-energy nexus and integration has been recently proposed to minimize water-energy footprint of an industrial park. It is required to develop a systematic approach for water-energy network and interconnections among the processes. Previous research work has presented the general superstructure and approach to develop economically optimal water networks that achieve a specified footprint target. In this work, the previous approach for water network has been extended with cooling systems options in order to capture the linkages between water and energy within industrial cities. The objective of this paper is to develop a framework for optimizing energy and water resources from processes that have a surplus of energy at various qualities. A systematic procedure is developed for optimizing and maximizing the benefits of these nexuses, considering power generation from a net surplus of waste heat energy from each plant by accounting for different sustainability metrics. The developed approach includes the use of composite curve analysis to first identify the potential for excess heat and then used to develop the combined water-energy network. A superstructure is generated to embed various configurations and related optimization formulation is solved to obtain an optimal process that economically satisfies the demand for water and energy considering some environmental metrics. Special emphasis is placed on capturing the synergy potentials from utilizing excess process heat and synergies across cooling and desalination systems, as well as synergies with the surroundings in terms of power and water exports from the industrial cluster. The work considers multiple objectives to explore trade-offs between minimum total annual cost and environmental sustainability metrics. A case study of an industrial cluster of typical processes operating in Qatar is presented to highlight the benefits of integration. It is shown how economically very attractive solutions across the nexus are identified by the proposed optimization-based approach. The results indicate that by water-energy integration the footprint reduction can be significant while economically is attractive too. Therefore, there is a great potential for savings water-energy resources by water-energy integrations. The work is contributed to sustainable development such as less pollution and resource minimization.

DEDICATION

To my parents

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NOMENCLATURE

Indices:

p	Plant/Process
i	Water Source
j	Water Sink
i'	Energy Source
j'	Energy Sink
r	Decentralized treatment
s	Centralized Treatment
l	Freshwater Type
t	Central Treatment Type
c	Contaminant

Parameters:

$z_{cj,p}^{min}$	Minimum permissible pollutant c composition in sink j, plant p (ppm)
$z_{c,jp}^{max}$	Maximum permissible pollutant c composition in sink j, plant p (ppm)
G_{jp}	Flowrate required in sink j, plant p (kg/h)
W_{ip}	Flowrate available in source i, plant p (kg/h)
$x_{c,ip}^{Source}$	Pollutant c composition in source i, plant p (ppm)
$x_{c,l}^{FRESH}$	Pollutant c composition in External Freshwater of type *l* (ppm)
L	

R_{rp} Water recovery factor in decentralized treatment r, plant p

R_{st} Water recovery factor in centralized treatment s, type t

$RR_{c,rp}^{REM\_1}$ Removal Ratio of pollutant c associated with Stage 1 of decentralized treatment r, plant p

$RR_{c,rp}^{REM\_2}$ Removal Ratio of pollutant c associated with Stage 2 of decentralized treatment r, plant p

$RR_{c,st}^{REM\_1}$ Removal Ratio of pollutant c associated with Stage 1 of centralized treatment s, type t

$RR_{c,st}^{REM\_2}$ Removal Ratio of pollutant c associated with Stage 2 of centralized treatment s, type t

$x_c^{WW\_Max}$ Maximum permissible discharge concentration of pollutant c in wastewater discharge

$x_c^{B\_Max}$ Maximum permissible discharge concentration of pollutant c in brine discharge

a Coefficient associated with piping cost calculations

b Power coefficient associated with piping cost calculations

C^{WW} Cost of Wastewater Discharge ($/kg)

C^{BRINE} Cost of Brine Discharge ($/kg)

C_l^{FR} Cost of Freshwater of type l ($/kg)

C^{STR} Cost of Buffer Storage ($/kg)

H_y Operating hours per year (h/yr)

K_F Treatment Cost Annualization Factor (yr^{-1})

N^{DAYS} Buffer Storage Capacity (days)

C_{rp}^{INV} Decentralized treatment r in plant p CAPEX ($)

C_{st}^{INV} Centralized treatment s, type t CAPEX ($)

C_{rp}^{REM} Cost of mass removed in decentral treatment r, plant p ($/kg)

C_{st}^{REM} Cost of mass removed in central treatment s, type t ($/kg)

γ Cost Annualization Factor (yr^{-1})

α Power coefficient associated with capital cost calculations for treatment units

ρ Density (kg/m^3)

μ Viscosity (kg/m s)

Sets:

P Set of Plants/Processes in Industrial City

SU_p Set of Water Sources in Plant p

SN_p Set of Water Sinks in Plant p

R Set of Decentralized Treatment

S Set of Central Treatment Locations

T Set of Central Treatment Types

L Set of Freshwater Types

C Set of Contaminants/Pollutants

Variables:

C^{Fresh} Total Freshwater Costs ($)

$C^{Treatment}$ Total Central and De-central Treatment Costs ($)

C^{Pipes} Total Piping Costs ($)

$C^{Storage}$ Total Water Buffer Storage Costs ($)

C^{Waste} Total Wastewater Handling Costs ($)

$z_{c,jp}^{in}$ Pollutant c Composition in sink j, plant p (ppm)

$M_{ip,jp'}$ Water flowrate from source i, plant p to sink j plant p'(kg/h)

$F_{l,jp}$ External freshwater flowrate of type l required in sink j, plant p (kg/h)

D_{ip} Wastewater flowrate discharged by source i, plant p (kg/h)

$T_{ip,rp}^{Inlet}$ Water flowrate from source i, plant p into decentral treatment r in plant p (kg/h)

$T_{ip,st}^{Inlet}$ Water flowrate from source i, plant p into central treatment s of type t (kg/h)

$T_{rp,jp}^{Treated}$ Treated water flowrate produced by decentral treatment r in plant p sent to sink j, plant p (kg/h)

$T_{st,jp}^{Treated}$ Treated water flowrate produced by central treatment s of type t sent to sink j, plant p (kg/h)

$D_{rp}^{Treated}$ Treated water flowrate sent to waste by decentral treatment r, in plant p (kg/h)

$D_{rp}^{Untreated}$ Untreated (brine) water flowrate sent to brine waste by decentral treatment r, in plant p (kg/h)

$D_{st}^{Treated}$ Treated water flowrate sent to waste by central treatment s, of type t (kg/h)

$D_{st}^{Untreated}$ Untreated (brine) water flowrate sent to brine waste by central treatment of type t (kg/h)

WW^{total} Total Wastewater Discharge (kg/h)

B^{total} Total Brine Discharge (kg/h)

y_{st} Binary variable associated with the selection of treatment type t, in a centralized treatment location s

$x_{c,rp}^{Treated}$ Concentration of contaminant c in the treated water stream produced by decentralized treatment r, in plant p (ppm)

$x_{c,st}^{Treated}$ Concentration of contaminant c in the treated water stream produced by centralized treatment s, of type t (ppm)

$x_{c,rp}^{REM}$ Intermediate concentration between Stages 1&2 in decentralized treatment r, plant p (ppm)

$x_{c,st}^{REM}$ Intermediate concentration between Stages 1&2 in centralized treatment s, type t (ppm)

$x_{c,rp}^{TOTAL\ REM}$ Total mass of contaminant c removed in decentralized treatment r, palnt p (ppm)

$x_{c,st}^{TOTAL\ REM}$ Total mass of contaminant c removed in centralized treatment s, type t (ppm)

$x_{c,rp}^{Treated}$ Concentration of contaminant c in permeate stream produced by decentral treatment r, plant p (ppm)

$x_{c,rp}^{Untreated}$ Concentration of contaminant c in brine stream produced by decentral treatment r, plant p (ppm)

$x_{c,st}^{Treated}$ Concentration of contaminant c in permeate stream produced by central treatment s, type t (ppm)

$x_{c,st}^{Untreated}$ Concentration of contaminant c in brine stream produced by central treatment s, type t (ppm)

$x_{c}^{WW\_Discharge}$ Total wastewater discharge concentration of contaminant c

$x_{c}^{B\_Discharge}$ Total brine discharge concentration of contaminant c

$L_{ip\,jp'}$ Length of pipe from source i, plant p to sink j plant p' (m)

L_{ip} Length of pipe carrying unused wastewater from source i, plant p to mainstream waste (m)

$L_{l,jp}$ Length of pipe carrying type l freshwater from mainstream to sink j, plant p (m)

$L_{ip,rp}$ Length of pipe from source i, plant p to decentral treatment r plant p (m)

$L_{ip,st}$ Length of pipe from source i, plant p to central treatment s of type t (m)

$L_{rp,jp}$ Length of pipe from decentral treatment r plant p to sink j, plant p (m)

$L_{st,jp}$ Length of pipe from central treatment s of type t to sink j, plant p (m)

$L_{wz,jp}$ Length of pipe from central treatment w of type z to sink j, plant p (m)

L_{rp} Length of pipe carrying unused wastewater from decentral treatment r, plant p to mainstream waste (m)

L_{st} Length of pipe carrying unused wastewater from central treatment s, type t to mainstream waste (m)

$DI_{ip\,jp'}$ Diameter of pipe from source i, plant p to sink j plant p' (m)

DI_{ip} Diameter of pipe carrying unused wastewater from source i, plant p to mainstream waste (m)

$DI_{l,jp}$ Diameter of pipe carrying type l freshwater from mainstream to sink j, plant p (m)

$DI_{ip,rp}$ Diameter of pipe from source i, plant p to decentral treatment r plant p (m)

$DI_{ip,st}$ Diameter of pipe from source i, plant p to central treatment s of type t (m)

$DI_{rp,jp}$ Diameter of pipe from decentral treatment r plant p to sink j, plant p (m)

$DI_{st,jp}$ Diameter of pipe from central treatment s of type t to sink j, plant p (m)

$DI_{wz,jp}$ Diameter of pipe from central treatment w of type z to sink j, plant p (m)

DI_{rp} Diameter of pipe carrying unused wastewater from interceptor r, plant p to mainstream waste (m)

DI_{st} Diameter of pipe carrying unused wastewater from central interceptor s, type t to mainstream waste (m)

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1. INTRODUCTION & MOTIVATION

Based on the statistics, global population expected at 8.5 billion in 2030. By that, water and energy footprints are increasing steadily. Industrial clusters have high energy and water footprints, esp. in the GCC. There are strong interactions and linkages among energy and water within the processing facilities. Water is used for cooling, extraction, fuel production, biofuels, and hydropower. On the other hand, energy is required for water pumping, desalination, transport, and treatment.

Any chemical process can be divided into different subsystems, such as reaction-separation network, utility system, energy network, and a water-wastewater network. Process and water streams and all the hot-cold utilities are connected in these subsystems within and between processes. The main objective of a chemical process is to convert raw materials into the preferred products, with minimum water and energy consumption and waste generation into the environment. Therefore, as mentioned the global consumption of water and energy is growing and it has been predicted that this trend will remain in the future [1]. Due to the water properties, which make it essential for producing energy and on the other hand energy requirement for water treatment and distribution, flows of energy and water are physically interconnected. Therefore, there are strong interactions and linkages among energy and water within the processing facilities. For example, in thermoelectric power generation, large amount of water uses for cooling and dissipates significant amounts of energy. The intensity of water and energy consumption depends on the generation and cooling technology. In general, it takes energy to provide water and it takes water to produce energy. Optimization of the freshwater efficiency of energy production, and electricity generation and optimization of the energy efficiency of water use, treatment, and distribution are the main two pillars of water and energy nexus.

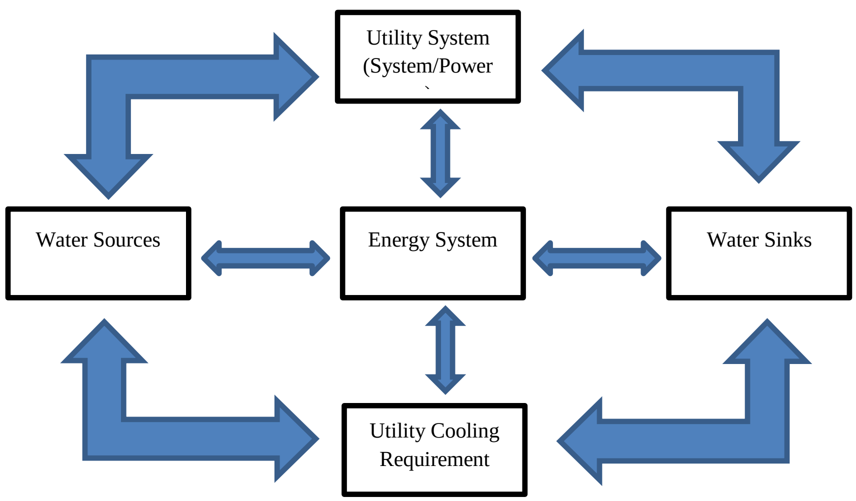

Figure 1: Water-Energy nexus

Developing systematic and applicable tools for the optimal design and operation of energy and water systems counting usage, generation/consumption, allocation, transformation, and discharge. There are different examples, which can be addressed in this field such as integration of excess industrial heat, solar energy, zero-liquid discharge, and process optimization of water and energy management technologies.

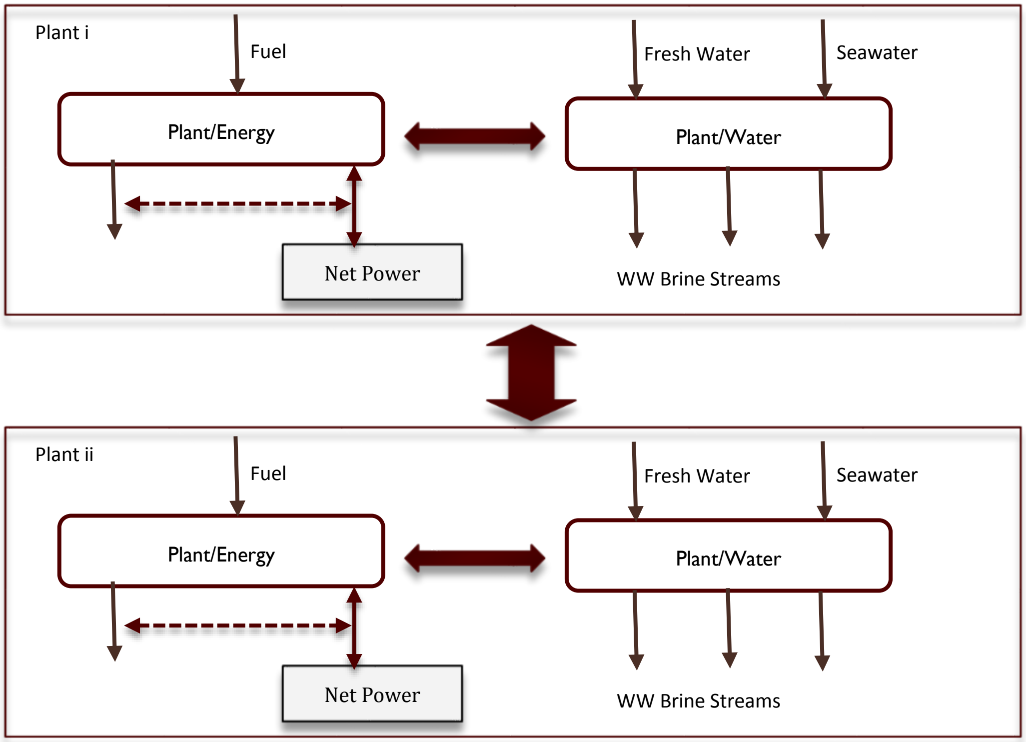

Figure 2: Water-Energy integration concept

As it is shown in Figure 2, each plant has an energy and a water network, which they can be interconnected (intra plant connection). Moreover, integration across the water-energy nexus can be done between different plants (inter plants connections).

In this paper, the work will investigate the water-energy nexus intra and inter plants and how they can be integrated in order to improve the sustainability of industrial processes and to reduce water and energy footprint.

2. LITERATURE REVIEW

It is well known that energy and water management can be achieved by the mass and energy integration methods. Energy integration was flashed by the development of the pinch point analysis, through which aims for minimum heating and cooling demand are established (Hohmann [2]; Linnhoff and Flower [3]; Umeda et al. [4]). The development of mass integration techniques was sparked by an extension of pinch concepts (El-Halwagi [5] and Manousiouthakis [6]). Other structures were developed for mass integration, such as process equipment as sinks to design direct recycle networks (ElHalwagi et al. [7]; El-Halwagi, [8] ; El-Halwagi [5] and Spriggs [9]). A number of works have proposed network optimization approaches for water-energy networks. Although the WNs and HENs integration has been done in several studies, but previous works have mainly focused on water and energy integration independently and there are few works, which covers the water-energy nexus. They can be classified as the following; mass/water integration and water-energy integration which can be within or/and across processes.

In general, in most of the works previously water and wastewater treatment networks are only used within the same plan but over recent years inter-plant water networks considering direct and indirect integration (via utility systems) have been analyzed and studied. In these networks water integration is well studied thought-out different plants (Chew et al. [10]; Foo [11]; Chen et al. [12]; Chen et al. [13]) including continuous and batch units (Chen et al. [14]) or considering retrofitting of water networks (Rubio-Castro et al. [15]).

Initial works have been reported for the development of approached that simultaneously integrate mass and energy. Simultaneous optimization of energy and water networks was done by Savulescu and Smith [16] and Savulescu et al. [17] using a linear programming formulation approach. Bagajewicz et al. [18] used an optimization-based approach for non-isothermal mixing simultaneous optimization of energy and water networks. Advanced, Bogataj and Bagajewicz [19], Bogataj and Bagajewicz [20] modeled energy efficient water utilization systems in process plants using superstructure optimization and MILP model. The combination of HENS approach previously introduced by Yee et al. [21] and a water network was done in their work for both single and multiple contaminants. Xiao et al. [22] utilized an optimization model considering sequential and simultaneous solution procedures for single and multiple impurities. In general, Bagajewicz [18] and Foo [11] provided the first comprehensive analysis papers on the matter of water network synthesis and integration using mathematical programming and pinch analysis. The main purpose of those papers was water integration without any heat integration. Bagajewicz [23], Foo [11] [24], Jezowski [25], Khor et al. [26], and books by Mann and Liu [27], Smith [28], Klemes et al. [29], El-Halwagi [30], and Klemes [31] are good references for details and recent progress within isothermal water networks. Jezowski presented his work on the water network synthesis considering isothermal and non-isothermal networks. Chen [32] presented an analysis on the synthesis of heat, mass, and work exchange networks, and emphasized that multi-objective optimization of these networks can be future work in this field. Benedetto et al. [33], included work on water footprint considering life cycle analysis and provided an overview of the topics on water, wastewater minimization, and finally combined water and energy minimization. Moreover, he showed the benefits of methods based on pinch analysis and mathematical programming and how the significant improvements in water and energy minimization were obtained.

Boix et al. [34] came up with a mathematical programming method to solve a water and a heat exchanger network considering multiple objectives such as minimization of fresh water and energy consumptions and the number of heat exchangers. Azeez et al. [35] presented new approach to improve superstructures including heat exchanger networks and mass exchanger networks. They used the supply temperature and composition and the target temperature and composition in the HENS and MENS to specify the intervals of their superstructures. Ahmetovic and Kravanja [36] came up with a framework in which direct and indirect heat exchange, heating and cooling and the freshwater and wastewater flow rates are considered. Later, this work was extended to include process-to-process streams for heat integration (Ahmetovic and Kravanja [37]). Grossman [38], in his paper provided an assessment on optimization models for the integrated water networks, which consume large amounts of water. The importance and significant impact of simultaneous optimization, heat and water integration was flashed out as well in his paper.

Jiménez-Gutiérrez et al. [39] combined water networks with a simultaneous integration of energy, mass and properties. The optimization objective function is minimizing the total annual costs subjected to energy, mass and property constraints.

Liu et al. [40] presented a new methodology in his paper for simultaneous integration of water and energy in heat-integrated water allocation networks. The model benefits you to capture the trade-off between freshwater consumption, utility usage and direct heat transfer by non-isothermal mixing. Moreover, it can significantly decrease the difficulty of subsequent HEN design. Finally, it is operative for simultaneous integration of water and energy in large-scale water and heat exchanger network systems. This is extremely valuable for any industrial application.

Gabriel et al. [41] developed a systematic methodology in order to maximize the benefits of water-energy nexus, considering a net surplus of heat energy in industrial processes. Using proposed procedure, the power and water generation potential for the process should be monitored. Beside the process water streams, in this work seawater desalination is included as a source. Based on the constructed superstructure, the model formulation is solved to optimize the Water-Energy nexus to integrate water, heat, and power considering power and water exportation constraints.

Therefore, there are significant interactions and trade-offs exist across the Water-Energy Nexus and an efficient superstructure and formulation covering all of those interactions is required. Every plant has a minimum cooling requirement, which needs to be satisfied by cooling options, which can be connected to water network. As mentioned earlier this water-energy interaction is not well studied specially inter and intra plants. Mainly research works have focused on water and energy integration independently. Moreover, there are few works on the Water-Energy nexus. However, they consider only a single plant with few sources and sinks. Therefore, Solutions need to be developed for high performance with respect to sustainability dimensions for an industrial park, esp.

economics. This work presents a novel superstructure and mathematical model. The problem is formulated as an MINLP model in Excel sheet.

3. RESEARCH SCOPE & OBJECTIVE

- Design a systematic approach to explore efficient strategies and designs for integrated water and energy management

- Capture the trade-offs between economic and sustainability metrics

- Generate a representation to capture water and energy management options as well as important water-energy interactions, especially considering (1) Process cooling requirements and Cooling systems incl. Air Coolers, Cooling Towers and Once-through Seawater systems, (2) Desalination systems for freshwater production, and (3) Treatment systems

- Develop an optimization model to systematize the search of the representation

- Solving an illustrative case study

4. A SYSTEMATIC APPROACH FOR DESIGNING INDUSTRIAL ENERGY-WATER INTEGRATION NETWORK

4.1 Overall Synthesis Approach

The overall synthesis approach is to develop a systematic network of water-energy interconnections among the processes considering sustainability metrics to support decision-making by the cluster. This is achieved by generating water and energy network superstructure in order to implement different linkages among them. The following section describes the generation of the superstructures employed for water and energy. Firstly, the superstructure should be optimized in order to get the optimal design with high performance. Moreover, alternative designs can be implemented for comparison of different scenarios.

4.2 Superstructure Representations

To start the problem, a network superstructure with full connectivity between all elements is generated to ensure that all possible design alternatives are included in the network. In order to do that an existing water network problem has been expanded from Sabla et al [42], [43], [44]. The Previous work has laid out the general representation and approach to develop economically optimal water networks that achieve a specified footprint target. In this work, the objective is to design a systematic approach to explore efficient strategies and designs for integrated water and energy management. The previous approach for water network has been extended to generate a representation to capture water and energy interactions, especially considering three units; (1) process cooling requirements and cooling systems including Air Coolers, Cooling Towers, and Once-Through Seawater systems, (2) Treatment systems, and (3) Desalination systems for freshwater production. Figure 3 shows different elements of a single plant, which are sources and sinks for the process itself, treatment units, desalination plants and cooling systems.

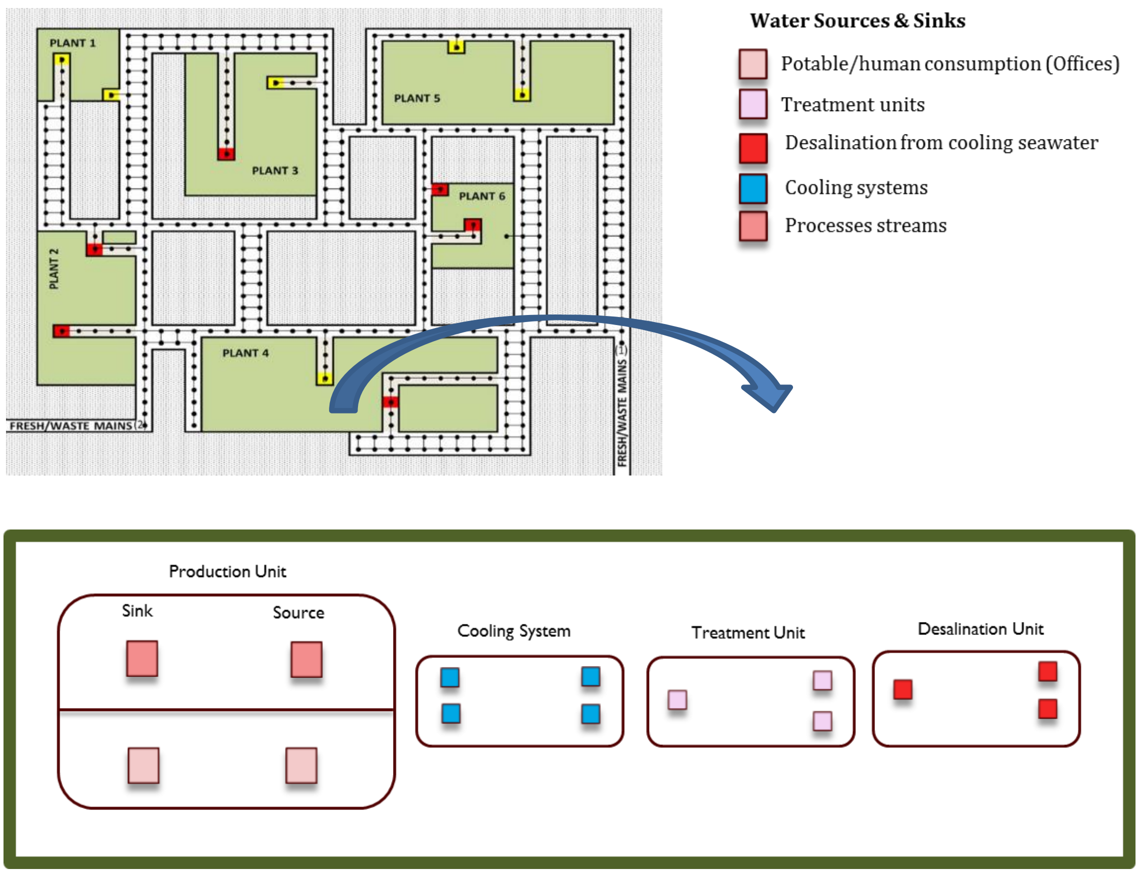

Figure 3: Elements of a single plant

Table 1: Different elements in figure 3

	Box Name	**Description**
	Offices sinks/sources	-Offices sinks can receive only fresh water from KAHRAMAA or desalination plants -Offices source can be sent to any sinks such as treatment units, reused directly, or discharged as wastewater
	Process Treatment sinks/sources	-Process treatment sinks receive wastewater from process - Process treatment source can be used in any water sinks except offices use
	Desalination sinks/sources	-Desalination units sinks can receive seawater either directly from seawater or used once-through cooling seawater -Desalination units source can be used for any water sinks
	Cooling systems sinks/sources	- Type 1 cooling systems sinks receive water from sea and the source can be either discharged back to sea or sent to desalination plant -Type 2 cooling systems (Cooling Tower) sinks receive only potable water and their source can be treated or used directly or discharged.
	Processes sinks/source	- Process sinks can receive any water source which satisfies their required contaminant concentrations - Processes sources can be sent to any sinks such as treatment units, reused directly, or discharged as wastewater

As it shown in Figure 3, an industrial park includes number of plants and each plant can be divided into the following elements; production unit, cooling systems, treatment, and desalination units. Production unit contains process streams and offices requirements. Each element is represented in terms of sources and sinks. For example in desalination unit, sink is concentrated water which gives two sources; potable water and brine stream. In Figure 4, it is clear that the infrastructure for the problem includes number of sources and sinks, which can be connected in different designs depending on the case study and objective function. Source-sink, source-treatment-sink, and source-discharge to environmental are three different ways in order to meet contaminants specification for different streams.

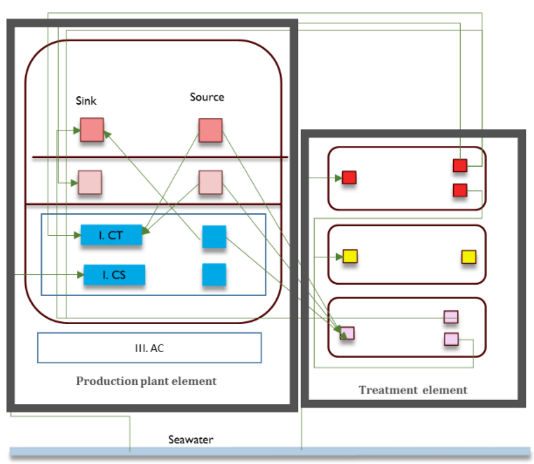

Figure 4: Synergy between Energy and Water Integration for a Plant

By combining synthesis elements to capture all interactions within and across water, the following water superstructure and integration network has been generated (example of two plants, one central treatment, one desalination by utility, one central desalination). Only decentral connection is shown. Boxes on the top and down represent sinks and sources, respectively. There are centralized and decentralized treatment units, which consist of different treatment plants such as processes treatments, and desalination units. Decentralized treatment options only handle wastewater from within the plant itself.

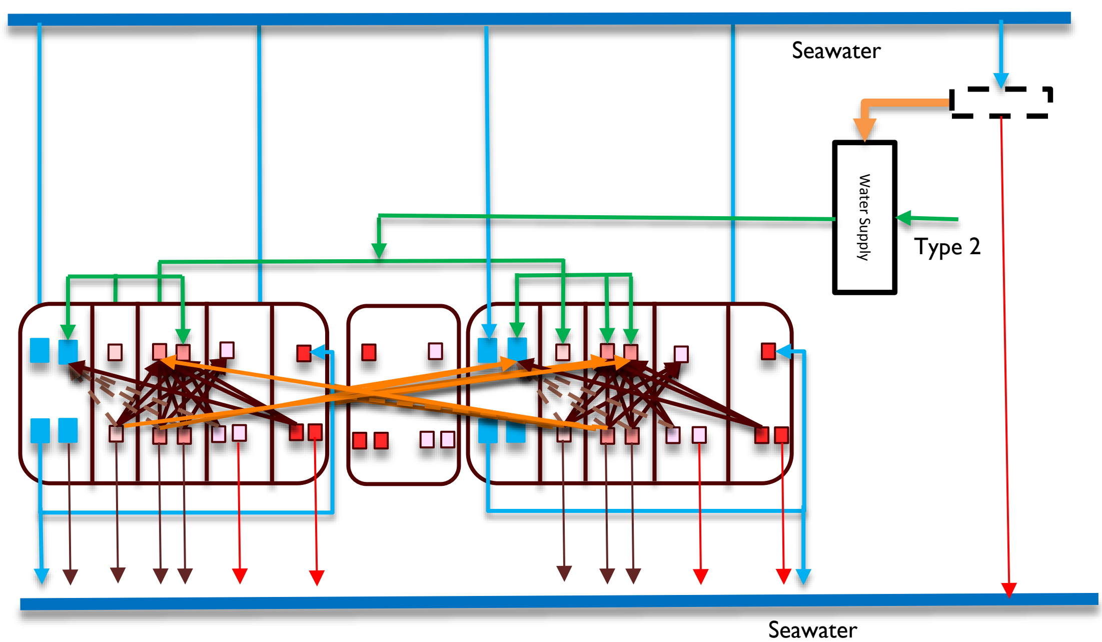

Figure 5: Water integration network superstructure

Moreover, no wastewater from the plant is allowed to be sent for treatment to other units outside the plant. On the other hand, centralized options receive water from the entire city and any plant. As it is shown on the superstructure, freshwater demand can be satisfied by the following options; external utility (desalination plant), natural potable resources, desalinated water produced directly from sea, and desalinated water produced from cooling seawater. Therefore, the once-through cooling seawater can be used as source water for the seawater desalination plant and therefore, desalinated water might be used in other sinks. On the other hand, seawater directly might be a source for desalination units in every plant

From the energy integration perspective, the energy management system is connected to net power and the minimum cooling requirement. The minimum cooling needs to be cooled down using one of the cooling systems options; air cooler, cooling towers, and once-through cooling seawater. In this work, one of the assumptions is that Q minimum cooling can be converted to power/electricity, which efficiency depends on the grade of heat. It can be used in any treatment, desalination, and cooling units. Moreover, the power in each plant can be exported or imported subjected to policies, regulations and infrastructure.

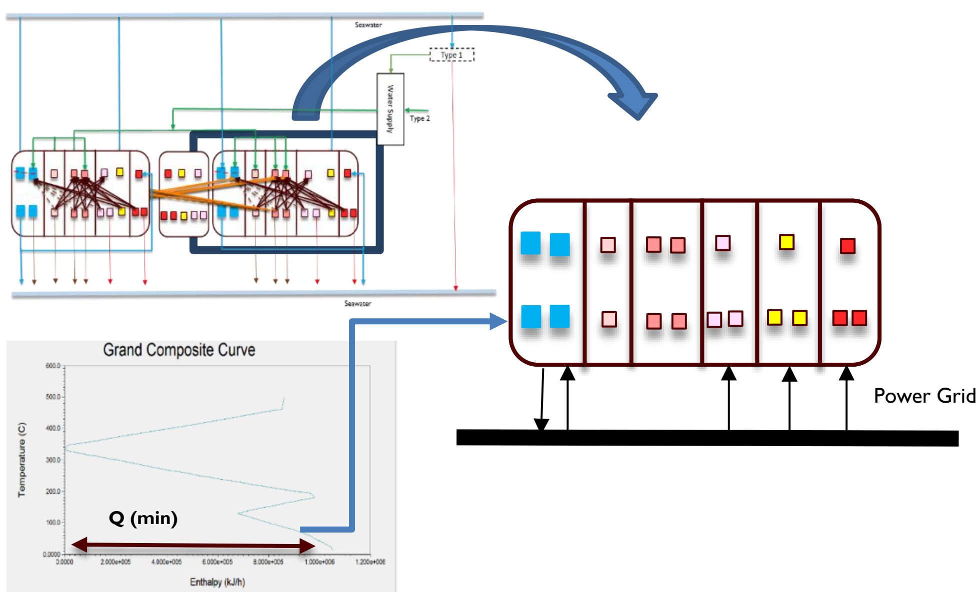

Figure 6: Water-Energy linkages through minimum cooling concept

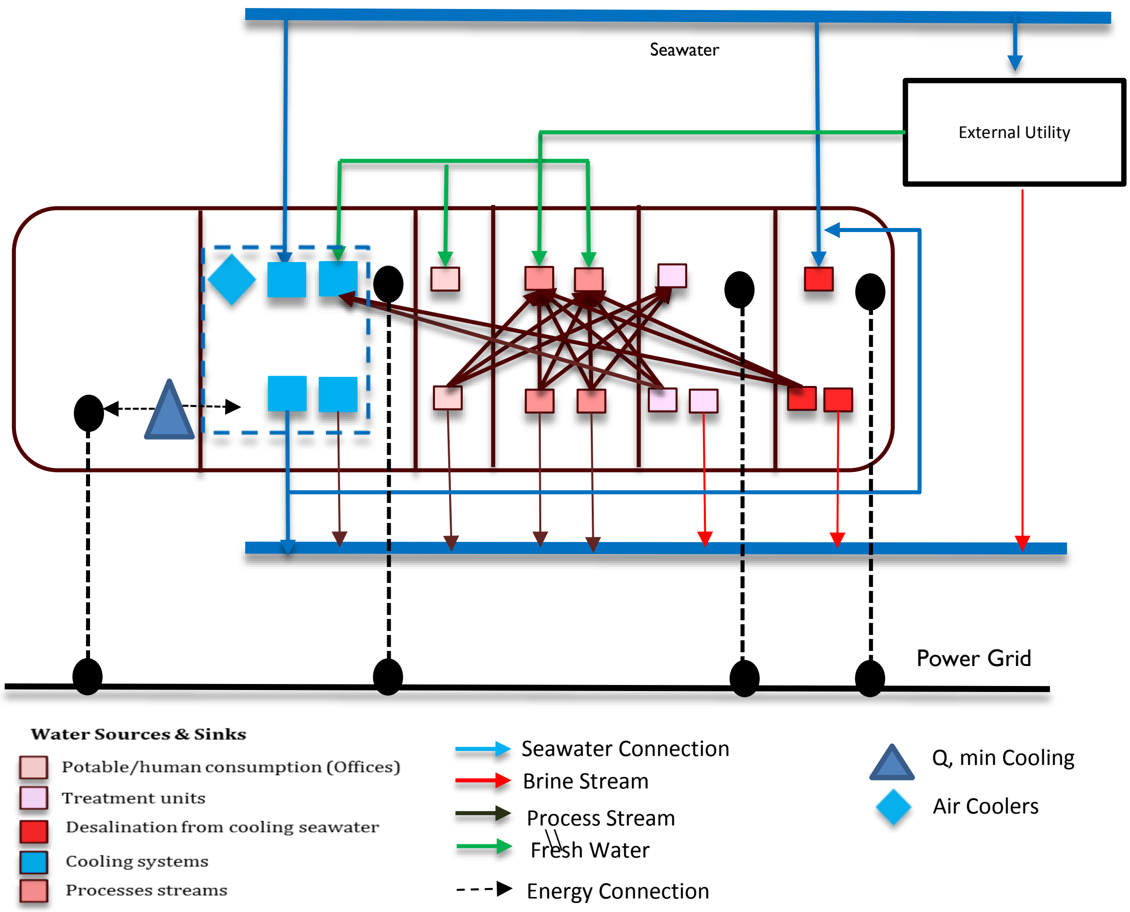

Figure 7: Water-Energy Interactions for a Single Plant

By combining synthesis elements to capture all interactions within and across water, the following Water-Energy superstructure and integration network has been generated (example of two plants, one central treatment, one desalination by utility, one central desalination). In Figure 7, only decentral treatment to plants connections has been shown for the water network. There are centralized and decentralized treatment units, which consist of different treatment plants such as processes treatments, and desalinations units. Decentralized treatment options only handle wastewater from within the plant itself.

Moreover, no wastewater from the plant is allowed to be sent for treatment to other units outside the plant. On the other hand, centralized options receive water from the entire city and any plant. For the energy integration as it was shown in Figure 7, for each plant the minimum heat can be cooled down by cooling systems or can be converted partially to power. For two or more plants, it can be shown as Figure 8 in terms of power grid.

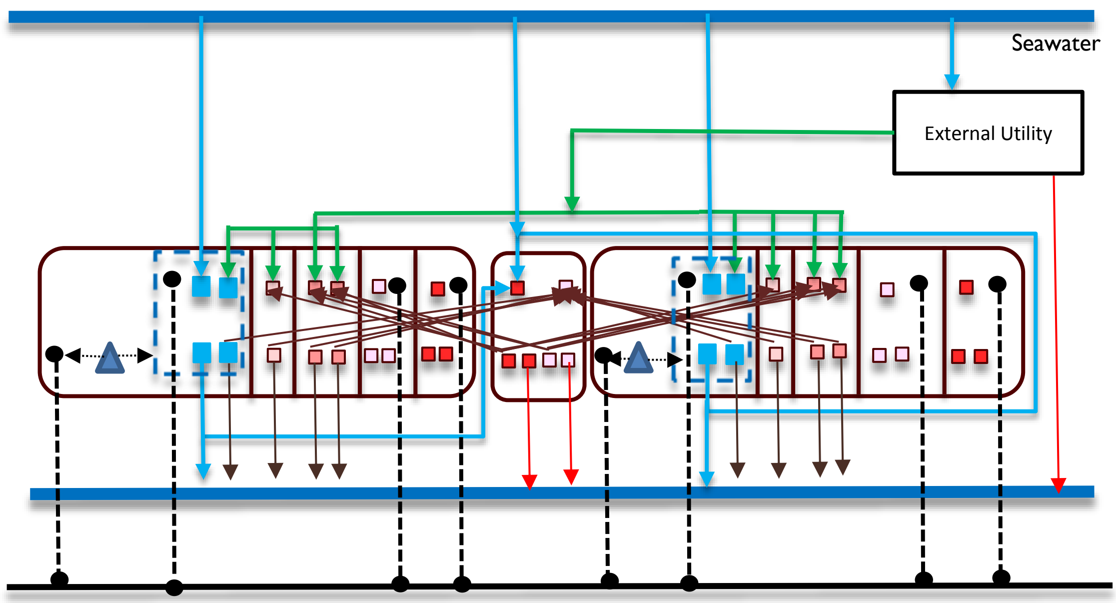

Figure 8: Water-Energy Interaction & Integration for an industrial park

5. PROBLEM STATEMENT

Given a set of water source and sink data for an industrial city including number of plants, central treatment units, and central desalination plant it is required to come up with an approach, which determines a network of water-energy interconnections among the processes. Heating, cooling, and water demand for each plant are known so that the composite curve of the plants can be generated. The problem then needs to perform a systematic search of possible solutions to find best performing with respect to the optimization objective. The objective is getting minimum total cost by the simultaneous minimization of the freshwater usage and the energy consumption of the whole system.

<u>Minimizing O1 (Total Annual Cost of Network):</u>

Minimize:

$$C^{Fresh} + C^{Seawater} + C^{Treatment} + C^{Pipes} + C^{Storage} + C^{Waste} + C^{Desalination} + C^{Cooling\ systems} + C^{WHP} \qquad (1)$$

Subject to:

g(x,y) <0 Inequality constraints → purities, flowrates, capacities

h(x,y) = 0 Equality constraints → mass balances, energy balances

Variables: x (continuous), y (integer)

Methodology for water-energy interaction design includes the following steps:

Step 1: problem assessment

- Describe the system boundaries and answer the following question
    - What are the main and existing linkages between water and energy resources?
- Data extraction for the case study water source/sink (flow rates, contaminants concentration, their minimum and maximum limit, environmental regulation) and energy (Temperature, minimum cooling requirement, …)

Step 2: problem targeting

- Generate resource utilization profiles for water and energy
- Energy composite curve / Energy pinch analysis

Step 3: problem design

- Construct water network superstructure and water allocation network
- Add direct and indirect energy linkages to water network (will be shown in next section)
- Mathematical Formulation of the problem

Sep 4: optimization

- Minimizing the total annual cost (operating, equipment, piping, and pumping, energy)
- Trade off analysis (Economic versus environmental metrics)

6. NETWORK OPTIMIZATION

For a given number of water sources and sinks for an industrial park, the synthesis goal is to determine the optimum design from the network superstructure, which achieves best options in terms of economics considering environmental metrics. This section includes the mathematical formulation of the network superstructure optimization problem.

The main objective of the network optimization is to minimize the total annualized cost of the network (TC) which is subjected to some inequality and equality constraints such as mass and energy balances, purities, flow rates and capacities and some environmental metrics constraints.

6.1 Mathematical Formulation

The mathematical formulation of this problem consists of two different networks; water network and energy network, which should be integrated simultaneously. The following sections describe the network formulation.

As mentioned before an existing water network problem has been expanded by adding cooling options, and desalination units.

The following tables summarizes all the equations, which have been used from Sabla et al. [42], [43], [44].

Table 2: Cost calculation equations

	Equation
Freshwater cost	$C^{Fresh} = H_y \sum_{l\in L} \sum_{p\in P} \sum_{j\in SN_p} F_{l,jp} C_l^{FR}$ (2)
Treatment Cost	$C^{Treatment} = K_F \sum_{p\in P} \sum_{r\in R} \left(T_{rp}^{total}\right)^{\alpha} C_{rp}^{INV} + K_F \sum_{s\in S} \sum_{t\in T} (T_{st}^{total})^{\alpha} C_{st}^{INV} + H_y \sum_{p\in P} \sum_{r\in R} \sum_{c\in C} T_{rp}^{total} x_{c,rp}^{TOTAL\ REM} C_{rp}^{REM} + \sum_{s\in S} \sum_{t\in T} \sum_{c\in C} T_{st}^{total} x_{c,st}^{TOTAL\ REM} C_{st}^{REM}$ $C^{Desalination} = K_F \sum_{p\in P} \sum_{m\in R} \left(T_{rp}^{total}\right)^{\delta} C_{mp}^{INV} + K_F \sum_{n\in S} \sum_{k\in T} (T_{st}^{total})^{\delta} C_{nk}^{INV} + H_y \sum_{p\in P} \sum_{m\in R} \sum_{c\in C} T_{rp}^{total} x_{c,mp}^{TOTAL\ REM} C_{mp}^{REM} + \sum_{n\in S} \sum_{k\in T} \sum_{c\in C} T_{st}^{total} x_{c,nk}^{TOTAL\ REM} C_{nk}^{REM}$ (3)
Wastewater Discharge Cost	$C^{Waste} = H_y\left(C^{WW} WW^{total} + C^{BRINE} B^{total}\right)$ (4)

Total cooling system costs involve summation terms for all types of cooling systems used and each includes capital and operating costing terms. For operating cost, it is mainly the power required by different cooling systems.

$$C^{cooling\ system} = \sum_{p\in P} CC^{AC}{}_p + \sum_{p\in P} CC^{CT}{}_p + \sum_{p\in P} OC^{AC}{}_p + \sum_{p\in P} OC^{CT}{}_p + \sum_{p\in P} OC^{CS}{}_p \qquad (5)$$

Total Waste heat to power system (WHP) cost depends on the capacity of the system, which includes summation terms of capital (turbine and boilers) and maintenance cost.

$$C^{Waste\ heat\ to\ power} = K_F \sum_{p\in P} PW_p\, CC^{WHP} + H_y \sum_{p\in P} PW_p\, OC^{WHP} \quad (6)$$

Moreover, the formulation also includes a set of mass balances with some inequality constraints for each of the water sources, sinks, and treatment units.

Table 3: Mass balances & inequality equations

	Equation
Source Balance	$\sum_{p,p'\in P}\sum_{j\in SN_p} M_{ip,jp'} + \sum_{p\in P}\sum_{r\in R} {M^{CT}}_{ip,jp'} + \sum_{p\in P}\sum_{r\in R} T^{Inlet}_{ip,rp} + \sum_{s\in S}\sum_{t\in T} T^{Inlet}_{ip,st} + \sum_{p\in P}\sum_{r\in R} T^{Inlet}_{ip,rp} + \sum_{s\in S}\sum_{t\in T} T^{Inlet}_{ip,st} + D_{ip} = W_{ip} \quad (7)$ $\forall p \in P\,;\ \forall i \in SU_p$
/Sink Balance	$\sum_{p,p'\in P}\sum_{i\in SU_p} M_{ip,jp'} + \sum_{p,p'\in P}\sum_{i\in SU_p} {M^{CT}}_{ip,jp'} + \sum_{p\in P}\sum_{r\in R} T^{Treated}_{rp,jp} + \sum_{s\in S}\sum_{t\in T} T^{Treated}_{st.jp} + \sum_{p\in P}\sum_{r\in R} T^{Desalinated}_{rp,jp} + \sum_{s\in S}\sum_{t\in T} T^{Desalinated}_{st.jp} + \sum_{l\in L} F_{l,jp} = G_{jp} \quad (8)$ $\forall p \in P\,;\ \forall j \in SN_p$

Table 3: Continued

Sink Contaminant Equality	$\sum_{p,p' \in P} \sum_{i \in SU_p} M_{ip,jp'} x_{c,ip}^{Source} + \sum_{p \in P} \sum_{r \in R} T_{rp,jp}^{Treated} x_{c,rp}^{Treated} + \sum_{s \in S} \sum_{t \in T} T_{st,jp}^{Treated} x_{c,st}^{Treated} + \sum_{l \in L} F_{l,jp} x_{c,l}^{FRESH} = G_{jp} z_{cjp}^{in}$ (9) $\forall p \in P;\ \forall j \in SN;\ \forall c \in C_p$
Sink Pollutant Concentration Inequality	$z_{c,jp}^{min} \le z_{c,jp}^{in} \le z_{c,jp}^{max}$ (10) $\forall p \in P;\ \forall j \in SN_p;\ \forall c \in C$
Decentral Treatment Balance	$\sum_{p \in P} \sum_{i \in SU_p} T_{ip,rp}^{Inlet} = \sum_{p \in P} \sum_{j \in SN_p} T_{rp,jp}^{Treated} + \sum_{p \in P} \sum_{v \in V} T_{rp,vp}^{Untreated} + \sum_{w \in W} \sum_{z \in Z} T_{rp,wz}^{Untreated} + D_{rp}^{Treated} + D_{rp}^{Untreated}$ (11) $\forall p \in P;\ \forall r \in R$
Central Treatment Balance	$\sum_{p \in P} \sum_{i \in SU_p} T_{ip,st}^{Inlet} = \sum_{p \in P} \sum_{i \in SU_p} T_{st,jp}^{Treated} + \sum_{w \in W} \sum_{z \in Z} T_{st,wz}^{Untreated} + D_{st}^{Treated} + D_{st}^{Untreated}$ (12) $\forall s \in S;\ \forall t \in T$
Decentral Treatment Recovery	$(1 - R_{rp}) \sum_{p \in P} \sum_{i \in SU_p} T_{ip,rp}^{Inlet} = \left(\sum_{p \in P} \sum_{v \in V} T_{rp,vp}^{Untreated} + \sum_{w \in W} \sum_{z \in Z} T_{rp,wz}^{Untreated} + D_{rp}^{Untreated}\right)$ (13) $\forall p \in P;\ \forall r \in R$
Central Treatment Recovery	$(1 - R_{st}) \sum_{p \in P} \sum_{i \in SU_p} T_{ip,st}^{Inlet} = \left(\sum_{w \in W} \sum_{z \in Z} T_{st,wz}^{Untreated} + D_{st}^{Untreated}\right)$ (14) $\forall s \in S;\ \forall t \in T$

Table 3: Continued

Total Wastewater Discharge	$WW^{total} = \sum_{p\in P}\sum_{i\in SU_p} D_{ip} + \sum_{p\in P}\sum_{r\in R} D_{rp}^{Treated} + \sum_{s\in S}\sum_{t\in T} D_{st}^{Treated}$ (15) $\forall c \in C$
Brine Discharge	$B^{total} = \sum_{p\in P}\sum_{r\in R} D_{rp}^{Untreated} + \sum_{s\in S}\sum_{t\in T} D_{st}^{Untreated}$ (16) $\forall c \in C$
Wastewater Discharge Load	$WW^{total} x_c^{WW\_Discharge} = \sum_{p\in P}\sum_{i\in SU_p} D_{ip}\, x_{c,ip}^{Source} + \sum_{p\in P}\sum_{r\in R} D_{rp}^{Treated} x_{c,rp}^{Treated} + \sum_{s\in S}\sum_{t\in T} D_{st}^{Treated} x_{c,st}^{Treated}$ (17) $\forall c \in C$
Brine Discharge Load	$B^{total} x_c^{B\_Discharge} = \sum_{p\in P}\sum_{r\in R} D_{rp}^{Untreated}\, x_{c,rp}^{Untreated} + \sum_{s\in S}\sum_{t\in T} D_{st}^{Untreated} x_{c,st}^{Untreated}$ (18) $\forall c \in C$

From the energy integration perspective, as mentioned earlier each plant has heating processes, which requires cooling. The concept of water and energy reduction footprint in this work has been approached by using minimum cooling requirement for each plant. All the cooling demands can be satisfied by cooling systems or part of it can be used for other purposes. The excess heat of a plant can be either exchanged across processes through different steam levels or converted directly to power through a cycle and use it in different units in an industrial park. In this work, the excess heat is only converted to power since the transportation is easier. The power generated can be used in any unit and any plants

(Central or decentral). Sinks can be any treatment, desalination, and cooling systems (Figure 3).

Therefore, in the second part of the problem beside water network superstructure with all added cooling options, an energy integration network is generated as well. For energy network, the formulation also includes a set of mass and energy balances with some inequality constraints for each of the water and energy sources, sinks, and interceptors.

It can be obtained by the following steps:

1. By generating composite curve for each plant, Q-min cooling can be obtained.

Convert this Q-min cooling to the maximum power which can be generated (in the next paragraph it will be explained).

As mentioned earlier, the minimum cooling Q of each plant can be converted to power. In this work by using the composite curve for each interval, the Carnot efficiency (maximum efficiency) was calculated.

$$\boldsymbol{\eta_{carnot} = 1 - \frac{T_{Cold}}{T_{Hot}}} \qquad (19)$$

The maximum work generated is calculated using the following equation and then the summation of all intervals gives the maximum power.

$$\boldsymbol{PW_{Max} = \eta_{carnot} \times Q} \qquad (20)$$

Since in practice this work cannot be generated, an efficiency of 50% was assumed in order to calculate the actual amount of power, which can be generated from waste heat [45].

$$\boldsymbol{PW_{Actuall} = \frac{W_{max}}{\eta}} \qquad (21)$$

2. This converted power can be used in any unit and any plants (Central or decentral). Sinks can be any treatment, desalination, or cooling systems.
3. The obtained superstructure can be optimized simultaneously with water network superstructure.

As it is shown in Equation 22, in this case, the submission of all heat removed from all cooling systems and converted waste heat to power (WHP) must be equal to the Q-min cooling obtained from the corresponding process composite curve for each.

$$\sum_{p\in P} Q^{AC}{}_{p} + \sum_{p\in P} Q^{CT}{}_{p} + \sum_{p\in P} Q^{CS}{}_{p} + \sum_{p\in P} Q^{WHP}{}_{p} = \mathrm{Q}^{min,cooling}{}_{\mathrm{p}} \quad (22)$$

For this phase of the problem, the formulation also includes a set of mass and energy balances with some inequality constraints for each of the water and energy sources, sinks, and interceptors (treatments and desalination units).

By converting Q minimum cooling of each plant to maximum power that can be generated, the energy model formulation includes a set of power balances for each of the process sources and sinks as described by Equations below. Sinks can be any treatment, desalination, or cooling systems. Therefore, the summation of process power source-to-treatment units (both de-central ($PW_{ip,rp}^{treatment}$), and central $PW_{ip,st}^{treatment}$)), source-to-desalination unit (both de-central ($PW_{ip,rp}^{Desalination}$), and central $PW_{ip,st}^{Desalination}$)), source-to-Air coolers $\left(PW^{AC}{}_{ip,jp\prime}\right)$, source-to-Cooling towers $\left(PW^{CT}{}_{ip,jp\prime}\right)$, and source-to-cooling seawater system $\left(PW^{CS}{}_{ip,jp\prime}\right)$ rates must be less than or equal the total power $\left(PW_{p}\right)$ available for each corresponding process power source.

$$\sum_{p\in P}\sum_{r\in R} PW^{treatment}_{i\prime p,rp} + \sum_{s\in S}\sum_{t\in T} PW^{treatment}_{i\prime p,st} + \sum_{p\in P}\sum_{r\in R} PW^{Desalination}_{i\prime p,rp} + \sum_{s\in S}\sum_{t\in T} PW^{Desalination}_{i\prime p,st} + \sum_{p\in P}\sum_{r\in R} PW^{CT}{}_{i\prime p,j\prime p} + \sum_{p\in P}\sum_{r\in R} PW^{CS}{}_{i\prime p,j\prime p} + \sum_{p\in P}\sum_{r\in R} PW^{AC}{}_{i\prime p,j\prime p} \le PW_{i\prime p} \qquad (23)$$

Moreover, the power rates to each of these sinks must not exceed the required power with each sink, which has been calculated before as follows. The remaining should be satisfied by external utilities.

$$\sum_{p\in P}\sum_{r\in R} PW^{treatment}_{i'p,r'p} \le \sum_{p\in P}\sum_{r\in R} PW^{treatment,calculated}_{i'p,r'p} \qquad (24)$$

$$\sum_{s\in S}\sum_{t\in T} PW^{treatment}_{i'p,s't} \le \sum_{s\in S}\sum_{t\in T} PW^{treatment,Calculated}_{i'p,s't} \qquad (25)$$

$$\sum_{p\in P}\sum_{r\in R} PW^{Desalination}_{i'p,r'p} \le \sum_{p\in P}\sum_{r\in R} PW^{Desalination,Calculated}_{i'p,r'p} \qquad (26)$$

$$\sum_{s\in S}\sum_{t\in T} PW^{Desalination}_{i'p,s't} \le \sum_{s\in S}\sum_{t\in T} PW^{Desalination,Calculated}_{i'p,s't} \qquad (27)$$

$$\sum_{p\in P}\sum_{r\in R} PW^{CT}{}_{i'p,j'p} \le \sum_{p\in P}\sum_{r\in R} PW^{CT,Calculated}{}_{i'p,j'p} \qquad (28)$$

$$\sum_{p\in P}\sum_{r\in R} PW^{CS}{}_{i'p,j'p} \le \sum_{p\in P}\sum_{r\in R} PW^{CS,Calculated}{}_{i'p,j'p} \qquad (29)$$

$$\sum_{p\in P}\sum_{r\in R} PW^{AC}{}_{i'p,j'p} \le \sum_{p\in P}\sum_{r\in R} PW^{AC,Calculated}{}_{i'p,j'p} \qquad (30)$$

An economic objective was used to assess the overall network performance. The objective function consists of the minimization of a total annualized cost, which includes the costs of fresh water, wastewater treatment, piping, waste disposal, desalination systems, seawater, and cost associated with cooling systems which are capital and operating cost and waste heat to power conversion cost. The objective function is described by Equation 1 below:

$$\boldsymbol{Minimize.}\ \boldsymbol{C^{Fresh}} + \boldsymbol{C^{Seawater}} + \boldsymbol{C^{Treatment}} + \boldsymbol{C^{Pipes}} + \boldsymbol{C^{Storage}} + \boldsymbol{C^{Waste}} + \boldsymbol{C^{Desalination}} + \boldsymbol{C^{Cooling\ systems}} + \boldsymbol{C^{WHP}}$$

Both phases (without and with waste heat utilization) of the problem have been formulated as a Mixed Integer Non-Linear Problem (MINLP). The objective function given by Equation 1 involves the minimization of total annualized cost, subject to equality constraints, as well as inequality constraints. Then they are solved using the "*what'sBest*" Mixed-Integer Global Solver for Microsoft Excel by LINDO Systems Inc.

7. SUSTAINABILITY METRICS

7.1 Introduction

There are different sustainability metrics and methods available nowadays. Sustainability metrics mainly is divided into three different categories; economical, environmental, and social impacts. Concerns that are addressed by these metrics include the following [46]:

- Economics Concerns: Profit, Value, Tax
- Environmental Concerns: Resource usages, Emissions, and Waste
- Safety and Health Concerns: Workplace, Society (safety such as flammability, temp, pressure, corrosively, or health damage)

Sustainability metrics might have different indicators. Indicators mainly clarify the sustainability impacts on individuals who might not be very well-informed on the subject. Economic indicators measure economic advance of the society. They measure economic enhancement, which can be obtained over a period. Environmental indicators determine the positive progress which have been observed regarding to the environmental concerns. Ecological health, water quality, and air quality are examples of this indicator. Social indicator measure concerns related to the safety and health such as number of people who were affected by environmental emissions, and number of families living below the poverty line [47].

Today researchers have proposed different sustainability metrics in order to quantify processes emissions. There are number of limitations in the existing approaches such as complexity, time consuming and not covering all the dimensions of sustainability. In addition, process design for sustainability involves complicated decision-making scenarios and this makes it difficult to explore the tradeoffs using existing methods.

Accordingly, in this work the objective is to introduce a methodology for designing sustainable chemical and petroleum processes during early stages of design. The methodology should incorporate the three dimensions of sustainability into an optimization framework and ensures that the most sustainable process is designed while taking into account profitability, environmental impacts and social issues such as health and safety.

7.2 Proposed Sustainability Metrics and Indicators

Sustainability metrics and indicators quantify and qualify the economic, environmental, and social impacts, which helps in decision-making [48]. Understanding the features of each sustainability metrics is an essential factor in choosing them for a specific process. Examples of the criteria can be as the following [49]:

- Easily available and accessible
- Analytical
- decision making tool
- Economically attractive
- Applicable to numerous process

Sustainability metrics are expressed in ratios for different categories. For example, in case of economic and environmental metrics, the numerator is typically the resource consumption or contaminant emission while the denominator is physical or financial impact. On the other hand, the social metrics are usually represented by percentages. Most of the sustainability metrics focus on quantifying the environmental and economic impacts rather than the social [50].

Over the years, researchers have suggested many metrics and indicators but most of the metrics cover only one of the aspects. Table 4 summarizes the main proposed sustainability metrics and highlights the main concerns with using them [51].

Table 4: Summary of sustainability metrics and indicators

AIChE Sustainability Index ("AIChE Sustainability Index: Strategic Commitment to Sustainability," 2008)	It can be used for performance comparison but since most of the indices are qualitative, it cannot be used in early stage of design.
Sustainability Indices (Tugnoli et al., 2008b)	Useful in terms of calculating the sustainability of chemical processes alternatives.
Three Dimensional Sustainability Metrics (Martins et al., 2007)	Environmental Metrics is presented however the direct correlation between operating conditions, the risk and environmental impact is not included.
BRIDGES to Sustainability Metrics (Tanzil and Beloff, 2006)	Only addresses one dimension of the susytainability metrics which is Environmental impact.
Global Environmental Risk Assessment (GERA) Index (Achour et al., 2005)	Economic and environmental concerns are not addressed. Useful in terms of health and safety risks.

Table 4: Continued

IChemE Sustainability Metrics (IChemE Metrics, 2002)	Very useful one in economic and environmental emissions calculations. Social impact is not well correlated with the process parameters.
Indicators of sustainable production (Krajnc and Glavic, 2003)	Not applicable in the early stage of the design but useful in evaluating the metrics for an operating unit.
Green Metrics (Constable et al., 2002)	Evaluates the efficiency of a chemical reaction. Rather than that does not address any other sustainability concerns.
BASF Socio-Eco-efficiency Metrics (Saling et al., 2002)	Useful in evaluating the impact of products and process during detailed design but requires significant data and information. In terms of social impact is not well correlated with parameters.
ALCHE/ CWRT Sustainability Metrics (AIChE Center for Waste Reduction Technologies (CWRT), 2000)	Covers the environmental impact of chemical processes. Only addresses the environmental impact of the sustainability metrics in terms of global warming, and acidification.
Dow Jones Sustainability Index (Knoepfel, 2001)	Useful for performance comparison but since most of the indices are qualitative, it cannot be used in early stage of design.
Sustainability Indicators (Afgan et al., 2000)	Indicator system has limited applications as it has been tailored towards accessing the impact of energy systems.
Inherent Process Safety Index (Heikkila, 1999)	Only addresses the safety concerns and impact.

In this work since the water-energy integration and optimization will not change the industrial city design and layout, these types of simulations do not affect the social metrics such as safety and health issues and their change can be negligible. Moreover, as mentioned earlier the main optimization objective is total annual cost minimization, which mean the economic metrics has been covered in the objective. Finally, the environmental metrics is the one, which needs to be calculated. For that, the TRACI metrics has been selected for this work that more details about it is provided in the following section.

7.3 TRACI Metrics

The Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI) was developed in 2002 by the Environmental Protection Agency. It is one of the environmental impact assessment software available with different characterization factors to assess life cycle assessment and sustainability metrics. Characterization factors measure the potential impacts [52].

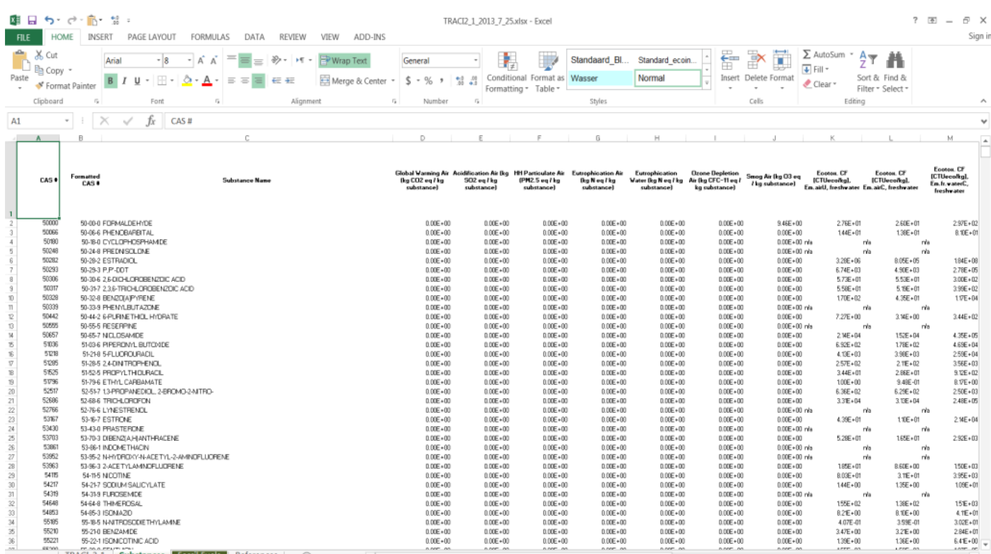

Figure 9: TRACI metrics sheet

The TRACI software can be divided into four main groups: inventory of stressors, impact categories, characterization and overall effect. The impact categories include the followings:

- Ozone Depletion
- Global Warming
- Acidification
- Eutrophication
- Smog Formation
- Human Health (Particulate, Cancer, Non-cancer)
- Eco-toxicity
- Fossil Fuel Use
- Land Use
- Water Use

Table 5: Different media affected by different categories in TRACI [52]

Impact Category	Media
Ozone Depletion	Air
Global Climate	Air
Acidification	Air, Water
Eutrophication	Air, Water
Smog Formation	Air
Human Health Particulate	Air
Human Health Cancer	Urban Air, Nonurban Air, Freshwater, Seawater, Natural Soil, Agricultural Soil
Human Health Noncancer	Urban Air, Nonurban Air, Freshwater, Seawater, Natural Soil, Agricultural Soil
Ecotoxicity	Urban Air, Nonurban Air, Freshwater, Seawater, Natural Soil, Agricultural Soil

More explanations about each impact can be found in the Appendix. TRACI is one of the most applicable software, which is used in industry. It has been used by many researchers in their work (Kim and Dale [53]; Bare et al. [54]; Guereca et al. [55]; Singh et al. [56]; Morris and Bagby, [57]; Zhou and Schoenung [58]).

7.4 Implementing Methodology

Figure 10 shows the methodology in order to calculate the sustainability metrics for the proposed water-energy networks.

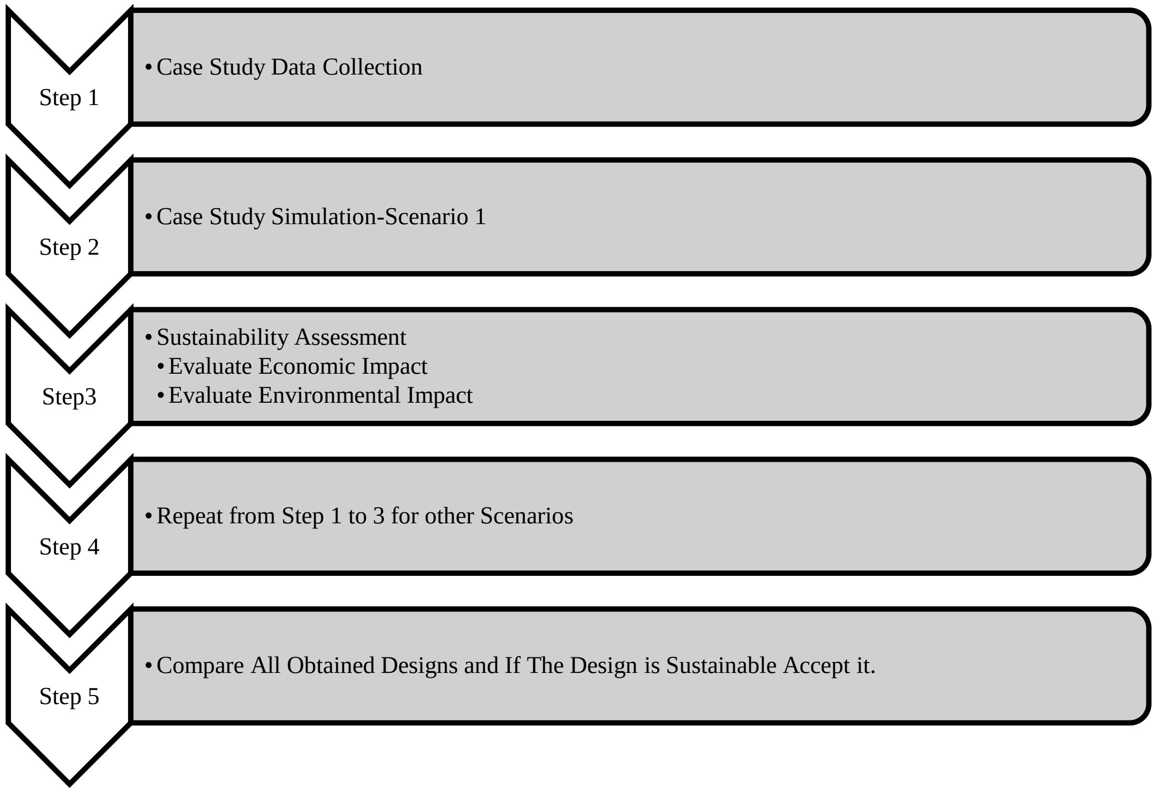

Figure 10: Implemented methodology

The case study is simulated and integrated using collected data from the literature and real sustainability reports. As will be mentioned later, in this work, water-energy data was collected for three plants using different sources. For WhatsBest to calculate the objective function and other required information for any design and superstructure, the following are the basic inputs into the simulator:

- Contaminants components available in water streams
- Contaminants compositions
- Flow rates for water streams
- Mass balance equations

- Concentration inequalities
- Energy balance equations

7.5 Sustainability Assessment

In this work, TRACI sustainability metrics has been selected to be calculated. This metrics addresses economic, environmental, and safety concerns in the early stage of the design. This is a Microsoft Excel based tool, which uses mass flows as inputs to evaluate the sustainability of a process. In order to quantify emission impacts the following equation has been used [59]:

$$I^i = \sum_{xm} CF^i_{xm} * M_{xm} \qquad (31)$$

Where:

I^i= The potential impact of all chemicals (x) for a specific impact category of concern (i)

CF^i_{xm}= The characterization factor of chemical (x) emitted for impact category (i)

M_{xm}= The mass of chemical (x) emitted

In this work, some assumptions have been made in order to calculate theses sustainability metrics.

- The goal in every industrial plants is to maximize profits or to minimize the total annual cost of the plant. The process is not sustainable if it is not economically attractive. Therefore, in order to address the economic concern, the total annual cost has been calculated by completing economic analysis. (Covered by O1)

- As mentioned earlier, Water-energy integration and optimization problems will not change the industrial city design and layout. Safety and health metrics are not affected by these types of simulations and can their change can be negligible. So, for the Safety and Health Concerns: Health impact covered in O2, solutions neutral on other aspects)
- The environmental waste and emissions for the proposed problem were analyzed as shown in Figure 12. The environmental emissions can be divided as solid waste, atmospheric impact, and aquatic impact. In the next step different impacts of these groups has been taken from TRACI metrics and been quantified.

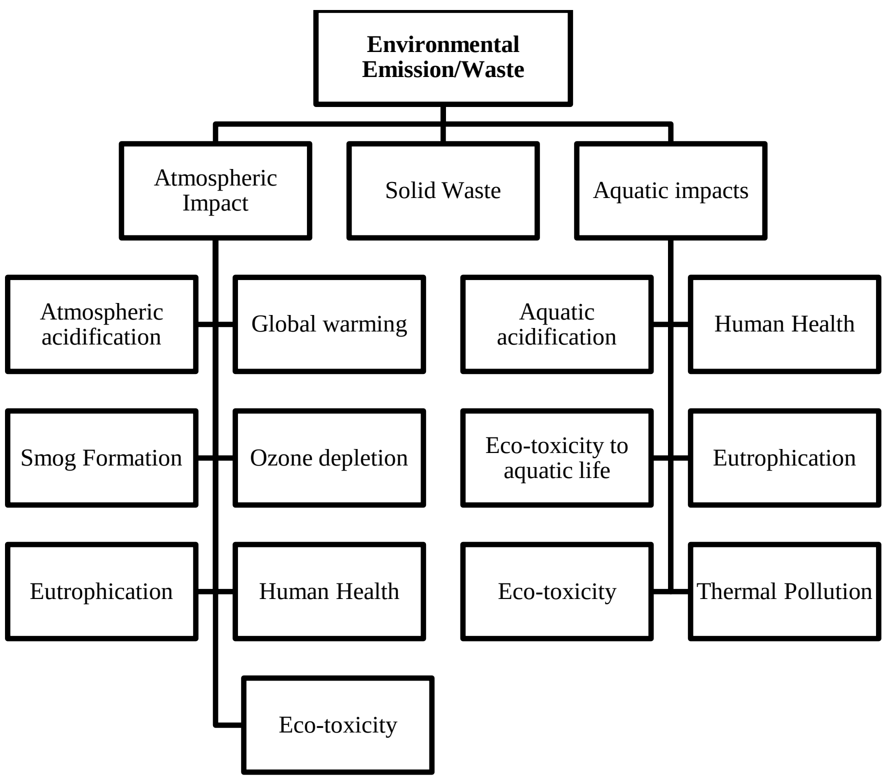

Figure 11: Environmental emissions categories in TRACI

Some of the examples of contributors in the proposed problem are:

- Brine discharge (Salinity)
- Power consumption (Atmospheric Impact)
- Biocide in seawater intake (Aquatic Impact)
- Sludge from treatment (Solid wastes)
- Thermal pollution by cooling processes (Aquatic Impact)
- Biocide Consumption

It was more simplifies based on the current optimize problem in order to decrease number of impacts as it is shown in Figure 12.

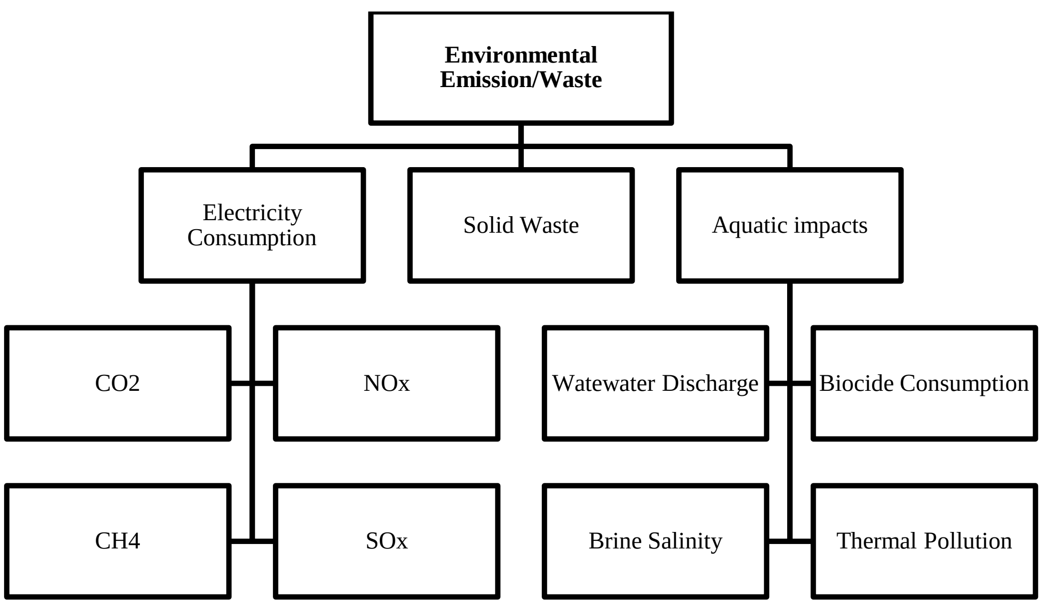

Figure 12: Detailed environmental emissions corresponding to the defined problem

Therefore, in this research work since there are only some atmospheric emissions (CO2. NOx. SOx, CH4) and biocide consumption for the cooling seawater, only two categories have been quantified. Global Warming and Eco-Toxicity are those two, which have been included in sustainability metrics.

7.6 Missing Emissions in Environmental Metrics

Warming of seawater by thermal discharges, such as cooling water releases from process cooling systems or power plants, can Affect the aquatic environments and. In this work, cooling systems are one of the main aspects of the problem. Once through cooling seawater might be one of the options selected for the optimized solution. Therefore, there will be an impact of Brine discharge back to seawater, which due to thermal pollution aquatic species might be affected. Temperature of the seawater usually differs from 10℃ to 25℃ that rises about 60℃ to 40℃ close to the area of the brine disposal [60]. Unfortunately, to date the impact of thermal pollution has not been covered by any of sustainability metrics or LCA. Therefore, in this work, it has not been quantified in the metrics but it is well addressed as of the main emissions of the model.

8. ILLUSTRATIVE CASE STUDY

The proposed approach is illustrated with a case study with three different plants. Water data with selected four contaminants (TDS, Organics, Ammonia, and Nitrogen) has been collected from different sources such as papers [61], and design reports [62], [63]. For WhatsBest to calculate the objective function some of the basic data are required as input such as water flowrates, contaminants compositions, mass balances, energy balances, and concentration inequalities. We have solved different scenarios to compare the differences between applying energy concept with and without WHP and conclude how this water-energy integration can change the economics significantly.

The case study contains three plants; Ammonia, Methanol, and GTL. The problem has six water sources, seven water sinks, and central and decentral treatment and desalination units. The shortest distance between different units for pipeline calculations (Table of distances can be found in Appendix) has been calculated. All central and decentral treatment options utilized in this problem represent a single treatment unit, each with a specified removal ratio, which is shown in Table 8. In addition, Figure 3 shows the composite curve of GTL plant, which is used in this case study.

Table 6: Energy data of the selected plants [61, 62, 63]

Plants	**Q min Cooling (MW)**
Ammonia	237
Methanol	105
GTL	983

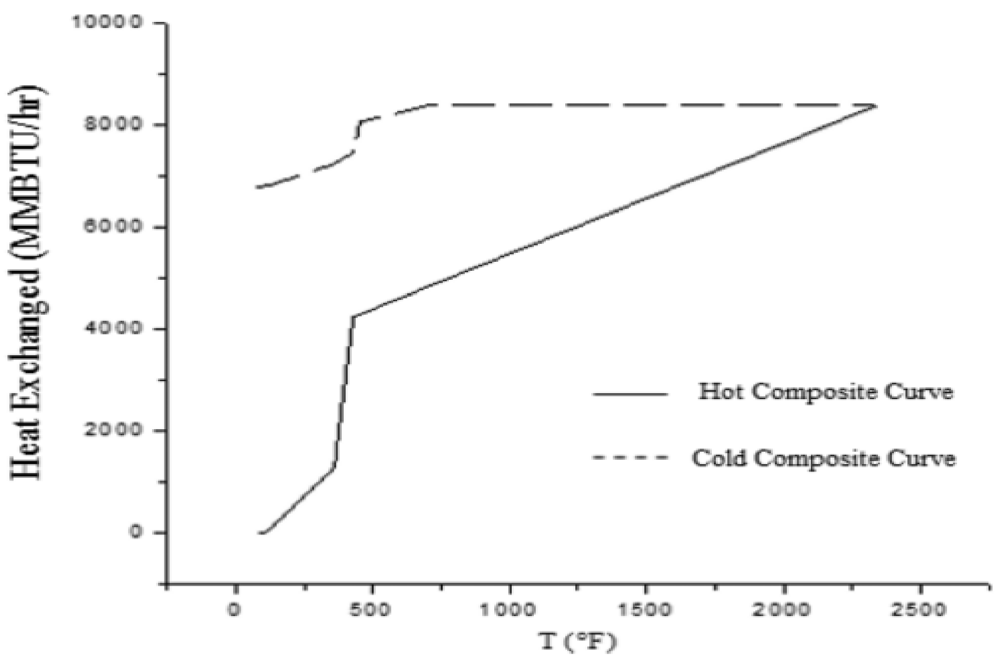

Figure 13: Pinch diagram for GTL process [61]

Table 7: Water flow calculation for different cooling systems

Plants units	Power/Electricity
Cooling Tower (kwh/m3)	17
Air Coolers (kw/MW)	48
Once-Through (kwh/m3)	0.058
RO Treatment (kwh/m3)	4.2
NF Treatment (kwh/m3)	0.53

Table 8: Power/Electricity required for different units [64, 66, 67]

Cooling System	**Avg Water Use (m3/h/MW) [64]**	**Cost of water QAR/m3 [65]**
Once Through	171	5.4 (KAHRAMAA)
Wet Cooling Tower	2	
Dry Air Coolers	0	

Table 9: Water sink data of the selected plants

SOURCE	FLOW	TDS	Organics	Ammonia	Nitrogen
	ton/d	ppm	ppm	ppm	ppm
P1D1	2,571	500	4.00	0.5	21
P1D2	840	200	4.00	0.5	5
P2D1	1,912	500	4.00	0.5	21
P2D2	500	200	4.00	0.5	5
P3D1	7,115	500	4.00	0.5	21
P3D2	163	200	4.00	0.5	5

Table 10: Water source data of the selected plants

SINK	FLOW	FLOW	TDS	Organics	Ammonia
	ton/d	ppm	ppm	Ppm	ppm
P1S1	45	50	4.0	1.00	50
P1S2	154	250	20	2.5	25
P1S3	400	550	15	25	40
P2S1	281	500	100	0.5	5
P2S2	115	250	20	2.5	25
P2S3	500	550	15	25	40
P3S1	16,648	500	46	0.5	5
P3S2	147	550	15.00	25	40

There are different technologies used in treatment units depending on the contaminant composition and water sink data. The technologies used in this case study are Nano-Filtration and Reverse Osmosis (with recovery of 40% for seawater and 90% for process wastewater) since they satisfy all the sink contaminants concentration. Moreover, as we are dealing only with power generated fhuytfrom waste heat for the desalination units, reverse osmosis has been selected for desalination units.

Table 11: Treatment technologies data [66], [67]

TR	**NF**	**RO**
Recovery Ratio %	90	40
OPEX ($/m3)	0.0868	0.528
CAPEX ($/m3)	0.185	0.181
TDS RR	90	99.7
Organics RR	90	95
Ammonia RR	75	80
Nitrogen RR	75	80

Moreover, all the flows discharged are satisfied by environmental regulations.

Table 12: Environmental regulations [68]

	TDS	Organics	Ammonia	Nitrogen
DISCHARGE (ppm)	1500	46	3	100

The amount of power that can be generated from waste heat for different plants has been calculated and summarized in the following table.

Table 13: Waste heat to power conversion cost elements [69]

Cost Component	
Installed Costs ($/kW)	2750
O&M Costs ($/kWh)	0.0125
Fresh water Type 1 Cost ($/m3)	1.5
Seawater Cost ($/m3)	0.02

9. RESULTS & DISCUSSION

The given case study has been simulated and optimized for different cooling system options and the following results were obtained for different scenarios.

9.1 Scenario 1: Water Network without Waste Heat Utilization

In the first scenario, the modified water network has been optimized without including waste heat utilization concept. In this case, all cooling demands are satisfied by cooling systems. The best objective showed that the value of objective function for the network with air coolers has the lowest total annual cost (33.8 MM$ per year) and is the optimal design as shown in the following tables. The most expensive scenario is selecting once-through cooling seawater as option.

Table 14: Sources to sinks flow rates – scenario 1, air coolers

	P1D1	P1D2	P2D1	P2D2	P3D1	P3D2
	ton/d	ton/d	ton/d	ton/d	ton/d	ton/d
P1S1	0	0	0	0	22	0
P1S2	0	0	0	0	153	0
P1S3	0	0	0	0	3	0
P2S1	0	0	0	0	0	0
P2S2	100	0	0	0	15	0
P2S3	0	0	0	0	0	0
P3S1	47	0	0	0	161	0
P3S2	0	0	0	0	0	0

Table 15: Sources to treatments flow- scenario 1, air coolers

	Decentral Treatment Units			Central Treatment Unit	
	TR1	TR2	TR3	TRc	Discharge
	ton/d	ton/d	ton/d	ton/d	ton/d
P1S1	0	0	0	22	0
P1S2	0	0	0	0	0
P1S3	0	397	0	0	0
P2S1	0	0	0	281	0
P2S2	0	0	0	0	0
P2S3	0	0	0	500	0
P3S1	0	0	9396	7043	0
P3S2	0	0	0	147	0

Table 16 : Treated water to sinks flow- scenario 1, air coolers

	P1D1	P1D2	P2D1	P2D2	P3D1	P3D2	Discharge
	ton/d	ton/d	ton/d	ton/d	ton/d	ton/d	ton/d
TR1	0	0	0	0	0	0	0
TR2	0	0	0	0	357	0	0
TR3	741	0	1912	0	5804	0	1211
TRc	0	0	0	0	0	0	548

Table 17: Sources to sinks flow rates – scenario 1, cooling towers

	P1D1	P1D2	P2D1	P2D2	P3D1	P3D2
	ton/d	ton/d	ton/d	ton/d	ton/d	ton/d
P1S1	0	0	0	0	45	0
P1S2	0	0	0	0	0	0
P1S3	0	0	0	0	0	0
P2S1	0	0	0	0	0	0
P2S2	0	0	0	0	114	0
P2S3	0	0	0	0	0	0
P3S1	156	0	116	0	362	0
P3S2	0	0	0	0	0	0

Table 18: Sources to treatments flow- scenario 1, cooling towers

	Decentral Treatment Units			Central Treatment Unit	
	TR1	TR2	TR3	TRc	Discharge
	ton/d	ton/d	ton/d	ton/d	ton/d
P1S1	0	0	0	0	0
P1S2	0	0	0	154	0
P1S3	0	400	0	0	0.05
P2S1	0	281	0	0	0
P2S2	0	0.503	0	0	0
P2S3	0	500	0	0	0.05
P3S1	0	0	12924	3090	0
P3S2	0	0	147	0	0.05

Table 19 : Treated water to sinks flow- scenario 1, cooling towers

	P1D1	P1D2	P2D1	P2D2	P3D1	P3D2	Discharge
	ton/d	ton/d	ton/d	ton/d	ton/d	ton/d	ton/d
TR1	1059	0	787	0	347	0	244
TR2	0	0	0	0	0	0	118
TR3	0	0	0	0	0	0	1360
TRc	1356	0	0	0	6246	0	1390

Table 20: Sources to sinks flow rates – scenario 1, cooling seawater

	P1D1	P1D2	P2D1	P2D2	P3D1	P3D2
	ton/d	ton/d	ton/d	ton/d	ton/d	ton/d
P1S1	0	0	0	0	45	0
P1S2	0	0	0	0	154	0
P1S3	0	0	0	0	0	0
P2S1	0	0	27	0	0	0
P2S2	104	0	2	0	0	0
P2S3	0	0	14	0	0	0
P3S1	45	0	0	0	189	0
P3S2	0	0	0	0	0	0

Table 21: Sources to treatments flow- scenario 1, cooling seawater

	Decentral Treatment Units			Central Treatment Unit	
	TR1	TR2	TR3	TRc	Discharge
	ton/d	ton/d	ton/d	ton/d	ton/d
P1S1	0	0	0	0	0.088
P1S2	0	0	0	0	0
P1S3	0	363	0	37	0
P2S1	0	0	0	254	0.05
P2S2	0	0	0	8.5	0
P2S3	0	0	0	486	0
P3S1	0	0	7606	8808	0
P3S2	0	0	69	78	0.05

Table 22 : Treated water to sinks flow- scenario 1, cooling seawater

	P1D1	P1D2	P2D1	P2D2	P3D1	P3D2	Discharge
	ton/d	ton/d	ton/d	ton/d	ton/d	ton/d	ton/d
TR1	0	0	0	0	0	0	0
TR2	0	0	0	0	326	0	36
TR3	303	0	879	0	5725	0	767
TRc	2118	0	991	0	675	0	967

Table 23: Summary of cooling systems comparison

	Air-Coolers	**Once-Through Cooling Seawater**	**Cooling Towers**
Total Intake Seawater (T/d)	3,006	1,405,753	95,754
Total Wastewater Discharge (T/d)	1,778	1,771	3,111
Treated Water (T/d)	17,787	17,710	31,118

9.2 Scenario 2: Water Network with Waste Heat Utilization

In this scenario, portion of Q cooling is converted to power and remaining goes to cooling systems. In this scenario, the summation of all cooling systems Q and the WHP should be equal to minimum Q cooling.

Table 24: Networks energy use for coolings after waste heat utillization-scenario 2

Cooling Systems	TAC (MM$/yr)		Power Imported (kW) Before WHP		Power Generated (kW) by WHP	
	Before WHP	After WHP	Cooling System	Treatment Units	Cooling System	Treatment Units
Air Coolers	34.1	30.6	63576	390	57973	390
Once-Through Cooling Seawater	48.2	46.1	13241	393	12974	390
Cooling Towers	44.8	43.6	46357	690	43604	670

Similar observation has been noticed after applying WHP concept for water-energy integration in the second scenario, as shown in Table 24. It shows that networks with air coolers are more cost-effective compared to other cooling systems. Moreover, the total annual cost of the network including air coolers reduced by almost 10% which results from cheaper energy cost and lowering cooling demand. The power generated from waste heat was found to be 0.027 $/kWh while the external utility is 0.0219 $/kWh. Beside the advantage of being cheaper, using electricity generated from waste heat does not have any environmental emissions.

In all systems power amount required from external utilities decrease to zero. It means that this amount can be satisfied by the WHP system without any emissions.

9.3 Exploration of Other Scenarios

As it was shown by waste heat utilization the total annual cost decreases since the converted waste heat to power is cheaper than external utility. However, the cooling system decision did not changed and air coolers remained to be the most cost effective option. Furthermore, other scenarios were explored in order to see the difference and how this decision could be changed.

9.3.1 Scenario 3: Desalinating Used Once-Through Cooling or Direct Seawater

In the third scenario, once-through cooling system has been forced into the problem and the approach includes the direct connection of the desalination plant intake to the discharge outfall of a nearby located once-through cooling seawater plant. Therefore, cooling water is used as source water for the seawater desalination plant and this blending reduce the salinity of the desalination plant concentrate prior to the discharge to the ocean. It means that it decreases its impact on the environment. Furthermore, water intake for a desalination plant contains 5-20% of the total plant construction expenditure. Hence, by co-location the economics of seawater desalination can be improved. In case of using reverse osmosis plant, the RO membrane separation of seawater, which is on average 10

°C warmer, requires approximately 5-8% lower feed pressure, so lower energy use and power costs for seawater desalination.

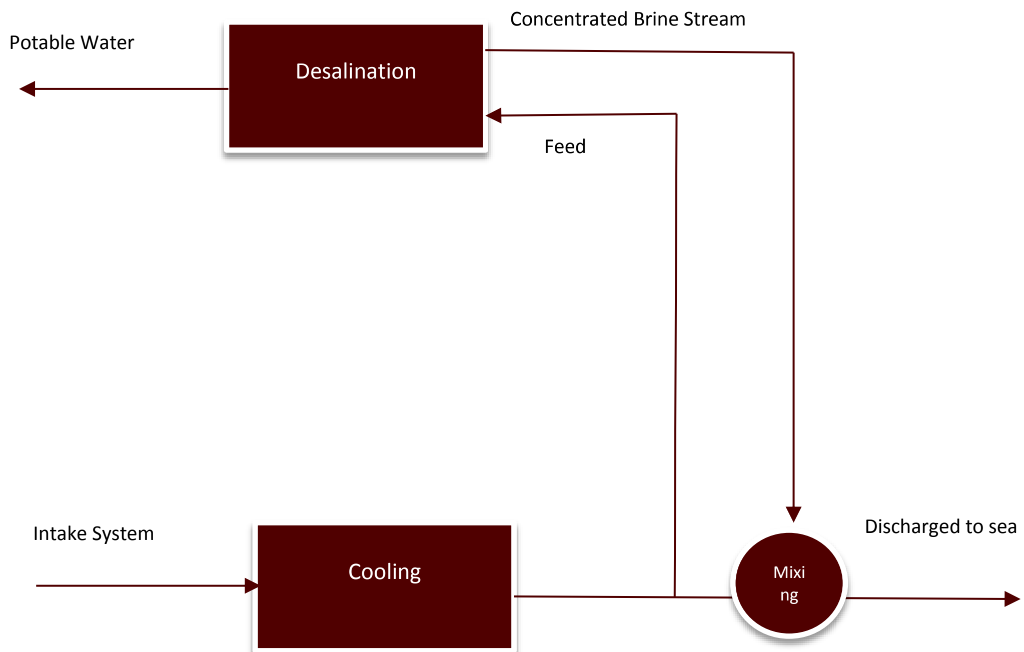

Figure 14: Co-Location

In this scenario, freshwater demand from any external utility will be zero, the water demand for offices use is satisfied by desalinating seawater directly, and the remaining is fulfilled by desalinating cooling seawater after cooling process. As it is shown in the following table, total annual cost decreases again in this case since the capital and operating cost drops as mentioned earlier.

Table 25: Results of scenario 3

TAC (MM$/yr)	44.6
Desalinated water directly from sea (Ton/d)	510
Desalinated water from cooling seawater(Ton/d)	993
Fresh Water from External Utility (Ton/d)	0
Power Generated from Waste Heat (MW)	20.6

By eliminating freshwater consumption from external utility, treatment cost increases (which includes both desalination cost and process treatment cost). Since freshwater produced from own, desalination is cheaper than the one from external utility, the total annual cost decreases.

9.3.2 Scenario 4: Exporting Desalinated Water from Once-Through Cooling Seawater

By desalinating cooling seawater and supplying water from own desalination water there is an opportunity of exporting water. The amount of water, which can be exported, was subjected to the constraints of being less than 500 m3 per day, which is one third of water production by the external utility. By adding this option to the previous scenario, it was found that in this case the objective value is negative. The negative value represents the annual profit, which is gained by exporting water. Furthermore, by exporting water the cooling system decision changes switches from air coolers to a combination design of once-through cooling seawater and air coolers with a significant difference.

Table 26 summarizes the obtained results and how cooling system option can change with different scenarios.

Table 26: Case comparison results of different scenarios

	Cooling System	**TAC (MM$/yr)**	**External Power Imported (MW)**
Scenario 1	Air Coolers	33.8	63
Scenario 2	Air Coolers	30.6	0
Scenario 3	Once-Through Cooling Seawater	44.6	0
Scenario 4	Once-Through Cooling Seawater + Air Coolers	-109.2	0

9.4 Sustainability Metrics

So all the results were without considering sustainability metrics especially environmental emissions. By adding environmental emissions to the objective function as a constraint, the trade-offs between economic and sustainability metrics were captured by developing Pareto front for the multi-objective optimization problem.

9.4.1 Without Waste Heat Utilization

As it is shown in Table 27, different trials have been done using different objectives. As mentioned earlier the minimum TAC cost results having a design with air coolers. If the objective function changes to minimum global warming, once through cooling seawater is the optimized solution. Finally, air coolers are the most sustainable solution in case of having minimum aquatic eco-toxicity.

Table 27: Compassion of different optimization objectives

	Cooling System	TAC (MM$/yr)	Global Warming (kg CO2-eq)	Eco-Toxicity
Min Global Warming	CS+CT	43.1	**1.05E+05**	1.3E+13
Min Eco-Toxicity	Both AC	35.6	3.46E+05	**8.84E+08**
Min TAC	Both AC	**33.8**	3.49E+05	9.00E+08

Different scenarios have been optimized without the waste heat utilization in order to get the trades-off between the total annual cost and different categories in sustainability metrics. The environmental emissions (Global Warming) decreases the total annual cost of the design increases, Obtained trend makes sense since in order to have more sustainable solution it is required to for the design to be more expensive. From Figure 14, it can be noticed:

- Scenario A

  Scenario A corresponds to the optimal economic solution where the TAC is minimized.

- Scenario F corresponds to the optimal economic solution where the global warming impact has the minimum value.

- Scenario B,C,D, and E

  three intermediate points with minimizing TAC

As it is shown in Table 28, as the cooling system design changes from air coolers to cooling seawater the global warming impact reduces since the power consumption in case of cooling seawater is the minimum. Moreover, the water network design changes by changing the cooling systems, which means amount of reused water, discharged water and other flow rates. In general, the total annual cost increases by decreasing the global warming impact, since more treatment is done and therefore more water reuse. Adding treatment actually means adding the cost. This trend consists with the theory.

Table 28: Total annual cost versus global warming impact before WHP

	Scenarios					
	A	**B**	**C**	**D**	**E**	**F**
Cooling System	Both AC	Both AC	AC+CS	AC+CS	CS+CT	CS
TAC (MM $/yr)	34.4	34.6	35.1	37.1	43.1	48.4
Global Warming (kg CO2-eq)	3.49E+05	3.30E+05	3.00E+05	2.00E+05	1.15E+05	1.05E+05

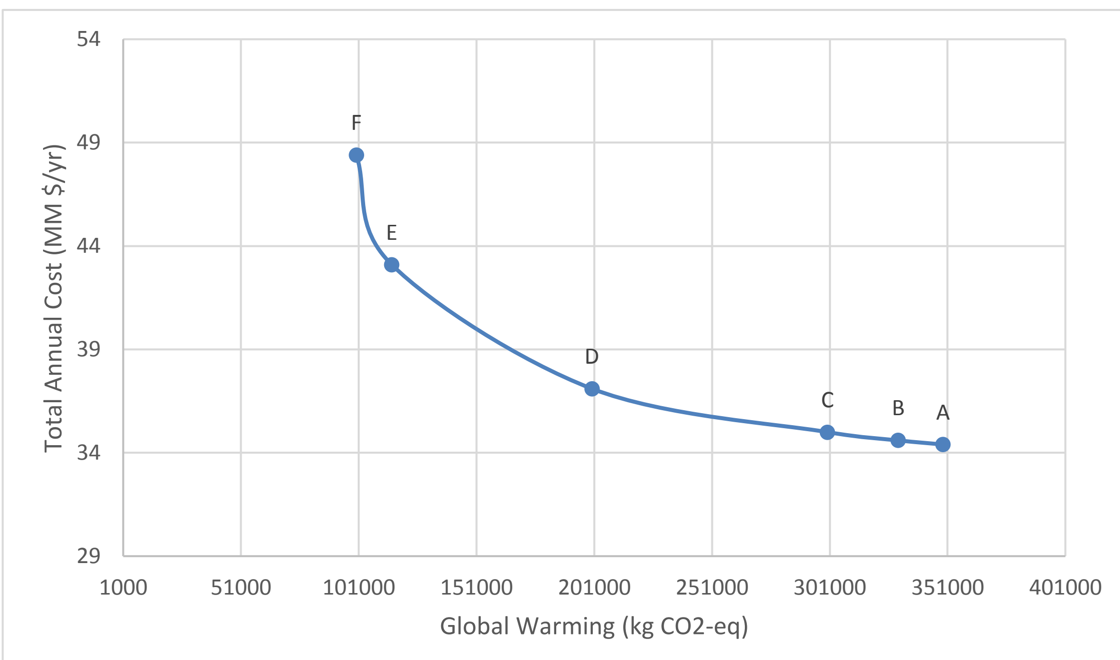

Figure 15: TAC versus GW impact (without waste heat utilization)

For the eco-toxicity influence (Aquatic impact), the same trials have been solved which is summarized in Table 29.

Table 29: TAC versus eco-toxicity impact (without waste heat utilization)

	Scenarios			
	A	**B**	**C**	**D**
Cooling System	Both CS	Both CS	Both CT	Both AC
TAC (MM $/yr)	48.2	49.3	44.8	35.6
Eco-Toxicity (CTUs)	1.42E+13	1.31E+13	2.27E+09	8.84E+08

For the optimal solution, which is selecting Air Coolers there is no difference in the impact by doing different trials since the contaminants included in the case study are not in the Aquatic eco-toxicity categories in TRACI metrics and in the Air Cooler design there is no flow for water.

If we force the design to select other cooling options, it can be noticed that as the cooling system option changes from the Air Coolers to Once-Through Cooling Seawater the eco-toxicity increases with total annual cost. Once-Through Cooling Seawater has the maximum impact because of the Biocide components (**Seawater Chlorination).** For the cooling seawater option only, as we treat wastewater more, less impact can be obtained. Adding treatment units means higher cost as it is clear from scenario A to B.

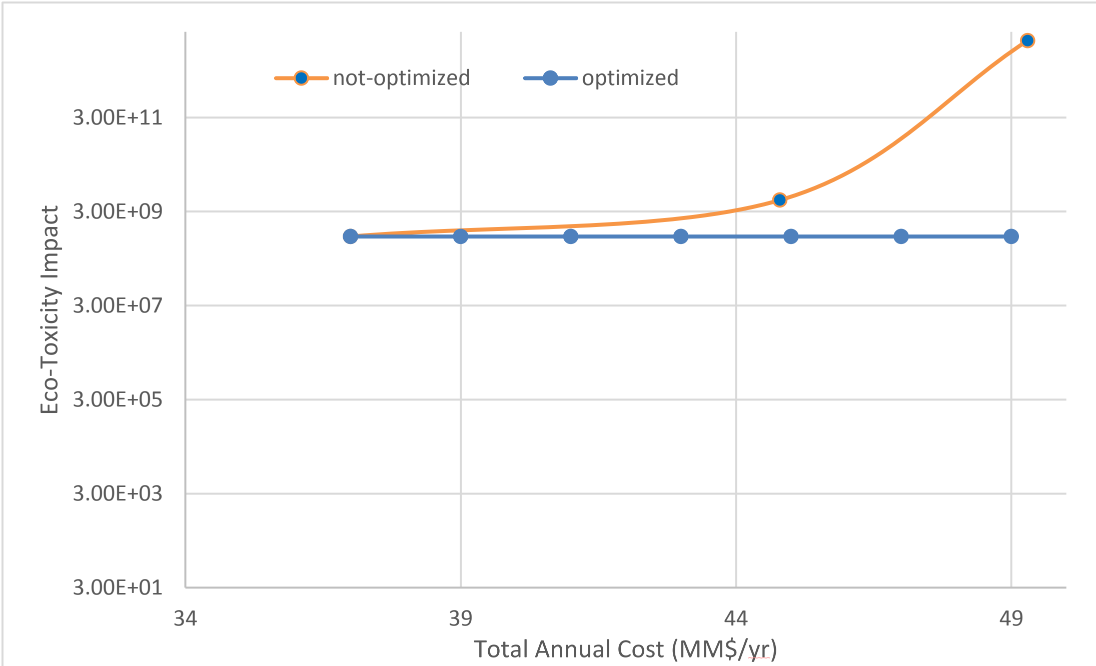

Figure 16: Total annual cost versus eco-toxicity (without waste heat utilization)

9.4.2 With Waste Heat Utilization

In the next section, the sustainability metrics were quantified and compared for the scenario with waste heat utilization and without. As it is shown in Table 30, the global warming affect decreased by almost 90 percent while the total annual cost is reduced by 10 percent. The remaining 10 percent of global warming impact is emission related to the external utility, which is counted in the formulation (KAHRAMAA).

Table 30: Global warming effect for air coolers before and after WHP

Cooling Systems	TAC (MM $/yr)	Global Warming (kg CO2-eq)
Air Coolers/Without WHP	33.8	3.49E+05
Air Coolers/With WHP	30.6	3.89E+04

In order to get the Pareto front curve for air coolers, same as the previous section (without waste heat utilization) different trials have been done for the case with WHP option as it is shown in Figure 15. As it is clear by waste heat utilization the annual cost decreases a little. However, the change in the emissions impact is significant (around 90%), which means the result is lower cost, lower emission.

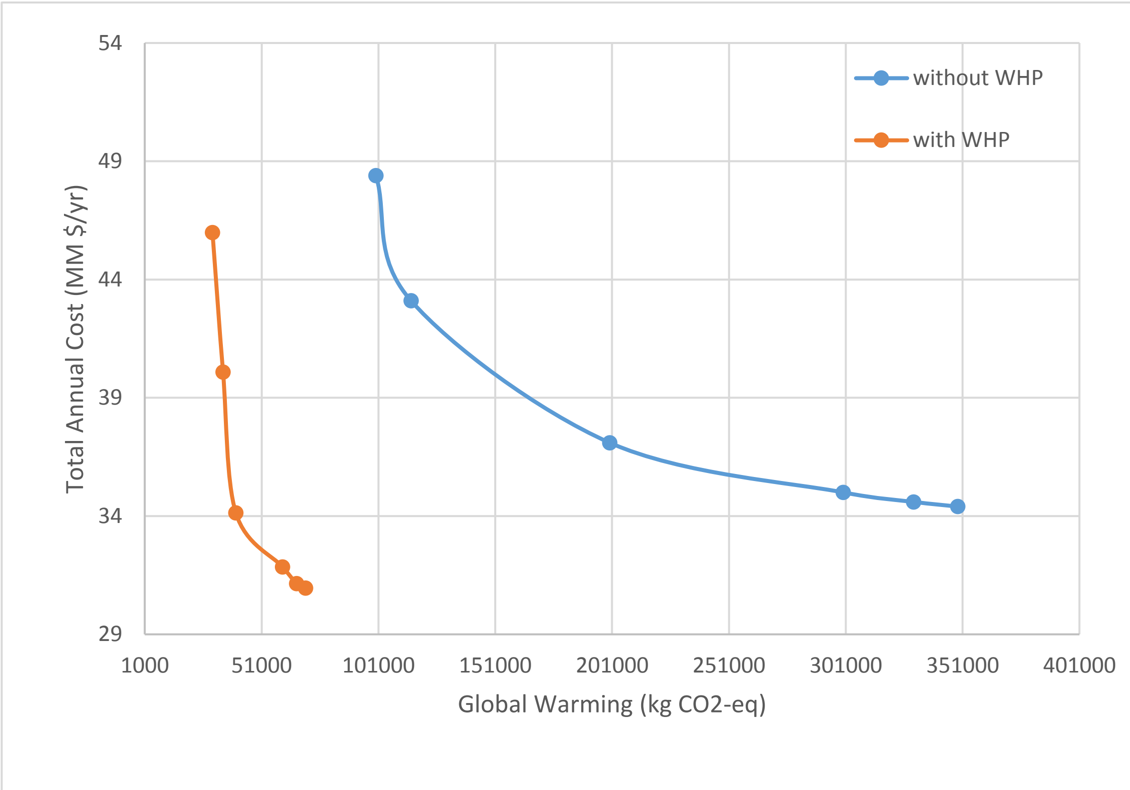

Figure 17: Global warming impact comparison before and after WHP

Figure 17 indicates that the obtained trend shows that in the case of air coolers the maximum benefits is obtained for the global warming impact. It can be justified since the air coolers have the maximum power consumption compared to other cooling system options. The change in the total annual cost is not significant since the power-generated cost from the waste heat is almost the same as the external power cost. However, since part of the waste heat is converted to the power, the minimum cooling requirement load decreases, which means lower cost.

10. CHALLENGES & FUTURE WORK

Challenges involved in this research work:

- From the energy perspective, only power generation was considered rather than power and steam.
- Multi-resource problems means more formulation involves and therefore more complex problem, which is difficult to get the optimal solution using current tools (LINDO).
- Pareto curve was generated considering two objectives only not more.
- Time horizon is not considered.

Recommendations for future work can be:

- Adding Utility systems in order to include the option of converting waste heat to steam (power and heat co-generation)

  Defining different objective function and multi-objective programming such as Reliability to improve the overall network performance
- Expanding the superstructure to create a basic platform for combined Water, Energy, and Carbon Network problem

  Multi-resource problems are larger in size and complexity and formulation involves more complex problem (Boolean Expressions, non-linear functions).
- Using Stochastic Solvers for its flexibility to handle element models especially in treatment systems.
- Extension and implementation of multi-period framework

11. CONCLUSION

This work presents a systematic approach for integration of industrial parks across the water-energy nexus. A new representation has been generated and added to the previous superstructure by adding cooling systems, and desalination plants, which captures design options across water and energy management. The objective of this paper is to develop a framework for optimizing energy and water resources from processes that have a surplus of energy at various qualities. A systematic procedure is developed for optimizing and maximizing the benefits of these nexuses, considering power generation from a net surplus of waste heat energy from each plant by accounting for different sustainability metrics. The developed approach includes the use of composite curve analysis to first identify the potential for excess heat and then used to develop the combined water-energy network. Furthermore, a case study was used to illustrate the approach and compare different scenarios for developing water-energy strategies. The results showed that significant reduction in water and energy footprint can be obtained by integration, which are economically attractive too. It was shown that how capturing the synergy potential from waste heat utilization, or water/power export scenario can be attractive. The work includes multiple objectives to explore trade-offs between minimum total annual cost and environmental sustainability metrics.

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