OPTIMIZATION OF WATER-ENERGY NETWORKS USING STOCHASTIC ALGORITHMS

A Dissertation

by

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ABSTRACT

Water – Energy nexus problem continues to gain traction and provides a comprehensive picture accounting for the nexuses which are generally omitted in isolated analysis. Several works have been dedicated to synthesis of optimal water and heat network but more work needs to been done to model the synergies between two networks thereby harnessing them for more efficient networks and adding the utility network into the model to make it more inclusive. This work presents an effort to analyze and mathematically model these nexuses, add the utility network to the model thereby making it more representative of actual scenario and synthesize an efficient water-energy network.

Apart from the work water-energy network, the work focusses on development of new tools to solve resource optimization problem. This work develops an alternative and novel search technique and utilizes stochastic algorithms Simulated Annealing (SA) and Tabu Search (TS) in developing solvers for Water - Energy Nexus problems. The architecture of the solver together with its components have been defined and presented in detail and their performance has been analyzed. The combined water-heat network synthesis problem has been formulated into a Mixed Integer Non-Linear Programming (MINLP) and solved using the solvers developed. Illustrative case study representing different policies on water-energy interaction have been solved and the tradeoffs across the networks have been analyzed.

DEDICATION

Dedicated to my late grandfather, my mother, my Neeta Aunty and my sister Neha.

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Contributors

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NOMENCLATURE

$F_{i(p1)}^{Process}$	Total flowrate of water discharged at process sources.
$F_{j(p2)}^{Process}$	Total flowrate of water required at process sources.
$F_{i(p1),env}$	Flowrate of water between i^{th} source in plant p1 to environment.
$F_{i(p1),j(p2)}$	Flowrate of water between i^{th} source in plant p1 to j^{th} sink in plant p2.
$F_{i(p1),d(p2)}$	Flowrate of water between i^{th} source in plant p1 to d^{th} decentral treatment unit in plant p2.
$F_{i(p1),r}$	Flowrate of water between i^{th} source in plant p1 to central treatment unit r.
$F_{j(p2)}^{Freshwater}$	Flowrate of water between fresh water source to j^{th} sink of plant p2.
$F_{r,j(p2)}$	Flowrate of water between r^{th} central treatment unit to j^{th} sink of plant p2.
$F_{cond(p1),j(p2)}$	Flowrate of water between condensate site(at the site of steam exchange)of plant p1 unit to j^{th} sink of plant p2.
$F_{d(p2)}^{in}$	Inlet flowrate of water at d^{th} decentral treatment unit of plant p2.
$Recovery_{d(p2)}$	Recovery ratio d^{th} decentral treatment unit of plant p2.
$F_{d(p2)}^{out}$	Outlet flowrate of water at d^{th} decentral treatment unit of plant p2.
$C_{cn,i(p1)}$	Concentration of contaminant cn in the i^{th} source of plant p1.

$C_{cn,d(p2)}$ Concentration of contaminant cn in the dth decentral unit of plant p2.

$F_{d(p1),CT(sink)(p2)}$ Flowrate of water at dth decentral treatment unit of plant p1 to cooling tower of plant p2.

$F_{d(p1),BFW(p2)}$ Flowrate of water at dth decentral treatment unit of plant p1 to boiler feed water in plant p2.

$F_{d(p1),env}$ Flowrate of water at dth decentral treatment unit of plant p1 to waste water discharge.

F_r^{in} Inlet flowrate of water at rth central treatment unit.

$Recovery_r$ Recovery ratios rth central treatment unit.

F_r^{out} Outlet flowrate of waterat rth central treatment unit.

$C_{cn,r}^{in}$ Inlet concentration of contaminant cn at central unit r.

$F_{r,CT(sink)(p2)}$ Flowrate of water from rth central treatment unit to cooling tower of plant p2.

$F_{r,BFW}$ Flowrate of water at rth central treatment unit to boiler feed water.

$F_{r,env}$ Flowrate of water at rth central treatment unit to environment.

F_{env} Flowrate of water discharged into environment.

$C_{cn,env}$ Concentration of contaminant cn at environment discharge.

$C_{cn,r}^{out}$ Concentration of contaminant cn at the outlet of rth central 9treatment unit.

$F_{d(p1),env}$	Flowrate of water from d[th] decentral treatment unit to environment.
$C_{cn,d}^{out}$	Concentration of contaminant cn at the outlet of d[th] decentral treatment unit.
F_{p2}^{BFW}	Flowrate at boiler feed water sink of plant p2.
$F_{fw,BFW(p2)}$	Flowrate from freshwater from boiler feed water of plant p2.
$F_{r,BFW(p2)}$	Flowrate from r[th] central treatment unit to boiler feed water of plant p2.
$F_{d(p1),BFW(p2)}$	Flowrate from d[th] decentral treatment unit of plant p1 to boiler feed water of plant p2.
$F_{desal(p1),BFW(p2)}$	Flowrate from desalination unit of plant p1 to boiler feed water of plant p2.
$F_{p2}^{CT(sink)}$	Flowrate at cooling tower sink of plant p2.
$F_{fw,CT(p2)}$	Flowrate from freshwater to cooling tower in plant p2.
$F_{r,CT(sink),(p2)}$	Flowrate at r[th] central treatment unit to cooling tower of plant p2.
$F_{desal(p1),CT(p2)}$	Flowrate from desalination unit of plant p1 to cooling tower of plant p2.
$F_{cond(p1),CT(p2)}$	Flowrate from condensate of steam exchange site at plant p1 to cooling tower in plant p2.
$F_{p1}^{CT(source)}$	Flowrate discharged from cooling tower source of plant p1.
$F_{p1}^{CT(sink)}$	Flowrate required at cooling tower sink of plant p1.

$F_{CT(p1),env}$ Flowrate from cooling tower source of plant p1 to environment.

$F_{CT(p1),r}$ Flowrate from cooling tower source of plant p1 to r^{th} central treatment unit.

$F_{CT(p1),d(p2)}$ Flowrate from cooling tower source of plant p1 to d^{th} decentral treatment unit of plant p2.

$F_{p1}^{OTSW(source)}$ Flowrate from once through sea water source at plant p1.

F_{env}^{OTSW} Flowrate from once through sea water source at plant p1 to environment.

$F_{p1,desal(p2)}^{OTSW}$ Flowrate from once through sea water source at plant p1 to environment to desalination unit in plant p2.

$F_{p1}^{OTSW(sink)}$ Flowrate required at once through sea water cooling sink in plant p1.

$F_{desal(p1)}^{Out}$ Outlet flowrate at desalination unit of plant p1.

$Recovery_{desal(p1)}$ Recovery ratio at desalination unit of plant p1.

$F_{desal(p1)}^{In}$ Inlet flowrate at desalination unit of plant p1.

$Q_{a(p1)}$ Waste heat from heat source a in plant p1.

$Q_{a(p1),b(p2)}$ Waste heat flow from source a in plant p1 to sink b of plant p2.

$Q_{a(p1),dectrpower(p2)}$ Waste heat flow from source a in plant p1 to decentral power generation unit in plant p2.

$Q_{a(p1),Cooling(p1)}$ Waste heat flow from source a in plant p1 to cooling units of plant p1.

$Q_{b(p2)}$ Heat requirement at sink b of plant p2.

$Q_{Fuel,b(p2)}$ Heat supplied by burning fuel to sink b in plant p2.

$P_{p1}^{Decentral}$ Power generated at decentral units of plant p1.

$P_{p1}^{Steam\,Turbine}$ Power generated by steam turbines of plant p1.

P_{p1}^{Import} Power imported by plant p1.

P_{p1}^{Export} Power exported by plant p1.

P_{p1}^{Equip} Power required by equipment of plant p1.

$P_{p1}^{Treatment}$ Power required by treatment units of plant p1.

$P_{p1}^{Cooling}$ Power required by cooling units of plant p1.

$P_{p1}^{Desalination}$ Power required by desalination units of plant p1.

$Q_{a(p1),Cooling(p1)}^{AC}$ Waste heat discharged from heat source a in plant p1 through air cooler cooling option in plant p1.

$Y_{a(p1),}^{AC}$ Fraction of discharged waste heat (cooling options) for heat source a to be discharged through air cooler cooling option.

$Q_{a(p1),Cooling(p1)}^{CT}$ Waste heat discharged from heat source a in plant p1 through cooling tower cooling option in plant p1.

$Y_{a(p1)}^{CT}$ Fraction of discharged waste heat (cooling options) for heat source a to be discharged through cooling tower cooling option.

$Q_{a(p1),Cooling(p1)}^{OTSW}$ Waste heat discharged from heat source a in plant p1 through once through seawater cooling option in plant p1.

$Y_{a(p1)}^{OTSW}$ Fraction of discharged waste heat (cooling options) for heat source a to be discharged using once through seawater cooling option.

P_{p1}^{AC} Power required by air cooler units in plant p1.

P_{p1}^{CT} Power required by cooling tower units in plant p1.

P_{p1}^{OTSW} Power required by once through seawater units in plant p1.

$P_{p1}^{Treatment(k)}$ Power required by treatment units in plant p1.

$F_{p1}^{Treatment(k)}$ Flowrate at treatment unit k in plant p1.

$P^{Steam\ turbine}$ Power generated by steam turbine units in plant p1.

m^{steam} Flowrate of steam through steam turbine.

$F_{desal(p1),export}$ Flowrate of water exported from desalination units of plant p1.

$F_{p1}^{Desalination}$ Flowrate at desalination unit in plant p1.

$F_{desal(p1),j(p2)}$ Flowrate at water from desalination units of plant p1 to sink j of plant p2.

$F_{desal(p1),CT(p2)}$ Flowrate at water from desalination units of plant p1 to cooling tower units of plant p2.

$F_{desal(p1),BFW(p2)}$ Flowrate at water from desalination units of plant p1 to boiler feed water units of plant p2.

$m_{VHP,p1}$ Flowrate of very high-pressure steam through steam turbine in plant p1.

Q_b^{Fuel} Amount of fuel burnt at heat sink b

Δh^{gen}	Concentration of j[th] sink in time period t
η_{turb}	Efficiency of heat generation turbine.
$\mathrm{DI}^{c}_{i(p1),j(p2)}$	Diameter of the pipe between source i of plant p1 to sink j of plant p2
$\mathrm{DI}^{c}_{i,bfw}$	Diameter of the pipe between sources and boiler feed water
$\mathrm{DI}^{c}_{desal,BFW}$	Diameter of the pipe between desalination units and boiler feed water
$\mathrm{DI}^{c}_{desal,p(CT)}$	Diameter of the pipe between desalination units and cooling towers in various plants.
$\mathrm{DI}^{c}_{desal,j}$	Diameter of the pipe between desalination units and sinks.
$\mathrm{DI}^{c}_{i(p1),r}$	Diameter of the pipe between sink i of plant p1 and central treatment units.
$\mathrm{DI}^{c}_{r,j(p2)}$	Diameter of the pipe between central interceptor r of to sink j of plant p2.
$\mathrm{DI}^{c}_{i(p1),d}$	Diameter of the pipe between sink i of plant p1 to decentral interceptor d.
$\mathrm{DI}^{c}_{d,j(p2)}$	Diameter of the pipe between decentral interceptor d to sink j of plant p2.

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1. INTRODUCTION

Water and Energy are the two important resources in modern industry inefficient utilization of which could lead to economic and environmental damages. Apart from the burdening the finances of the industry, inefficient water, and energy network generate a lot of wastewater and an enhanced level of carbon emission. With tight environmental regulations coming into play due to emphasis on sustainability and for financial consideration, a balance needs to be struck. Optimization of water and heat network have been going for the past several years for striking this balance but harnessing of the synergies have not been addressed rigorously. Designing an efficient water - energy network has economic, environmental and social impact. It helps the industries in reducing their carbon and wastewater emission and enables investments for the society from the financial savings.

A real-life manifestation of the above-mentioned concept is that of Eco-Industrial Parks (EIPs). This concept started as exchange of resources between heavy industries in industrial complexes. Since then, it has been extended to another relevant type of industrial park, the so-called mixed industrial park, which consists of various small- and medium-sized enterprises, sometimes complemented by a small number of larger industries. Very little work has been done on the combined water-energy problem and the complications involved in solving it. One of the major problems encountered while solving these class of problems is the performance of solvers in the face of enhanced size and complexity of the problem.

Alternatives to currently available tools for solving optimization problems have been investigated with comparison being made in each of them. The aim of this work is twofold:

(1) Develop an enhanced representation for the water-energy network model by adding utility system and utilization of waste heat in form of steam and power, modeling the nexuses between water and energy network and quantifying the impact of both networks on each other.

(2) Define an alternative form of search strategy for these kinds of resource optimization and develop solvers based on stochastic algorithms like Simulated Annealing (SA) and Tabu Search (TS). The modular architecture will be incorporated in the solvers to make it flexible for the user to make any changes to it.

When it comes to defining the enhanced energy – network, this works model the water-energy nexuses, adds utility network to the model with its associated heat, power balances and mathematical models. Equations for linking water-energy elements like dual usage of water (both as energy carrier in form of steam and raw material), dependence of water footprint on waste heat discharge technology, effect of adding steam(generated from waste heat) on boiler feed water balance, use of water for heating(steam) purpose, decentral power generation related models and balances and then the condensate being used at cooling tower and models for calculating power for various units in plants have modelled and incorporated into the overall optimization model.

Apart from improving and making the water-energy network problem more overarching and inclusive to formulate a problem closer to real scenarios and exploit the nexuses which have not been looked in earlier works, a considerable amount of research has been focused on the development of tools for solving these kinds of problems. Stochastic algorithms SA and TS have been used to develop these solvers. Although stochastic algorithms have been used extensively in solving various problems in different fields, it is the first time they have been used to solve these kinds of resource optimization problems. These methods are reliable and perform robustly in handling larger and more complex problems. The solver developed in this work has been designed in a modular way. This allows the user to incorporate the changes (objective function, balances, constraints) easily into the solver without much effort going into customization of the tool. SA and TS are the two stochastic algorithms chosen because they are simple in philosophy and have found to perform robustly in other optimization problems. Apart from robustness and flexibility, the tool enables the user to store multiple optimal solutions. This data created enables the user to study the tradeoffs across various structures, helps the user to find multiple structures with similar performance and enables the user to understand which elements of structure always provide a better solution. The data generated can be used for training the solver thereby enhancing the performance of solver with each run by incorporating the elements of machine learning.

This work aims to fill the gaps in both problem formulation and the framework required to solve a bigger and more complicated multi-resource optimization problem encompassing both energy and water network and demonstrate the benefits of exploiting the nexus between them. Though the focus has been to solve the combined water-energy problem, the implementation and the modular architecture of the solver have been fashioned in a way that it can be utilized to solve problems having more resources. Several illustrative scenarios reflecting different policies about the exchange of water and energy have been presented. The results indicate great potential for achieving considerable savings of resources and reduced environmental footprint if both networks are studied in unison rather than separately. Apart from this, the effectiveness of stochastic algorithms in solving these problems and valuable insights gained across the designs have been demonstrated.

2. LITERATURE REVIEW

This section reviews the work done in the area of process integration, early methods and then its development across years, and its successful application in the area of resource network optimization. Works related to water, energy and combined network till now have also been summarized and a brief review on the gap in current approaches has also been presented. It also summarizes the work done in areas of stochastic algorithms and their application in chemical engineering.

2.1. Process Integration & Resource Network Optimization

The concept of Process integration is defined as “a holistic approach to process design, retrofitting and operation which emphasizes the unity of the process (El-Halwagi [1]). It is an approach towards minimizing resource consumption by designing and planning utility networks within industrial process plants. Water and Energy integration within and across processes presents a practical approach to reduce the respective footprints of processing systems and increase profitability. Work in areas of process integration was first developed in the 1970s when Linnhoff and Flower [2] first published their work on the synthesis of the heat exchanger network using a graphical technique called pinch analysis. Linnhoff and Eastwood [3] then applied this technique for Total Site Integration.

Following the application of pinch technology in heat exchanger networks, El-Halwagi and Manuosiouthakis [4], as well as Wang and Smith [5] implemented it for the water treatment, exchange and integration within a single plant. Apart from these, Liu et al [6], Kuo and Smith [7], Hallale [8], El-Halwagi et al [9], Shenoy and Bandyopadhyay [10] developed a process-based graphical approach for simultaneous targeting and design of water networks. Recent works in graphical techniques include Parand et al [11], Pombo et al [12] and Liu et al [13].

Graphical methods can be used for solving small scale problems, but with larger problems concepts of mathematical optimization are utilized to solve the problem. Takama et al [14] proposed a method for solving the planning problem of optimal water allocation combining all alternatives into an integrated system. El-Halwagi et al [15] presented a mathematical model to determine the optimal water usage and interception network while accounting for the process model. Chakraborty [16] has developed a source-sink equivalent of the above problem and proposed MINLP and MILP models. Karuppiah & Grossmann [17] proposed an MINLP formulation to optimize the synthesis of integrated wastewater systems considering different alternatives for wastewater treatment.

Lovelady et al [18] reported a systematic approach for the reduction of water usage and wastewater discharge in pulp and paper plants. Chew et al [19] proposed an MINLP formulation for the synthesis of direct and indirect inter-plant water networks but with limitations that type of treatment unit was not set as an optimization variable, direct discharge from source environment was not allowed and there was no restriction on the contaminant levels of the discharge. Lovelady et al [20] developed a property-integration optimization approach for designing eco-industrial parks that are constrained by properties. Montastruc et al [21] discussed the capacity of EIP to sustain sudden variations in the concentration level of pollutants. Alnouri et al ([22], [23], [24], [25]) developed water integration model for an industrial city considering the spatial representation of plants. Bishnu et al ([26], [27]) addressed the multi-period planning of water networks in EIPs.

Besides water network optimization, a lot of work has also been done in the area of energy integration using mathematical modeling. Čučeka et al [28] present approaches for retrofitting existing heat exchanger networks. Klemeš et al [29] present techniques of process integration and optimization for energy efficiency and savings. Arsenyeva et al [30] integrated the heat utilized from exhaust gases with the existing processes. Bohlayer & Zotti, G [31] worked on the integration of low-grade waste heat in distributed energy generation systems to minimize the cost. Chan et al [32] worked on the synthesis of energy-efficient chilled and cooling water networks by integrating waste heat recovery refrigeration systems. Chang et al [33] developed an efficient optimization algorithm for waste heat integration using a heat recovery loop between two plants. Chang et al [34] also developed an energy hub approach for direct interplant heat integration. Hipolito-Valencia et al [35] studied the optimal design for inter-plant waste energy integration. Kapil et al [36] developed methods for integration of low-grade heat in the process industry with district heating networks. Kralj et al [37] examined waste heat integration between processes. Song et al [38] applied waste heat integration techniques to a cellulosic ethanol production plant. Yu et al [39] worked on simultaneous heat integration and techno-economic optimization of the Organic Rankine Cycle (ORC).

A lot of work reviewing the application of water and energy networks have also been published. Klemeš et al [40] present recent development in Process Integration and its application across resource optimization problems. Ahmetovic [41] presents a review of work in the area of non-isothermal water network synthesis. Dunn & El-Halwagi [42] review the work done on heat and mass exchanger networks.

2.2. Water-Energy Nexus Optimization.

Simultaneous optimization of energy and water networks was done by Bagajewicz et al [43] who used an optimization-based approach for non-isothermal mixing simultaneous optimization of energy and water networks. Xiao et al [44] utilized an optimization model considering sequential and simultaneous solution procedures. Boix et al [45] came up with a mathematical programming method to solve water and a heat exchanger network considering multiple objectives such as minimization of freshwater and energy consumptions and the number of heat exchangers. Ahmetovic and Kravanja [46] proposed a framework in which direct and indirect heat exchange, gradual heating and cooling and the splitting of freshwater and wastewater streams are included. Jiménez-Gutiérrez et al [47] combined water networks with a simultaneous integration of energy, mass, and properties. Gabriel et al [48] focus on water-energy nexus targets in GTL plants.

Gabriel [49] optimizes the water-energy network for industrial processes coupled with hybrid thermal membrane desalination. El-Halwagi [50] described the water-energy nexus in a thermal desalination system. Fouladi & Linke [51] examined the problem of water and energy nexus problem for an Industrial Park. Bishnu et al [52] analyze the water and energy nexus problem using simulated annealing as the stochastic algorithm for synthesizing the network. DeeNooyer [53] worked on Integrating water resources and power generation and applied their method on an energy-water nexus case study in Illinois.

Guttierrez et al [54] developed an MINLP model for the simultaneous integration of energy, mass, and properties in water networks. Hickman, et al [55] examined the synergistic role of renewable energy integration into the unit commitment of the energy-water nexus. Hou et al [56] worked on simultaneous integration of water and energy on the conceptual methodology for both single and multi - contaminant problems. Huang, et al [57] synthesized an industrial combined heat and power plants compromising the water-energy nexus with dual objective optimization. Li et al [58] worked on sustainable water-energy networks and how ocean energy for seawater desalination can fit into the role. Maritn & Grossman [59] looked into the water-energy nexus in biofuels production and renewable-based power. Nikolakopoulos & Kokossis [60] applied the energy and water integration techniques for designing a sustainable textile waste refinery.

Garcia and You [61] present the modeling challenges and process systems engineering research opportunities in the area of Water-Energy-Food Nexus. Gao and You [62] address the optimal design of water networks for shale gas production. Garcia and You [63] present life cycle network modeling and optimization framework of energy-based products and processed using water and optimizes the water footprint. Garcia and You [64] review the nexus between the food-water-energy network and waste streams and highlight the research opportunities in process and supply chain design. Garcia and You [65] focus on the optimization of the water footprint in renewable fuel production.

2.3. Utility Network Modelling and Optimization.

Total Site Integration for water and energy networks generally take place through utility systems as it requires both fuel and water for the generation of steam and power. Work on optimization of complex water and energy network of utility system has been done. Varbanov et al [66] presented a utility system model for fossil fuel consumption and steam and power output. Wu et al [67] presented an optimization model for minimization of cost and environmental impact of the utility system. Hassiba et al [68] utilized the utility model in the simultaneous integration of heat and carbon dioxide in industrial parks. Mavromatis et al [69] optimized the utility networks for operational variations. These works look into the optimization of utility networks in isolation and overlook the linkages with overall water and energy networks. Utility network with huge water and energy footprint is a key building block in the overall network and this work incorporates it into the overall water-energy optimization model.

2.4. Gaps in Current Approaches.

The above-mentioned work in the area of the combined water-energy network is a step ahead but they lack many elements of the problem. Options like conversion of waste heat to steam & power, the export of water & power and discharge of waste heat have not been incorporated together earlier. Utility network, which is a significant element in overall water – energy network, has been looked in isolation and not integrated with the network. The formulation presented in this work intends to present a more inclusive picture of the problem trying to model and incorporate all these options and account for the utility network as well. Solutions like water acting as a carrier of steam & acting as a raw material that has never been discussed in earlier works have modeled and accounted for the formulation presented in this work. Also, the steam levels and models for steam/gas turbine has been defined for utility network. Fuel and water consumption in the utility system has also been quantified in the integrated model.

Since the problem is of a quite considerable size and complexity, a conscious decision about the selection of solver which is flexible and robust had to be made. Currently available tools had been compared with each other and were found to be lacking in robustness as the size and complexity of the problem even for single resource problems. Angeli et al [70] presented a new methodology based on an MINLP formulation for the optimal design of reliable measurement system A comparison was made between BARON and Genetic Algorithm (GA) keeping time as a constraint and the latter performed better. Shi & You [71] developed techniques for global optimization of water supply scheduling with pump operation. The performance of the proposed algorithm was compared with solvers like BARON and SCIP and BARON was unable to return a feasible solution. Gao & You [72] focused on the optimal design of water supply chain networks for shale gas production using new algorithms and comparison was made with solvers like DICOPT, SCIP, SBB, and BARON. BARON and SCIP could not return a feasible solution.

This work proposes the development of novel search techniques based on solvers that integrate principles of stochastic algorithms for dealing with the complexity and size of the problem at hand. Stochastic algorithm-based solvers have been applied in other fields and have been found to perform robustly for a practically sized problem and can handle the complexities involved be it non-linearities in the objective function or the equations. A new approach to optimization has been developed and used in these solvers with the aim of making it user-friendly in terms of customization for trying out different models and expanding into different resources for integration.

2.5. Stochastic Algorithms

The application of stochastic techniques such as Simulated Annealing, Tabu Search for solving different optimization problems across several fields has shown the versatility of these methods. The approach utilized by these methods enables the user to use complicated and non-linear expressions to define their problem that in turn helps in defining the optimization problem incorporating the complex nature of the real problem in a better way. Despite these advantages, no significant work has been done in the area of water - energy integration networks using these methods. This work demonstrates the application of Simulated Annealing and Tabu Search. Compared to deterministic techniques, stochastic methods may be slow but they search the solution space thoroughly and provide multiple solutions, unlike deterministic solvers that just give one solution as output. The availability of multiple solutions allows us to compare solutions. Apart from this, it also lays the groundwork for solving a more complicated problem involving the integration of multiple resource networks in a single problem.

Different stochastic algorithms have been developed in the past and they have been extensively used in various fields. Some of the notable ones include Simulated Annealing (Metropolis et al [73], Kirkpatrick et al [74]), Tabu Search (Glover [75]), Genetic Algorithm (Goldberg [76], Holland [77]), Swarm based optimization methods like Particle Swarm Optimization (Hul [78], Kennedy [79], Poli [80]) and Ant Colony Optimization (Colorni [81], Dorigo [82]). These methods mimic different natural processes to search for an optimum solution and have the advantage of handling any kind of non-linear expression in the optimization problem. Simulated Annealing, application of which has been demonstrated further in the paper, mimics the process of annealing in which a heated body is allowed to cool slowly in a heat bath ensuring the molecules settle down in their lowest energy state. Tabu search is a metaheuristic-based algorithm that essentially prohibits visit to a particular solution so that the solver searches across other solutions across the search space. These algorithms when implemented are found to perform robustly when applied on various optimization problems.

2.6. Applications of Stochastic Algorithm in Chemical Engineering.

Stochastic algorithms have been previously applied in chemical engineering for various optimization problems. Lavric et al [83] utilized a genetic algorithm for the optimization of water consumption and wastewater network topology, Prakotpol and Srinophakun [84] developed a genetic algorithm toolbox for water pinch analysis, Shafiei et al [85] used genetic algorithm for synthesizing optimal water network for a pulp and paper mill and Jezowski et al [86] employed genetic algorithm for the optimization of water usage in chemical industry. Tan et al [87] developed a methodology for the design of efficient resource conservation networks using adaptive swarm intelligence. In addition to the above-mentioned fields, these methods have been used in chemical engineering in molecular design (Papadapolous and Linke [88], Berhane and Urmila [89]), Reaction Network Synthesis (Kokossis and Linke [90], Marcoulaki et al [91], Zhao and Marquardt [92]).

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3. OBJECTIVES OF THIS WORK

Various optimization models for water and energy network has been proposed looking at them separately. Besides that, the stochastic algorithms utilized in this work have also been used to solve various optimization problems. This work aims to fill the gaps in current approaches of water – energy optimization and achieve the following objectives:

- Develop a more comprehensive optimization model for the water-energy network by including the utility network into the model.
- Define and model the nexuses between the networks, model and incorporate them into the overall optimization problem
- Define the components of the SA and TS based solvers and describe the architecture used.
- Develop the novel solution search transition framework utilized by the solvers and their integration with stochastic algorithms.
- Use the solvers to solve illustrative case study representing various water-energy exchange policies and analyze the performance of the solvers and impact of the policies on the networks.

The novelty of this work lies in the fact that an alternative search technique has been developed and SA and TS have not been utilized as the basis for solvers custom-built to solve these kinds of problem. These algorithms have been chosen as they are simple in theory to implement, have a track record of performing robustly on optimization problems of other fields and ability to parallelize these solvers in order to speed up computation. This, in turn, lays the foundation for solving optimization problems for other resources having a similar structure.

Chapter 4 presents in detail the components of the solvers developed, the new transition framework and the architecture of both SA and TS solvers. The solvers developed have been utilized to solve the water network problem adapted Alnouri et al [23] and their performance has been analyzed. Chapter 5 expands the problem to include details of the utility network, cooling options, decentral power and steam generation from waste heat and the nexus associated with them. These nexuses were modeled and a new optimization problem is formulated. In chapter 6, solvers developed are in turn modified to cater for these changes (framework for solution generator, simulator, testing of solutions) and then an illustrative case study has been solved considering various scenarios in which steam/power exchange and export of water/power is allowed or prohibited. Chapter 7 looks into the multi-objective analysis of economics and the sustainability of these networks. The objective function for air and aquatic impact have been adapted from Fouladi [93] and multi-objective analysis studying the tradeoffs between cost and the above-mentioned objectives are studied. Chapter 8 lists the conclusion drawn from the optimization of the combined water-energy network and analysis of solver performance. Chapter 9 presents the future work that can be done on problem formulation and on the tools for optimization.

4. STOCHASTIC OPTIMIZATION OF WATER NETWORK

4.1. Objective.

This section defines various components of the solvers, their architecture for integrating the principles of SA and TS and then a case study on water network optimization is solved to demonstrate the effectiveness of these solvers. It adapts the water network formulation from Alnouri et al [23] and a case study from Fouladi [93] to demonstrate the robustness of the solvers and analyze their performance.

As mentioned in section 2.6, the choice of these algorithms has been influenced by their simplicity and track record for robustness. The subsequent section presents the formulation, layout component of the solver which has a modular architecture thereby enabling the user to customize it for problems of bigger size and more resources to be integrated. A new scheme of search is proposed in which the mass balances, constraints and objective function are handled separately. The solution space is searched using a transition framework that employs smart search to scan the space and seek out feasible solutions thereby making the search more efficient and effective. A simulation module that has been designed by keeping the degrees of freedom for the equations to be zero then simulates the newly generated solution and the feasibility and performance of the solution is evaluated using a separate module.

The solver is then tested while varying various parameters and running the search from a different point. Apart from this, the objective function is also modified and the problem solved to study how it impacts the performance of the solver.

4.2. Problem Statement and Formulation.

The water network problem solved has been adapted from Alnouri et al [23] and represented in figure 4.1. The infrastructure for the problem consists of several sources and sinks with the presence of two types of treatment units – Decentral units within individual plants and Central Treatment units which are located away from the plants. The treatment plant consists of several treatment units, having the capacity to remove various contaminants generally denoted by different regeneration ratios. The water network part of the optimization problem is set up with the help of information about wastewater streams (sources) and water using operations (sinks), contaminants present in those streams, and flowrate constraints in various connections.

The following sets have been defined as a basis for the water network formulation:

I {i = 1, 2, … $N_{sources}$ | I is a set of water sources}

J {j = 1, 2 … N_{sinks} | J is a set of water sinks}

R {r = 1, 2…N_{unit}| R is a set of treatment units in each stage}

P {p = 1, 2 … N_{plant} | P is a set of plant}

CN {cn = 1, 2 …$N_{contaminants}$ | CN is a set of contaminants}

D {d = 1, 2…N_{unit}| d is a set of decentral treatment units}

Each source can be split into several streams: (1) Source-to-Sink flows ($F_{i(p1),j(p2),}$) representing the flow from ith source of plant p1 to jth sink of plant p2 (p1,p2 ϵ P) , (2) Source-to-Interceptor flows ($F_{i(p1),\, r(s1)}$) which represents the flow from each source to treatment units of stage 1 and (3) Source-to-Environment flows ($F_{i(p1),\, env}$) which represents the flow from each source of plant p1 to environment for discharge.

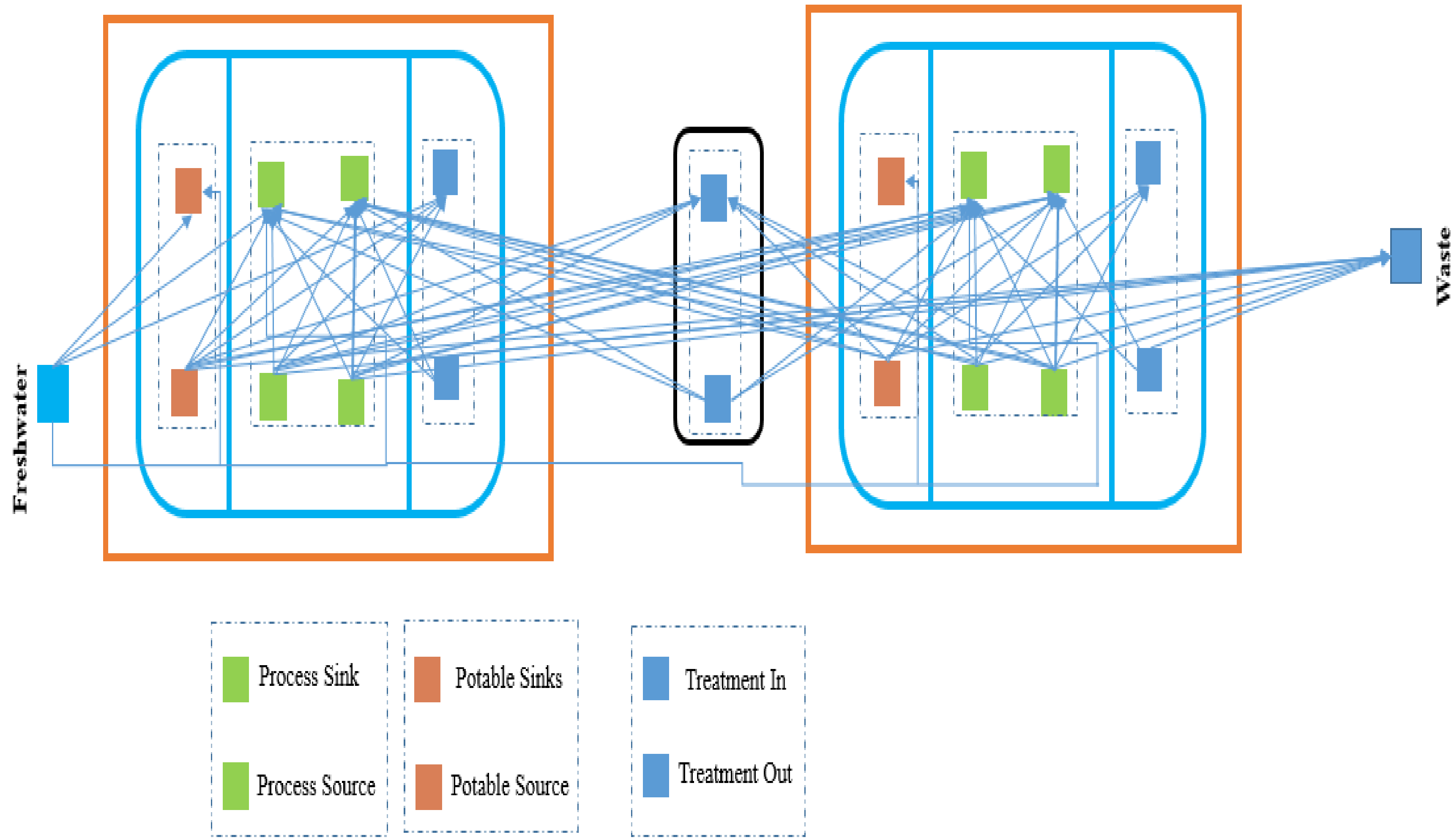

Figure 4.1 Water Network Superstructure

The following equations define the mass balances at various facilities:

$$F_{i(p1)}^{Process} = \sum_j F_{i(p1),j(p2)} + \sum_d F_{i(p1),d(p2)} + \sum_r F_{i(p1),r} + F_{i(p1),env} \quad (1)$$

$$F_{j(p2)}^{Process} = \sum_i F_{i(p1),j(p2)} + \sum_d F_{d(p1),j(p2)} + \sum_r F_{r,j(p2)} + F_{j(p2)}^{Freshwater} \quad (2)$$

Water sources can either be discharged to environment($F_{i,env}$), sent to a sink ($F_{i,j}$) or sent to inceptors ($F_{i,r}, F_{i,d}$). Requirement at sinks can be met by contaminant rich water from sources ($F_{i,j}$), fresh water ($F_j^{Freshwater}$) and treated water from the interceptor units ($F_{r,j}, F_{d,j}$) .

Mass balances for interceptors (decentral units) at inlet and outlet are described by equations (3)-(6).

$$F_{d(p2)}^{in} = \sum_i F_{i(p1),d(p2)} \quad (3)$$

$$F_{d(p2)}^{out} = Recovery_{(p2)} * F_{d(p2)}^{in} \quad (4)$$

$$F_{d(p2)} * C_{cn,d(p2)}^{in} = \sum_i F_{i(p1),d(p2)} * C_{cn,i(p1)} \quad (5)$$

$$F_{d(p1)}^{Out} = \sum_j F_{d(p1),j(p2)} + F_{d(p1),env} \quad (6)$$

Here $F_{i,d}$ represent flows from various sources to interceptors in treatment units and F_d is the amount of water that will be regenerated by each interceptor. Equation 3 accounts for the mass balance and equation 5 represents the component balance at the inlet of each treatment unit. In equation 5, $C_{cn,i(p1)}$ is the concentration of contaminant cn in source i of plant p1 and $C_{cn,r}^{in}$ is the inlet concentration of contaminant cn in interceptor r. The amount of water coming out of a treatment unit depends upon the recovery ratio ($Recovery_p$) and is calculated using equation 4. Water from interceptor units are can then be either used at process sinks($F_{d,j}$) or discharged into the environment ($F_{d,env}$) and has been modeled by equation 6. The same balances are shown for central treatment units in equations 7 to 10.

$$F_r^{in} = \sum_p \sum_i F_{i(p1),r} \quad (7)$$

$$F_r^{out} = Recovery_r * F_r^{in} \quad (8)$$

$$F_r * C_{cn,r}^{in} = \sum_p \sum_i F_{i(p1),r} * C_{cn,i(p1)} \quad (9)$$

$$F_r^{Out} = \sum_p \sum_j F_{r,j(p2)} + F_{r,env} \quad (10)$$

Inlet and outlet concentrations in treatment units (interceptors) are related using a removal ratio. The removal ratio is a parameter that accounts for the percentage of contaminants removed from a stream and depends on the type of treatment unit utilized. Equation (11) correlate the inlet and outlet concentrations of the interceptors (Central and Decentral).

$$C_{cn}^{out} = (1- RR_{cn}) * C_{cn}^{in} \quad (11)$$

Mass balances for discharge to the environment, is given by equations (12) and respective component balance for environmental discharge requirements is given by equation (13).

$$F_{env} = \sum_p \sum_d F_{d(p1),env} + \sum_r F_{r,env} + \sum_p \sum_i F_{i(p1),env} \quad (12)$$

$$F_{env} * C_{cn,env} = \sum_r F_{r,env} * C_{cn,r}^{out} + \sum_p \sum_i F_{i(p1),env} * C_{cn,i} +$$
$$\sum_p \sum_{d(p1)} F_{d,env} * C_{cn,d}^{out} \quad (13)$$

Water can be discharged into the environment from various sources ($F_{i,env}$) or from treatment units ($F_{r,env}$, $F_{d,env}$). $C_{cn,env}$ is the concentration of contaminant b in the environmental discharge. Apart from ensuring the balances, the constraints at sinks for maximum allowable concentration and the flowrate feasibility are checked. The above-mentioned constraints are as follows:

$$F_{j(p2)}^{Freshwater} * C_{cn,fw} + \sum F_{i(p1),j(p2)} * C_{cn,i(p1)} + \sum F_{r,j(p2)} * C_{cn,r} + \sum F_{d(p1),j(p2)} *$$
$$C_{cn,d(p1)} \leq F_{j(p2)} * C_{cn,j(p2)} \quad (14)$$

$C_{cn,fw}$ is the concentration of contaminant cn in freshwater, $C_{cn,i}$ is the concentration of contaminant cn in source i, $C_{cn,r}$ and $C_{cn,d}$ is the concentration of contaminant b in streams originating from the central and decentral interceptor. $C_{cn,j}$ is the concentration of contaminant cn in sink j.

$$C_{cn}^{env} \leq C_{cn}^{max} \quad (15)$$

$C_{cn}^{env}$the concentration of contaminant b is discharged into the environment and C_{cn}^{max} is the maximum concentration of contaminant b that can be discharged into the environment.

$$F_{i(p1),j(p2)} - M_{F_{i(p1),j(p2)}}^{max} \leq 0 \quad (16)$$

$$F_{i(p1),r} - M_{F_{i(p1),r}}^{max} \leq 0 \quad (17)$$

$$F_{i(p1),d(p2)} - M_{F_{i(p1),d(p2)}}^{max} \leq 0 \quad (18)$$

$$F_{r,j(d2)} - M_{F_{r,j(d2)}}^{max} \leq 0 \quad (19)$$

$$F_{d(p1),j(p2)} - M_{F_{d(p1),j(p2)}}^{max} \leq 0 \quad (20)$$

$$F_{r} - M_{r}^{max} \leq 0 \quad (21)$$

$$F_{d(p1)} - M_{F_{d(p1)}}^{max} \leq 0 \quad (22)$$

Equations (16) - (20) defines the existence of various streams from sources to sinks, sources to interceptors, interceptors to sinks and interceptors to environment. Equations (21) and (22) defines the existence of treatment units.

The evaluation function consists of the total cost of the water network and the energy network. The aim of the optimization is to minimize the cost. Water network costs consist of the cost of freshwater, piping cost, treatment, desalination cost and export cost of water. Energy network costs consist of total capital and operating costs of cooling systems.

The piping cost of the water network is given by the following expression:

$$\sum_{i\epsilon I}\sum_{j\epsilon J} a(DI^{c}_{i(p1),j(p2)})^{b} dis_{i,j} + \sum_{I}\sum_{R} a(DI^{c}_{i(p1),r})^{b} dis_{i,r} + \sum_{R}\sum_{J} a(DI^{c}_{r,j(p2)})^{b} dis_{r,j}$$

$$+ \sum_{I}\sum_{D} a(DI^{c}_{i,d})^{b} dis_{i,d} + \sum_{D}\sum_{J} a(DI^{c}_{d,j(p2)})^{b} dis_{d,j} \ .$$

$$\sum \quad \sum_{p1,p2\in P}(\sum_{i\epsilon I}\sum_{j\epsilon J} a(DI^{c}_{i(p1),j(p2)})^{b} dis_{i,j} \quad + \ \sum_{d\,\epsilon\, R}\sum_{j\epsilon J} a(DI^{c}_{d,j(p2)})^{b} dis_{d,j} +$$

$$Hy\ C^{fresh}\sum_{i\epsilon I}\sum_{t\in T} F_{Fw,j(p2),t} + \sum_{r\epsilon R} F_{r}\left(C_{r}^{oper} + C_{r}^{cap}\right) + \sum_{d\epsilon D} F_{d}(C_{d}^{oper} + C_{d}^{cap}))$$

(23)

where $DI^{c}_{i(p1),j(p2)}$ is the diameter of the pipe between source i of plant p1 to sink j of plant p2, , $DI^{c}_{desal,p(CT)}$is the diameter of the pipe between desalination units and cooling towers in various plants,$DI^{c}_{desal,j}$is the diameter of the pipe between desalination units and sinks, $DI^{c}_{i(p1),r}$ is the diameter of the pipe between sink i of plant p1 and central treatment units,

$DI^{c}_{r,j(p2)}$is the diameter of the pipe between central interceptor r of to sink j of plant p2, $DI^{c}_{i(p1),d}$ is the diameter of the pipe between sink i of plant p1 to decentral interceptor d , $DI^{c}_{d,j(p2)}$is the diameter of the pipe between decentral interceptor d of to sink j of plant p2. The capital cost is a function of the diameters of interconnecting pipes, which in turn is calculated based on the flow rate through the interconnection. The pipe Size (DI) is calculated as:

$$DI = 0.363((M)^{0.45} * \rho^{0.13}) \qquad (24)$$

This expression has been taken from Peters et al. [94], where M represents the volumetric flowrate given in m^3/s and ρ is the density of the stream. The pipe diameter obtained using the expression is rounded off up to one decimal place.

Treatment Cost:$C^{cap} * F^{treatment(k)} + C^{oper} * F^{treatment(k)}$. (25)

where C^{cap} is capital cost per m^3 of water treated and C^{oper} is operating cost per m^3 of water treated.

Freshwater Cost: $C^{fresh} * F^{freshwater}$ (26)

where C^{fresh} is cost per m^3 of freshwater.

4.3. Solver Development

Simulated Annealing (SA) and Tabu Search (TS) was chosen as the preferred algorithm as it has been proven to be robust across various fields. The benefit of developing a solver custom-built for the problem is it provides options for storing multiple solutions which help the user in understanding the complete picture across the solutions. Deterministic solvers provide only one solution at the end of the run and it doesn't help the user to understand variations across solutions. Also, it handles bigger size problem and nonlinearities quite effectively. To handle the complexities of the problem and to provide a complete picture of the system to the user, simulated annealing and tabu search based solvers have been developed. As mentioned in Section 2.5, SA and TS have been applied in chemical engineering in areas of molecular design and reaction network which were far more complex in terms of problem structure and size but the performance of this algorithm was found to be robust.

4.3.1. Solver Components

Figure 4.2 represents the major components that can be utilized in developing most of the metaheuristic-based stochastic solvers. It consists of mainly of a transition framework, a simulator module, feasibility testing module, evaluator for gauging the performance of the solution, metaheuristic principles integration toolbox that determines how the solution navigates from one solution to another based on specific algorithm rules and a termination toolbox that checks if the criteria for termination of the solver run is met. These components are an important part of developing solvers based on any meta-heuristic algorithm.

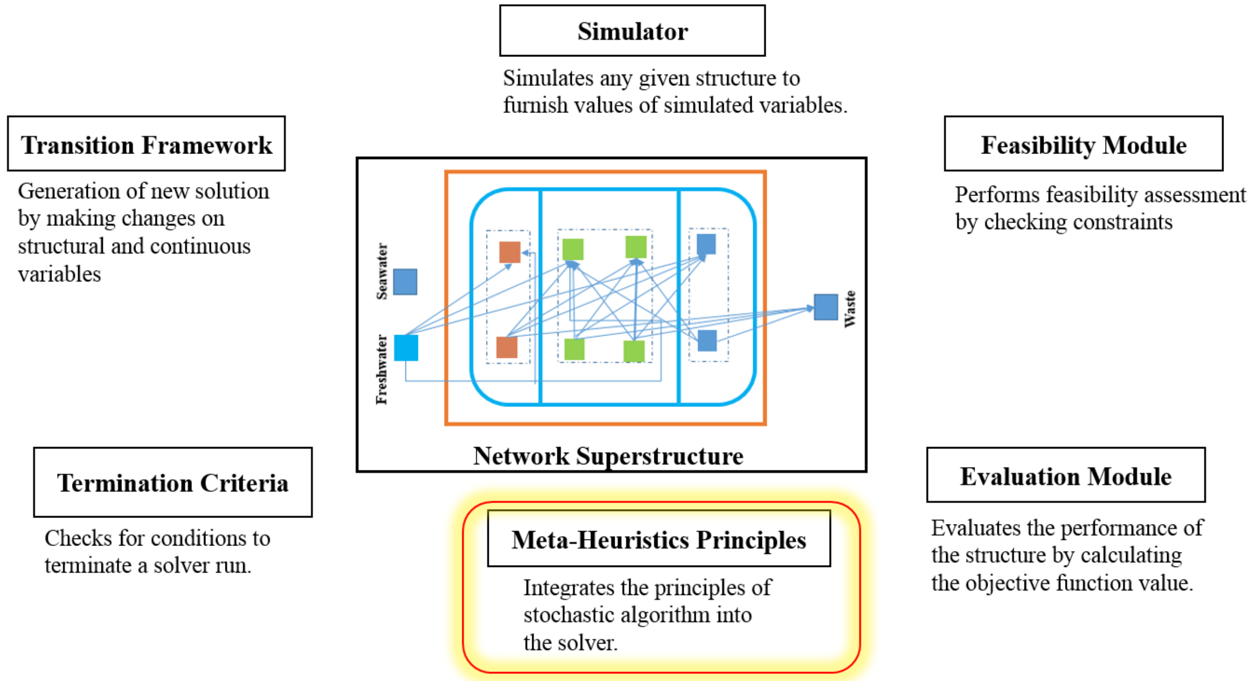

Figure 4.2 Solver Components

The architecture of the solvers utilizes all the above-mentioned components to develop solvers based on SA and TS. The metaheuristic module (highlighted in figure 4.2) is one of the most important components of the search. It guides the solver and its principles enable the solver in decision making in moving from one solution to another during the search This module varies for different algorithms and in essence integrates the principles of the metaheuristics with the solver.

SA and TS have simple philosophies and have performed robustly across optimization problems in different fields. Apart from that, they can be parallelized to enhance the speed of the solution search. Though there is a SA toolbox available in Matlab, it lacks the capability to incorporate constraints and store multiple solutions. The solver developed overcomes these limitations and is custom-built to solve the water network optimization problem. The solver has a modular structure thereby providing the user the flexibility to expand and integrate other resource networks (Energy, CO_2, H_2) as well.

Both SA and TS solver starts with an initial structure. This can be anything specified by the user. One of the common initial solutions is supplying all the sinks with freshwater and discharging all the water from sources to the environment. On this initial structure, various moves are made using a transition framework thereby generating a new solution. The new solution is then simulated and the flows are then evaluated using the evaluation subroutine. The evaluation here refers to the new flows being feasible and the calculation of objective function value. After the evaluation subroutine, the search is guided by algorithm-specific rules that are different for SA and TS. The solver then checks if the termination criteria have been met or not. Meeting of criteria means termination of the run else, the solver goes back to transition framework generating and evaluating new solutions. Subsequent subsections describe the elements in detail.

4.3.2. Transition Framework

During the search across solution space, new solutions are generated by successive transition from current state S^b to a new state S^* in its neighborhood ($S^* \in N(S^b)$). This is achieved by performing different transitional moves on the structure. These are performed randomly on any of the various connections in the superstructure, which have been characterized as adjustables i.e. their values can be modified along with the search and are not calculated using the simulation module.

Based on the nature of the moves, they have been broadly divided into two categories:

- Structural Transitions

- Redistribution Transitions

Figure 4.3 shows different kinds of transitions under these classes. Structural transitions refer to changes that alter the structure of the existing solution state by adding, deleting or reconnecting a stream. Redistribution transitions change the flowrate in the current structure.

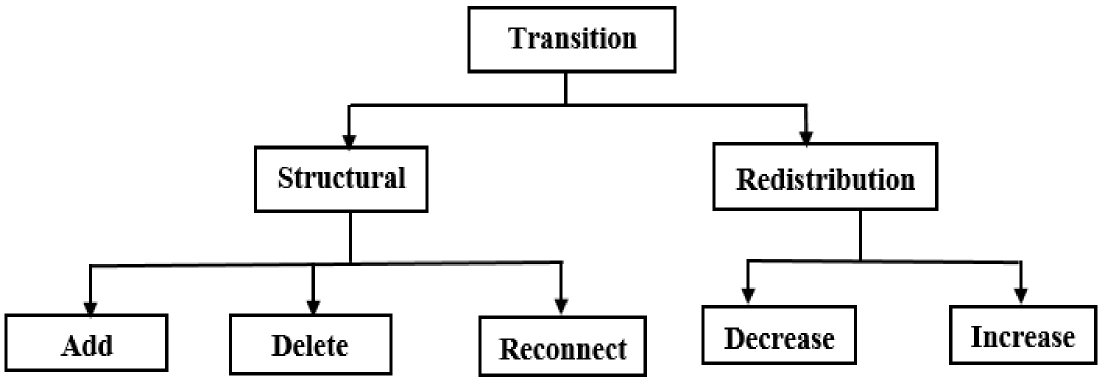

Figure 4.3 Structural and Redistribution Transitions

These transitions are performed on the connections between source to treatment units and sinks and connections between treatment units and sinks. Figure 4.4 represents the matrix form in which these connections have been modeled for the search. Modifications are carried out on these variables using the transition framework.

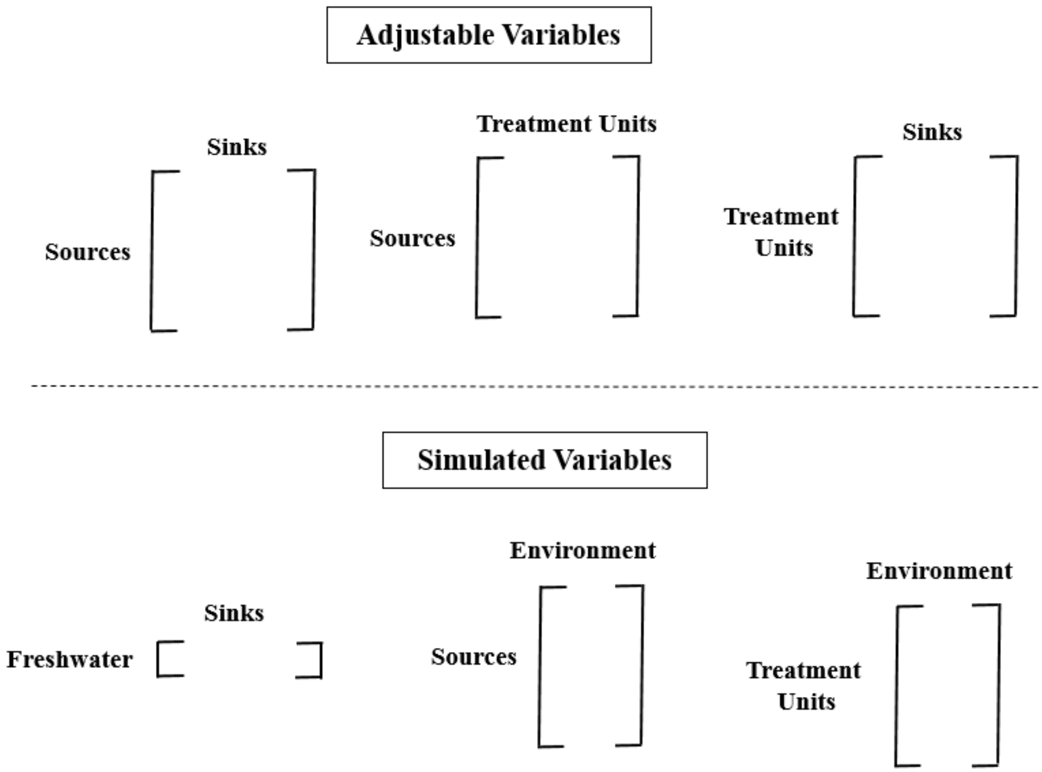

Figure 4.4 Adjustable & Simulated Variables for Transition Framework

The variables have been divided into two categories:

- Adjustable Variables
- Simulated Variables

Adjustable variables are the ones that can be altered by the transition module to generate new solutions. These variables include connections from sources to sinks, sources to treatment units and treatment units to sinks. These three groups of variables have been represented in the form of a matrix in the solver code and these matrices are operated upon by transition framework to navigate the solution space. A connection can be added, deleted or reconnected or the values of flowrate redistributed in these matrices to generate a new solution

The second set of variables namely the simulated variables includes the flows of freshwater to sinks, discharge of sources to the environment and discharge of treatment units to the environment. These variables are not operated upon by transition variables but are calculated using the equations of the optimization model using the simulator module. The adjustable and simulated variable has been defined in a way that the degree of freedom of the mass balance equations is zero and there is no chance of failure of the simulation module. Figure 4.5 presents the classification of flows into the above-mentioned categories.

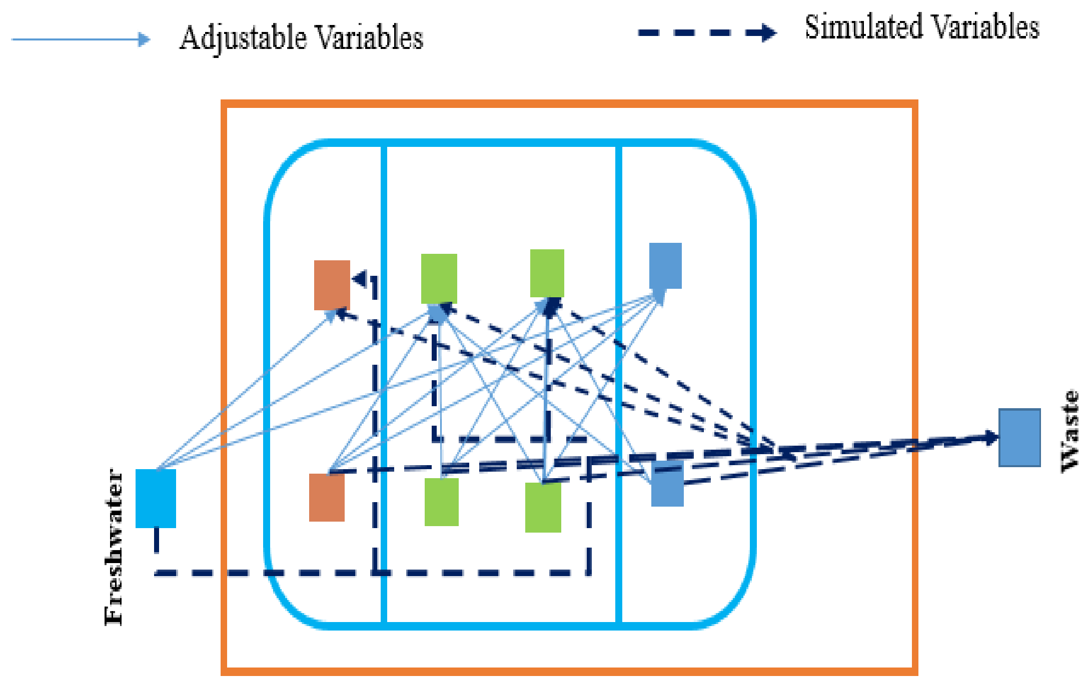

Figure 4.5 Classification of flows

The next section describes the algorithm for carrying out the structural and redistribution transition on the adjustable variables.

4.3.2.1. Structural Transition

Structural transitions are classified into three kinds of moves:

- Add
- Delete
- Reconnect.

Add: Figure 4.6 explains the algorithm for add move. In this move, the new connection is added at the selected adjustable variable.

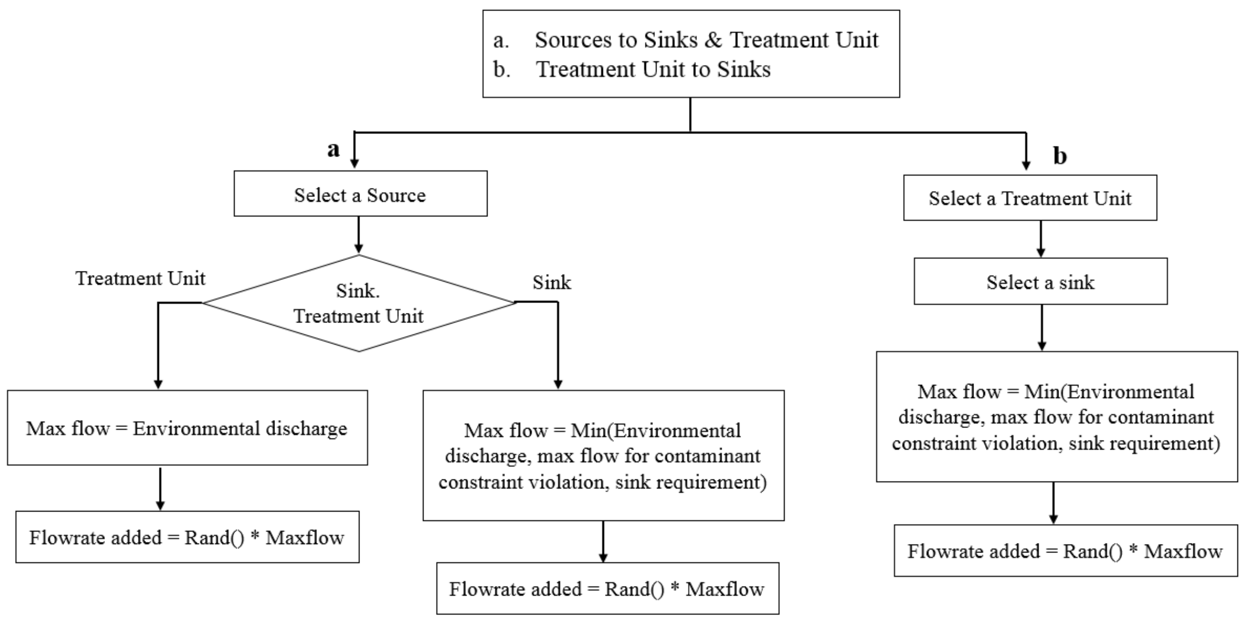

Figure 4.6 Add subroutine

When a connection is being added, the first step is to select the type of variable where it is to be added namely sources to sinks & treatment units and treatment units to sinks. Once the variable matrix is decided, the source or treatment unit is selected in those matrices. After the selection, a decision is made about the second point of the connection. It can be a sink or a treatment unit visit zero flowrate and is selected randomly. The maximum value that this connection can accommodate is calculated and a value between zero and this maximum value is added to the new connection.

Apart from the add move, there is add with redistribution move. The algorithm is almost similar to that of add subroutine except for the fact that flow added to the new connection comes from one of the existing connections.

The remaining algorithm for delete and reconnect moves are given in Appendix B.

4.3.2.2. Structural Transition

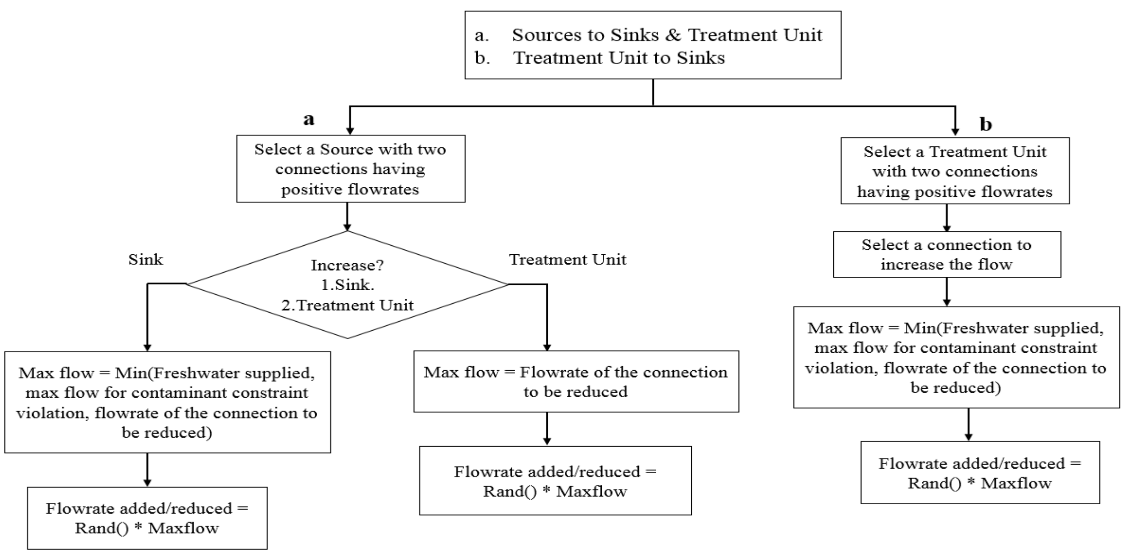

Figure 4.7 Redistribution Subroutine

The redistribution subroutine keeps the structure of the network intact and alters the flowrate. Two non-zero connections are selected in a matrix (randomly selected) and the flows are redistributed across them with flowrate increasing in one and decreasing in other to maintain the balance across the selected source or treatment unit. As a result of this perturbation, the freshwater requirement at sink changes. Figure 4.7 presents the algorithm used in executing this move. The algorithm description of other moves has been provided in Appendix A.

4.3.3. Simulation Module

The simulation module has been designed keeping the degrees of freedom of the equations zero. This ensures that it doesn't fail in any scenario. After generating the new solution which contains flowrates from sources and treatment units, values of remaining connections are calculated. As defined earlier, the flowrates from sources to sinks & treatment units, from treatment units to sinks, flowrates of waste heat for steam exchange, flowrates of waste heat for power exchange (generated using decentral generation units)are used to calculate the simulated variables. Simulated variables are the ones on which the search scheme cannot apply transitions as discussed earlier. Their values change due to change in values of adjustables (variables where perturbations are made). The variables simulated are as follows:

- Flowrate of freshwater to Sinks.
- Flowrate of wastewater discharge to the environment from different sources.
- Flowrate of wastewater discharge to the environment from treatment units.
- Amount of waste heat discharge using cooling options

The simulated variables are connected to the adjustable variables through the mass balance equations [1] – [13]. To demonstrate the functioning of the simulation module, equation 1 has been taken as an example.

$$F_i^{Process} = \sum_j F_{i,j} + \sum_d F_{i,d} + \sum_r F_{i,d} + F_{i,env} \quad (27)$$

This equation represents the mass balances at the sources. Here total flowrate from the sources ($F_i^{Process}$) is a constant and is presented in red color. The three variables in blue color scheme (flow from sources to sinks and from treatment units to sinks) are adjustables. These are the values that change as they are subjected to transition framework. Due to these changes, the value of flowrate from sources to environmental discharge ($F_{i,env}$) changes and is simulated using the above-mentioned equation. The simulated variables have been represented in green font. All the intermediary variables have been represented in black font.

The same can be applied for other mentioned simulated variables. The adjustables are chosen in a way that the simulated variables are the part of a set of linear equations. Also, the number of simulated variables is equal to the number of these linear equations. This ensures that there is no failure of simulation to converge and it gives a unique solution every time the simulation is run. Using the values obtained after simulating the given set of adjustables, the new structure is checked for constraints and its performance is evaluated. Equations 28 to 39 present the working of the simulator.

$$F_{j(p2)}^{Process} = \sum_i F_{i(p1),j(p2)} + \sum_d F_{d(p1),j(p2)} + \sum_r F_{r,j(p2)} + F_{j(p2)}^{Freshwater} \quad (28)$$

$$F_{d(p2)}^{in} = \sum_i F_{i(p1),d(p2)} \quad (29)$$

$$F_{d(p2)}^{out} = Recovery_{d(p2)} * F_{d(p2)}^{in} \quad (30)$$

$$F_{d(p2)} * C_{d(p2)}^{in} = \sum_i F_{i(p1),d(p2)} * C_{i(p1)} \quad (31)$$

$$F_{d(p1)}^{Out} = \sum_j F_{d(p1),j(p2)} + F_{d(p1),env} \quad (32)$$

$$F_r^{in} = \sum_p \sum_i F_{i(p1),r} \quad (33)$$

$$F_r^{out} = Recovery_r * F_r^{in} \quad (34)$$

$$F_r * C_{cn,r}^{in} = \sum_p \sum_i F_{i(p1),r} * C_{cn,i} \quad (35)$$

$$F_r^{Out} = \sum_p \sum_j F_{r,j(p2)} + F_{r,env} \quad (36)$$

$$C_{cn}^{out} = (1- RR_{cn}) * C_{cn}^{in} \quad (37)$$

$$F_{env} = \sum_p \sum_d F_{d(p1),env} + \sum_r F_{r,env} + \sum_p \sum_i F_{i(p1),env} \quad (38)$$

$$F_{env} * C_{cn,env} = \sum_r F_{r,env} * C_{cn,r}^{out} + \sum_p \sum_i F_{i(p1),env} * C_{cn,i} + \sum_p \sum_{d(p1)} F_{d,env} * C_{cn,d}^{out} \quad (39)$$

4.3.4. Evaluation Module

After the new structure has been generated and simulated, it is checked whether the solution obtained is feasible or not. The set of equations [14] – [22] defines the feasibility constraints of the optimization problem. These include constraints imposed on contaminants at sinks and the environment and the maximum allowable flowrate at various connections. If the constraints are satisfied, the value of objective function is calculated using equation [23].

4.3.5. Meta-Heuristic Principles

This module guides the search and provides the solver the direction to navigate through solution space. The decision to move from the current solution to the newly generated solution (by the transition framework) is made through this module. Different stochastic algorithms have different search guidance principles. Simulated Annealing utilizes Metropolis-Hastings criteria which makes the solver accept any improving solution straightaway but non-improving solutions may also be accepted based on probability. Decisions in Tabu Search are based on a set of metaheuristic principles. In Particle Swarm Optimization, the search moves towards a better performing solution. The same applies to Ant Colony Optimization where the search starts from the same point but the solver tends to go towards the better performing solution with different points communicating with each other. Genetic Algorithm utilizes metaheuristics of the bioinspired phenomenon of selection, mutation, and crossover and tends to move towards a better solution.

4.3.6. Termination Criteria

This module enables the solver to terminate its run once conditions for termination are satisfied. These conditions can be the total number of states evaluated, the time of the run, the total number of non-improving solutions evaluated or other specific parameters of the algorithm. For Simulated Annealing, the following conditions for termination of search are checked.

1. The annealing temperature falls below 0.
2. The number of not improving transitions exceeds more than a k^{max} . (3000 in this work).

For Tabu Search, the following termination criterions are checked:

1. Number of non-improving state visits should be 3000.
2. Total number of states evaluated should be a maximum of 150000.

4.4. Meta-Heuristics Selected: Simulated Annealing & Tabu Search

4.4.1. Simulated Annealing

Simulated Annealing is probabilistic that incorporates the concepts of artificial intelligence by mimicking the process of annealing. It has been used extensively to solve chemical engineering problems like reaction networks (Mehta & Kokossis[95],Cordero et al[96]),flowsheet optimization(Palmer & Realff[97],Weizhong et al[98]), Plant Layout Optimization(Alves et al[99]). SA reproduces various stages of the actual annealing process to find an optimum solution.

Annealing as a process brings down the molecules of a substance to their lowest energy state. A heated body has its atoms in various configurations each corresponding to a certain energy state. Heated atoms move freely and can attain any energy state. As the temperature decreases slowly, the mobility of the atoms is lost and they move to lower energy state after recalibrating at new temperature. The energy distribution of atoms becomes narrower and at T=0, it becomes the lowest when the system is completely frozen with all the atoms in their lowest energy state. It should be noted that to reach the lowest energy state, the cooling should be slow. Rapid cooling to T=0 can freeze the system anywhere between the state it occupies at high temperature to the state and the energy of the frozen state. This would mean that instead of getting a globally optimal solution, there is a high probability of getting a local optimum solution. Therefore, enough time must be given to the ensemble for cooling and recalibration.

In the water network problem, the system is allowed to attain all the states with equal probability. Starting from the initial state, transitions are made to a new solution and the system is allowed to move towards better and deteriorating states. As soon as a better state is encountered, the system moves towards it but the low-performance states are not rejected outright. They are accepted with a probability and it decreases as the system cools down further making it tougher for the system to move to low-performance states that in turn force it to move towards better states even though it is allowed to attain an inferior solution. At each temperature, the system is allowed to undergo random and reversible changes systemically for it to equilibrate. The phenomenon of equilibration at various temperatures is mimicked by incorporating the concept of Markov Chain.

Various cooling schedules have been proposed for reducing the temperature and a choice has to be made between speed and chances of getting a global solution. Theoretically, if a system is given an infinite amount of time to cool, it will attain a global optimum. Similarly, if it is allowed to undergo a very large number of transitions at various temperatures (very large Markov chain), the search will be more exhaustive. In reality, the solution time and Markov chain length are finite. So, a judicious choice has to be made about the cooling schedule and the

Markov chain length. The cooling schedule should not be too slow to take very long times and not too rapid to converge prematurely to a local optimum. In the same fashion, the Markov chain should not be too small which would mean incomplete coverage of solution space or too long which would slow down the search.

4.4.1.1. SA based Solver

Figure 4.8 presents the schematic of SA based solver. Both solvers start with an initial feasible solution that facilitates the generation of new structures by applying various transitions. For the water network problem, a simple initial solution is a linear structure in which all the contaminated water from the sources are discharged into the environment and the requirements of sinks are fulfilled by the usage of external supply of freshwater. The values of freshwater and environment discharge are then calculated using the simulator module

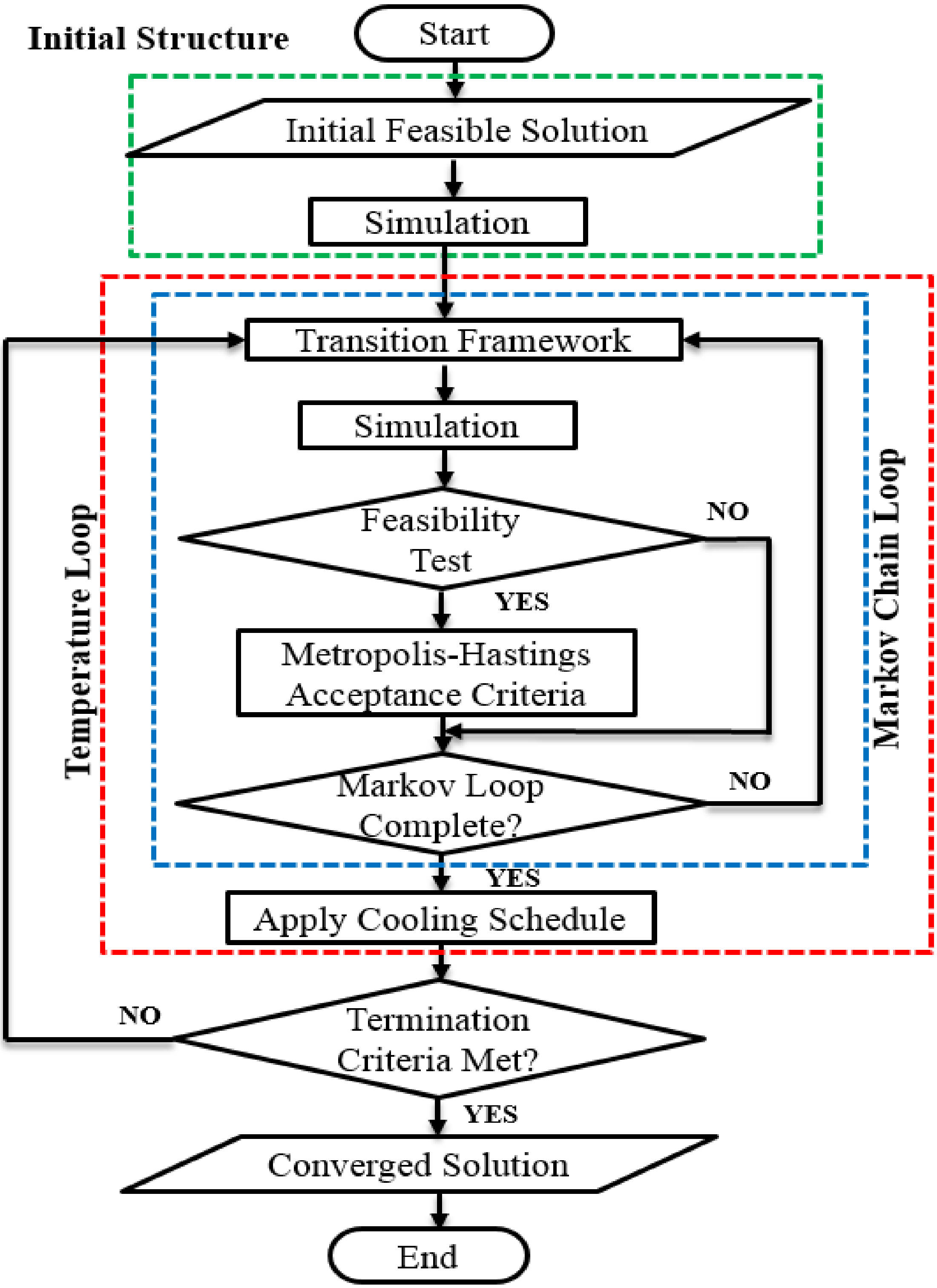

Figure 4.8 Schematic for SA solver

The aim of the SA scheme is an optimization of function J(S) over the domain D. Here D represents the set of various network structures that can be generated. An initial feasible solution, S^i belonging to set D, is provided and evaluated. After this, a new solution S* is generated (new design framework of the superstructure) in the neighborhood of the initial solution, $N(S^i)$. The process of generating solutions is probabilistic in nature in order to ensure a thorough search. The new solution now generated is evaluated for feasibility. If the new solution is feasible, the criteria for it to be accepted is checked. The solution remains the current state unless a new solution, which meets the acceptance criteria, is generated. To represent the calibration of the system at a particular temperature, the system undergoes a homogenous Markov chain of state transition in isothermal condition. This process is executed iteratively until the termination criteria are met and an optimal solution has been found (state corresponding to the zero energy state or perfect crystal).

The acceptance criteria is based on temperature and the difference between the objective function of the current state and the new solution(J(S*)-J(s)). The original Metropolis-Hastings acceptance criteria P(S*) has been applied in this work. If a solution generated is feasible and better than its predecessor, it is selected with a probability of 1. If it is of similar quality or worse than the current solution, it is accepted with a probability that is a function of temperature and objective function.

$$P(S^*) = \min\{1, \exp(-\frac{\Delta J}{T})\} \tag{40}$$

This acceptance criterion ensures that the search is biased towards a better solution as the acceptance probability for them is 1. It also allows the system to attain even worse states to explore the solution space. As the search progresses, it becomes tough for the system to move to a worse state as is evident by the expression.

After the Markov chain transition has been performed, the temperature in search is decreased using a cooling schedule. To mimic the process of cooling as the search progresses, a cooling schedule is introduced in the framework. The temperature decrease can be rapid in initial stages as equilibration is easy. It can rapidly cool down to freezing temperature range where slow cooling is required. To implement such behavior, a logarithmic cooling schedule suggested by Aarts and Van Laar [100] has been applied.

$$T_a^{n+1} = T_a^n \left[1 + \frac{T_a^n \ln(1+\gamma)}{3\sigma^n}\right]^{-1} \quad (41)$$

Here T_a^n is the current temperature, γ is the parameter that helps to control the cooling and σ^n is the standard deviation of the objective value across the Markov length.

After the temperature is reduced as per the cooling schedule, the criteria for termination of a run is checked. If the termination criteria are met, the solver ceases its search and returns the final solution else it goes back to transition module generating and evaluating new solutions.

4.4.2. Tabu Search

The word tabu (or taboo) comes from Tongan, a language of Polynesia, where it was used by the aborigines of Tonga Island to indicate things that cannot be touched because they are sacred. Apart from Simulated Annealing, Tabu Search has also been examined to test the effectiveness of the stochastic algorithm in solving the combined water-energy nexus problem.

Tabu Search is a metaheuristic-based algorithm which is based on an enhanced search around a solution. The embedded heuristic of the algorithm prevents the solver from getting stuck around a solution (cycling) which in turn enables it to conduct a thorough search of solution space. This method was developed by Fred C Glover in 1986. To solve a problem, which is larger and far more complex, stochastic algorithms were selected as the basis of the solver as they have been found to perform robustly for other optimization problems.

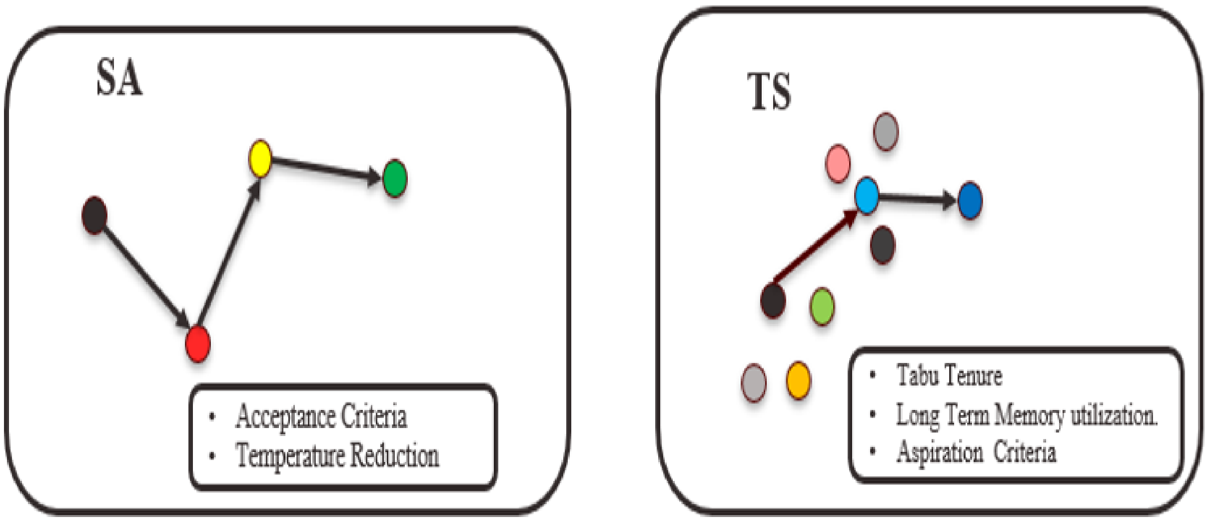

Figure 4.9 SA vs TS

Figure 4.9 shows a contrast between the two search techniques. While simulated annealing mimics the phenomenon of annealing process and explores the solution space based on the performance of the current solution and extent of the search, Tabu Search employs metaheuristics and search memory information thereby incorporating concepts of artificial intelligence.

Both algorithms employ a modular approach and the simulation, evaluation and solution generation platform is compartmentalized into different subroutines enabling the user to solve more complex and bigger problems. Unlike deterministic solvers provide only one solution at the end of the run, the solver developed using both these algorithms store multiple solutions that allow us to evaluate multiple solutions with similar performance.

4.4.2.1. SA based Solver

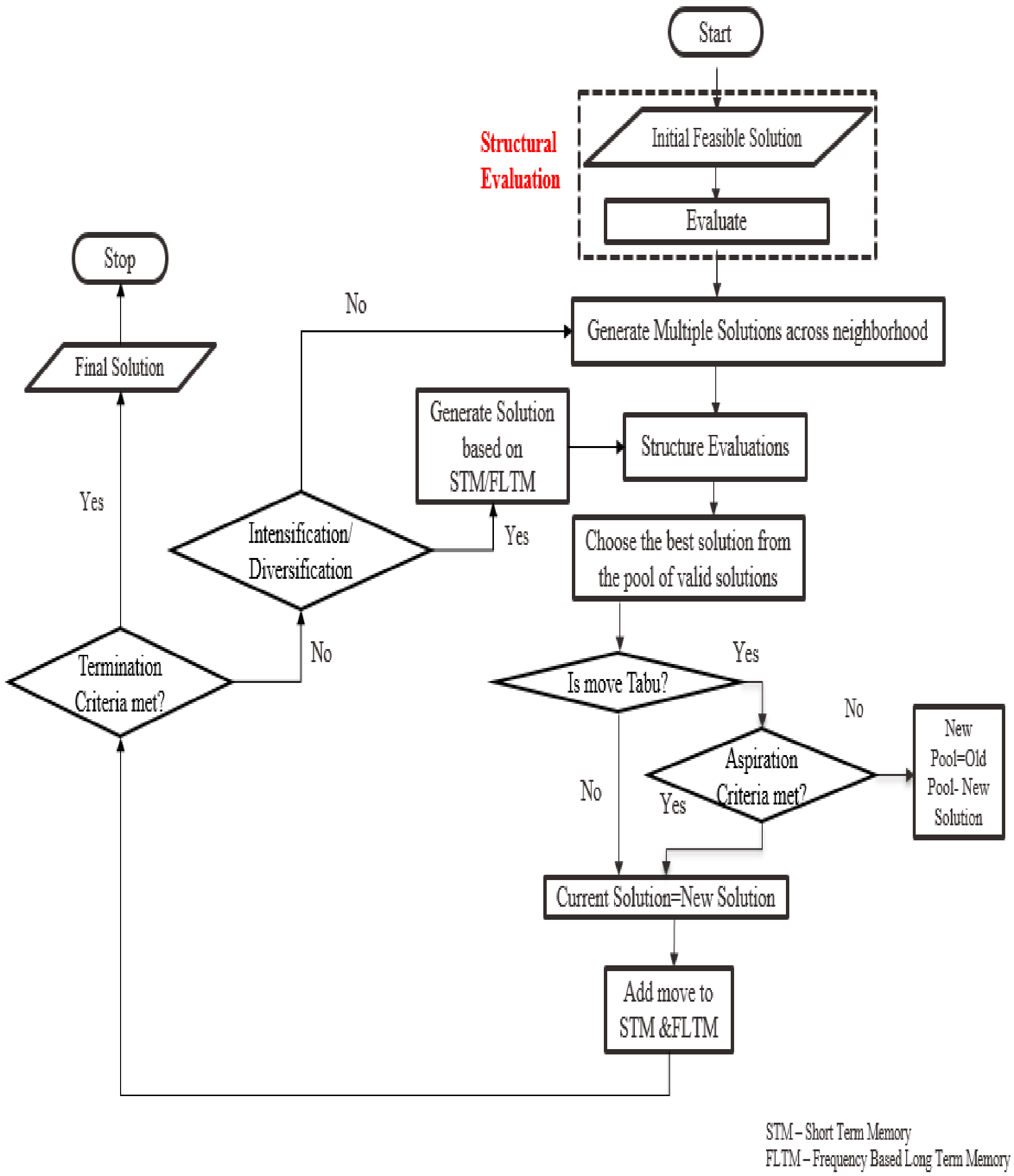

Figure 4.10 Schematic of Tabu Search Solver

Figure 4.10 shows the flow diagram for the Tabu Search solver. Most of the elements of this schematic are the same as that of SA as the initial structure, transition framework and simulation module stays unchanged except for the module where TS solution search principles are integrated into the solver thereby providing it with a different approach to navigate through the solution space.

As in the case of SA, the TS also starts with an initial structure on which changes are made by the transition framework to generate new solutions. The new solutions are simulated using the simulation module and the entire structure is then evaluated by checking for constraints and then calculating the objective function if the constraints are satisfied. After these steps, the solver implements the TS rules for the solution search.

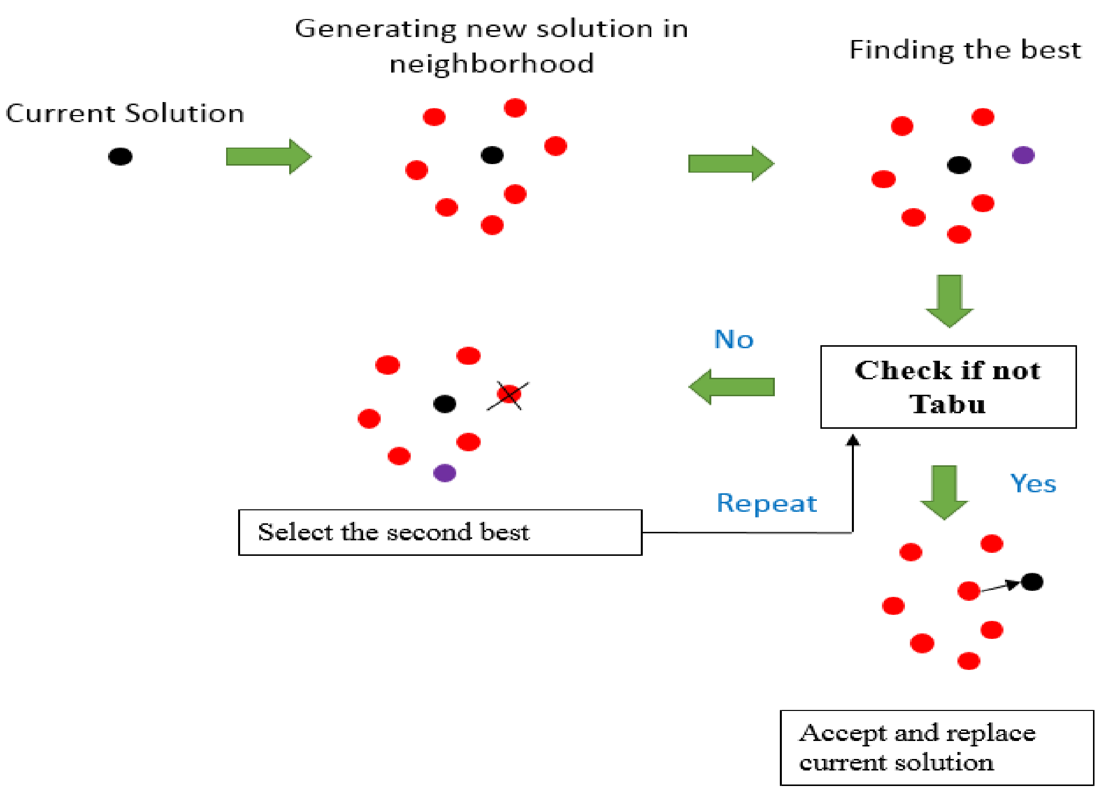

Figure 4.11 Tabu Search Transition

Figure 4.11 shows a Tabu Search transition from one solution to another in its neighborhood. Before the transition is allowed to be made, the following rules are followed:

- The transition should be allowed in this move (non-tabu).
- The solution selected should be the best in the neighborhood.
- If the best solution obtained is obtained due to a tabu move, the non-tabu move criteria can be relaxed (Aspiration Criteria).
- The search can also look into areas which have been frequently visited and given better solution (intensification) or areas which have been visited less (diversification)

Once a move has been made to generate solutions in the neighborhood, it becomes tabu for a certain period called tabu tenure. The tabu can be defined as prohibition in making changes to a particular aspect of solution or prohibiting a particular way to make changes in the solution.

All valid solutions from the neighborhood ensemble are evaluated and the design instance giving the best performance is scrutinized. If the move associated with its generation is not tabu, this solution becomes the current solution. The information about these tabu or non-tabu status of a move is stored in a circular list called tabu list. If a transition appears on this list, it stays there for a certain number of transitions during which it cannot be applied. This phase is called tabu tenure. TS uses the data stored in the short-term memory (STM) to execute this feature.

If the move is tabu, then we apply the above-mentioned criteria for the second-best solution. However, if the tabu move leads to the generation of better-performing solutions than the current state, this criterion is relaxed and the new solution becomes the current solution. This feature of tabu search is called aspiration criteria and enables the solver to get out of a solution if it gets stuck. The search is provided flexibility in exploring the solution space by not making the tabu criteria rigid in every case. If a better solution can be obtained by a transition that is prohibited during that particular search period, the tabu criteria can be relaxed and the newly generated solution becomes the current solution.

Apart from this, the search employs knowledge obtained through the database that stores the search history. It utilizes the knowledge obtained from Long Term Memory (LTM) during the search to shape a more efficient and thorough examination of the solution space. Intensification allows the solver to explore those regions that have given the promising solution. The information extracted from the search memory directs the solver to those regions and help zero in on good solutions. In this implementation, the solver checks which connections have given better performing solution and explore the region around those connections for intensification.

Apart from exploring the better performing region, the solver also searches around less-visited regions which have given fewer promising results. This feature is called diversification. The search is biased towards diversification to ensure a thorough search. This is done by using a modified objective function during performance comparison.

Modified Objective = Objective evaluated + k (Frequency of the connection perturbed). The modified objective penalizes intensification and encourages diversification.

Termination of the search requires the meeting of user-defined criterions. These can be the amount of time dedicated, number of non-improving moves, the number of states evaluated, etc. Once the termination criteria are met, the search freezes at the optimal solution.

4.5. Solver Development

This solver has been developed in MATLAB as the programming language on a laptop with the Intel Core i7 Duo processor, 16 GB RAM, and a 64-bit Operating System. The components needed to develop the solver can be coded in any other programming language as well. Separate subroutines have been coded for implementing various moves and for calculating objective function and checking constraints and these modules have been then placed as per the SA and TS solver algorithm explained in section 3.2 and 3.3. Several runs have been conducted for Markov chains of different length to study the behavior of the solver to change in parameters.

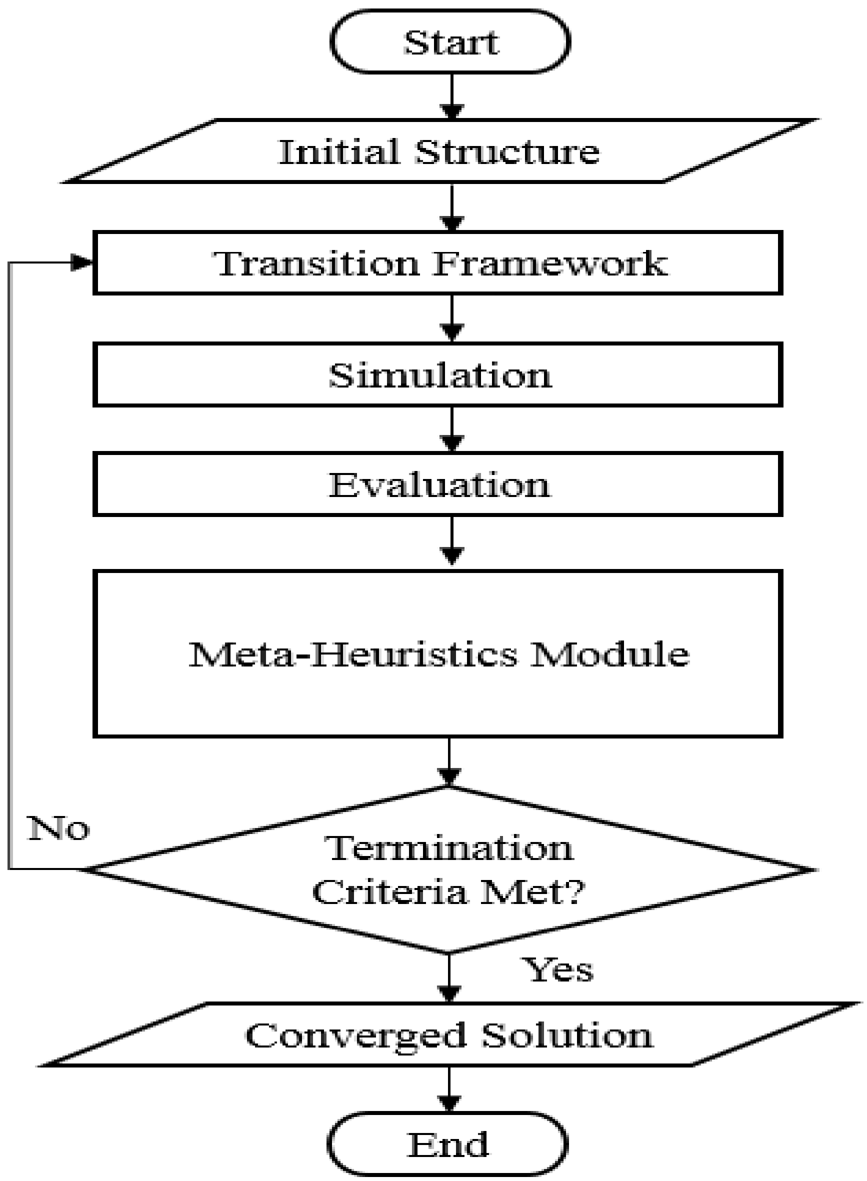

Figure 4.12 Solver Architecture

4.6. Case Study

The case study has been adapted from Fouladi [93] has been utilized to demonstrate the performance of the solvers. There are 11 sources, 9 sinks and 4 contaminants namely Total Dissolved Solids (TDS), Organics, Ammonia and Nitrogen have been considered in the system. In all case studies, the values of a,b and ρ are set to 696.58, 1.215 and 1000 kg/m^3 respectively. H_y is set to a value of 8760 h/y and the cost of freshwater C^{fresh} is set as $1.48/ton. Flowrate, concentration, and removal ratios data have been taken from various sustainability reports and open-source data. The case study input data are presented in Appendix A.

The data consists of source and sink flowrates and concentration, information about the treatment unit and the layout of the Eco-Industrial City. The case study presented in this work to demonstrate the application of SA on the water network integration problem consists of Methanol (600000 mtpy), Ammonia (2500 mtpd) and Gas to Liquid (50600 bblpd) plants. Four major contaminants namely TDS, Organics, Ammonia, and Nitrogen are present in the water streams. Water is discharged from sources like offices, reformers and other process streams where it gets produced. There is the requirement of water at these process facilities and offices. These constitute the sinks inside the plant. Freshwater is supplied externally. There are decentral treatment facilities at each plant and a central treatment facility located away from them. Each of these houses three different kinds of technologies namely Nano-filtration (NF), Reverse Osmosis (R.O), Dissolved Air Floatation (D.A.F) and a combination of NF & DAF. The brine generated at these units is taken care of by external authority. Freshwater supply and wastewater discharge piping are also the responsibility of external authority.

The solution obtained has been compared with the linear structure in which all the wastewater is discharged into the environment. Tables 4.1 to 4.5 presents the data for the case study. The units for contaminants is parts per million (ppm).

Table 4.1 Source Data

Sources	Flowrate(t/h)	TDS	Organics	Ammonia	Nitrogen
P1S1	1.875	50	4	1	50
P1S2	6.41	2500	20	2.5	25
P1S3	16.67	550	15	25	40
CT1	101.54	1000	20	2.5	25
P2S1	11.71	500	100	0.5	5
P2S2	4.79	2500	20	2.5	25
P2S3	20.83	550	15	25	40
CT2	45	1000	20	2.5	25
P3S1	693.68	500	46.3	0.5	5
P3S2	6.13	550	15	25	40
CT3	421.1	1000	20	2.5	25
Fresh Water	-	200	4	0.5	5

Table 4.2 Sink Data

Sources	Flowrate(t/h)	TDS	Organics	Ammonia	Nitrogen
P1D1	107.12	500	4	0.5	21
P1D2	35	200	4	0.5	5
CT1	474	200	4	0.5	5
P2D1	79.67	500	4	0.5	21
P2D2	20.83	200	4	0.5	5
CT2	210	200	4	0.5	5
P3D1	296.45	500	4	0.5	21
P3D2	6.79	200	4	0.5	5
CT3	1965.42	500	4	0.5	5
Env	-	1500	46	3	100

Table 4.3 Treatment Cost Parameters

	Recovery (%)	Oper ($/ton)	Cap ($/ton)
NF	0.9	0.0869	0.1847
RO	0.9	0.1809	0.5277
DAF	0.9	0.374	0.5385
NF+DAF	0.81	0.4609	0.7232

Table 4.4 Removal Ratios

	TDS	Organics	Ammonia	Nitrogen
NF	90	75	66.7	95
RO	99.4	95	80	80
DAF	0	90	99	94
NF+DAF	90	97.5	96.6	97.6

Table 4.5 Freshwater & Seawater Cost

Water Type	**Cost ($/m3)**
Freshwater	1.48
Sea Water	0.02

4.7. Results

The case study has been run multiple times across various Markov chain lengths and neighborhood sizes for both SA and TS solver. This has been done to test the robustness of the search technique and to demonstrate the importance of the appropriate length of the Markov chain. Figures 4.13 & 4.14 presents a comparison of one of the solver runs for both SA and TS solver. Both the solvers converge to the optimal solution (with similar performance) asymptotically.

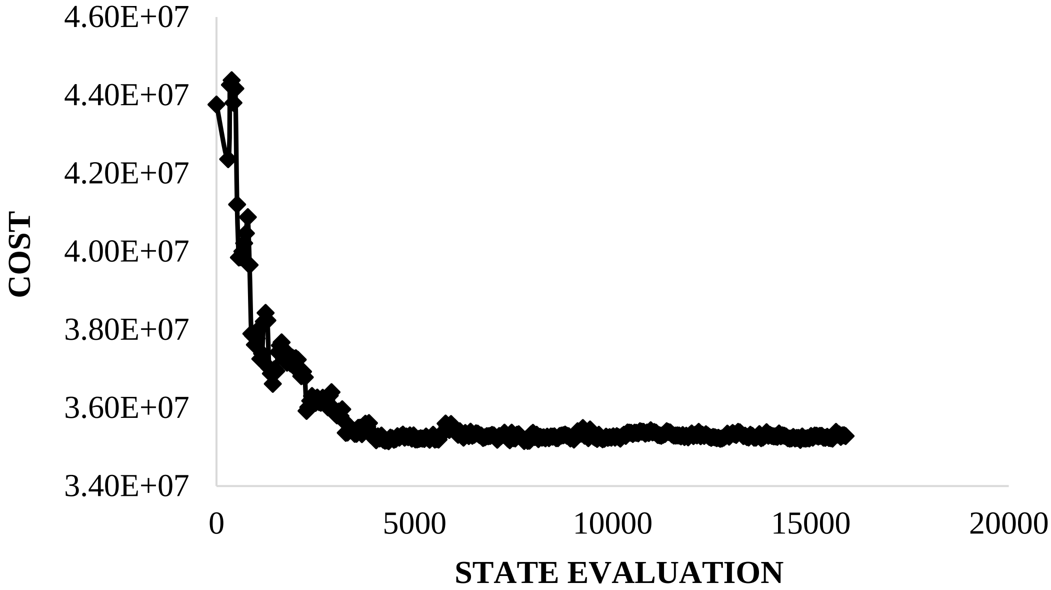

Figure 4.13 Asymptotic Convergence of SA solver

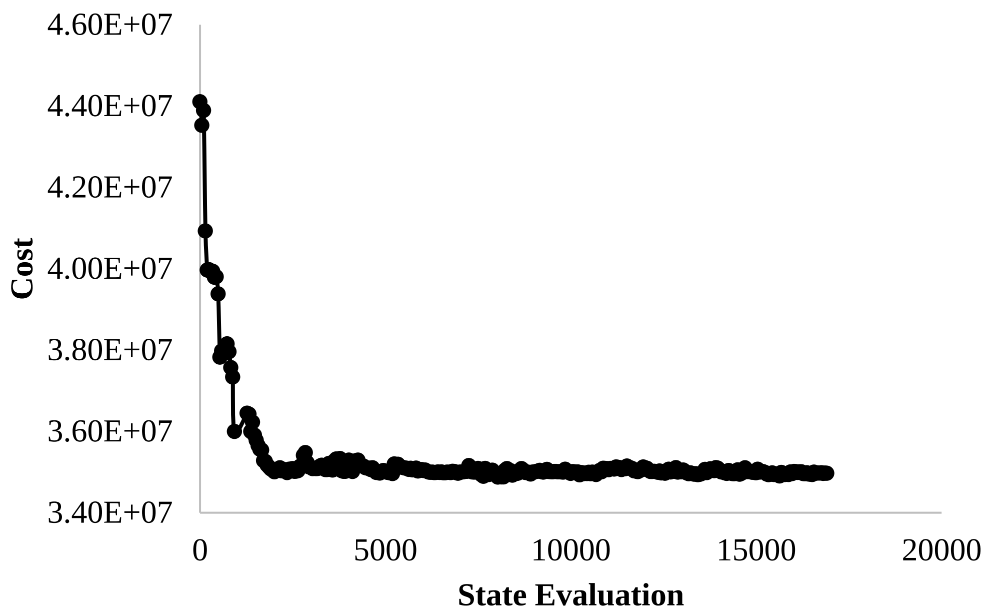

Figure 4.14. Asymptotic Convergence of TS solver

Figure 4.15 shows how the value of average, minimum and maximum for 10 runs varies with Markov chain length for SA solver and figure 4.16 presents the same data for TS solver for neighborhood size varying from 40 – 100. In case of shorter chain, the system is not allowed enough perturbation to explore its neighborhood. Therefore, the performance of the solution increases with the chain length.

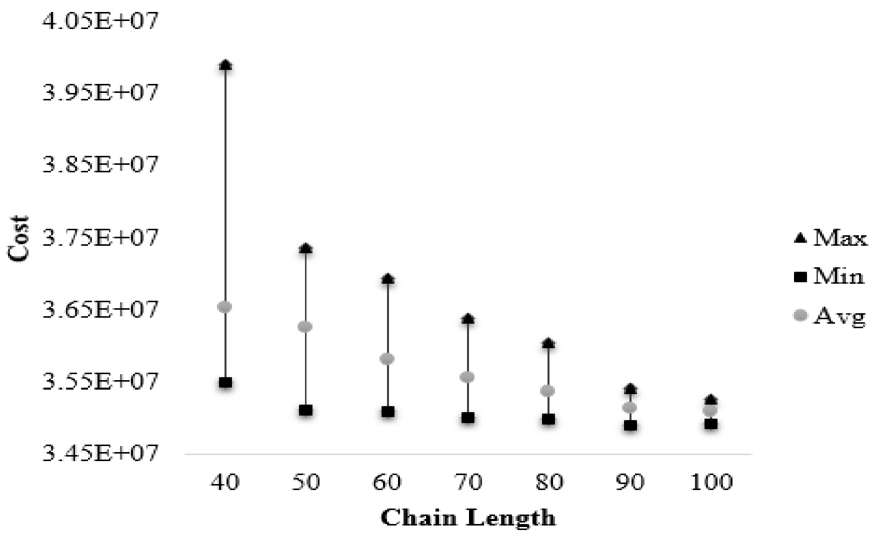

Figure 4.15 Objective Function Vs Chain Length (SA)

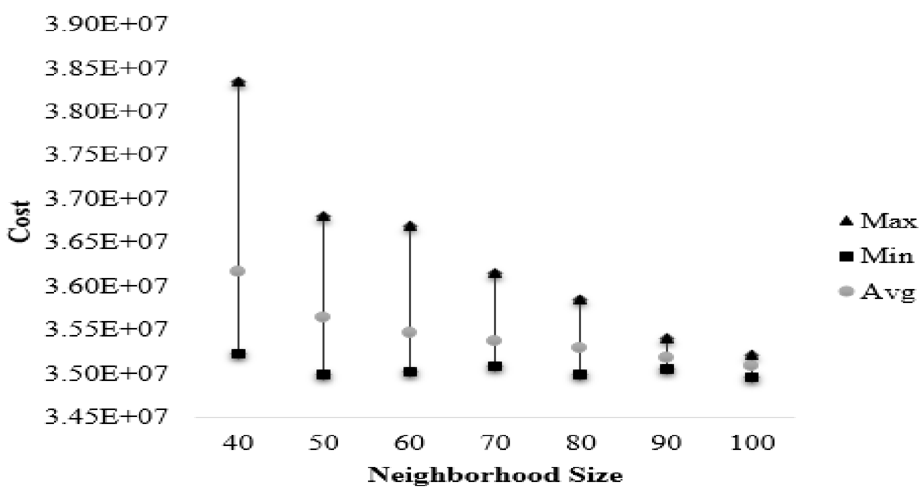

Figure 4.16 Objective Function vs Neighborhood Size (TS)

A similar observation is noticed for standard deviation as well. For each chain length, the solver is run for ten times and a standard deviation across the objective values is calculated. The standard deviation across the runs decreases with an increase in the chain length. This again is attributed to the fact that increased chain length allows for a more thorough search and thereby the solver converges to similar values across different runs. Figure 4.17 depicts this behavior across the chain/neighborhood size. 40 – 100 for SA and TS.

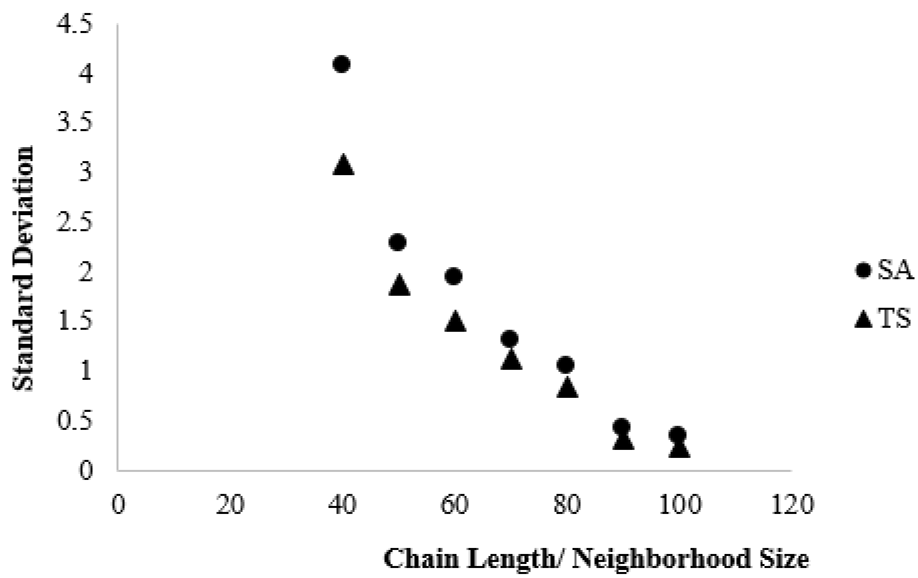

Figure 4.17 Standard Deviation vs Chain / Neighborhood Size

In both cases, the standard deviation decreases with an increase in chain size. However, for smaller chain sizes, TS has better performance than SA but as the chain /neighborhood size increases, they show a similar degree of robustness.Figure 4.18 represents the variation of state evaluation with chain length. For both SA and TS solver, the state evaluation increases with an increase in chain size. When a comparison is made between SA and TS, TS converges to an optimal solution faster than SA. Figure 4.19 shows the variation of standard deviation with state evaluation. In both cases, the standard deviation decreases with increasing chain/neighborhood size. When compared between the two, TS provides a more robust search with lesser state evaluations than SA.

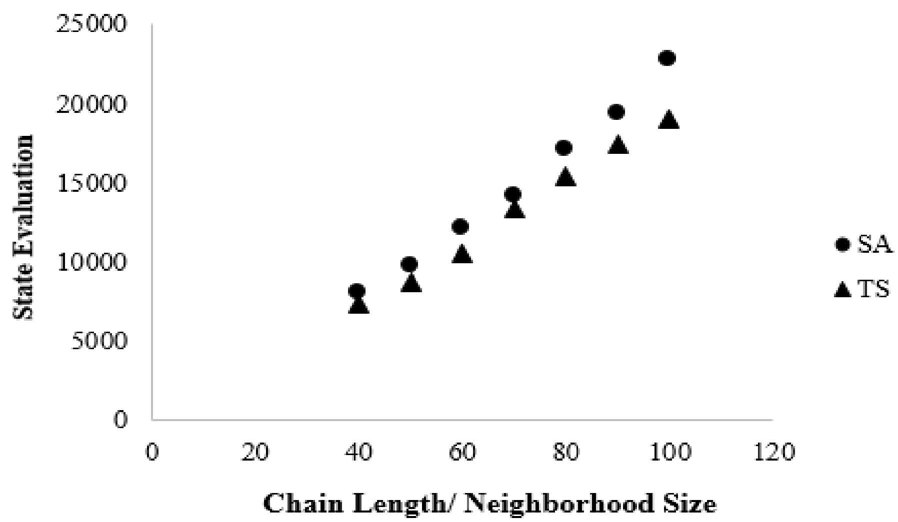

Figure 4.18 State Evaluations vs Chain / Neighborhood Size

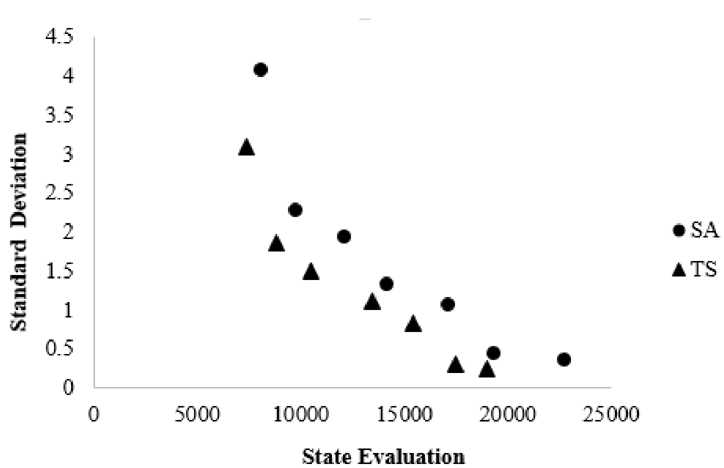

Figure 4.19 Standard Deviation vs State Evaluation

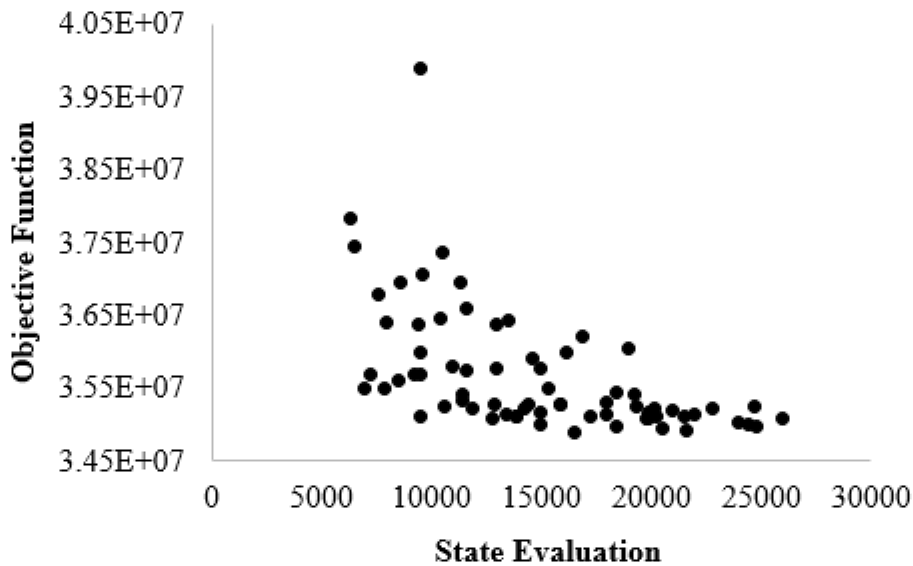

Figure 4.20 Objective Function vs State Evaluation (SA)

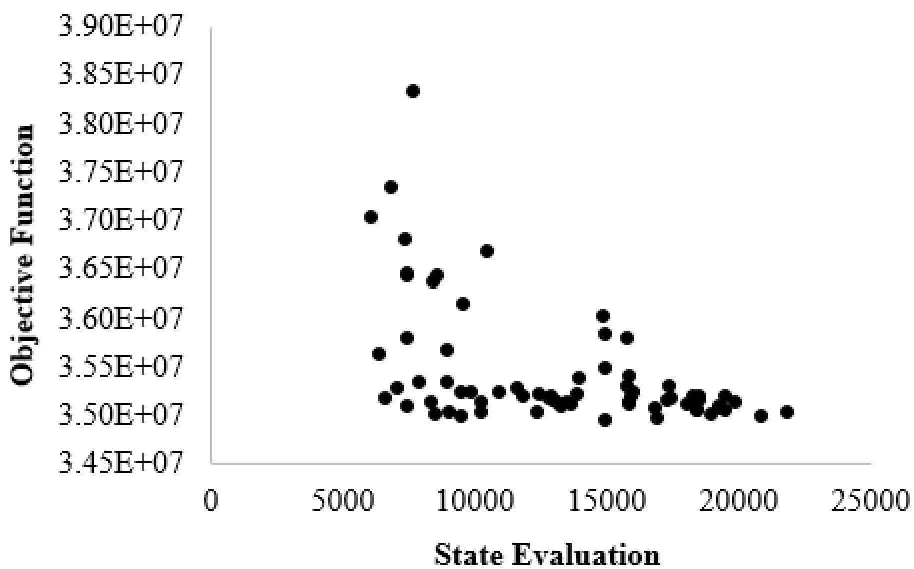

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Figure 4.21 Objective Function vs State Evaluation (TS)

Figures 4.20 and 4.21 presents all the data points generated across the campaign of runs for SA and TS solvers. Objective function is plotted against number of state evaluations for chain/neighborhood size of 40 – 100. The data presents the random nature of the search as more state evaluations doesn't necessarily mean a better solution in all instance. The opposite is also true as some objective functions are achieved in a lesser number of state evaluations. Despite the random nature of the search, the average performance of both solvers increases with an increasing number of state evaluations.

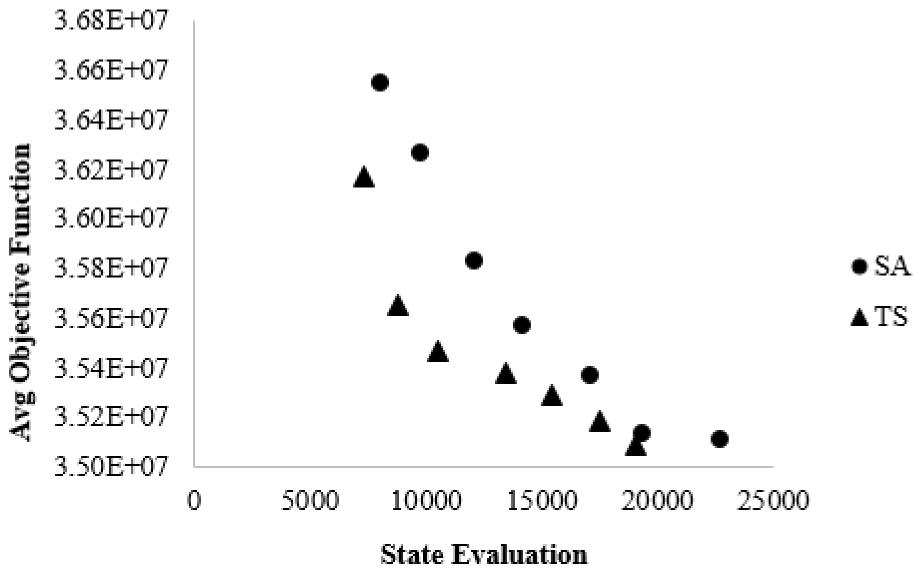


Figure 4.22 Average Objective Function vs State Evaluation

Figure 4.22 presents the variation of the average objective function with the average number of state evaluations for each chain/neighborhood size. As the average state evaluations increase, the performance of the objective function also increases. This is due to the fact that more state evaluations mean rigorous search of the solution space thereby enhanced the chance of finding a better solution.

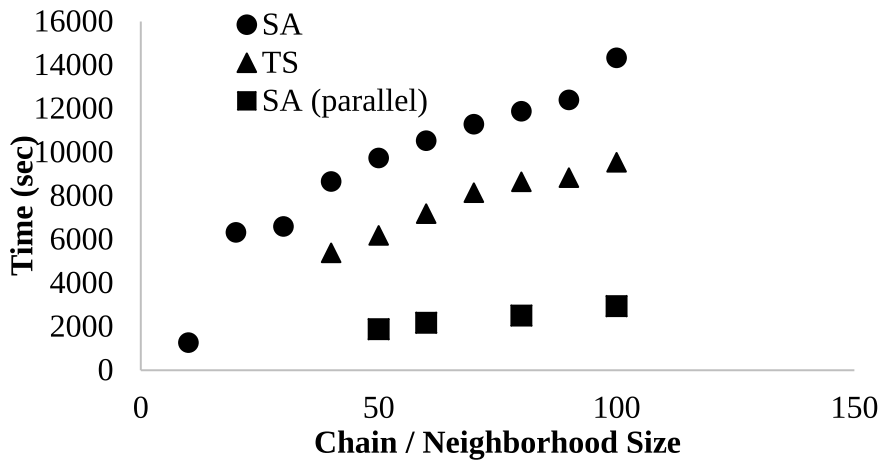


Figure 4.23 Time vs Chain / Neighborhood Size

Figure 4.23 shows variation time for SA, TS and SA solver run using 4 cores of a quad-core laptop. Between SA and TS, TS is faster. The average time for the SA run is two hours and 37 minutes whereas for TS it is around 1 hr 40 minutes. However, running the code in parallel configuration results in an increase in speed and the SA solver run in parallel configuration has an average runtime of 35 minutes.

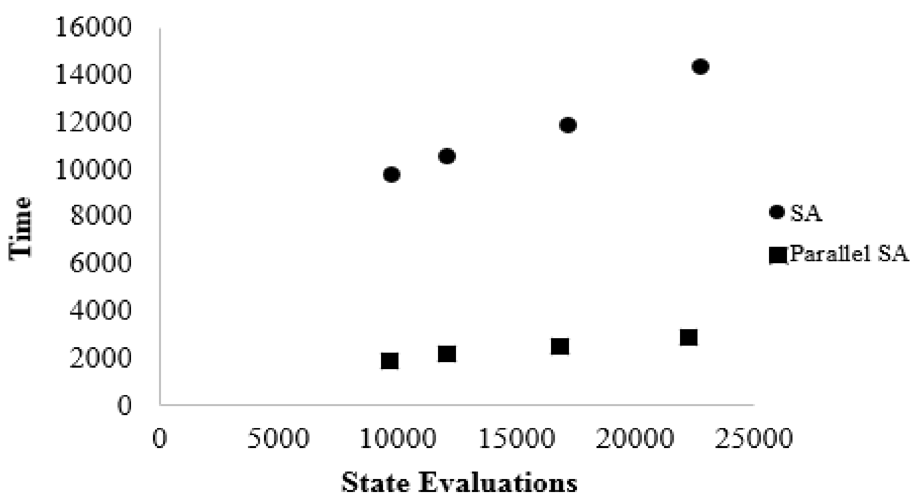


Figure 4.24 Time vs State Evaluations

Figure 4.24 presents how average time of state evaluation vary. As the state evaluation increases, the average time for the run increase. However, if the computing resources are increased, more states can be evaluated in lesser time thereby enhancing the pace of the run.

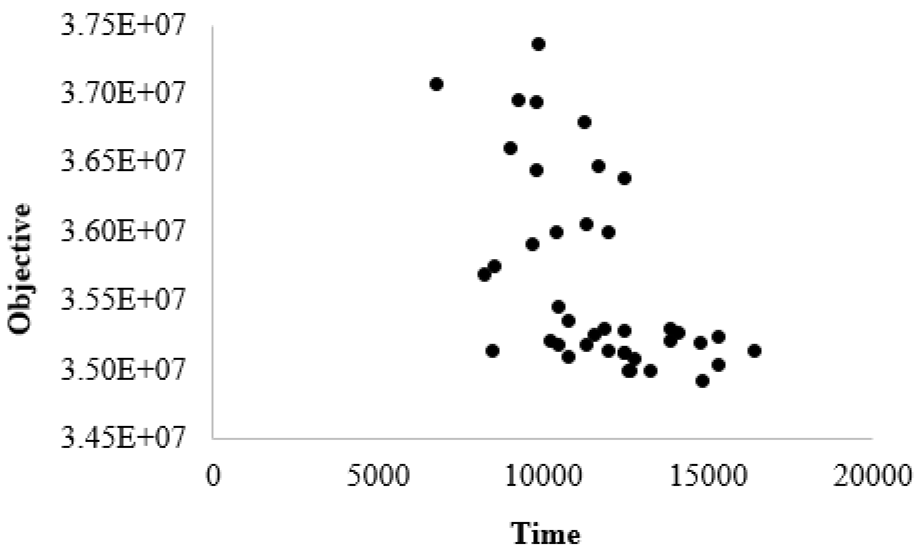


Figure 4.25 Objective vs Time (SA)

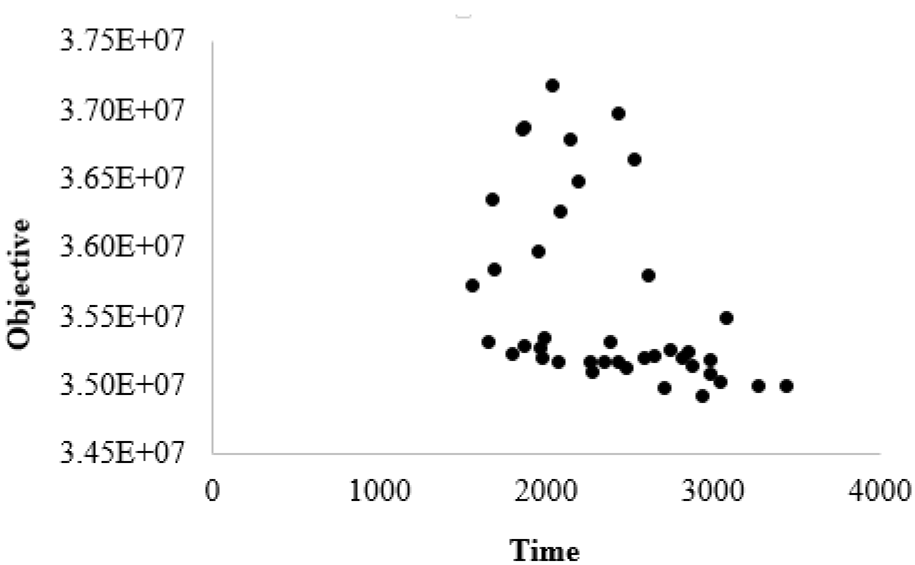


Figure 4.26 Objective vs Time (Parallel SA)

Figure 4.25 & 4.26 present the variation of objective function value for 40 runs for single and parallel simulated annealing. As observed, the quality of the solution is not impacted but the time is reduced if parallel computing resources are used. Also, the fuzzy nature of the plot reflects the random nature of the search.

Figure 4.27 provides a graphical presentation of the best performing optimal structure. It is the same for both SA and TS solver. However, the flowrates for some connections vary and are given in Tables 4.6 to 4.11. Recycling of water after using RO for treating wastewater from sinks has been observed in this case. The remaining requirement is met by an external supply of freshwater

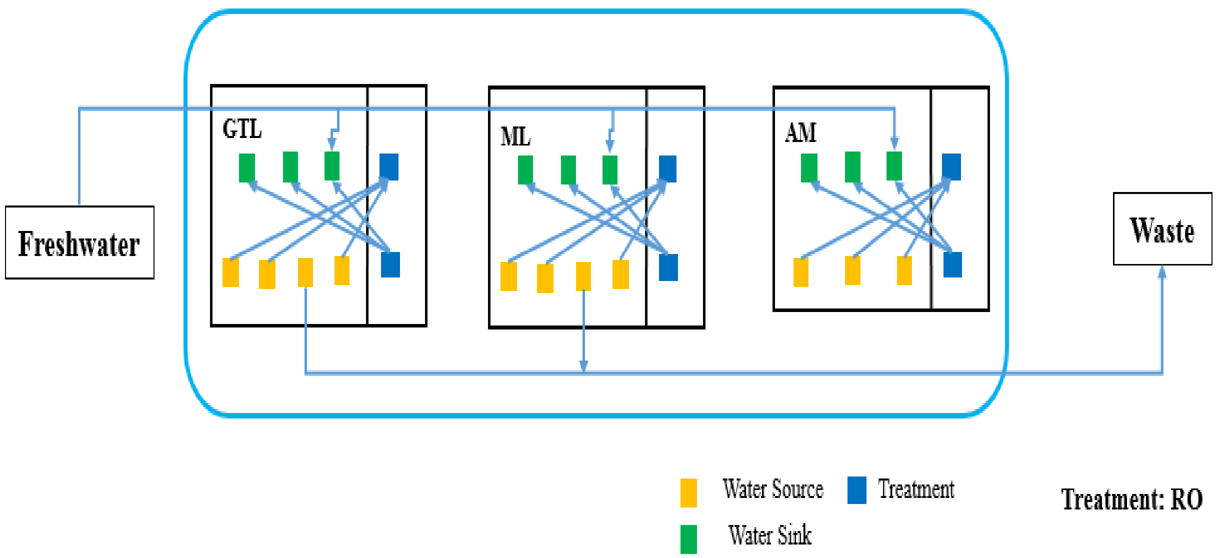


Figure 4.27 Best solution for SA & TS solvers

SA solver cost breakdown:

Total Network Cost: 34.9 MM$/yr

Water Treatment Cost: 9.16 MM$/yr

Piping Cost: 1.67 MM$/yr

Savings compared to initial structure (41.4 MM$/yr): 15.7%.

TS solver cost breakdown:

Total Network Cost: 34.95 MM$/yr

Water Treatment Cost: 9.16 MM$/yr

Piping Cost: 1.66 MM$/yr

Savings compared to initial structure (41.35 MM$/yr): 15.57%.

Table 4.6 Source to Treatment Units Map (SA)

	P1T1	**P2T1**	**P3T1**
P1S1	1.742	0	0
P1S2	6.31	0	0
P1S3	0	0	0
CT1	100.47	0	0
P2S1	0	11.36	0
P2S2	0	4.67	0
P2S3	0	0	0
CT2	0	44.16	0
P3S1	0	0	689.92
P3S2	0	0	5.81
CT3	0	0	420.8

Table 4.7 Treatment Units to Sinks Map (SA)

	P1D1	**P1D2**	**CT1**	**P2D1**	**P2D2**	**CT2**	**P3D1**	**P3D2**	**CT3**
P1T1	26.75	35	35.9	0	0	0	0	0	0
P2T1	0	0	0	12.77	20.83	20.57	0	0	0
P3T1	0	0	0	0	0	0	253.34	6.79	744.75

Table 4.8 Source to Treatment Units Map (Without Roundup Function)

	P1T1	P2T1	P3T1
P1S1	1.78	0	0
P1S2	6.23	0	0
P1S3	0	0	0
CT1	101.14	0	0
P2S1	0	11.45	0
P2S2	0	4.26	0
P2S3	0	0	0
CT2	0	44.67	0
P3S1	0	0	691.27
P3S2	0	0	6.11
CT3	0	0	420.34

Table 4.9 Treatment Units to Sinks Map (Without Roundup Function)

	P1D1	P1D2	CT1	P2D1	P2D2	CT2	P3D1	P3D2	CT3
P1T1	39.54	28.46	30.235	0	0	0	0	0	0
P2T1	0	0	0	23.58	12.63	18.132	0	0	0
P3T1	0	0	0	0	0	0	291.43	6.79	707.728

Table 4.10 Source to Treatment Units Map (TS)

	P1T1	P2T1	P3T1
P1S1	1.86	0	0
P1S2	6.39	0	0
P1S3	0	0	0
CT1	101.35	0	0
P2S1	0	11.64	0
P2S2	0	3.92	0
P2S3	0	0	0
CT2	0	44.8	0
P3S1	0	0	687.45
P3S2	0	0	6.09
CT3	0	0	421.07

Table 4.11 Treatment Units to Sinks Map (TS)

	P1D1	P1D2	CT1	P2D1	P2D2	CT2	P3D1	P3D2	CT3
P1T1	42.53	16.49	39.584	0	0	0	0	0	0
P2T1	0	0	0	7.46	14.59	32.274	0	0	0
P3T1	0	0	0	0	0	0	284.38	6.79	711.979

4.7.1. Observation

The optimized structure shows considerable improvement in cost when compared to a non-optimized structure with a 15% percent improvement. The solver converges asymptotically like SA solver and the performance of the most cost-effective structure is similar to that obtained by SA solver.

The solver performs robustly and it enables the user to define the problem in as complicated way as possible which means the optimization problem can be defined in more realistic in terms of cost approximation and constraints. The transition framework employed to search the transition framework utilizes the information from the constraints for an efficient search. This aspect of the search shows that engineering insights can be embedded in the search technique.

Since the stochastic solver performed well, the scope of the problem is enhanced to include the utility network as well. The problem is reformulated in subsequent section and models simulating power-generating turbines, boiler feed water, decentral power generation and steam generation from waste heat is included. The related energy and mass balance equations are formulated and the problem is solved thereby harnessing more nexuses across water and energy network.

5. WATER – ENERGY NETWORK REPRESENTATION

Section 5 demonstrates the effectiveness of SA and TS based solver to effectively handle resource optimization problem. In this section, the problem is expanded from water to water-energy network optimization. The modular architecture of the solvers developed makes it easier to customize to solve the combined problem. Apart from this, it provides the user with more insight into various other solutions with similar performance that can now be stored during the search.

The water-energy network formulated in Fouladi [93] added options for waste heat disposal and help choose the most cost-effective discharge option for it. The proposed formulation in this work expands on that problem and now includes waste heat utilization options and a model of the utility network in the optimization network. Waste heat can be used to generate steam and power which can then be exchanged across the plants. The utility network includes models for power generation for the plant requirements. Boiler Feed Water is accounted in the network and models calculating the steam and fuel requirements are incorporated. Apart from this, the modeling of water as both energy carrier and raw material is also explored. The new models account for more options of exploiting the water-energy nexus which provides the stakeholders new information about savings which can be achieved by integrating the water and energy network.

5.1. Problem Statement & Network Superstructure

The superstructure proposed in this work encapsulates the combined water-energy network along with the nexuses between them. The structure of the combined network shows how complex the problem becomes when both are considered together compared to considering each separately. Figure 5.1 & 5.2 represents the elements of water and energy networks.

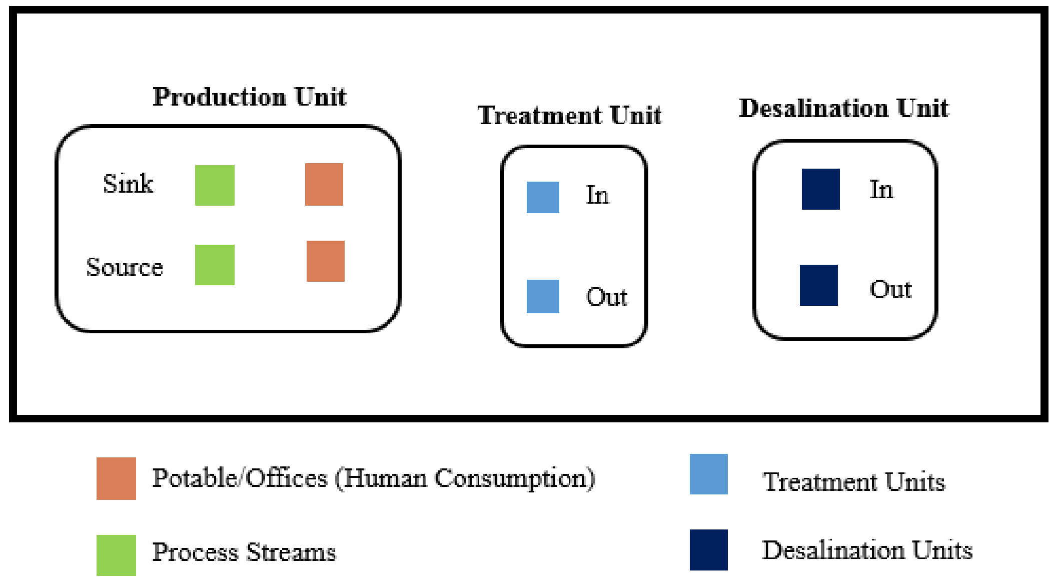


Figure 5.1 Elements of Water Network.

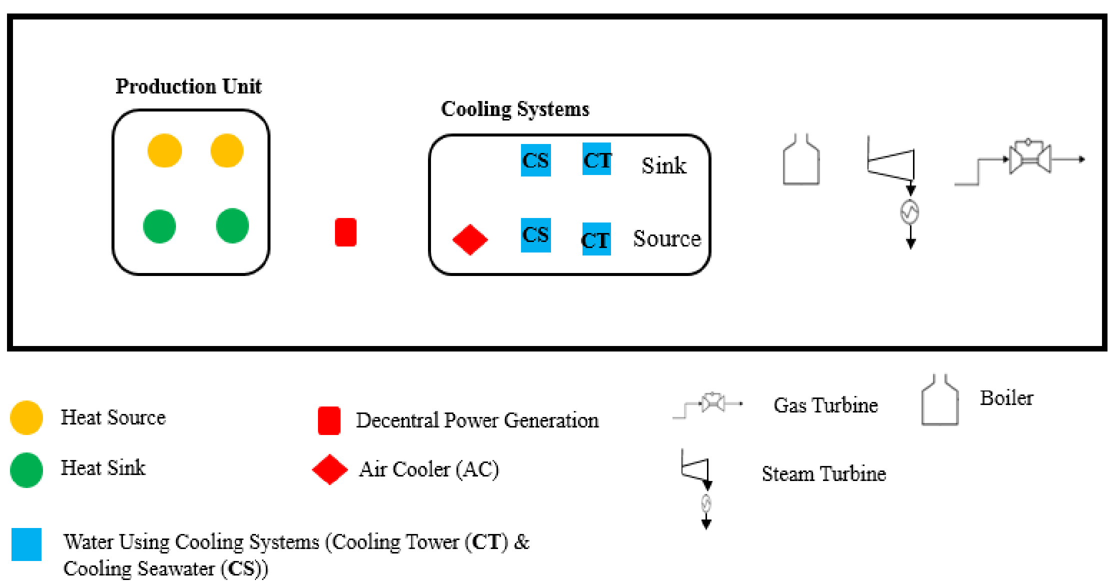


Figure 5.2 Elements of Energy Network

The water network used in this network has been adapted from Alnouri et al [25] and consists of water sources, sinks, treatment units, desalination units, and external freshwater supply. Sinks can be supplied with water from sources, treatment units, desalination units, and freshwater supply. Water sources and sinks have been classified into process streams and potable water. Water from sources can be discharged into the environment or used at sinks or can be treated and then used at sinks.

The energy network has been adapted from Fouladi [93] and consists of heat sources, sinks, cooling systems namely air cooler, cooling tower and seawater cooling. The heating requirement at sinks is met by steam generated from the utility system or from waste heat. Apart from steam generation for heating, excess heat can be used to generate power at decentral power generation units in each plant. This power can be exported to utilities, treatment units in various plants, exported to the external grid and send to cooling options like air cooler, cooling tower and once-through cooling seawater. The remaining heat is dumped into these cooling options. Figure 5.3 presents the complex superstructure generated when water and energy networks are considered simultaneous optimization for a single plant.

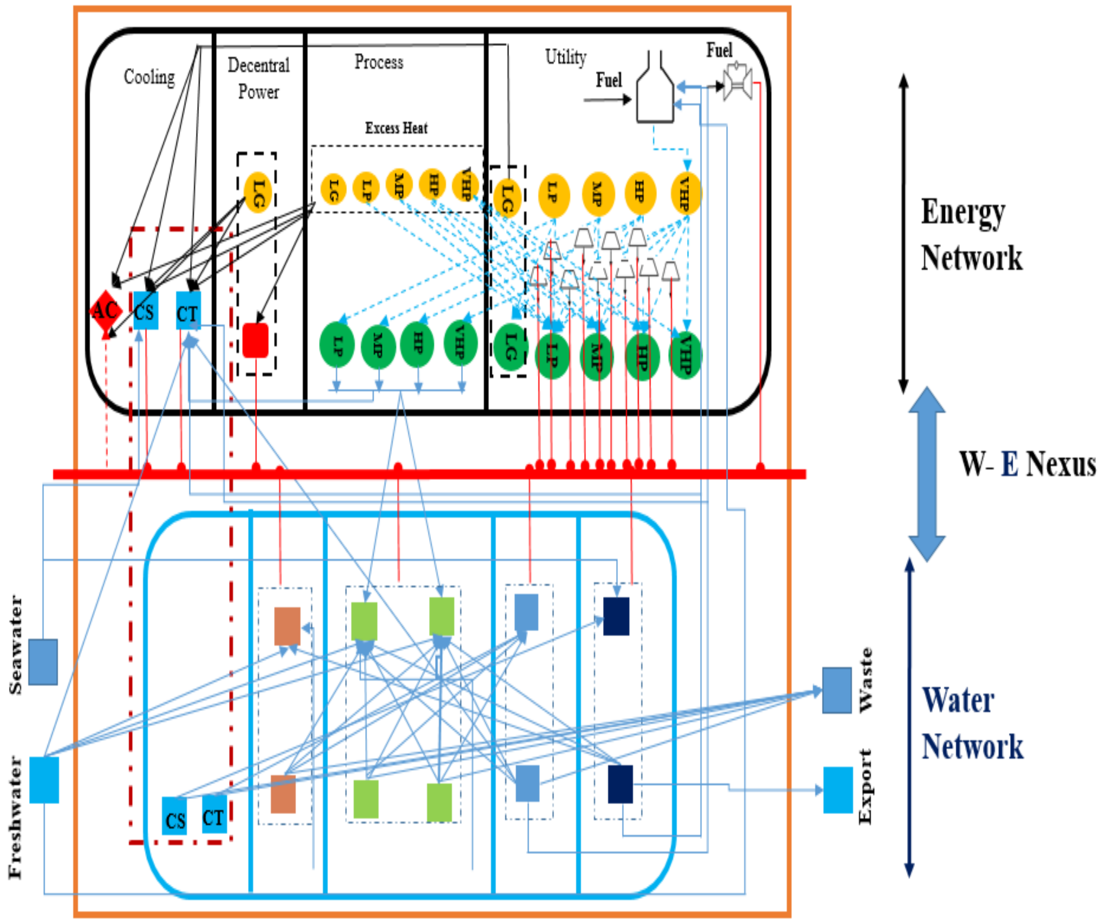


Figure 5.3 Water-Energy Superstructure for Single Plant

5.1.1. Utility Network

The utility network presented in figure 5.4 is a general utility network with all possible levels of steam connected with a turbine and generating power.

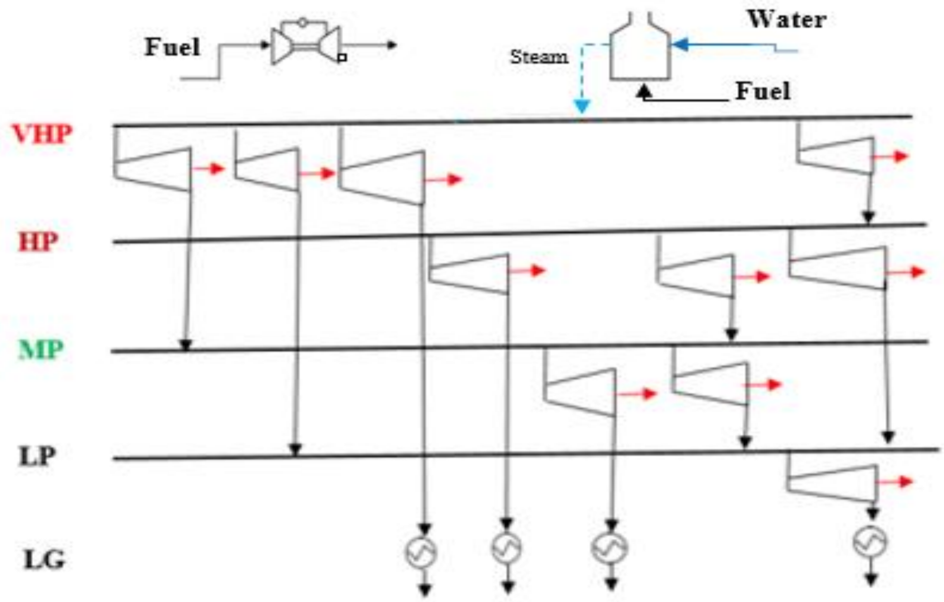


Figure 5.4 Utility System Configuration

The utility system provides power and steam for various operations of the plant. It generates power using gas or steam turbine and produces steam by burning fuel and heating water. This process generates very high-pressure steam which is then brought down to appropriate levels by using steam turbines generating the desired level steam and electricity. The general utility configuration accounts for all possible combinations of turbines. Steam levels are have been classified into Very High Pressure (VHP), High Pressure (HP), Medium Pressure (MP) and Low Pressure (LP). This classification has been done on the basis of temperature and pressure and varies for different plants. The utility system has major energy and water footprint and a key element in the combined water-energy network. This work integrates utility systems with energy and water network and explores links between the two rather than being optimized in isolation. Figure 5.5 presents part of the combined representation where the utility system is placed.

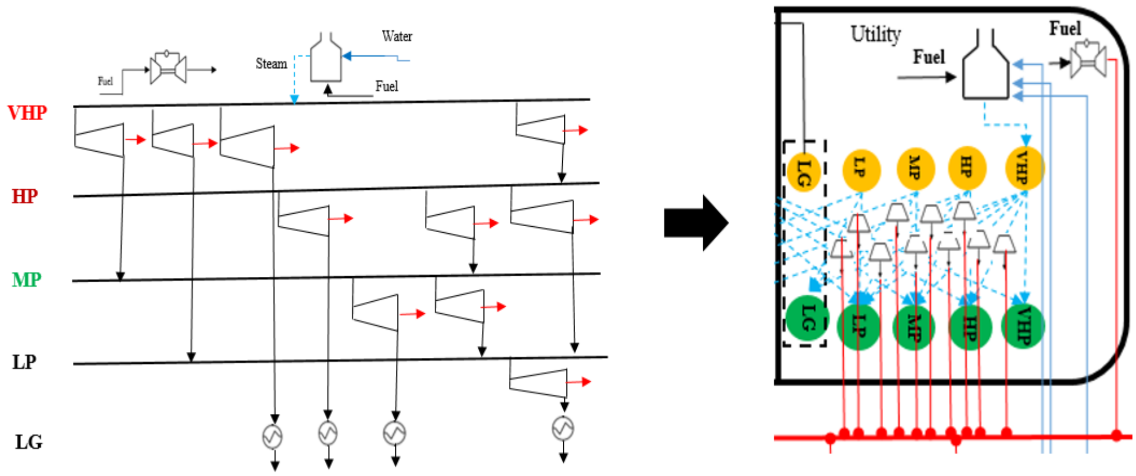


Figure 5.5 Utility System placement in Water-Energy Network

5.1.2. Decentral and Central Configuration

Figure 5.6 represents inter and intra-plant superstructure with all possible options for excess heat utilization and discharge and interlinkages between water and energy networks considering the decentral setup of treatment and power generation elements.

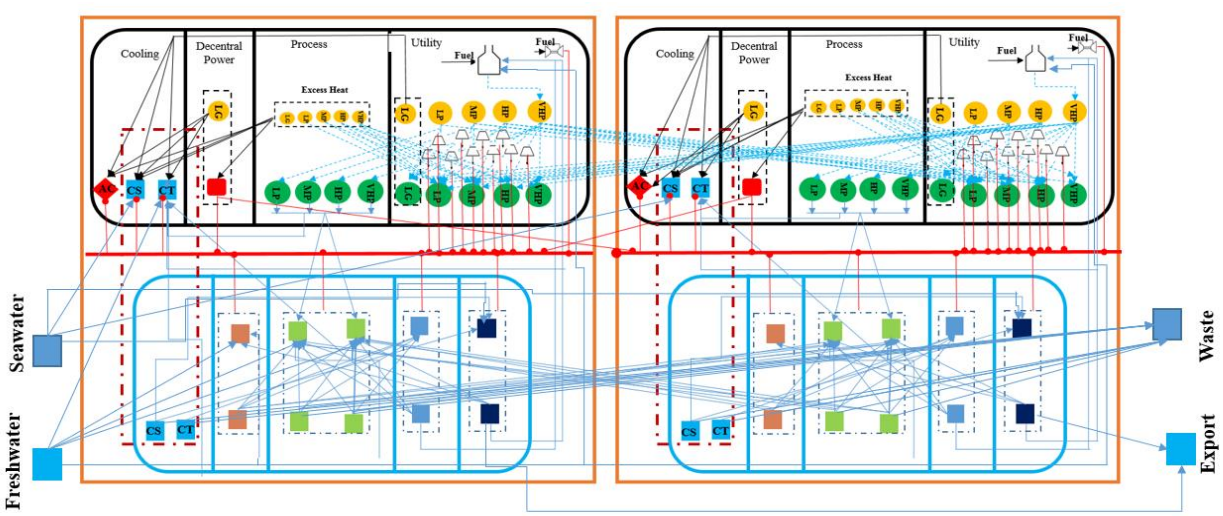


Figure 5.6 Illustration of Inter & Intra plant Water-Energy Superstructure (Decentral Treatment & Utility) - 2 plants

When considered together, heat sinks also become water sources as there is a discharge of water due to condensation. A similar observation can be made for cooling towers and seawater cooling. Also, water condensation at heat sinks can be used at cooling towers or other water sinks as raw material thereby reflecting the dual usage of water.

Figure 5.7 represents the inter-plant water – energy network with central treatment & utility setup.

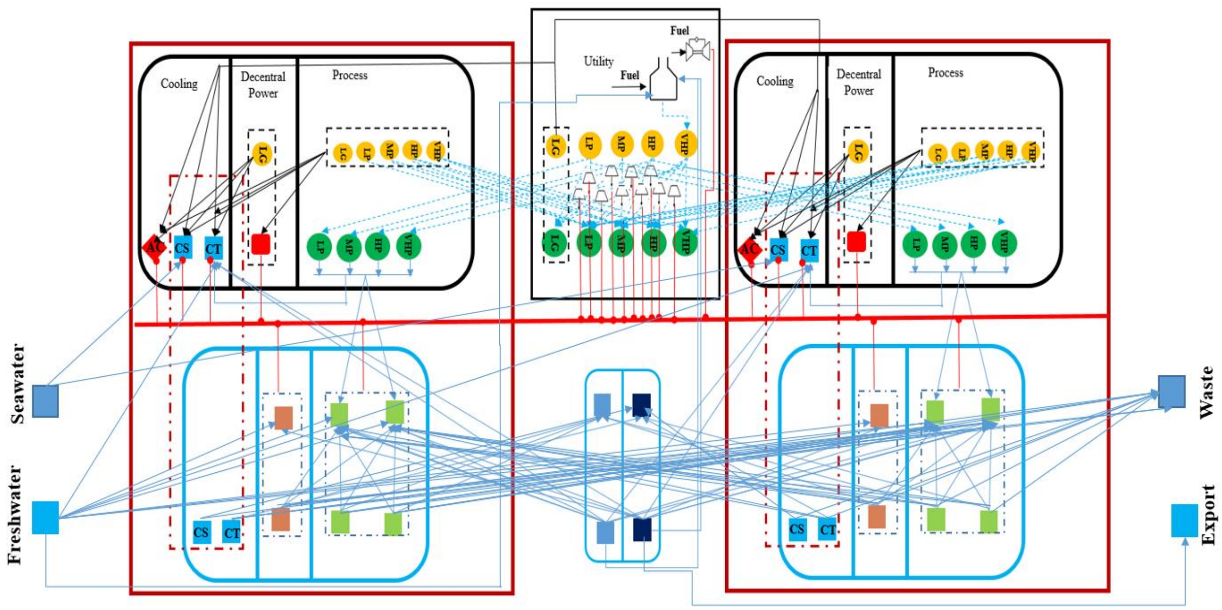


Figure 5.7. Illustration of Inter & Intra plant Water-Energy Superstructure (Central Treatment & Utility) – 2 plants

The combined superstructure also shows interlinks between the two networks. Heat sinks can also be modeled as water sources as condensation of steam generates a discharge of water which can be used at other water sinks. Here water acts as both energy carrier and raw material.

The choice of cooling technologies used also impacts the water footprint of the network. Outflowing water from seawater cooling can be desalinated and then exported. The power generated from decentral power generation impacts the boiler feedwater consumption. Subsequent sub-sections describe these nexuses in detail.

5.2. Waste Heat Utilization

5.2.1. Steam Exchange

Steam can be generated at High Pressure (HP), Medium Pressure (MP) and Low Pressure (LP) levels of the plant. These levels are defined relative to each plant and have varying values of temperature and pressure in each plant. The matching of the sinks with sources is done based on the temperature and pressure criteria. A transfer of steam generated at a source in plant (P1) in a particular level to a heat sink in another plant (P2) can take place if the temperature and pressure at the heat source are greater than that of the heat sink. Any transfer of steam generated from waste heat between sources and sinks impacts the energy usage in the overall system.

5.2.2. Decentral Power Generation

Waste heat can be utilized to generate power using technologies such as Organic Rankine Cycle (ORC). These power-producing processes are similar to the Rankine cycle except for the fact that the working fluids in them are different mixtures of organics. These technologies efficiently harness the power generation potential of low-grade heat compared to the normal Rankine cycle and are also efficient in the high-grade heat extraction and power generation. These cycles have different efficiencies for different temperature ranges.

Apart from steam and power generation, waste heat can be discharged from cooling options like Air Cooler (AC), Cooling Tower (CT) and Once through Seawater (OTSW).

5.2.3. Cooling Options

Seawater cooling requires seawater and power as input. Seawater comes into the plant to extract heat and it leaves extracting the excess heat. Cooling tower needs freshwater and power as input. Both seawater and cooling tower option increase the water footprint of the plant. Air coolers need air and power as input for its operations. The use of air coolers reduces the water footprint of the combined network. Selection of each of these options has varying impact on energy and water network of the system.

5.2.4. Synergies

Several synergies have been mapped and then exploited to generate a better-combined water- heat network. The following list provides an overall summary of various linkages found in the water-energy network:

Energy System

- Water used as heat carrier and working fluid
- Cooling may involve water use (e.g. cooling tower)

Water System

- Energy used in water treatment
- Energy used for transporting water
- Energy can be used to replace water for heat exchange purposes (Air Coolers).

The following nexuses have been looked into modeled in this work:

- Use of water as heat carrier (steam exchange) and then as freshwater in the water network.
- Impact of the addition of power generated from the decentral unit.
- Impact of various cooling options on water and energy footprint of the network.

5.2.5. Impact of Steam & Power Exchange

This section addresses the gap in modeling the impact of water and energy network on each other and the utility system with boiler feed water, fuel requirements and power generated.

Steam of various grade is generated at heat sources and subsequently supplied to various heat sinks. The amount of steam condensate at heat sinks creates a new water source that can be used for integration in the water network. Water in the form of steam acts as an energy carrier. Apart from that, it can then be condensed and then reused in the water network for meeting the requirements of water sinks thereby filling the gap of modeling duel usage of water as an energy carrier and as raw material. Figure 5.8 highlights this synergy in the main superstructure.

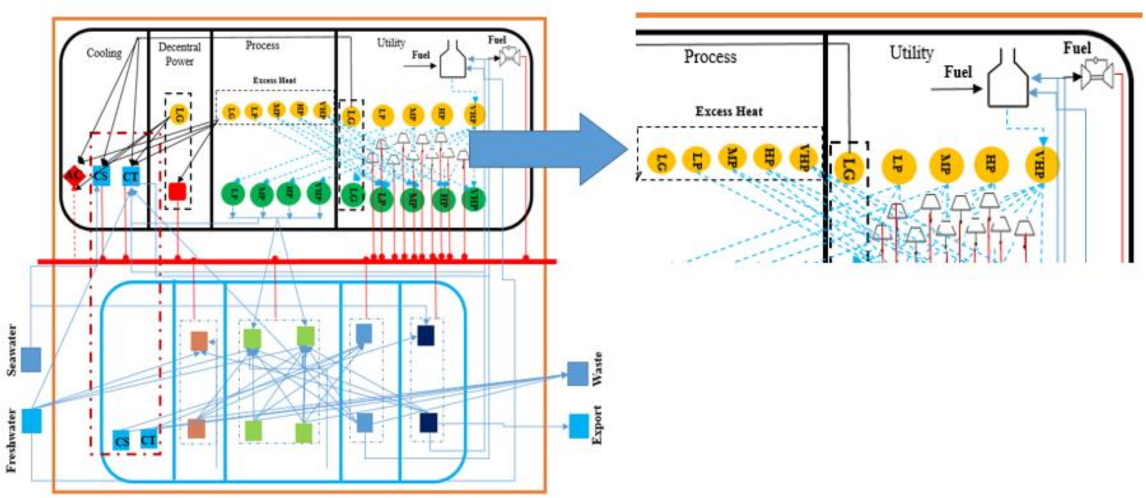


Figure 5.8 Steam Exchange Synergy

Exchange of steam also affects the water and fuel balances at the turbines generating power for the plant receiving the steam. Figure 5.9 shows the impact on water and energy network due to changes caused by the supply of steam generated from excess heat.

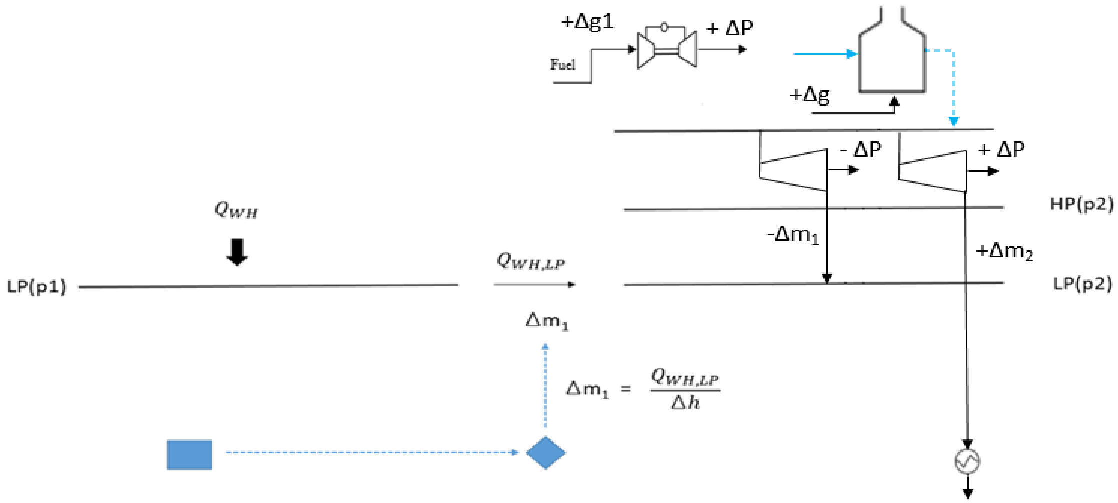


Figure 5.9 Impact of steam addition on the network

In figure 5.9, steam generated from excess heat (Q_{WH}) is added into the network at Low Pressure (LP) steam level. Due to this excess water Δm_1 is added into the system. To compensate for this excess water, the steam flowrate at LP level is reduced by the same amount. This reduction in flowrate translates into a reduction in power generated (-ΔP). The power balance is then maintained by producing the same amount of power at different turbines leading to a change in fuel (+Δ g in case of steam turbine and +Δg1 in case of a gas turbine) and water balances (+Δm_2).

The exchange of power generated from excess heat by decentral power generation units affects the water balance in the reboiler which produces steam and the fuel requirements at both steam and gas turbines for power generation in the plants.

As part of power, the requirement is supplied by a decentral unit, the recipient plant needs to produce less power. This translates into an impact on the energy and water balances at the turbine. Figure 5.10 highlights the power exchange in the superstructure.

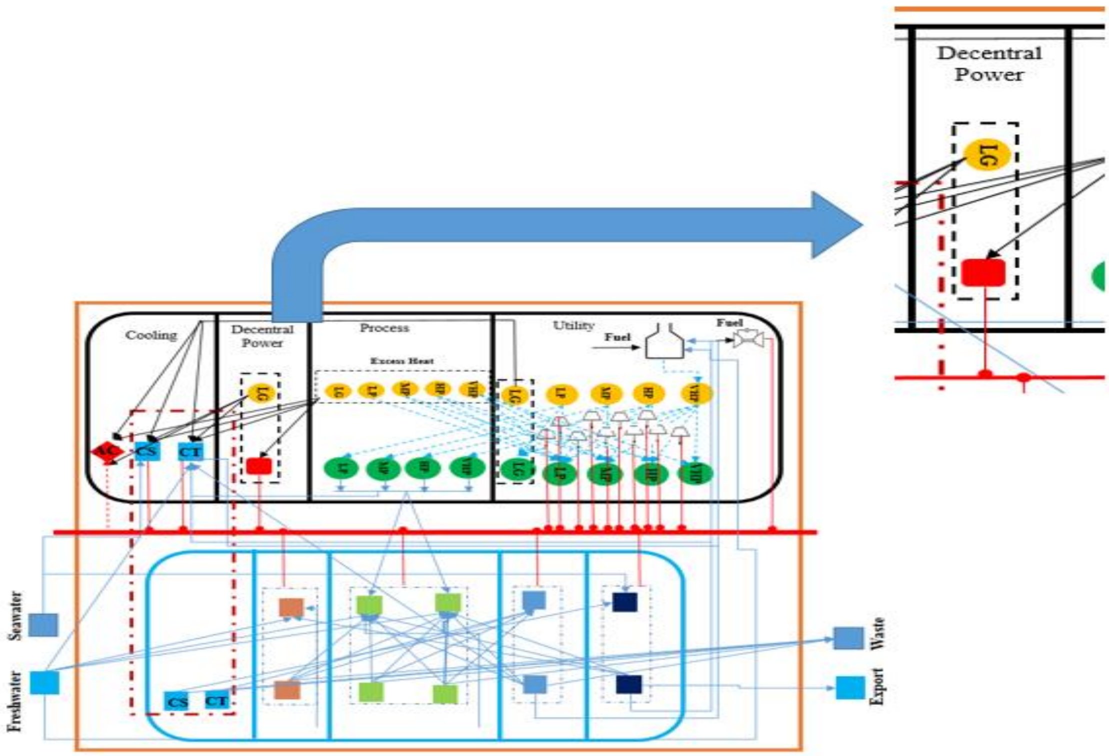


Figure 5.10 Power Exchange Synergy

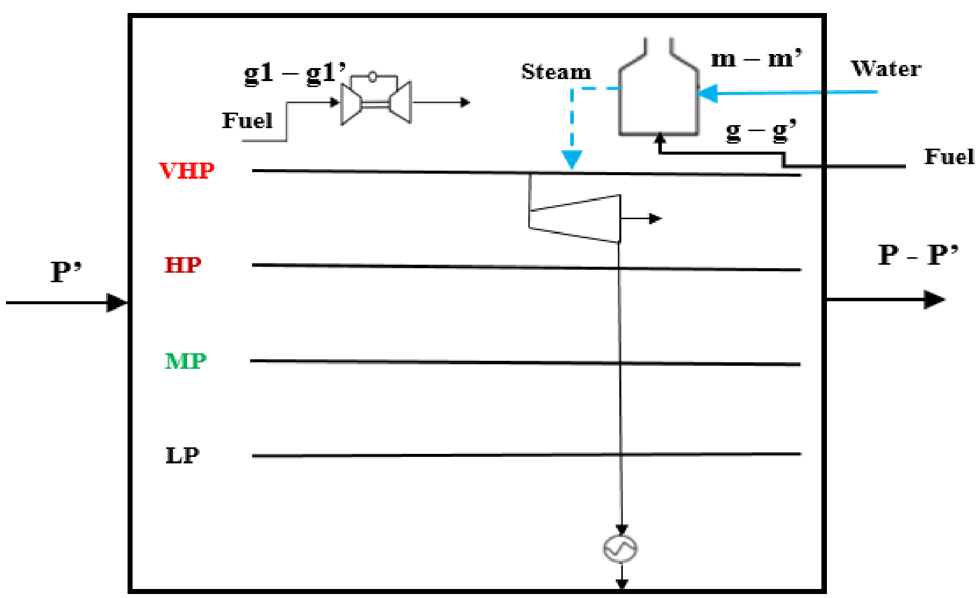


Figure 5.11 Impact of adding power from decentral power generation units.

Figure 5.11 explains the impact of decentral power generation in the combined network. As power (P') from the decentral generation unit is added to the utility network, P'is reduced to maintain the power balance. Due to this, there is a reduction in water consumption at boiler feed water (m-m') and fuel consumption (g-g') at the steam turbine. The same is true in the case of the gas turbine as the fuel requirement changes (g1-g1').

5.3. MINLP Problem Formulation.

The Water Network problem solved from this work has been adapted from Alnouri et al [25]. The following sets have been defined as a basis for the water network formulation:

I {i = 1, 2, … $N_{sources}$ | I is a set of water sources}

J {j = 1, 2 … N_{sinks} | J is a set of water sinks}

R {r = 1, 2…N_{unit}| R is a set of treatment units in each stage}

P {p = 1, 2 … N_{plant} | P is a set of plant}

CN {cn = 1, 2 …$N_{contaminants}$ | CN is a set of contaminants}

D {d = 1, 2…N_{unit}| d is a set of decentral treatment units}

Each source can be split into several streams: (1) Source-to-Sink flows ($F_{i(p1),j(p2),}$) representing the flow from i^{th} source of plant p1 to j^{th} sink of plant p2 (p1,p2 ϵ P) , (2) Source-to-Interceptor flows ($F_{i(p1), r(s1)}$) which represents the flow from each source to treatment units of stage 1 and (3) Source-to-Environment flows ($F_{i(p1), env}$) which represents the flow from each source of plant p1 to environment for discharge.

The following equations define the mass balances at various facilities:

$$F_{i(p1)}^{Process} = \sum_j F_{i(p1),j(p2)} + \sum_d F_{i(p1),d(p2)} + \sum_r F_{i(p1),r} + F_{i(p1),env} \quad (42)$$

$$F_{j(p2)}^{Process} = \sum_i F_{i(p1),j(p2)} + \sum_d F_{d(p1),j(p2)} + \sum_r F_{r,j(p2)} + F_{j(p2)}^{Freshwater}$$

$$+ \quad \sum_{cond} F_{cond(p1,j(p2)} \tag{43}$$

Water sources can either be discharged to environment($F_{i,env}$), sent to a sink ($F_{i,j}$) or sent to inceptors ($F_{i,r}, F_{i,d}$). Requirement at sinks can be met by contaminant rich water from sources ($F_{i,j}$), fresh water ($F_j^{Freshwater}$) and treated water from the interceptor units ($F_{r,j}, F_{d,j}$) .

Mass balances for interceptors (decentral units) at inlet and outlet are described by equations (44)-(47).

$$F_{d(p2)}^{in} = \sum_i F_{i(p1),d(p2)} \tag{44}$$

$$F_{d(p2)}^{out} = Recovery_{d(p2)} * \ F_{d(p2)}^{in} \tag{45}$$

$$F_{d(p2)} * \ C_{cn,d(p2)}^{in} \ = \sum_i F_{i(p1),d(p2)} * \ C_{cn,i(p1)} \tag{46}$$

$$F_{d(p1)}^{Out} = \sum_j F_{d(p1),j(p2)} + \sum_{CT(sink)} F_{d(p1),CT(sink)(p2)} \ + \ \sum F_{d(p1),BFW(p2)}$$

$$+ F_{d(p1),env} \tag{47}$$

Here $F_{i,d}$ represent flows from various sources to interceptors in treatment units and F_d is the amount of water that will be regenerated by each interceptor. Equation 44 accounts the mass balance and equation 46 represents the component balance at the inlet of each treatment unit. In equation 46, $C_{cn,i(p1)}$ is the concentration of contaminant cn in source i of plant p1 and $C_{cn,r}^{in}$ is the inlet concentration of contaminant cn in interceptor r. The amount of water coming out of a treatment unit depends upon the recovery ratio ($Recovery_d$) and is calculated using equation 4.Water from interceptor units are can then be either used at process sinks($F_{d,j}$), cooling tower ($F_{d,CT(sink)}$), boiler feed water ($F_{d,BFW}$) or discharged into environment ($F_{d,env}$).The same balances are shown for central treatment units in equations 48 to 51.

$$F_r^{in} = \sum_p \sum_i F_{i(p1),r} \tag{48}$$

$$F_r^{out} = Recovery_r * F_r^{in} \tag{49}$$

$$F_r * C_{cn,r}^{in} = \sum_p \sum_i F_{i(p1),r} * C_{cn,i(p1)} \tag{50}$$

$$F_r^{Out} = \sum_p \sum_j F_{r,j(p2)} + \sum_{p2} F_{r,CT(sink)(p2)} + \sum_{p2} F_{r,BFW(p2)} + F_{r,env} \tag{51}$$

Inlet and outlet concentrations in treatment units (interceptors) are related using a removal ratio. The removal ratio is a parameter that accounts for the percentage of contaminant removed from a stream, and depends on the type of treatment unit utilized. Equation (52) correlate the inlet and outlet concentrations of the interceptors (Central and Decentral).

$$C_{cn}^{out} = (1- RR_{cn}) * C_{cn}^{in} \tag{52}$$

Mass balances for discharge to the environment, is given by equations (53) and respective component balance for environmental discharge requirements is given by equation (54).

$$F_{env} = \sum_p \sum_d F_{d(p1),env} + \sum_r F_{r,env} + \sum_p \sum_i F_{i(p1),env} \tag{53}$$

$$F_{env} * C_{cn,env} = \sum_r F_{r,env} * C_{cn,r}^{out} + \sum_p \sum_i F_{i(p1),env} * C_{cn,i} + \sum_p \sum_{d(p1)} F_{d,env} * C_{cn,d}^{out} \tag{54}$$

Water can be discharged into the environment from various sources ($F_{i,env}$) or from treatment units ($F_{r,env}$, $F_{d,env}$). $C_{cn,env}$ is the concentration of contaminant b in the environmental discharge. The balance at steam turbine is given by the following equation.

$$F_{p2}^{BFW} = 0.92F_{p2}^{BFW} + \sum_{p2} F_{fw,BFW(p2)} + \sum_r F_{r,BFW(p2)} + \sum_p \sum_d F_{d(p1),BFW(p2)} + \sum_{p1} F_{desal(p1),BFW(p2)} \tag{55}$$

The amount of water needed at the reboiler (boiler feed water) of the turbine can be met by the recycled water, supply of freshwater, supply of water from decentral and central treatment units or from desalinated water. Balances of cooling tower sources and sinks are given by following equations

$$F_{p2}^{CT(sink)} = F_{fw,CT(p2)} + \sum_r F_{r,CT(p2)} + \sum_{p1} \sum_d F_{d(p1),CT(p2)} + \sum_{p1} F_{desal(p1),CT(p2)}$$

$$+ \sum_{p1} F_{cond(p1),CT(p2)} \quad (56)$$

$$F_{p1}^{CT(source)} = 0.9 * F_{p1}^{CT(sink)} \quad (57)$$

$$F_{p1}^{CT(source)} = F_{CT(p1),env} + \sum_r F_{CT(p1),r} + \sum_{p2} \sum_d F_{CT(p1),d(p2)} \quad (58)$$

Water requirement at cooling tower sinks can be met by freshwater ($F_{fw,CT(j)}$), treated water from central ($F_{r,CT(j)}$) and decentral units ($F_{d,CT(j)}$), desalinated water ($F_{desal,CT(j)}$) or condensate ($F_{cond,CT(j)}$) produced at heat sinks. Water from cooling tower sources can either be sent to central ($F_{p(CT),r}$) or decentral ($F_{p(CT),d}$) units or can be discharged as wastewater ($F_{p(CT),env}$).

Balances at once through seawater sources and sinks are given below

$$F_{p1}^{OTSW(source)} = F_{env}^{OTSW} + \sum_p F_{,desal(p1)}^{OTSW} \quad (59)$$

$$F_{p1}^{OTSW(sink)} = F_{p1}^{OTSW(source)} \quad (60)$$

$$F_{desal(p1)}^{Out} = Recovery_{desal(p1)} * F_{desal(p1)}^{In} \quad (61)$$

Seawater can be desalinated and used in the plant or for export apart from being used for cooling purposes. Apart from ensuring the balances, the constraints at sinks for maximum allowable concentration and the flowrate feasibility are checked. The above-mentioned constraints are as follows:

$$F_{j(p2)}^{Freshwater} * C_{cn,fw} + \sum F_{i(p1),j(p2)} * C_{cn,i(p1)} + \sum F_{r,j(p2)} * C_{cn,r} + \sum F_{d(p1),j(p2)} * C_{cn,d(p1)} \leq F_{j(p2)} * C_{cn,j(p2)} \quad (62)$$

Where $C_{cn,fw}$ is the concentration of contaminant cn in freshwater, $C_{cn,i}$ is the concentration of contaminant cn in source i, $C_{cn,r}$ and $C_{cn,d}$ is the concentration of contaminant b in streams originating from central and decentral interceptor. $C_{cn,j}$ is the concentration of contaminant cn in sink j.

$$C_{cn}^{env} \leq C_{cn}^{max} \tag{63}$$

Where $C_{cn}^{env}$the concentration of contaminant b is discharged into the environment and C_{cn}^{max} is the maximum concentration of contaminant b that can be discharged into the environment.

$$F_{i(p1),j(p2)} - M_{F_{i(p1),j(p2)}}^{max} \leq 0 \tag{64}$$

$$F_{i(p1),r} - M_{F_{i(p1),r}}^{max} \leq 0 \tag{65}$$

$$F_{i(p1),d(p2)} - M_{F_{i(p1),d(p2)}}^{max} \leq 0 \tag{66}$$

$$F_{r,j(d2)} - M_{F_{r,j(d2)}}^{max} \leq 0 \tag{67}$$

$$F_{d(p1),j(p2)} - M_{F_{d(p1),j(p2)}}^{max} \leq 0 \tag{68}$$

$$F_r - M_r^{max} \leq 0 \tag{69}$$

$$F_{d(p1)} - M_{F_{d(p1)}}^{max} \leq 0 \tag{70}$$

Equations (64) - (68) defines the existence of various streams from sources to sinks, sources to interceptors, interceptors to sinks and interceptors to environment. Equations (69) and (70) defines the existence of treatment units.

Constraint on export:

$$\sum_p F_p^{Export} \leq 0.33 * \text{Kahramaa Capacity (0.48 million tons/d).} \tag{71}$$

Heat network considered in this work consists of utilities across all the plants and the waste heat discharged from them. The discharged heat can be converted into steam of various grades (depending on the temperature and pressure profile), power using various decentral power generation units or can be discharged into the environment using seawater cooling, cooling towers, and air coolers. The exchange of power and steam and the choice of different cooling options affects the water and energy balances that can be calculated using the equations below. Heat network part of the optimization problem is set up with the help of information about the waste heat profile of the plant, their heating, and power requirements and the temperature and pressure profile of various grades of steam that can be generated.

The following additional sets have been defined as a basis for the heat network formulation:

A {a = 1, 2 … $N_{sources}$ | A is a set of steam levels in heat sources}

B {b = 1, 2 … N_{sinks} | B is a set of steam levels in heat sinks}

Excess heat can be redistributed within itself across various levels of steam that can be generated. Figure 5.12 represents a grand composite curve of a plant outline the kind of excess heat that can be extracted and classified as per the steam generation specification.

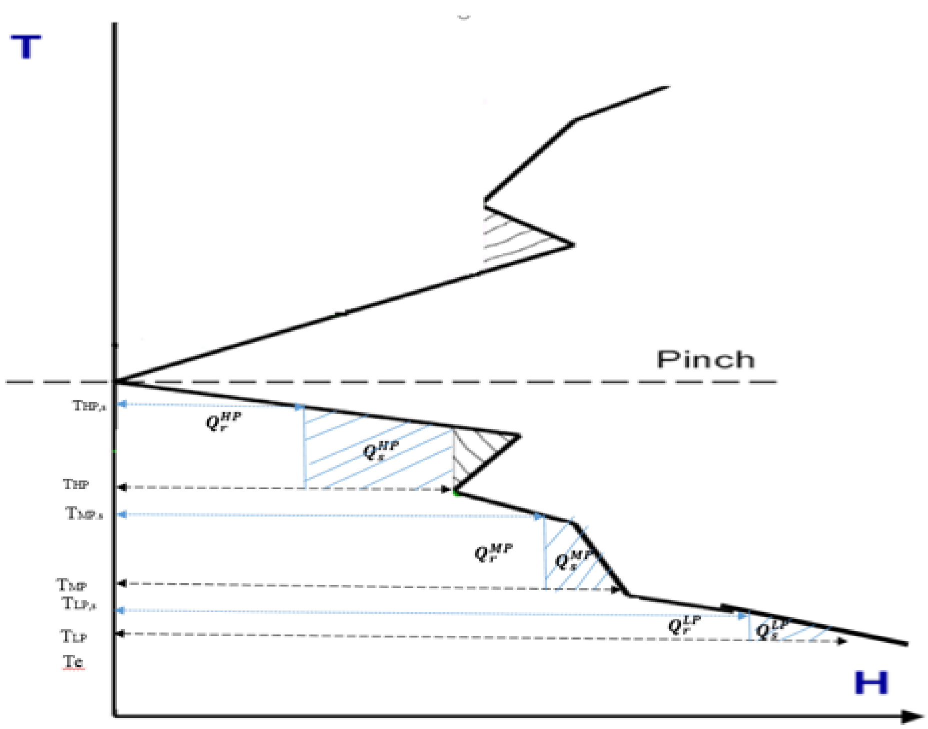


Figure 5.12 Grand Composite Curve of a representational plant

Excess heat can be classified into various level of steam extraction levels namely Very High Pressure (VHP) steam, High Pressure (HP) steam, Medium Pressure (MP) steam and Low Pressure (LP) steam. Across these levels, the heat can be redistributed as follows.

$$Q_{VHP} = Q^{steam(VHP)} + Q_{VHP \to HP} + Q_{VHP \to MP} + Q_{VHP \to LP} \quad (72)$$

$$Q_{HP} = Q^{steam(HP)} + Q_{HP \to MP} + Q_{HP \to LP} \quad (73)$$

$$Q_{MP} = Q^{steam(MP)} + Q_{MP \to LP} \quad (74)$$

Excess heat from very high-pressure level can be extracted in form of steam or can be redistributed to the lower levels to be utilized there. The same balance holds true for other levels as well

Excess heat from steam levels A in heat sources of I can be converted to steam and supplied to steam levels B in heat sinks of J ($Q_{a(p1),b(p2)}$), converted to power in decentral power generation units($Q_{a(p1),dectrpower(p2)}$),sent to cooling options ($Q_{a(p1),Cooling(p1)}$) or redistributed internally as reflected in equations 72 -74. Heat requirements of steam level B of heat sink of J can either be met from steam supply from steam levels A of heat sources of I ($Q_{a(p1),b(p2)}$) and by burning extra fuel ($Q_{Fuel,b(p2)}$).

Equations (75) and (76) describe the mass balances at heat sources and sinks

$$Q_{a(p1)} = \sum_{p2} \sum_{b} Q_{a(p1),b(p2)} + \sum_{p2} Q_{a(p1),dectrpower(p2)} + Q_{a(p1),Cooling(p1)}$$
$$+ \sum_{b} Q_{a(p1),b(p1)} \quad (75)$$

$$Q_{b(p2)} = \sum_{p1} \sum_{a} Q_{a(p1),b(p2)} + Q_{Fuel,b(p2)} \quad (76)$$

Part of waste heat of steam level A of heat source of J to discharged from cooling options ($Q_{a(p1),Cooling(p1)}$) can either be discharged from once through seawater ($Q^{AC}_{a(p1),Cooling(p1)}$), cooling towers ($Q^{CT}_{a(p1),Cooling(p1)}$) and air coolers ($Q^{OTSW}_{a(p1),Cooling(p1)}$).

$$Q^{AC}_{a(p1),Cooling(p1)} = Y^{AC}_{a(p1),} * Q_{a(p1),Cooling(p1)} \quad (77)$$

$$Q^{CT}_{a(p1),Cooling(p1)} = Y^{CT}_{a(p1)} * Q_{a(p1),Cooling(p1)} \quad (78)$$

$$Q^{OTSW}_{a(p1),Cooling(p1)} = Y^{OTSW}_{a(p1)} * Q_{a(p1),Cooling(p1)} \quad (79)$$

$$Y^{AC}_{a(p1)} + Y^{CT}_{a(p1)} + Y^{OTSW}_{a(p1)} = 1 \quad (80)$$

Here Y represents the fraction of waste heat allotted to each cooling option.

Each plant runs down the different masses of steam to required steam levels to meet the heating requirements. Any excess power requirement is met through running the steam down to the condensate level.

Equation (81) represents the overall power balance around the turbine

$$\sum P^{Decentral}_{p1} + \sum P^{Steam\ Turbine}_{p1} + P^{Import}_{p1} - P^{Export}_{p1} = \sum P^{Equip}_{p1} + \sum P^{Treatment}_{p1} + \sum P^{Cooling}_{p1} + \sum P^{Desalination}_{p1} \quad (81)$$

The power requirement for plant for equipment (P^{Equip}_{p1}), treatment ($P^{Treatment}_{p1}$), cooling ($P^{Cooling}_{p1}$) and desalination ($P^{Desalination}_{p1}$) is met through power exchange from decentral power generation units ($P^{Desalination}_{p1}$), power generated by steam turbines ($P^{Steam\ Turbine}_{p1}$) and power imported ($P^{Steam\ Turbine}_{p1}$). Any excess power generated is exported (P^{Export}_{p1}).

Power for cooling consists of power required by air coolers, cooling towers and once through seawater.

$$P^{Cooling} = P^{AC} + P^{CT} + P^{OTSW} \quad (82)$$

$$P^{AC}_{p1} = C_1 * Q^{AC}_{a(p1),Cooling(p1)} \quad (83)$$

$$P^{CT}_{p1} = C_2 * Q^{CT}_{a(p1),Cooling(p1)} \quad (84)$$

$$P^{OTSW}_{p1} = C_3 * Q^{OTSW}_{a(p1),Cooling(p1)} \quad (85)$$

Here C_1, C_2 and C_3 are constants.

Power requirement for treatment is given by the following equation

$$P_{p1}^{Treatment(k)} = C_4 * F_{p1}^{Treatment(k)} \quad (86)$$

Here C_4 is a constant.

Power requirement for desalination is given by the following equation

$$P_{p1}^{Desalination} = C_5 * F_{p1}^{Desalination} \quad (87)$$

Here C_5 is a constant.

Power generated by a steam turbine depends on the mass of the steam passed through it and is calculated by the equation 43. It has been adapted from Hassiba et al ([68], [101]).

$$P^{turb} = c_1^{turb} * m^{steam} - c_2^{turb} \quad (88)$$

Water requirement at cooling tower and once through seawater is given by the following relationship

$$F_p^{CT} = K_2 * Q_{a(p1),Cooling(p1)}^{CT} \quad (89)$$

$$F_p^{OTSW} = K_3 * Q_{a(p1),Cooling(p1)}^{OTSW} \quad (90)$$

The desalinated water can either be exported or used in the plants at sinks or as boiler feed water.

$$F_{desal}^{Out} = F_{desal,export} + \sum_j F_{desal,j(p2)} + \sum_j F_{desal,CT(p2)} + \sum_i F_{desal,BFW(p2)} \quad (91)$$

The condensate produced at heat sink j is sum total all the steam flowrate from the sources to the sink and the flowrate of the steam from the turbine that meets the deficit demand.

$$m_j^b = \sum_{i,a} m_{i(a),j(b)} + m_{VHP,j(b)} \quad (92)$$

The amount of fuel needed to generate steam is calculated by the following relationship

$$Q_j^{Fuel} = (\Delta h^{gen} * m^{steam}) / (\eta_{turb}) \quad (93)$$

Capacity constraint at decentral power generation units

$$\sum_p P_{p1}^{Decentral} \leq \sum P_{p1}^{Equip} + \sum P_{p1}^{Treatment} + \sum P_{p1}^{Cooling} + \sum P_{p1}^{Desalination} \quad (94)$$

If the export of power disallowed, the following constraint is applicable.

$$P_{p1}^{Decentral} \leq W_{max,power}^{Steam} \quad (95)$$

The power generated by the decentral power generation units cannot exceed the plant requirement if the export of power is prohibited. The technology utilized in converting excess heat to power considered in this work in Organic Rankine Cycle (ORC). Unlike conventional turbines, ORC uses working fuel composed of organic molecules with the vapor - liquid phase change occurring at lower temperatures compared to water – steam system. Figure 5.13 presents a schematic representation of ORC.

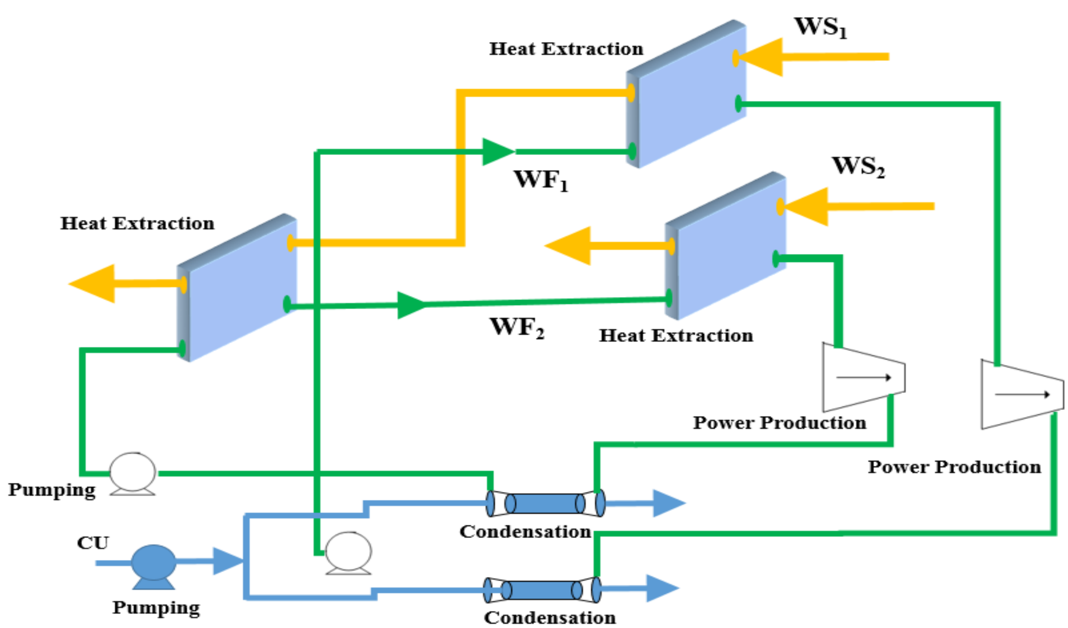


Figure 5.13 Representational Decentral Power Generation Unit

Excess heat from plants is passed through the Rankine cycle which makes the working liquid to evaporate. The vapor generated is passed through a turbine which brings down the vapor temperature to low-temperature reservoir liquid level thereby generating electricity. The amount of power which can be generated depends on the grade of the heat supplied. Heat levels with higher temperatures are more efficient in power generation compared to lower heat levels. Equation 1 describes the relationship for power generated and the temperature levels.

$$W_{max} = CP\ (T_i\ - T) - CP\ T_L\ \left[ln \frac{T_i}{T}\right] \tag{96}$$

Here W_{max} is the maximum power that can be generated, T_i is the initial temperature (the greatest temperature of the interval) and T_f is the final temperature of interval. T_L is the reservoir temperature. The amount of decentral power generated for the allocated heat (Q) from the interval is calculated by the following equation:

$$W = \frac{Q}{Q_{max}}\ x\ W_{max} \tag{97}$$

Constraints on heat exchange are as follows:

$$T_b^{Steam} \leq T_a^{Steam} \tag{98}$$

$$p_b^{Steam} \leq p_a^{Steam} \tag{99}$$

Steam exchange between a source and sink can take place only if the temperature and pressure at the source is greater than that of the sink.

Constraint on export of power is as follows.

$$\sum P_{export} \leq 0.33 * \text{Kahramaa Capacity (38963 Gwh)}. \tag{100}$$

Objective function: The evaluation function consists of total cost of water network and the energy network. The aim of the optimization is to minimize the cost.

Total Cost of the combined water energy network: Cost of Water Network + Cost of Energy Network

$$\text{Cost} = C^{Freshwater} + C^{Piping} + C^{Seawater} + C^{Oper\ (Treatment)} + C^{Cap\ (Treatment)} + C^{Oper\ (Desalination)} + C^{Cap\ (Desalination)} + C^{Export} + C^{Oper\ (Air\ Cooler)} + C^{Cap\ (Air\ Cooler)} + C^{Oper\ (Cooling\ Tower\ )} + C^{Cap\ (Cooling\ Tower)} + C^{Oper\ (Treatment)} + C^{Steam} + C^{Steam\ Pipeline} + C^{Oper\ (Decentral\ Power)} + C^{Cap\ (Decentral\ Power)} + C^{Fuel} \quad (101)$$

Water network costs consists of following components:

- Cost of freshwater
- piping cost
- Capital and Operating costs of treatment,
- Capital and Operating costs of desalination cost
- Seawater Cost
- Export cost of water.

Energy network costs consists of total energy cost of the system,

- Capital and Operating costs of cooling systems
- Steam generation (excess heat) cost.
- Steam Pipeline Cost
- Capital and Operating costs of decentral power generation units.
- Fuel Cost.

Table 5.1 presents the detailed expression of each component.

Table 5.1 Cost Components

Cost	Equation
Freshwater	$\mathrm{Hy}\ \mathrm{C}^{\mathrm{fresh}} \sum_{i\in I} \sum_{t\in T} F_{Fw,j(p2),t}$
Piping	$\sum_{\mathrm{i\epsilon\, I}} \sum_{\mathrm{j\epsilon J}} \mathrm{a}(\mathrm{DI}^{\mathrm{c}}_{\mathrm{i(p1),j(p2)}})^{\mathrm{b}} dis_{i,j} + \sum_{\mathrm{i\epsilon\, I}} \sum_{\mathrm{BFW}} \mathrm{a}(\mathrm{DI}^{\mathrm{c}}_{\mathrm{i,bfw}})^{\mathrm{b}} dis_{i,bfw} +$ $\sum_{\mathrm{desal}} a\left(\mathrm{DI}^{\mathrm{c}}_{\mathrm{desal,BFW}}\right)^{\mathrm{b}} dis_{desal,bfw} +$ $\sum_{desal} a(\mathrm{DI}^{\mathrm{c}}_{\mathrm{desal,p(CT)}})^{\mathrm{b}} dis_{desal,P(CT)} +$ $\sum_{\mathrm{desal}} a\left(\mathrm{DI}^{\mathrm{c}}_{\mathrm{desal,j}}\right)^{\mathrm{b}} dis_{desal,j} + \sum_{\mathrm{I}} \sum_{\mathrm{R}} \mathrm{a}(\mathrm{DI}^{\mathrm{c}}_{\mathrm{i(p1),r}})^{\mathrm{b}} dis_{i,r} +$ $\sum_{\mathrm{R}} \sum_{\mathrm{J}} \mathrm{a}(\mathrm{DI}^{\mathrm{c}}_{\mathrm{r,j(p2)}})^{\mathrm{b}} dis_{r,j}$ $+ \sum_{\mathrm{I}} \sum_{\mathrm{D}} \mathrm{a}(\mathrm{DI}^{\mathrm{c}}_{\mathrm{i,d}})^{\mathrm{b}} dis_{i,d} + \sum_{\mathrm{D}} \sum_{\mathrm{J}} \mathrm{a}(\mathrm{DI}^{\mathrm{c}}_{\mathrm{d,j(p2)}})^{\mathrm{b}} dis_{d,j}$ $+\sum\ \ \sum_{p1,p2\in P}(\sum_{\mathrm{i\epsilon\, I}} \sum_{\mathrm{j\epsilon J}} \mathrm{a}(\mathrm{DI}^{\mathrm{c}}_{\mathrm{i(p1),j(p2)}})^{\mathrm{b}} dis_{i,j} +$ $\sum_{\mathrm{desal}} a\left(\mathrm{DI}^{\mathrm{c}}_{\mathrm{desal,BFW}}\right)^{\mathrm{b}} dis_{fw,j}\ \sum_{\mathrm{desal}} a\left(\mathrm{DI}^{\mathrm{c}}_{\mathrm{desal,BFW}}\right)^{\mathrm{b}} dis_{fw,j} +$ $\sum_{\mathrm{desal}} a(\mathrm{DI}^{\mathrm{c}}_{\mathrm{desal,p(CT)}})^{\mathrm{b}} dis_{desal,P(CT)} +$ $\sum_{\mathrm{desal}} a\left(\mathrm{DI}^{\mathrm{c}}_{\mathrm{desal,j}}\right)^{\mathrm{b}} dis_{desal,j} + \sum_{\mathrm{I}} \sum_{\mathrm{R}} \mathrm{a}(\mathrm{DI}^{\mathrm{c}}_{\mathrm{i(p1),r}})^{\mathrm{b}} dis_{i,r} +$ $\sum_{\mathrm{r\epsilon R}} a\left(\mathrm{DI}^{\mathrm{c}}_{\mathrm{r,env}}\right)^{\mathrm{b}} dis_{r,env} + \sum_{\mathrm{r\epsilon\, R}} \sum_{\mathrm{j\epsilon J}} \mathrm{a}(\mathrm{DI}^{\mathrm{c}}_{\mathrm{r,j(p2)}})^{\mathrm{b}} dis_{r,j} +$ $\sum_{\mathrm{i\epsilon\, I}} \sum_{\mathrm{d\epsilon D}} \mathrm{a}(\mathrm{DI}^{\mathrm{c}}_{\mathrm{i,d}})^{\mathrm{b}} dis_{i,d} + \sum_{\mathrm{d\epsilon D}} a\left(\mathrm{DI}^{\mathrm{c}}_{\mathrm{d,env}}\right)^{\mathrm{b}} dis_{d,env} +$ $\sum_{\mathrm{d\,\epsilon\, R}} \sum_{\mathrm{j\epsilon J}} \mathrm{a}(\mathrm{DI}^{\mathrm{c}}_{\mathrm{d,j(p2)}})^{\mathrm{b}} dis_{d,j}$ where $\mathrm{DI}^{\mathrm{c}}_{\mathrm{i(p1),j(p2)}}$ is the diameter of the pipe between source i of plant p1 to sink j of plant p2, $\mathrm{DI}^{\mathrm{c}}_{\mathrm{i,bfw}}$ is the diameter of the pipe between sources and boiler feed water, $\mathrm{DI}^{\mathrm{c}}_{\mathrm{desal,BFW}}$is the

Table 5.1 Continued

	diameter of the pipe between desalination units and boiler feed water, $\mathrm{DI}^{c}_{desal,p(CT)}$ is the diameter of the pipe between desalination units and cooling towers in various plants, $\mathrm{DI}^{c}_{desal,j}$ is the diameter of the pipe between desalination units and sinks, $\mathrm{DI}^{c}_{i(p1),r}$ is the diameter of the pipe between sink i of plant p1 and central treatment units, $\mathrm{DI}^{c}_{r,j(p2)}$ is the diameter of the pipe between central interceptor r of to sink j of plant p2, $\mathrm{DI}^{c}_{i(p1),d}$ is the diameter of the pipe between sink i of plant p1 to decentral interceptor d , $\mathrm{DI}^{c}_{d,j(p2)}$ is the diameter of the pipe between decentral interceptor d of to sink j of plant p2. The capital cost is a function of the diameters of interconnecting pipes, which in turn is calculated based on the flow rate through the interconnection. The pipe Size (DI) is calculated as: DI = $0.363((M)^{0.45} * \rho^{0.13})$ This expression has been taken from Peters et al. [94], where M represents the volumetric flowrate given in m^3/s and ρ is density of the stream. The pipe diameter obtained using the expression is rounded off up to one decimal place.

Table 5.1 Continued

Treatment Cost	$(\sum_{r\epsilon R} F_r(C_r^{oper} + C_r^{cap}) + \sum_{d\epsilon D} F_d(C_d^{oper} + C_d^{cap}))* H_y$
Desalination Cost	$(C_{desal}^{oper} + C_{desal}^{cap})* F^{desalination} * H_y$
Seawater Cost	$C^{seawater}\ F^{seawater} * H_y$
Export Cost of water	$C_{water}^{export} * F^{export} * H_y$
Air Cooler	**Operating Cost:** $C_{Oper}^{AC} * P^{AC} * H_y$ **Capital Cost:** $C_{cap}^{AC} * P^{AC}$
Cooling Tower	**Operating Cost:** $C_{Oper}^{CT} * P^{CT} * H_y$ **Capital Cost:** $C_{cap}^{CT} * P^{CT}$
Steam Generation Cost	$C_{steam}^{oper} + C_{steam}^{cap})* F^{steam} * H_y$
Steam Pipeline Cost	$C^{pipe} * D^{a,b}$(Stijepovic et al [102]) $C_{i,j,k,l}^{pipe}$ (\$/m) = $A_1 * wt_{pipe} + A_2 * D_{out}^{0.48} + A_3 + A_4 * D_{out}$ A_1= pipe cost per unit weight (0.82 \$/kg), wt_{pipe} = weight of the pipe per unit length(kg/m), A_2 = installation cost (185 \$/$m^{0.48}$), D_{out} = outside diameter of the pipe (m), A_3= right-of-way cost (6.8 \$/m) A4 -insulation cost (295 \$/m). $D_{inner} = \sqrt{\frac{4*m_{i,j,k,l}}{u*\rho_{i,j,k,l}*\pi}}$

Table 5.1 Continued

	$m_{i,j,k,l}$ - mass flow rate of utility generated in the match with process stream j in plant i which is transferred to plant k to utility rank l (kg/sec) $\rho_{i,j,k,l}$ - density of utility generated in the match with process stream j in plant i which is transferred to plant k to utility rank l (kg/m^3) u - velocity (m/s), D_{inner} - inner diameter. We assume that velocity in the pipeline of 45 m/s for medium and high-pressure steam and of 20 m/s for low-pressure steam. In order to evaluate the outside diameter and the weight per unit length of pipeline, we assume that low and medium pressure steam is transported in stainless steel pipes of schedule 40, while high-pressure steam is transported in stainless steel pipes of schedule 80. Data from ASME B36.19M -2004 stainless steel standards are regressed in order to determine the outside diameter and weight per unit length with respect to the inner diameter of the pipe. The outside diameters and the weight per unit length are calculated as:

Table 5.1 Continued

	$D_{outer}(m)$ = 1.052*$D_{inner}(m)$ + 0.005251 (Schedule 40) wt_{pipe}(kg/m) = 644.3*$D_{inner}(m)^{2}$ + 1.052*$D_{inner}(m)$ + 0.00521 (Schedule 40) $D_{outer}(m)$ = 1.101*$D_{inner}(m)$ + 0.006349 (Schedule 80) wt_{pipe}(kg/m) = 1330*$D_{inner}(m)^{2}$ + 75.18*$D_{inner}(m)$ + 0.9268 (Schedule 80)
Decentral Power Cost	$(C_{orc}^{oper} + C_{orc}^{cap})* P^{decentral} * H_y$
Fuel Cost	$C^{fuel} * Q^{fuel}$

6. STOCHASTIC OPTIMIZATION OF WATER – ENERGY NETWORK

The solver developed for the combined water-energy network optimization problem shares many components with stochastic solvers developed for water networks (Section 3). The solution generation platform for water network remains the same and new platform for making perturbation in heat network is added. Simulation and Evaluation modules are modified to include the added equations and related models.

6.1. Solver Development

6.1.1. Transition Framework

Transition framework for water network remains the same with boiler feed water and condensate option added into the transition. In case of heat networks, the transition module are similar but the logic used in making those changes are different. In case of heat network, there are three categories of decision where these perturbations are allowed:

- Exchange of Steam.
- Exchange of Power.
- Perturbation in cooling options.

When a decision to allow exchange of steam is made, the feasible connections between sources and sinks are looked into. If a connection is to be added, then the maximum value that added is calculated as minimum of waste heat discharge and heat sink requirement. Then a random value between zero and maximum value is chosen and added. Same logic applies when the amount of steam exchange has to be increased. To disallow steam exchange, select a sink-source matching and assign the value to it as zero.

The same logic applies while making reducing the amount of heat exchange. A value between zero and the current value is chosen and reduced from the given connection. In case of reconnection of given source, disallow a steam exchange at a particular connection and allow it with some other sink. It must be ensured that there is at least one more potential place where steam can be allocated apart from the current allocation. The same moves are applicable for power exchange as well with values of power being considered instead of steam.

In case of cooling options, the amount of heat that is to be discharged stays constant for a move. The way it is distributed across the cooling option is changed. Moves include the addition of a cooling option, deleting a cooling option, increasing the value for heat discharged from a particular cooling option or decreasing the value.

6.1.2. Simulation Module

Variables representing boiler feedwater, steam condensate, waste heat to steam and power generation are added and the equations are formulated accordingly.

$$F_i^{Process} = \sum_j F_{i,j} + \sum_d F_{i,d} + \sum_r F_{i,d} + F_{i,env} \tag{102}$$

$$F_{j(p2)}^{Process} = \sum_i F_{i(p1),j(p2)} + \sum_d F_{d(p1),j(p2)} + \sum_r F_{r,j(p2)} + F_{j(p2)}^{Freshwater} + \sum_{cond} F_{cond(p1,j(p2)} \tag{103}$$

$$F_{d(p2)}^{in} = \sum_i F_{i(p1),d(p2)} \tag{104}$$

$$F_{d(p2)}^{out} = Recovery_{d(p2)} * F_{d(p2)}^{in} \tag{105}$$

$$F_{d(p2)} * C_{d(p2)}^{in} = \sum_i F_{i(p1),d(p2)} * C_{i(p1)} \tag{106}$$

$$F_{d(p1)}^{Out} = \sum_j F_{d(p1),j(p2)} + \sum_{CT(sink)} F_{d(p1),CT(sink)(p2)} + \sum F_{d(p1),BFW(p2)} + F_{d(p1),env} \tag{107}$$

$$F_r^{in} = \sum_p \sum_i F_{i(p1),r} \tag{108}$$

$$F_r^{out} = Recovery_r * F_r^{in} \quad (109)$$

$$F_r * C_{cn,r}^{in} = \sum_p \sum_i F_{i(p1),r} * C_{cn,i} \quad (110)$$

$$F_r^{Out} = \sum_p \sum_j F_{r,j(p2)} + \sum_{p2} F_{r,CT(sink)(p2)} + \sum_{p2} F_{r,BFW(p2)} + F_{r,env} \quad (111)$$

$$C_{cn}^{out} = (1- RR_{cn}) * C_{cn}^{in} \quad (112)$$

$$F_{env} = \sum_p \sum_d F_{d(p1),env} + \sum_r F_{r,env} + \sum_p \sum_i F_{i(p1),env} \quad (113)$$

$$F_{env} * C_{cn,env} = \sum_r F_{r,env} * C_{cn,r}^{out} + \sum_p \sum_i F_{i(p1),env} * C_{cn,i}$$

$$+ \sum_p \sum_{d(p1)} F_{d,env} * C_{cn,d}^{out} \quad (114)$$

$$F_{j(p2)}^{BFW} = 0.92 F_{j(p2)}^{BFW} + \sum_{p2} F_{fw,BFW(p2)} + \sum_r F_{r,BFW(p2)} + \sum_p \sum_d F_{d(p1),BFW(p2)} +$$

$$\sum_{p1} F_{desal(p1),BFW(p2)} \quad (115)$$

$$F_p^{CT(sink)} = F_{fw,CT(j)} + \sum_r F_{r,CT(j)} + \sum_d F_{d,CT(j)} + \sum F_{desal,CT(j)} + \sum F_{cond,CT(j)} \quad (116)$$

$$F_p^{CT(source)} = 0.9 * F_p^{CT(sink)} \quad (117)$$

$$F_{p2}^{CT(sink)} = F_{fw,CT(p2)} + \sum_r F_{r,CT(p2)} + \sum_{p1} \sum_d F_{d(p1),CT(p2)} + \sum_{p1} F_{desal(p1),CT(p2)}$$

$$+ \sum_{p1} F_{cond(p1),CT(p2)} \quad (118)$$

$$F_{p1}^{CT(source)} = F_{CT(p1),env} + \sum_r F_{CT(p1),r} + \sum_{p2} \sum_d F_{CT(p1),d(p2)} \quad (119)$$

$$F_{desal}^{Out} = Recovery_{desal} * F_{desal}^{In} \quad (120)$$

$$F_{i(p1)}^{OTSW(source)} = F_{i(p1),env}^{OTSW} + \sum_p F_{i(p1),desal(p1)}^{OTSW} \quad (121)$$

$$F_p^{OTSW(sink)} = F_p^{OTSW(source)} \quad (122)$$

$$Q_{a(p1)}^P = \sum_{p2} \sum_b Q_{a(p1),b(p2)} + \sum_{p2} Q_{a(p1),dectrpower(p2)} + Q_{a(p1),Cooling(p1)} \quad (123)$$

$$Q_{b(p2)}^P = \sum_{p1} \sum_a Q_{a(p1),b(p2)} + Q_{Fuel,b(p2)} \quad (124)$$

$$\sum P_p^{Decentral} + \sum P_p^{Steam\,Turbine} + P_p^{Import} - P_p^{Export} = \sum P_p^{Equip} + \sum P_p^{Treatment} + \sum P_p^{Cooling}$$

$$+ \sum P_p^{Desalination} \quad (125)$$

$$Q_{a(p1),Cooling(p1)}^{AC} = Y_{a(p1),}^{AC} * Q_{a(p1),Cooling(p1)} \quad (126)$$

$$Q_{a(p1),Cooling(p1)}^{CT} = Y_{a(p1)}^{CT} * Q_{a(p1),Cooling(p1)} \quad (127)$$

$$Q_{a(p1),Cooling(p1)}^{OTSW} Y_{a(p1)}^{OTSW} * Q_{a(p1),Cooling(p1)} \quad (128)$$

$$Y_{a(p1)}^{AC} + Y_{a(p1)}^{CT} + Y_{a(p1)}^{OTSW} = 1 \quad (129)$$

$$P_p^{AC} = C_1 * Q_{a(p1),Cooling(p1)}^{AC} \quad (130)$$

$$P_p^{CT} = C_2 * Q_{a(p1),Cooling(p1)}^{CT} \quad (131)$$

$$P_p^{OTSW} = C_3 * Q_{a(p1),Cooling(p1)}^{OTSW} \quad (132)$$

$$P^{Cooling} = P^{AC} + P^{CT} + P^{OTSW} \quad (133)$$

$$P_p^{Treatment(k)} = C_4 * F_p^{Treatment(k)} \quad (134)$$

$$F_p^{CT} = K_2 * Q_{p(a),cooling}^{CT} \quad (135)$$

$$P^{turb} = c_1^{turb} * m^{steam} - c_2^{turb} \quad (136)$$

$$F_p^{OTSW} = K_3 * Q_{p(a),cooling}^{OTSW} \quad (137)$$

$$P_p^{Desalination} = C_5 * F_p^{Desalination} \quad (138)$$

$$F_p^{Desalination} = F_p^{Export} + F_p^{BFW} + \sum_j F_{desal,j} \quad (139)$$

$$m_j^b = \sum_{i,a} m_{i(a),j(b)} + m_{VHP,j(b)} \quad (140)$$

$$Q_j^{Fuel} = (\Delta h^{gen} * m^{steam}) / (\eta_{turb}) \quad (141)$$

6.1.3. Evaluation Module

After the new structure has been generated and simulated, it is checked whether the solution obtained is feasible or not. The set of inequalities for both water and energy network define the feasibility constraints of the optimization problem. Also, the objective function consisting of the costs of water and energy network is used.

6.2. Case Study

The case study chosen to demonstrate the implementation of the method is a representative of Eco-Industrial Park. The water and heat data have been collected through various open-source, sustainability reports and simulations. Plants include in this case study are as follow:

1. GTL – Gas to Liquid Plant using Fischer Tropsh Process. Data generated using simulation.
2. Ammonia (AM) – Data and collected for the ammonia process using ASPEN simulation.
3. Refinery (RF) - Data collected for overall refinery processes from literature.
4. Methanol (ML) - Methanol Plant simulation used for data generation.
5. Aluminum (AL) – Water and Energy data collected from open sources.
6. Steel (SL) - Water and Energy data collected from open sources for overall plant.
7. Power Station(PS) - Water and Energy data collected from open sources for power generation plants.
8. NGL(NL) – This plant represents the Natural Gas to Liquid conversion plant. Water and Energy data collected from open sources
9. Polyethylene (PE) – Data for water and energy discharge/requirement for polyethylene plant collected from open sources.
10. LDPE. This plant produces low-density polyethylene. Data collected from open sources.

11. VCM. This plant produces Vinyl Chloride Monomer. Water and Energy data generated using simulation.

Tables 6.1 & 6.2 present the source and sink data respectively. The number of contaminants considered are 10 and consists of TDS, TSS, Nitrogen, Organics, Ammonia, Hardness, Sulfate, Total Petroleum Hydrocarbon (TPH), and Oil & Sulfur. There are a total of 17 sources and 14 sinks.

Table 6.1 Source Data

Type	Plant	Flow	TDS	TSS	Nitrogen	Organics	Ammonia	Hardness	Sulphate	TPH	Oil	Sulfur
Process	VCM	1350	1500	50	100	46.167	3	150	400	0	15	0
Sanitary	VCM	348	1750	50	75	150	5	150	400	0.5	10	0
Brine	VCM	840	3400	50	100	46.167	3	150	400	0	15	0
Blowdown	Steel	2354	1300	0.33	2.25	1	0.5	130	5	5E-07	0.01	0
Sanitary	Steel	182	1750	50	75	150	5	150	400	0.5	10	0
Process	LDPE	3376	1500	50	100	46.167	3	150	400	0	15	0
Process	Fuel Add	872	1500	50	100	46.167	3	150	400	0	15	0
Process	Urea	2500	1500	50	100	46.167	3	150	400	0	15	0
Sanitary	Urea	1000	1750	50	75	150	5	150	400	0.5	10	0
Process	PE	960	1500	50	100	46.167	3	150	400	0	15	0
Brine	PE	350	8500	0	100	0	3	0	400	0	15	0
Brine	PE	200	8500	50	100	46.167	3	150	400	0	15	0
Process	PE	600	1500	50	100	46.167	3	150	400	0	15	0
Process	NGL	332	1500	50	100	46.167	3	150	400	0	15	0
Sanitary	NGL	189	1750	50	75	150	0	0	400	0.5	10	0
Process	GTL	7656	12.8	0.33	5	229	0.5	0.33	5	5E-07	0.01	0
Process	GTL	10187	12.8	0.33	5	229	0.5	0.33	5	5E-07	0.01	0

Table 6.2 Sink Data

Type	Plant	Flow	TDS	TSS	Nitrogen	Organics	Ammonia	Hardness	Sulphate	TPH	Oil	Sulfur
Process	VCM	2850	500	1.33	21	4	0.5	120	50	1	1	64
Process	Steel	4649	500	1.33	21	4	0.5	120	50	1	1	64
Process	LDPE	2081	500	1.33	21	4	0.5	120	50	1	1	64
Process	LDPE	3114	500	1.33	21	4	0.5	120	50	1	1	64
Process	Fuel Add	3682	500	1.33	21	4	0.5	120	50	1	1	64
Process	Urea	5400	500	1.33	21	4	0.5	120	50	1	1	64
Process	Aluminum	840	500	1.33	21	4	0.5	120	50	1	1	64
Process	PE	3412.4	500	1.33	21	4	0.5	120	50	1	1	64
Process	PE	1701.5	500	1.33	21	4	0.5	120	50	1	1	64
Process	NGL	365	500	1.33	21	4	0.5	120	50	1	1	64
Irrigation	NGL	2200	1750	50	75	150	5	150	400	0.5	10	0.1
Process	Refinery	6405	500	1.33	21	4	0.5	120	50	1	1	64
Process	GTL	4956	500	1.33	21	4	0.5	120	50	1	1	64
Process	GTL	1211	500	1.33	21	4	0.5	120	50	1	1	64

The sources consist of various grades of water namely process, sanitary, irrigation and brine. Waste water discharged from sources can either be directly used in other sinks, discharged into the environment or can be sent to treatment and then reused at sinks. Table 6.2 represent the sink data used in the case study. The main categories of sinks considered in this case study are process and irrigation. It is assumed that regulation prohibit reuse of treated water in industrial cities in offices. The treatment option available are Reverse Osmosis (RO), Dissolved Air Floatation (DAF), Nano-Filtration (NF), Membrane Bio Reactor (MBR) and Activated Carbon (AC). Data for treatment technologies is attached in Appendix A.

Energy data available provides information about the amount of excess heat that is available and can be extracted in the form of steam and electricity. It lists out the utility requirement of the plants and the grade of heating. The data has been gathered from open sources and simulations. Table 6.3 provides excess heat data, power requirement for essential equipment heating requirements .and grades of steam that can be produced in plants.

Table 6.3 Heat Data

	Excess Heat (Mw)	Power (Mw)	Furnace Heating (Mw)	Steam Heating (Mw)	Steam Quality	T (C)	P(bars)
GTL	878	439.5	0	0	MP,LP	240,180	16,3.6
AM	426.04	110.6	0	0	LP	140	1.98
ML	427	162	355	0			
RF	113.6	750	0	340	LP	200	16
AL	78.6	1350	0	0	LP	100	1.02
PS	41.67	-	-	-			
NL	22.73	-	-	-			
PE	46	-	-	-			
VCM	26.4	-	-	-			

Initial Configuration

- All office sinks receive water must receive water from an external freshwater supply
- All office wastewater streams were assumed to be of irrigation quality
- Process wastewater streams were assumed at the environmental discharge limit (for all applicable contaminants that are handled within the process)
- Process Brine streams (both from in-plant desalination, as well as from and non-desalination activities) are discharged to the sea.
- No exchange of steam or power, no export of water or power takes place.

- Heat is discharged into the environment using Air Cooler, Cooling Tower and Once through seawater.

Table 6.4 Water – Energy Network (Initial Case)

Plant	Freshwater	Wastewater treatment	AC (Mw)	CT (Mw)	OTSW (Mw)
VCM	2850.0	1698.0	0	26.4	0
Steel	4649.0	2536.0	-	-	-
LDPE	5195.0	3776.0	-	0	0
Methanol	3682.0	872.3	427	0	0
Ammonia	5400.0	3500.0	426.04	0	0
Aluminum	840.0	150.0	78.6	0	0
PE	5114.0	2110.0	0	41.67	0
NGL	2565.0	521.0	0	22.7	0
Refinery	6405.0	-	113.6	0	0
GTL	6167.0	17853.0	0	0	878
PS	-	-	0	46	0

Cost Breakdown of water network for initial configuration is as follow:

Freshwater Cost: 23.91 MM$

Desalination Cost: 1.84 MM$

Treatment Cost: 3.36 MM$

Piping Cost: 1.42 MM$

Total Cost: 30.43 MM$

Cost breakdown of energy network:

Cooling Options:

Power: 58.87 Mw

Capital Cost: 12.54 MM$

Seawater Cost:26.03 MM$

Decentral Power Generation

Capacity:0

Capital Cost:0

Operating Cost:0

Excess heat to Steam

Steam Production Cost:0

Piping Cost:0

The aggregate analysis of water and energy networks are listed in Tables 6.5 and 6.6.

Table 6.5 Water network aggregate analysis (Initial Case)

Water Network Cost (MM$/yr)	30.43
Desalinated Water import/export (tons/d)	139171
Onsite Desalination(tons/d)	6167
Total Water Reuse (tons/d)	0

Table 6.6 Energy Network aggregate analysis (Initial Case)

Energy Network Cost (MM$/yr)	1307
Total Power Generation (Mw)	3211
Total Fuel (Gj/yr)	286×10^6
Power Export (Mw)	0

6.3. Results

6.3.1. Solver Performance

The first set of runs for the synthesis of the combined water-energy network is to demonstrate the ability and robustness of the simulated annealing implementation. The objective of the optimization is minimization of total cost. Exchange of both steam and power has been allowed and the plants can export excess freshwater & power generated. The solver has been coded and executed in Matlab using a laptop with the Intel Core i7 Quad-core processor, 16 GB RAM, and a 64-bit operating system.

The Markov chain length/neighborhood size selected varies from 10 – 100. Like water network solved in section, the performance of the two solvers are analyzed here. Figure 6.1 shows how the search progresses with number of state evaluations for one of the instances of SA solver & TS solver run. The solvers converge to an optimal solution in each instance asymptotically.

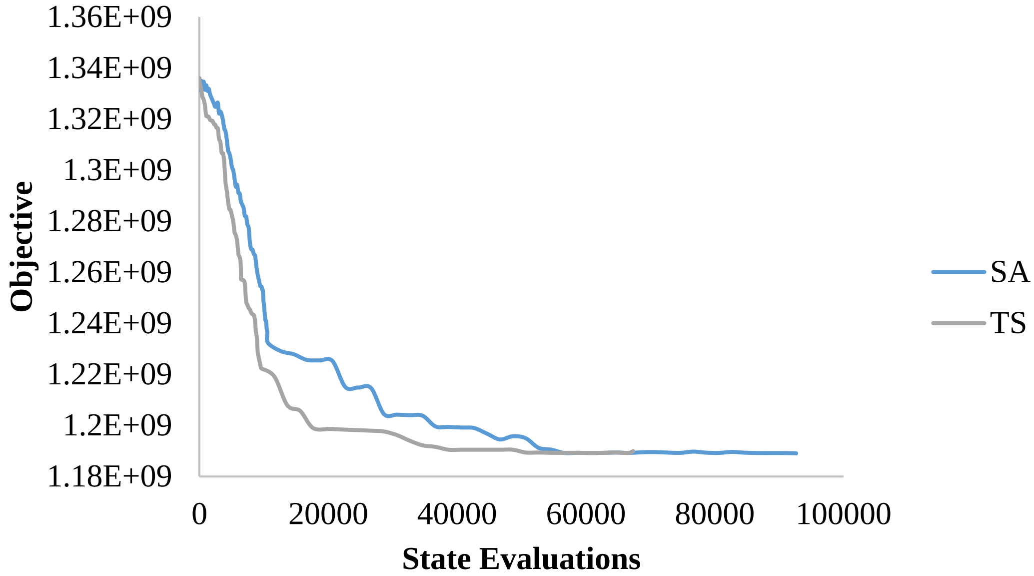


Figure 6.1 Cost vs State Progression (SA & TS)

Figure 6.2 & 6.3 show the average objective value (10 runs) for Markov chains/neighborhood size varying from 10 – 100 for SA & TS solver. As the chain size increases, the average objective function becomes better as a greater number of state evaluations are allowed.

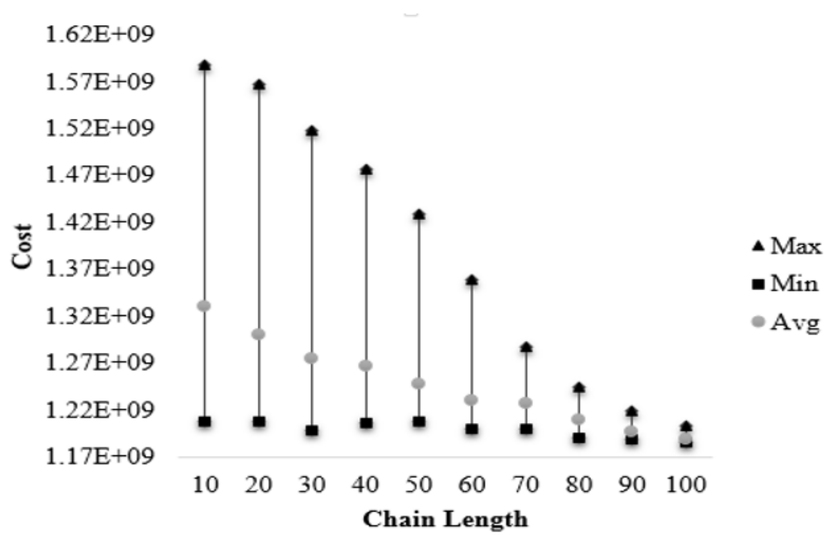


Figure 6.2 Cost vs Chain Length (SA)

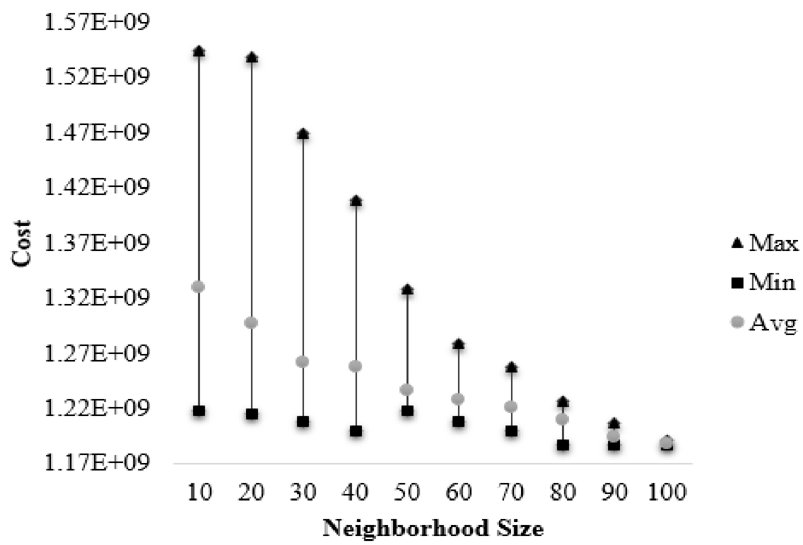


Figure 6.3 Cost vs Neighborhood Size (TS)

Figure 6.4 represents the variation of average objective function across the runs versus the numbers of state evaluated. It shows an improving trend for the objective function (lower cost) with increasing state evaluations. This shows the more the solver is allowed to search, the better the performance. TS solver on average is faster compared to SA solver as it requires lesser number of runs.

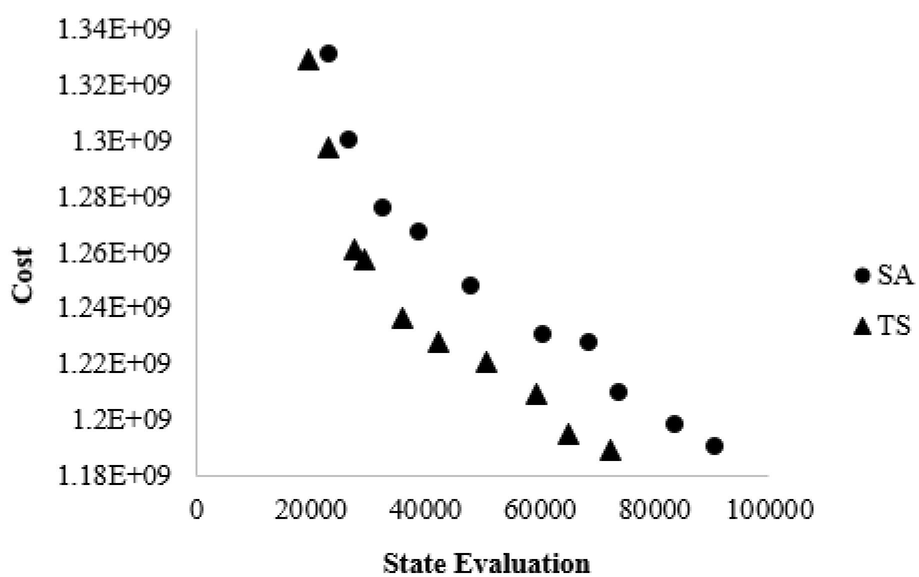


Figure 6.4 Cost vs State Evaluations (SA & TS)

Figure 6.5 presents the variation of state evaluations versus chain length/neighborhood size for SA and TS solver. The number of evaluations increases with chain length implying for a thorough search with an extensive exploration of solution space, the chain length should be larger.

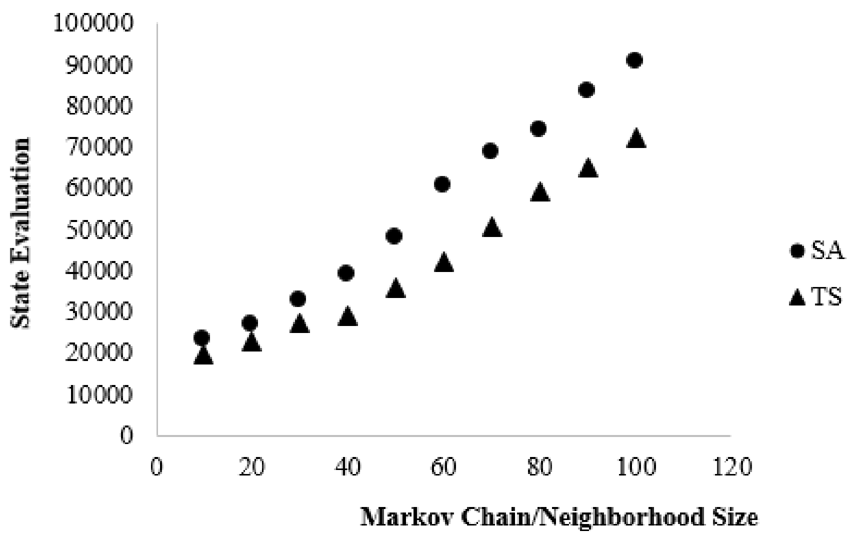


Figure 6.5 State Evaluations vs Markov Chain /Neighborhood Size (SA & TS)

Figure 6.6 shows the standard deviation across each Markov chain/neighborhood. The graph shows an improving trend with very low standard deviation for larger chain sizes. As the chain size is increased, the solver is enabled to search the solution space in more enhanced way thereby making the probability greater for generating the near-optimal solution.

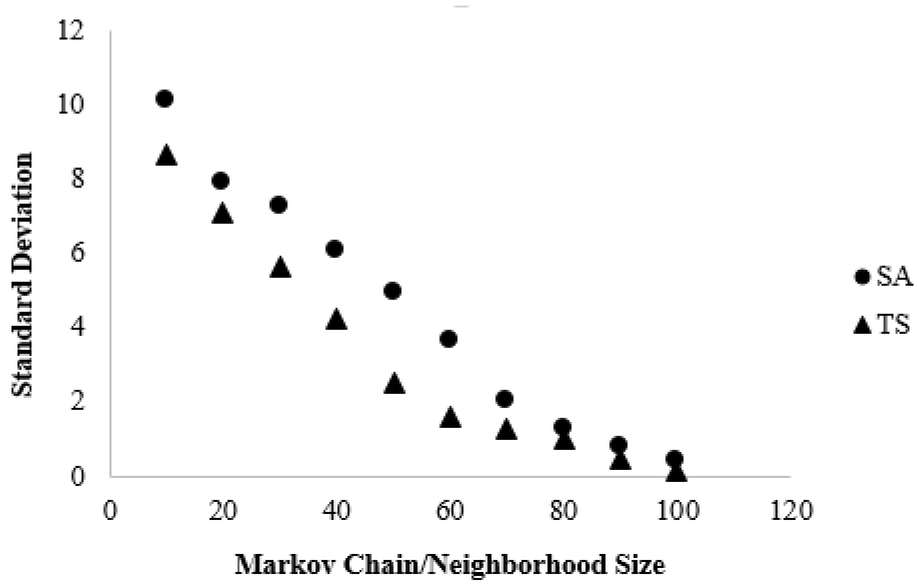


Figure 6.6 Standard Deviation vs Markov Chain/Neighborhood Size (SA & TS)

Figure 6.7 shows the variation of standard deviation with state evaluations. As the number of evaluations increase, the solver become more robust and converge to almost same solution. The number of evaluations correspond to increasing chain /neighborhood size and again highlights the fact that the solvers becomes more reliable with increasing chain/neighborhood size.

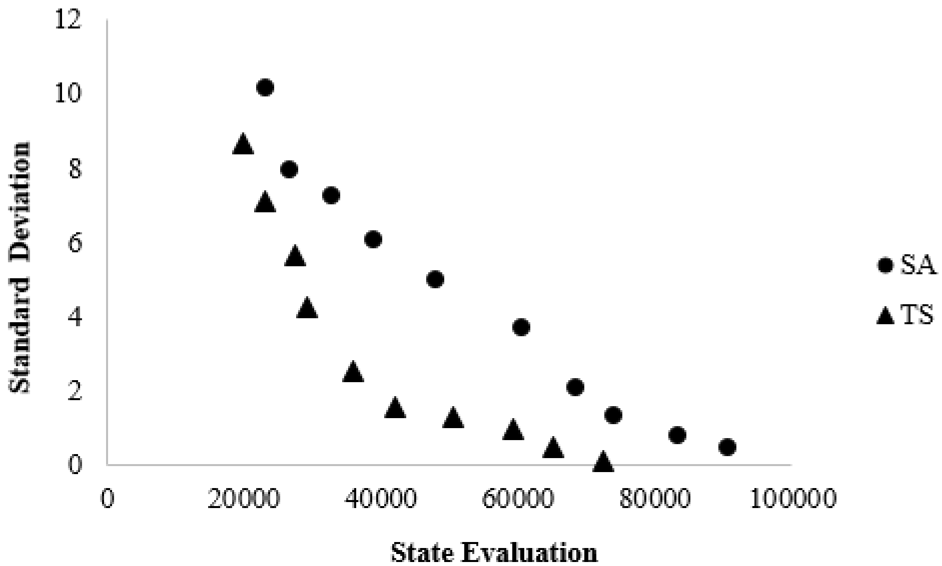


Figure 6.7 Standard Deviation vs State Evaluations (SA)

Figure 6.8 and 6.9 show the variation of cost with state evaluations across all the runs for SA and TS solver. The graph shows the randomness of the solver as more runs doesn't necessarily means better solution. However, as the number of evaluation increases, the probability of getting a better solution improves.

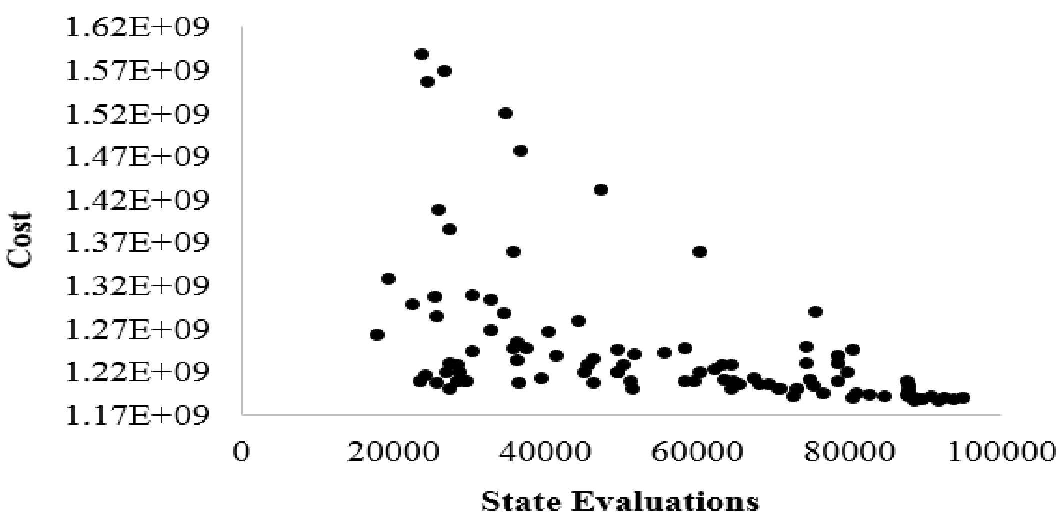


Figure 6.8 Cost vs State Evaluations (SA)

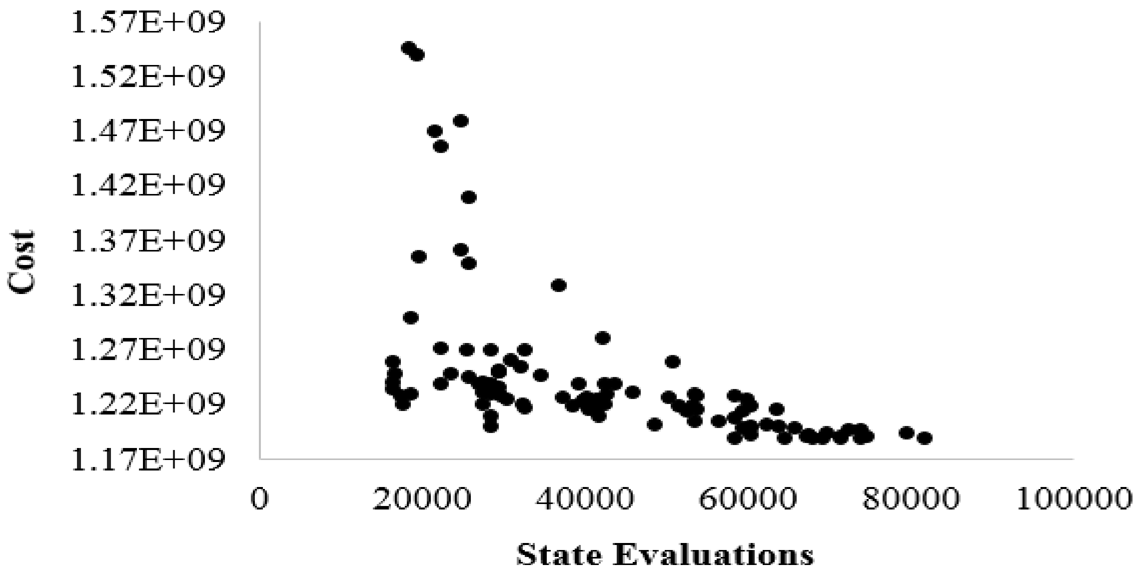


Figure 6.9 Cost vs State Evaluations (TS)

6.3.2. SA Result

The best performing water – energy network (listed below) has a net cost of 1187 MM$ pa for SA solver it took the solver 6-8 hours to converge to the solution.

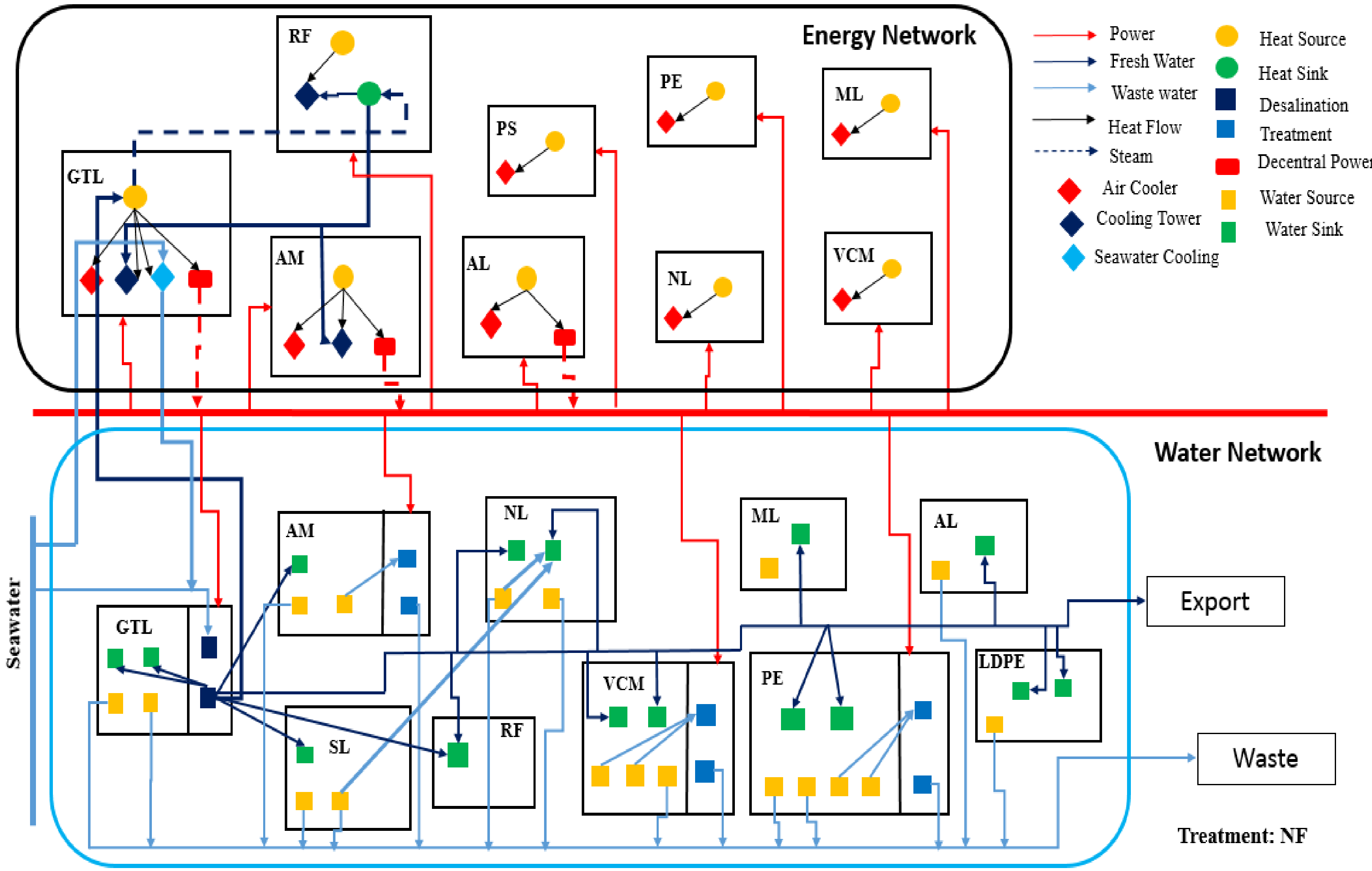


Figure 6.10 Water – Energy network with best performance (SA)

Table 6.7 Desalinated water across plants (Steam, Power exchange & export) – SA

Plant	Desalinated Water	Discharge
VCM	2850	1350.0
Steel	4649	816
LDPE	5195	3376.0
Methanol	3682	872.0
Ammonia	5400	2217.7
Aluminum	840	150
PE	5114	1560.0
NGL	2565	373.7
Refinery	6405	-
GTL	6167	17853.0

Table 6.8 Sources to Treatment Units (Steam, Power exchange & export) – SA

Connection	Flowrate (tons/d)
VCM to VCM	1188.0
Ammonia to Ammonia	1000.0
PE to PE	550.0

Table 6.9 Sources to Sinks (Steam, Power exchange & export) – SA

Connection	Flowrate (tons/d)
NGL to NGL	479.3
Steel to NGL	1720.7

Cost Breakdown of water network for initial configuration is as follow:

Freshwater Cost: 0 MM$

Desalination Cost: 17.6 MM$

Treatment Cost: 2.11 MM$

Piping Cost: 2.14 MM$

Export: -118.71 MM$

Total Cost: -97 MM$

Treatment technology selected: Nano-Filtration

The energy network consists of the following connections:

Table 6.10 Waste Heat to Cooling Systems (Steam, Power exchange & export) – SA

	AC (Mw)	CT (Mw)	OTSW (Mw)
GTL	415.48	41.63	197.34
Ammonia	291.67	0	95.06
Methanol	427	0	0
Refinery	0	113.6	0
Aluminum	78.6	0	0
Power Plant	41.67	0	0
NGL	22.7	0	0
PE	46	0	0
VCM	26.4	0	0

193.45 Mw of medium pressure steam produced from excess heat from GTL plant is transferred for heating purposes in Refinery.

Table 6.11 Decentral Power (Steam, Power exchange & export) - SA

Steam Levels	Plants				
	Refinery	Ammonia	GTL	Methanol	Aluminum
MP(GTL)	0	0	0	0	0
LP(GTL)	18.26	0	0	21.87	0
MP(Ammonia)	0	0	0	0	0
LP(Ammonia)	11.234	0	0	0	0
GTL (LG)	0	0	0	0	24.654
Ammonia (LG)	0	0	0	0	0
Aluminum	0	0	0	7.754	0

The cost breakdown of this network is as follow:

Cooling Options:

Power: 69.89 Mw

Capital Cost: 15.93 MM$/yr

Seawater Cost: 10.6 MM$/yr

Decentral Power Generation

Capacity: 83.77Mw

Capital Cost: 10.05 MM$

Operating Cost: 14.67 MM$

Waste Heat to Steam

Steam Production Cost: 4.84 MM$

Piping Cost: 0.078 MM$

The aggregate analysis of water and energy network is listed in Tables 6.12 & 6.13.

Table 6.12 Water network aggregate analysis (SA)

Water Network Cost (MM$/yr)	-97
Onsite Desalination(tons/d)	663379
Total Water Reuse (tons/d)	0
Water Export (tons/d)	480000

Table 6.13 Energy Network aggregate analysis (SA)

Energy Network Cost (MM$/yr)	1285.19
Total Power Generation (Mw)	3380.3
Total Fuel (Gj/yr)	289.1×10^6
Power Export (Mw)	0

Deviation of Cost from Initial Water Network: -127 43MM$

Deviation of Cost from Initial Energy Network: -21.81 MM$

Total Savings: 149.24 MM$ p.a.

The combined integrated water-energy network shows a saving of 13.6% when compared to an unintegrated network. Export of desalinated water, steam and power exchange provide big savings to the combined network.

Following features have been observed in the solution:

- A policy decision of exporting water and power makes the network profitable.
- Given the following policy, the solution gives a mixture of three options (Air Cooler, Cooling Tower, and Sea Water) as the optimal cooling option rather than one particular technology as reported by Fouladi [93].
- Plants having no export of desalinated water generally have Air Cooler as the cheapest option.

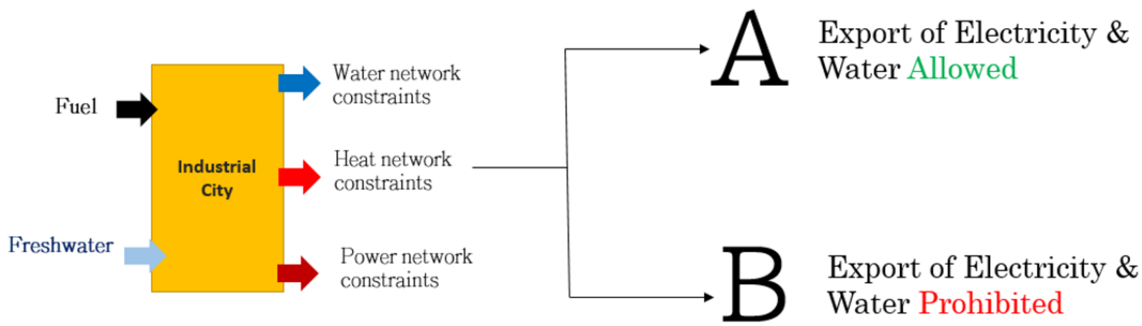
- Dual usage of steam is observed both as a carrier of energy and as raw material (water) at sinks in case of cooling towers of the refinery where steam used in transferring heat from GTL is then used in a cooling tower at the refinery.
- There is an increase in fuel usage from the initial case due to enhanced desalination requirements for export purposes.
- Decentral Treatment Units are preferred for treating wastewater.

For SA solver, the results show the effectiveness of this tool in solving a combinatorically challenging problem and it can handle non – linearities with ease due to the modular approach taken in the optimization of the problem. It shows robust performance and can provide the user with a near-optimal solution. Various analyses carried out across parameters like chain length, state evaluation provides results which are in line with a logical conclusion. The standard deviation for chains of larger value is really small and the solver robustly converges to an optimal solution. The solver shows improving performance with increasing chain size and state evaluation. For the 10 runs used, the solver is given different initial points and it converges to almost similar solutions. It shows asymptotic convergence for one of the runs and given the complexity and size of the problem, the performance shown here provides the user confidence in the solutions.

6.3.3. TS Result

Water – Energy network problem is solved using Tabu Search and the impact of various policies on the water-energy network are studied. The policies are associated with exchange of steam and power and the export of water and power. The objective in each case remains minimization of the total cost of the combined network.

Figure 6.11 presents a set of scenarios evaluated. In scenario 1, the exchange of both steam and power is allowed. It has a subsection allowing the export of water and power and disallowing it. In scenario 2, only the exchange of power is allowed with the same subsections.



Scenario 1: Exchange of both Steam and Power allowed

Scenario 2: Exchange of only Power allowed

Figure 6.11 Policy Scenarios

6.3.3.1. Scenario 1. Exchange of steam and power, export allowed

Scenario 1 deals with steam and Power exchange allowed and the export of water & power is also allowed. Most of the water requirement is met by freshwater produced at the desalination plant. There are direct water reuse connections between irrigation sink in NGL plant and sources in NGL, Steel, and Ammonia. All the sources are directly discharged into the sea but three sources from VCM, Ammonia, and Polyethylene (PE) plants are first treated to environmental discharge levels and then discharged. The treatment technology used is Nano-Filtration. The source water is not reused as its treatment for usage at sinks requires treatment by multiple treatment units in series which is costlier than producing water at the desalination plant

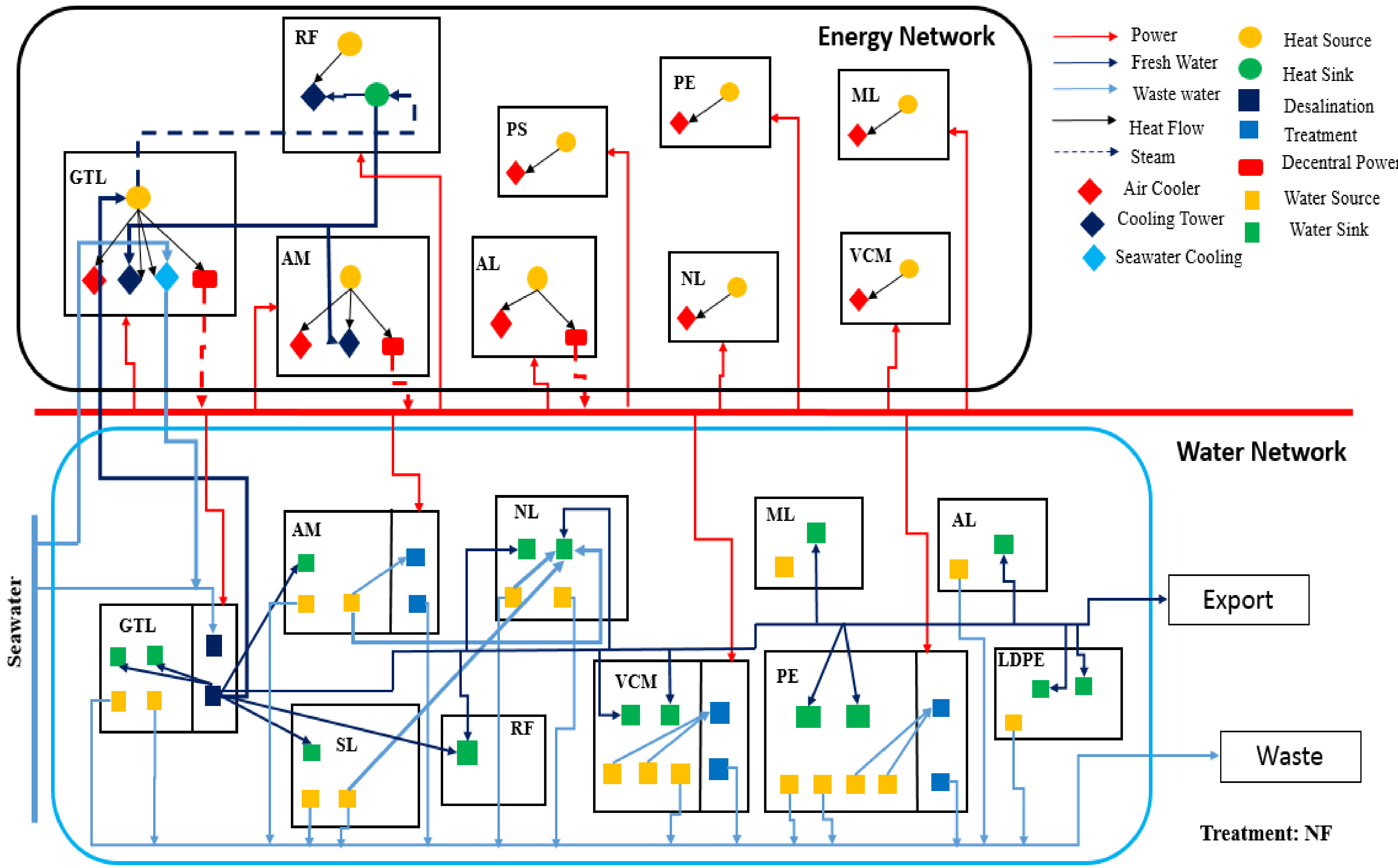


Figure 6.12 Water – Energy network with the best performance (Scenario 1) - TS

Tables 6.14 – 6.16 present the flowrates of the water network. All flowrates are in tons/day.

Table 6.14 Desalinated and wastewater across plants (Scenario 1)

Plant	Desalinated Water	Discharge
VCM	2850	1350.0
Steel	4649	823.2
LDPE	5195	3376.0
Methanol	3682	872.0
Ammonia	5400	2217.7
Aluminum	840	135
PE	5114	1560.0
NGL	2565	674.57
Refinery	6405	-
GTL	6167	17853.0

Table 6.15 Sources to Treatment (Scenario 1)

Connection	Flowrate (tons/d)
VCM to VCM	1188.0
Ammonia to Ammonia	1000.0
PE to PE	550.0

Table 6.16 Sources to Sinks (Scenario 1)

Connection	Flowrate (tons/d)
NGL to NGL	178.5
Ammonia to NGL	282.3
Steel to NGL	1712.8

Cost Breakdown of water network for is as follow:

Freshwater Cost: 0

Desalination Cost: 17.6 MM$

Treatment Cost: 2.11 MM$

Piping Cost: 2.12 MM$

Export: -118.81 MM$

Total Cost: -96.9 MM$

Treatment technology used: Nano-Filtration

194.78 Mw of medium pressure steam produced from excess heat from the GTL plant is transferred for heating purposes in Refinery. The condensate collected here is then reused at sinks at the cooling tower sinks in the same plant, Ammonia, and GTL. This aspect shows the dual use of water both as energy carriers and raw material. Part of excess heat is also used for generating power at decentral power generation units which is then used at various utilities in different plants. The remaining heat is discharged through cooling technologies. Although most of the heat is discharged through Air Cooler, a part of it is also disposed of through cooling tower and seawater cooling. Water transported in the form of steam and then used at the cooling tower makes it a cheaper option than air cooler for that amount of water. Also allowing export incentivizes the use of seawater cooling because the outgoing seawater can be desalinated and exported for profit. Due to constraints on export quantity, a fixed amount of heat can be discharged using this method. Tables 6.17 and 6.18 present the heat flows across the plants.

Table 6.17 Excess heat to Cooling Systems (Scenario 1)

	AC (Mw)	CT (Mw)	OTSW (Mw)
GTL	300.46	25.55	292.4
AM	397.95	16.85	0
ML	427	0	0
RF	0	113.6	0
AL	70.8	0	0
PS	41.67	0	0
NL	22.7	0	0
PE	46	0	0
VCM	26.4	0	0

Table 6.18 Decentral Power Generation (Scenario 1)

Steam Levels	Plants				
	Refinery	Ammonia	GTL	Methanol	Aluminum
MP(GTL)	0	0	0	0	0
LP(GTL)	12.52	0	15.54	0	12.16
MP(AM)	0	0	0	0	0
LP(AM)	0	8.876	0	2.358	0
GTL (LG)	0	0	24.654	0	0
AM(LG)	0	0	0	0	0
AL	0	5.408	2.346	0	0

The cost breakdown of this network is as follow:

Cooling Options:

Power: 70.45 Mw

Capital Cost: 17.58 MM$/yr

Seawater Cost: 8.83 MM$/yr

Decentral Power Generation

Capacity: 83.77 Mw

Capital Cost: 10.05 MM$/yr

Operating Cost: 14.67 MM$/yr

Excess heat to Steam

Steam Production Cost: 4.85 MM$/yr

Piping Cost: 0.078 MM$/yr

The aggregate analysis of water and energy network is listed in Tables 31 & 32:

Table 6.19 Water network aggregate analysis (Scenario 1)

Water Network Cost (MM$/yr)	-96.9
Onsite Desalination(tons/d)	663362
Total Water Reuse (tons/d)	2200
Water Export (tons/d)	480000

Table 6.20 Energy Network aggregate analysis (Scenario 1)

Energy Network Cost (MM$/yr)	1285.3
Total Power Generation (Mw)	3382.1
Total Fuel (Gj/yr)	289.34×10^6
Power Export (Mw)	0

Deviation of Cost from Initial Water Network: -127 33MM$

Deviation of Cost from Initial Energy Network: -21.7 MM$

Total Savings: 149.03 MM$ p.a.

6.3.3.2. Scenario 2. Exchange of steam and power allowed, export not allowed

Scenario 2 deals with steam and Power exchange allowed but export of water & power is prohibited. Figure 6.13 shows the overall network of the optimal solution. Like in the previous scenario, the water network remains unchanged. Most of the water requirement is met by freshwater produced at the desalination plant. There are direct water reuse connections between irrigation sink in NGL plant and sources in NGL and Steel. All the sources are directly discharged into the sea but three sources from VCM, Ammonia, and Polyethylene (PE) plants are first treated to environmental discharge levels and then discharged. The treatment technology used is Nano-Filtration.

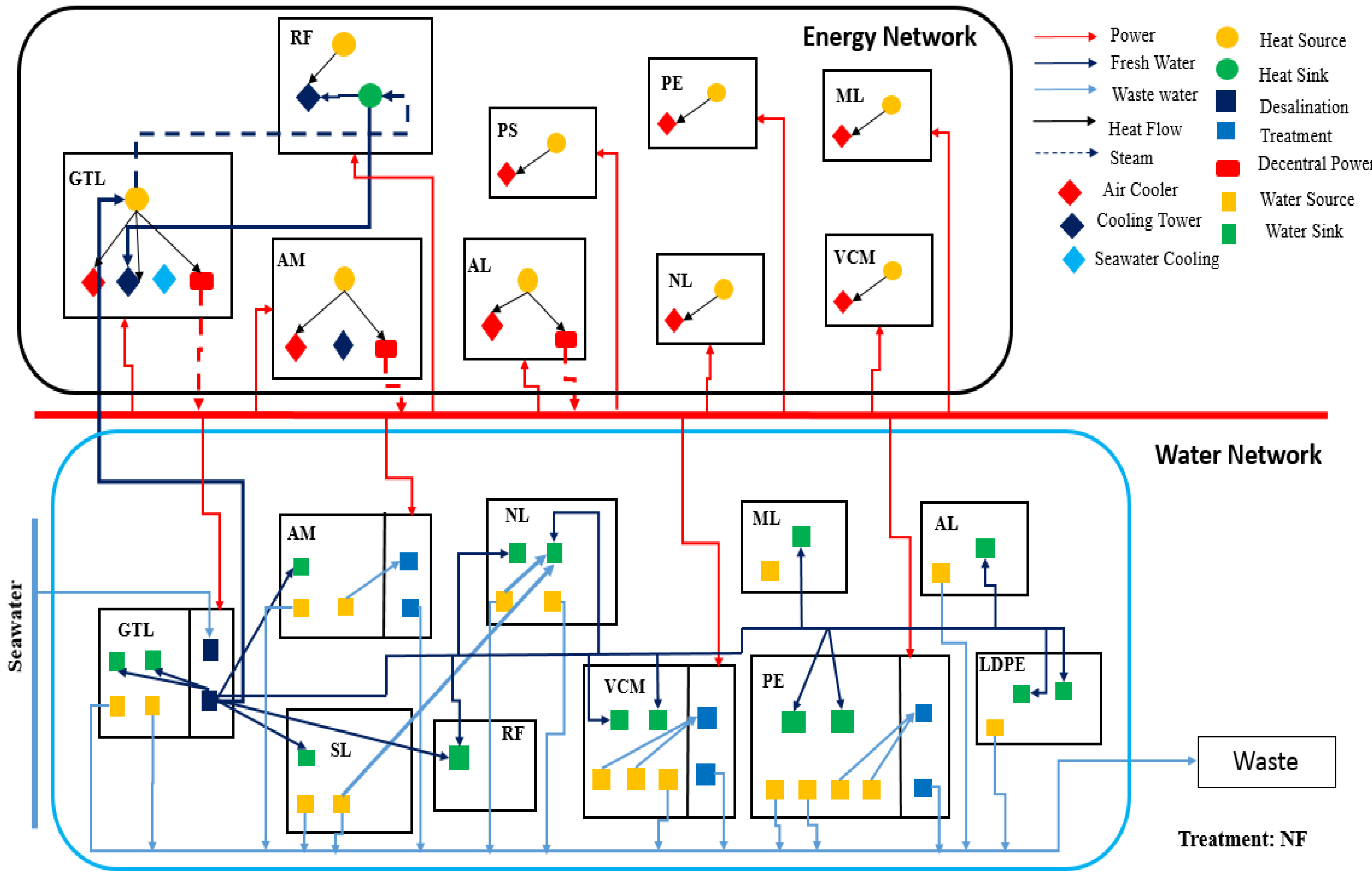


Figure 6.13 Water – Energy Network (Scenario 2)

Tables 6.21 – 6.23 present the flowrates of the water network.

Table 6.21 Desalinated and wastewater across plants (Scenario 2)

Plant	Desalinated Water	Discharge
VCM	2850	1350.0
Steel	4649	857
LDPE	5195	3376.0
Methanol	3682	872.0
Ammonia	5400	2508.0
Aluminum	840	135
PE	5114	1560.0
NGL	2565	332
Refinery	6405	-
GTL	6167	17853.0

Table 6.22 Sources to Treatment (Scenario 2)

Connection	Flowrate (tons/d)
VCM to VCM	1188.0
Ammonia to Ammonia	1000.0
PE to PE	550.0

Table 6.23 Sources to Sinks (Scenario 2)

Connection	Flowrate (tons/d)
NGL to NGL	521
Steel to NGL	1679

Cost Breakdown of the water network is as follow:

Freshwater Cost: 0

Desalination Cost: 18.23 MM$

Treatment Cost: 2.12 MM$

Piping Cost: 2.94 MM$

Export: 0 MM$

Total Cost: 23.29 MM$

Treatment technology used: Nano-Filtration

193.62 Mw of medium pressure steam produced from excess heat from the GTL plant is transferred for heating purposes in Refinery. The condensate collected here is then reused at sinks at cooling tower sinks in the same plant and in GTL highlighting the dual usage of water. Excess heat which cannot be used for steam generation but is of power generation grade is utilized for generating power at decentral power generation units which is then used at various utilities in different plants. Heat which cannot be used for either purpose is discharged through Air Cooler and Cooling Tower. Most of the heat is discharged through Air Cooler and a small portion through Cooling Tower. Since the export of water is prohibited, heat is not discharged through seawater cooling. Tables 6.24 and 6.25 present the heat flows across the plants.

The energy network consists of the following connections:

Table 6.24 Excess heat to Cooling Systems (Scenario 2)

	AC (Mw)	CT (Mw)	OTSW (Mw)
GTL	583.98	40.67	0
Ammonia	413.66	0	0
Methanol	427	0	0
Refinery	0	113.6	0
Aluminum	70.8	0	0
Power Plant	41.67	0	0
NGL	22.7	0	0
PE	46	0	0
VCM	26.4	0	0

Table 6.25 Decentral Power Generation (Scenario 2)

Steam Levels	Plants				
	Refinery	Ammonia	GTL	Methanol	Aluminum
MP(GTL)	0	0	0	0	0
LP(GTL)	0	0	0	34.419	0
MP(Ammonia)	0	0	0	0	0
LP(Ammonia)	0	9.4531	0	0	3.234
GTL (LG)		0	20.216	0	5.23
Ammonia (LG)	0	0	0	0	0
Aluminum	4.54	0	0	0	3.32

The cost breakdown of this network is as follow:

Cooling Options:

Power: 78.153 Mw

Capital Cost: 19.06 MM$/yr

Seawater Cost: 0 MM$/yr

Decentral Power Generation

Capacity: 86.01 Mw

Capital Cost: 10.84 MM$/yr

Operating Cost: 13.54 MM$/yr

Excess heat to Steam

Steam Production Cost: 4.84 MM$/yr

Piping Cost: 0.078 MM$/yr

The aggregate analysis of water and energy network is listed in Tables 6.26 & 6.27.

Table 6.26 Water network aggregate analysis (Scenario 2)

Water Network Cost (MM$/yr)	23.29
Onsite Desalination(tons/d)	115961
Total Water Reuse (tons/d)	2200
Water Export (tons/d)	0

Table 6.27 Energy Network aggregate analysis (Scenario 2)

Energy Network Cost (MM$/yr)	1259.31
Total Power Generation (Mw)	3107
Total Fuel (Gj/yr)	278.38×10^6

Deviation of Cost from Initial Water Network: -7.14 MM$

Deviation of Cost from Initial Energy Network: -48.05 MM$

Total Savings: 55.19 MM$ p.a.

The combined integrated water-energy network shows a saving of 55.19 MM$ when compared to an unintegrated network. Steam and power exchange lead to savings but disallowing freshwater export makes the structure less profitable. The freshwater needs of the plants are met by onsite desalination.

6.3.3.3. Scenario 3. Exchange of power allowed, export allowed

Scenario 3 deals with only power exchange allowed and export of water & power is allowed. Figure 6.14 shows the overall water network of the optimal solution. The water network remains unchanged like in previous scenarios. Tables 6.28 – 6.30 present the flowrates of the water network.

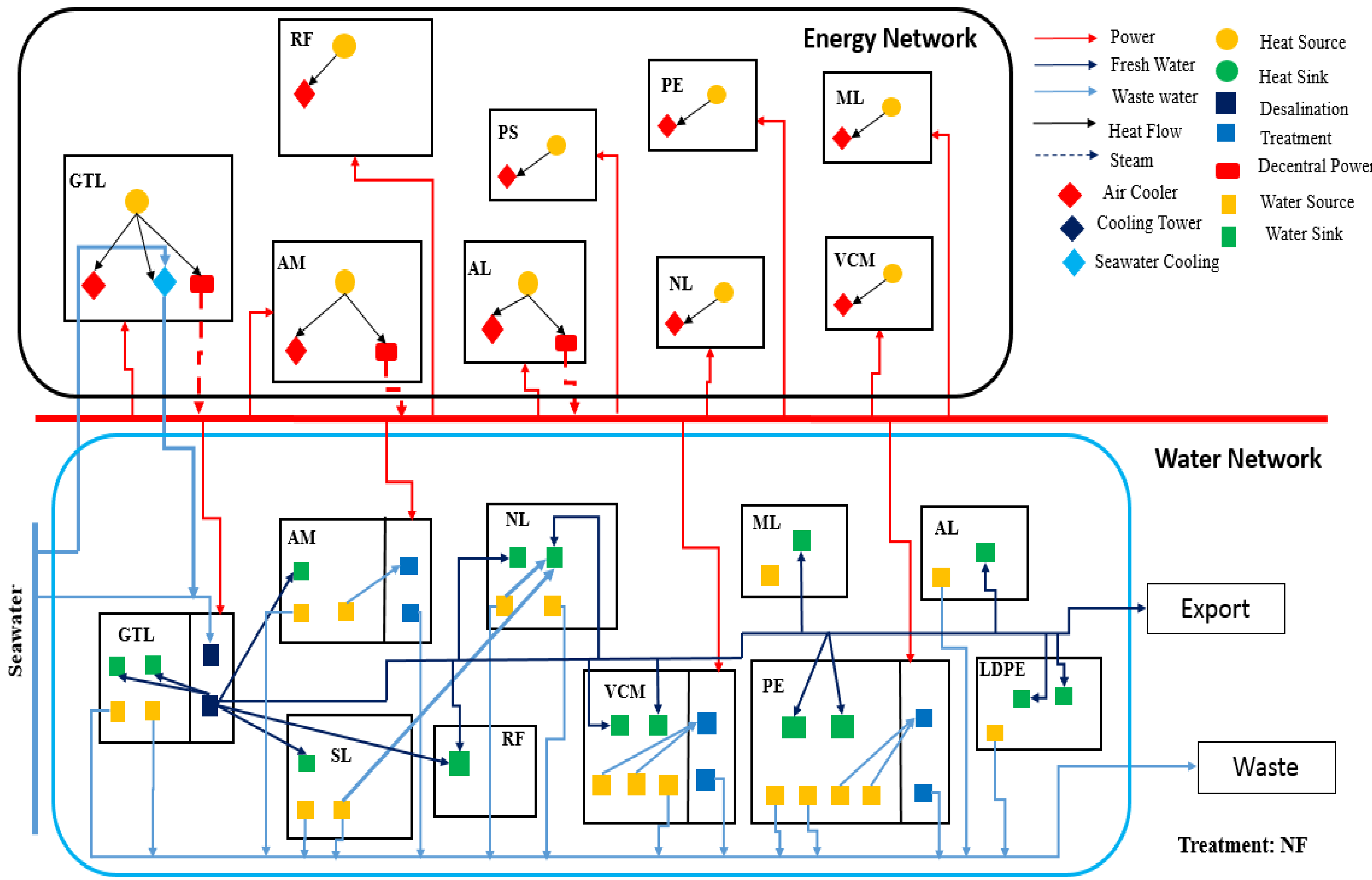


Figure 6.14 Water – Energy Network (Scenario 3)

Table 6.28 Desalinated and wastewater across plants (Scenario 3)

Plant	Desalinated Water	Discharge
VCM	2850	1350.0
Steel	4649	762.68
LDPE	5195	3376.0
Methanol	3682	872.0
Ammonia	5400	2508.0
Aluminum	840	135
PE	5114	1560.0
NGL	2565	359.45
Refinery	6405	-
GTL	6167	17853.0

Table 6.29. Sources to Treatment (Scenario 3)

Connection	Flowrate (tons/d)
VCM to VCM	1188.0
Ammonia to Ammonia	1000.0
PE to PE	550.0

Table 6.30. Sources to Sinks (Scenario 3)

Connection	Flowrate (tons/d)
NGL to NGL	494.24
Steel to NGL	1773.32

Cost Breakdown of the water network is as follow:

Freshwater Cost: 0

Desalination Cost: 19.36 MM$

Treatment Cost: 2.12 MM$

Piping Cost: 2.23 MM$

Export: -118.81 MM$

Total Cost: -95.1 MM$

Since no exchange of steam is allowed, all of the heat which can be converted to medium pressure steam in the GTL plant is also converted to power along with the lower grade of excess heat. The remaining heat is discharged through Air Cooler and Seawater Cooling. Portion of heat is discharged through water cooling and the outflowing seawater is desalinated and exported. Tables 6.31 and 6.32 present the heat flows across the plants.

The energy network consists of the following connections:

Table 6.31 Excess heat to Cooling Systems (Scenario 3)

	AC (Mw)	**CT (Mw)**	**OTSW (Mw)**
GTL	478.13	0	292.4
Ammonia	413.71	0	0
Methanol	427	0	0
Refinery	113	0	0
Aluminum	70.8	0	0
Power Plant	41.67	0	0
NGL	22.7	0	0
PE	46	0	0
VCM	26.4	0	0

Table 6.32 Decentral Power Generation (Scenario 3)

Steam Levels	Plants				
	Refinery	**Ammonia**	**GTL**	**Methanol**	**Aluminum**
MP(GTL)	0	0	27.455	14.246	0
LP(GTL)	0	22.853	0	16.767	0
MP(Ammonia)	0	0	0	0	0
LP(Ammonia)	0	0	0	12.321	0
GTL (LG)	0	0	0	0	25.421
Ammonia (LG)	0	0	0	0	0
Aluminum	0	0	2.045	0	4.945

The cost breakdown of this network is as follow:

Cooling Options:

Power: 72.7 Mw

Capital Cost: 17.29 MM$/yr

Seawater Cost: 10.65 MM$/yr

Decentral Power Generation

Capacity: 121.13 Mw

Capital Cost: 15.12 MM$/yr

Operating Cost: 22.08 MM$/yr

Excess heat to Steam

Steam Production Cost: 0 MM$/yr

Piping Cost: 0 MM$/yr

The aggregate analysis of water and energy network is listed in Tables 6.33 & 6.34:

Table 6.33 Water network aggregate analysis (Scenario 3)

Water Network Cost (MM$/yr)	-95.1
Onsite Desalination(tons/d)	732975
Total Water Reuse (tons/d)	2200
Water Export (tons/d)	48000

Table 6.34 Energy Network aggregate analysis (Scenario 3)

Energy Network Cost (MM$/yr)	1391.29
Total Power Generation (Mw)	3285.34
Total Fuel (Gj/yr)	283.6×10^6
Power Export (Mw)	0

Deviation of Cost from Initial Water Network: -122.1 MM$

Deviation of Cost from Initial Energy Network: 84.29 MM$

Total Savings: 37.81 MM$ p.a.

The combined integrated water-energy network shows a saving of 37.81 MM$ when compared to an unintegrated network. Export of desalinated water, power exchange provide savings but lack of steam exchange makes this structure less profitable. Treatment technology used in this structure is Nano-Filtration and onsite desalination is used to supply fresh water for the plant.

6.3.3.4. Scenario 4. Exchange of power allowed, export not allowed

Scenario 4 deals with only power exchange allowed but the export of water & power is allowed. Figure 6.15 presents the water-energy network for this scenario.

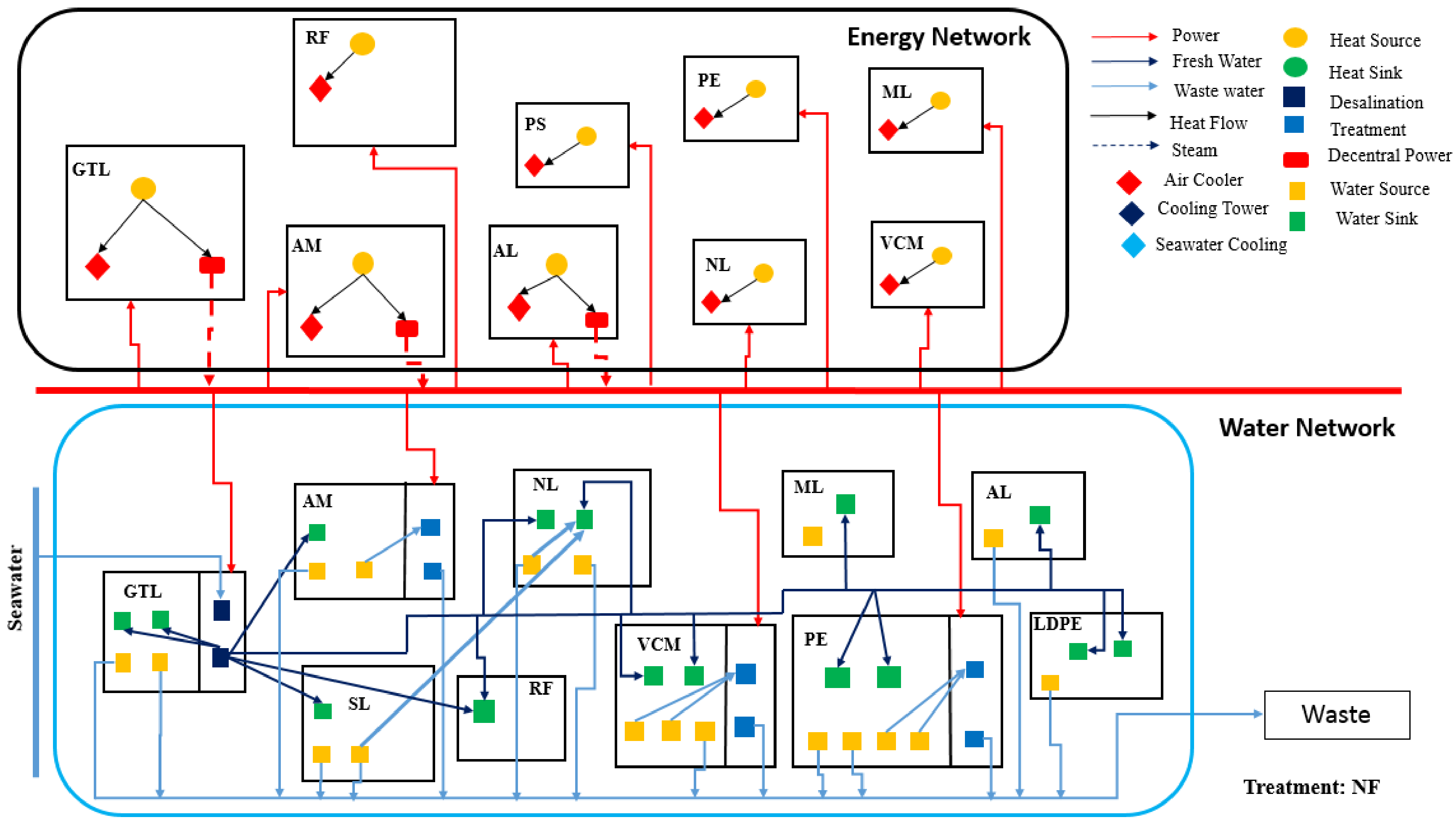


Figure 6.15 Water – Energy Network (Scenario 4)

The water network remains unchanged like in previous scenarios. Tables 35 – 37 present the flowrates of the water network.

Table 6.35 Desalinated and wastewater across plants (Scenario 4)

Plant	Desalinated Water	Discharge
VCM	2850	1350.0
Steel	4649	742.77
LDPE	5195	3376.0
Methanol	3682	872.0
Ammonia	5400	2500
Aluminum	840	135
PE	5114	1560.0
NGL	2565	380.62
Refinery	6405	-
GTL	6167	17853.0

Table 6.36 Sources to Treatment (Scenario 4)

Connection	Flowrate (tons/d)
VCM to VCM	1188.0
Ammonia to Ammonia	1000.0
PE to PE	550.0

Table 6.37 Sources to Sinks (Scenario 4)

Connection	Flowrate (tons/d)
NGL to NGL	472.38
Steel to NGL	1793.23

Cost Breakdown of water network for initial configuration is as follow:

Freshwater Cost: 0

Desalination Cost: 18.22 MM$

Treatment Cost: 3.26 MM$

Piping Cost: 2.87 MM$

Total Cost: 24.15MM$

All steam and power generation grade heat is converted to power using a decentral power generation system. Remaining excess heat is discharged through Air Coolers and since there is no exchange of steam or export of water allowed, cooling towers and seawater cooling is not used. Tables 6.38 and 6.39 present the heat flows across the plants.

The energy network consists of the following connections:

Table 6.38 Excess heat to Cooling Systems (Scenario 4)

	AC (Mw)	CT (Mw)	OTSW (Mw)
GTL	769.84	0	0
Ammonia	413.66	0	0
Methanol	113.6	0	0
Refinery	427	0	0
Aluminum	70.8	0	0
Power Plant	41.67	0	0
NGL	22.7	0	0
PE	46	0	0
VCM	26.4	0	0

Table 6.39 Decentral Power Generation (Scenario 4)

Steam Levels	Plants				
	Refinery	**Ammonia**	**GTL**	**Methanol**	**Aluminum**
MP(GTL)	0	0	32.55	0	8.804
LP(GTL)	0	0		21.343	17.694
MP(Ammonia)	0	0	0	0	0
LP(Ammonia)	0	12.15	0	0	0
GTL (LG)	24.674	0	0	0	0
Ammonia (LG)	0	0	0	0	0
Aluminum	0	0	0	0	7.734

The cost breakdown of this network is as follow:

Cooling Options:

Power: 87.4 Mw

Capital Cost: 17.29 MM$/yr

Seawater Cost: 10.65 MM$/yr

Decentral Power Generation

Capacity: 121.05 Mw

Capital Cost: 15.03 MM$/yr

Operating Cost: 21.98 MM$/yr

Excess heat to Steam

Steam Production Cost: 0 MM$/yr

Piping Cost: 0 MM$/yr

The aggregate analysis of water and energy network is listed in Tables 6.40 & 6.41:

Table 6.40 Water network aggregate analysis (Scenario 4)

Water Network Cost (MM$/yr)	24.15
Onsite Desalination(tons/d)	732935
Total Water Reuse (tons/d)	2200
Water Export (tons/d)	0

Table 6.41 Energy Network aggregate analysis (Scenario 4)

Energy Network Cost (MM$/yr)	1289.3
Total Power Generation (Mw)	3061.3
Total Fuel (Gj/yr)	275.59×10^6
Power Export (Mw)	0

Deviation of Cost from Initial Water Network: -2.9 MM$

Deviation of Cost from Initial Energy Network: -17.7 MM$

Total Savings: 20.6 MM$ p.a.

The combined integrated water-energy network shows a saving of 20.6 MM$ when compared to an unintegrated network. Inhibiting steam exchange and export makes the structure least profitable among the scenarios considered. All the usable waste heat is converted to decentral power which is then used at various power sinks across the industrial city. The water requirement is met using desalinated water and the irrigation water requirement is met by direct reuse of water. Most of the water from the sources is discharged directly into the environment and two streams are treated using Nano-filtration technology to bring them to the discharge level.

6.4. Conclusion

Scenarios, where the export of water and exchange of both water and power is allowed, generate the most cost-effective results. Considerable savings are achieved if these policies are incorporated into planning. The solver performs robustly and multiple solutions with similar performance are obtained thereby giving insight into the tradeoffs between various elements of the structure. The solver shows asymptotic convergence in one of the runs. Its performance increases as (Lower Cost and Standard Deviation) the Markov chain length increases. Compared to SA, TS takes a lesser number of state evaluation to attain the desired result. Also, TS has better standard deviation compared to SA for lower Markov chains but it becomes similar for higher neighborhood sizes.

7. MULTI-OBJECTIVE ANALYSIS OF SUSTAINALIBILITY AND ECONOMICS

Sustainability refers to the idea of meeting our own needs without compromising the ability of future generations to meet their own needs. The whole idea impinges on the philosophy of minimal impact on the environment. Sustainability can be represented using different methods and the concern represented by them is broadly categorized into economic, environment and social impact.

Despite the lack of consensus over the term, over the last few decades, the idea of sustainability evolved from a vague concept to precise definitions that attempt to present sustainability in quantitative terms and indicators. The sustainability matrix and indices help to define and quantify sustainability. It generally involves quantification of the impact on the environment across various indicators. Some of the indicators are economic, environmental, ecological, water quality and air quality. Apart from these, social indicators show the overall well-being of the people in society.

Very many methods for quantifying sustainability have been proposed. Though many researchers have tried quantifying the effects, they lack in covering all dimensions. The methodology developed by Fouladi [93] utilizing sustainability metrics has been adapted here for designing a sustainable water-energy network which covers the multidimensionalal aspect of profitability and environmental impacts.

7.1. Sustainability Metrics

Sustainability metrics quantify the economic, environmental and social impact which help in decision making by understanding the tradeoffs. Extensive work has been done over the years by researches across several fields to come up with a framework which covers all aspects of sustainability. Some of the examples are:

- AIChE Sustainability Index. ("AIChE Sustainability Index: Strategic Commitment to Sustainability," 2008)
- Sustainability Indices (Tugnoli et al., [103])
- Three-Dimensional Sustainability Metrics (Martins et al [104])
- BRIDGES to Sustainability Metrics (Tanzil and Beloff, [105])
- Global Environmental Risk Assessment (GERA) Index (Achour et al [106])
- IChemE Sustainability Metrics (IChemE Metrics [107])
- Indicators of sustainable production (Krajnc and Glavic [108])
- Green Metrics (Constable et al [109])
- BASF Socio-Eco-efficiency Metrics (Saling et al [110])
- AICHE/ CWRT Sustainability Metrics (AIChE Center for Waste Reduction Technologies (CWRT) [111])
- Sustainability Indicators (Afgan et al [112])
- Inherent Process Safety Index (Heikkila [113])

In this work, we adapt the work of Fouladi [93] for quantifying the sustainability parameter. Since water-energy network optimization doesn't change the industrial city layout, the social impact is minimal. Economic and Environmental impact is the one that is sought out for and the trade-off between the two is studied. This work utilizes TRACI metrics for environmental impact calculation. The expression of cost as an objective function has been accounted for in previous sections.

7.2. TRACI Metrics

TRACI stands for Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts. Environmental Protection Agency (EPA) developed it. It has been developed for sustainability metrics, life cycle impact assessment, industrial ecology, and process design impact assessment. It enables the user to quantify ozone depletion, global warming, acidification, eutrophication, photochemical smog formation, human health particulate effects, human health cancer, human health non-cancer, eco-toxicity, and fossil fuel depletion effects.

7.2.1. Methodology

For quantifying the impact of a chemical emission, TRACI utilizes the amount of the chemical emission and the estimated potency of the stressor. The estimated potency is based on the best available models and data for each impact category. For some impact categories (e.g., ozone depletion potentials, global warming potentials), there is an international consensus on the relative potency of the chemicals listed. For other impact categories, the relative potency may be dependent on models related to chemical and physical principles and/or experimental data.

The calculation of impact factor is done using following equation:

$$I^i = \sum_{xm} CF_{xm}^i M_{xm} \tag{142}$$

Where:

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

CF_{xm}^i = the characterization factor of chemical (x) emitted to media(m) for impact category(i)

M_{xm} = the mass of chemical (x) emitted to media (m).

For emission-related categories, characterization factors are available for media listed in Table 7.1.

Table 7.1 Eco - characterization and respective media.

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, Non-urban Air, Freshwater, Seawater, Natural Soil, Agricultural Soil
Human Health Non-cancer	Urban Air, Non-urban Air, Freshwater, Seawater, Natural Soil, Agricultural Soil
Eco-toxicity	Urban Air, Non-urban Air, Freshwater, Seawater, Natural Soil, Agricultural Soil

The following assumptions have been made for calculation of these sustainability metrics

- Safety and health metrics are not affected as the industrial city design or layout doesn't change.
- Environmental emissions can be divided as solid waste, atmospheric impact and aquatic impact. Values for these groups has been taken from TRACI metrics and quantified. Figure 7.1 presents these groups

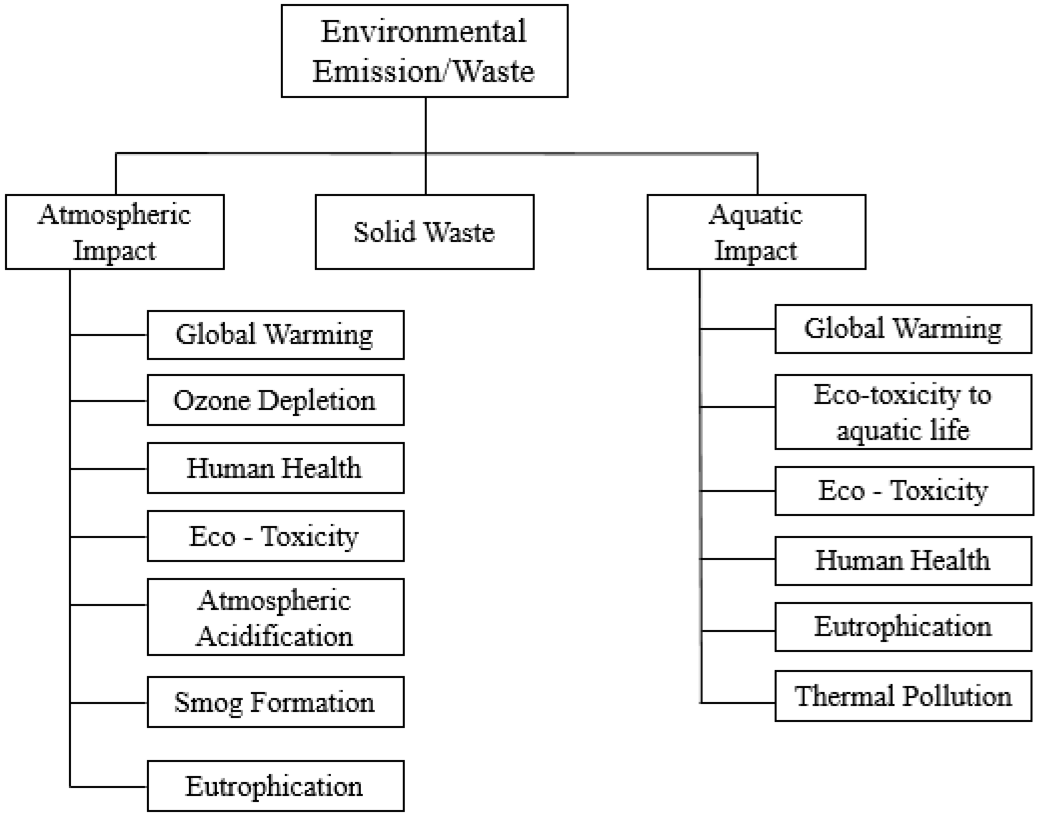


Figure 7.1 Elements of TRACI metrics

Contributors assumed for this problem as mentioned in Fouladi [93] are as follows:

- 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

Figure 7.2 provides a detailed picture of the contributors assessed in the problem. This work quantifies only two categories of impact: Atmospheric Impact and Aquatic Impact.

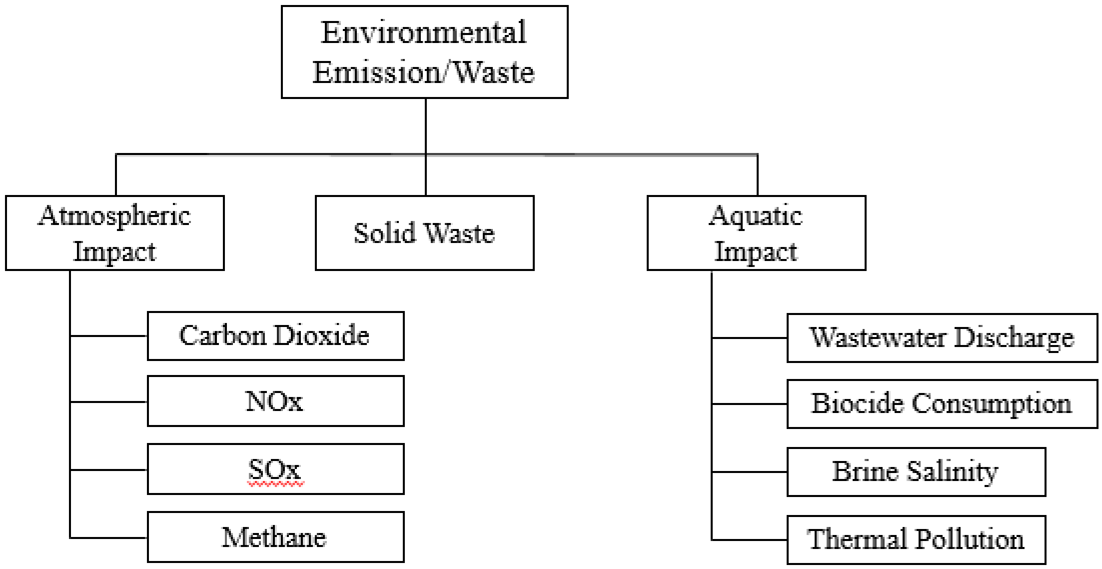


Figure 7.2 Elements of TRACI metrics assessed.

7.3. Solver Customization & Multi-Objective Analysis

All the elements of the Tabu Search solver in section 5 have been used here with modification in the evaluation module. Two objectives namely global warming and aquatic impact have been defined and solved for the optimal structure.

The multi-objective analysis has been carried out between atmospheric and aquatic impact versus cost. The structure has been first optimized for minimizing atmospheric impact and the corresponding cost of the structure has been calculated. Atmospheric impact for the cost-effective structure is calculated and plotted on a graph between cost and atmospheric impact. In both cases, there is an exchange of power and power and the export of water and power is allowed. The above mentioned two points present the two extremes of the plot: the least cost and least atmospheric impact. The constraint for atmospheric impact is relaxed by certain percentages and then the structure is optimized for cost. The data generated is then plotted to generate the cost vs atmospheric impact Pareto curve. A similar analysis is also carried out for the aquatic impact objective as well.

7.3.1. Atmospheric Impact

The atmospheric impact consists of global warming, atmospheric acidification, and ozone depletion. Firstly, the emission of CO_2, CH_4, SO_2, and NOx are calculated by the following expression:

Emission (Tons/yr) : Power x Conversion Factor x 0.001 x 24 x 365 (143)

Conversion factor the above-mentioned pollutants are as follows:

Table 7.2 Conversion Factor

Pollutant	Conversion Factor
CO_2	1.22
CH_4	72×10^{-7}
SO_2	24×10^{-3}
NOx	275×10^{-7}

The environment burden (EB) is then calculated for global warming, atmospheric acidification, and ozone depletion is calculated using the following expression:

EB = Potency Factor (PF) x Emission (tons/yr). (144)

Table 7.3 Global Warming

Pollutant	Potency Factor
CO_2	1
CH_4	21
N_2O	40
NOx	310

Table 7.4 Atmospheric Acidification

Pollutant	Potency Factor
SO_2	1
N_2O	0.7

Table 7.5 Ozone Depletion

Pollutant	Potency Factor
CO_2	1
CH_4	21
N_2O	40
NOx	310

7.3.2. Aquatic Impact

Here the impact of chloride and manganese due to discharge of wastewater into water bodies is evaluated. The chloride and manganese discharge are calculated by the following expression:

Discharge (Tons/yr) = Load Discharge x Conversion Factor x 365. (145)

The conversion factor for chloride and manganese are 0.5423 and 0.03606 respectively. The environmental burden of these contaminants is calculated by the equation mentioned in the atmospheric impact section. The impact factor of chloride and manganese are 0.5 and 0.1.

For multi-objective analysis, cost vs atmospheric /aquatic impact is mapped. The best structure for atmospheric/aquatic impact has a higher cost than the cost-optimal structure. As the constraints of global warming and aquatic impacts are relaxed, the structure moves towards the optimal cost structure.

7.4. Case Study

The case study used to demonstrate the above-described method is the same as the one used for the demonstration of Simulated Annealing and Tabu Search. Only the objective function changes in the formulation and instead of cost, atmospheric impact and aquatic impact are chosen as objective. This study aims to analyze the trade-offs between economics and sustainability.

7.5. Results

7.5.1. Atmospheric Impact

The first objective function evaluated is global warming. The entire framework of the solver remains the same except for the objective function. The objective function calculates the amount of CO_2, SO_x, NO_x, and CH_4 is released into the atmosphere and the impact. Figure 7.3 presents the optimal structure for minimizing the atmospheric impact.

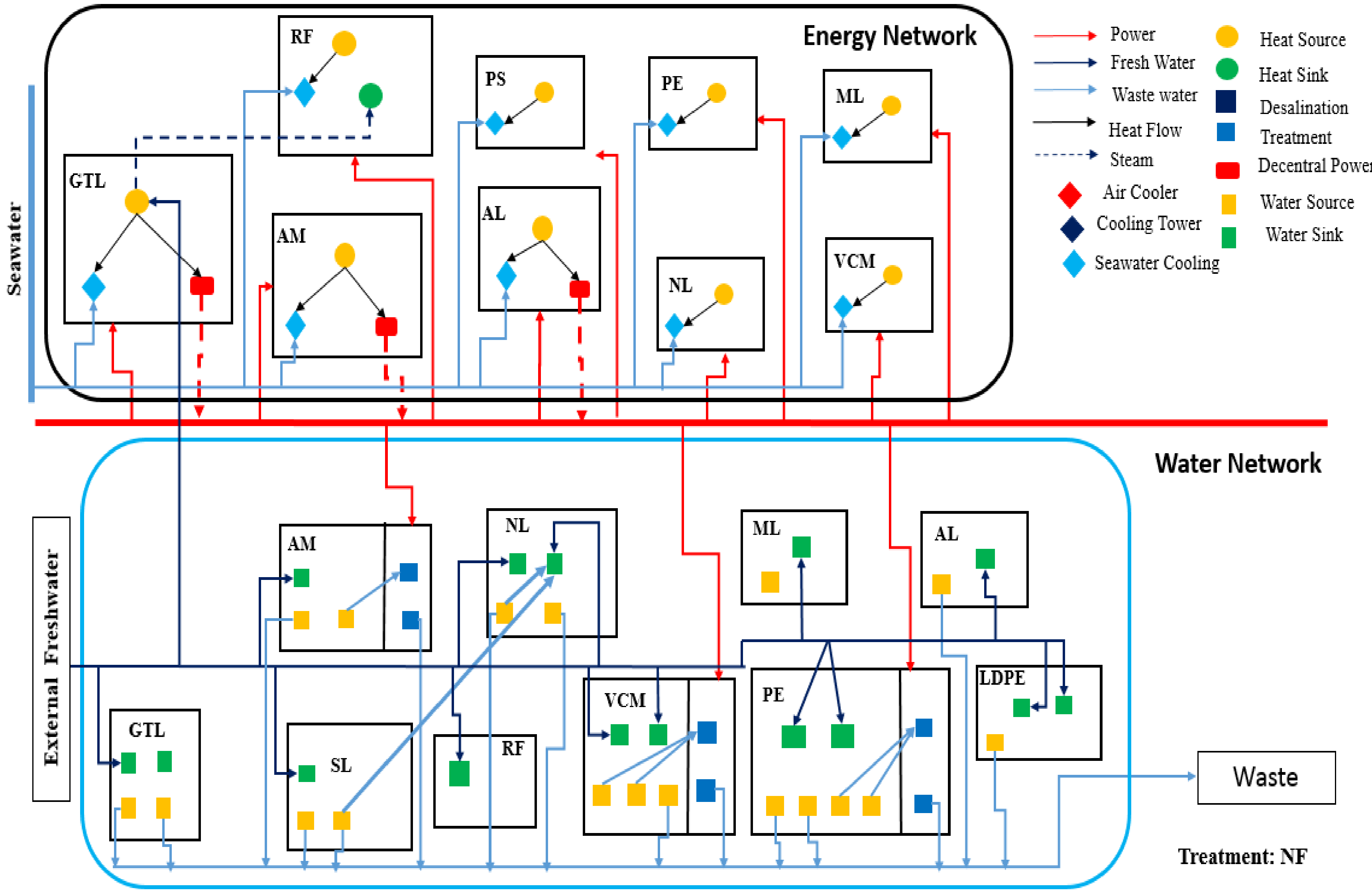


Figure 7.3 Water- Energy Network (Atmospheric Impact)

Table 7.6 Freshwater usage across plants (Atmospheric Impact)

Plant	Flowrate (tons/d)
VCM	**2850**
Steel	4649
LDPE	5195
Fuel Additives	3682
Ammonia	5400
Aluminum	840
PE	5114
NGL	365
Refinery	6405
GTL	6167

Table 7.7 Source to Waste (Atmospheric Impact)

Plant	Flowrate (tons/d)
VCM	1350.0
Steel	2081.4
LDPE	3376.0
Methanol	872.0
Ammonia	2508.0
Aluminum	135
PE	1560.0
NGL	332
GTL	17853.0

Table 7.8 Sources to Sinks (Atmospheric Impact)

Connection	Flowrate (tons/d)
NGL to NGL	489.345
Steel to NGL	1710.24

Freshwater Cost: 21.96 MM$

Desalination Cost: 0 MM$

Treatment Cost: 2.12 MM$

Piping Cost: 2.93 MM$

Total Cost: 27.06 MM$

The energy network consists of the following connections:

Table 7.9 Waste Heat to Cooling Systems (Atmospheric Impact)

	AC (Mw)	CT (Mw)	OTSW (Mw)
GTL	0	0	617.27
Ammonia	0	0	413.66
Methanol	0	0	113.6
Refinery	0	0	427
Aluminum	0	0	70.8
Power Plant	0	0	41.67
NGL	0	0	22.7
PE	0	0	46
VCM	0	0	26.4

195 Mw of medium pressure steam produced from excess heat from GTL plant is transferred for heating purposes in Refinery.

Table 7.10 Decentral Power Generation (Atmospheric Impact)

Steam Levels	Plants				
	Refinery	Ammonia	GTL	Methanol	Aluminum
MP(GTL)	0	0	0	0	0
LP(GTL)	20.56	0	7.35	12.315	0
MP(Ammonia)	0	0	0	0	0
LP(Ammonia)	4.85	0	0	0	7.531
GTL (LG)	8.93	7.45	6.607	2.56	0
Ammonia (LG)	0	0	0	0	0
Aluminum	0	1.574	0	0	6.0798

Cooling Options:

Power: 17.79 Mw

Capital Cost: 0 MM$/yr

Seawater Cost: 53.76 MM$/yr

Decentral Power Generation

Capacity: 85.08 Mw

Capital Cost: 10.32 MM$/yr

Operating Cost: 13.17 MM$/yr

Waste Heat to Steam

Steam Production Cost: 4.85 MM$/yr

Piping Cost: 0.78 MM$/yr

The aggregate analysis of water and energy network is listed in Tables 7.11 & 7.12.

Table 7.11 Water network aggregate analysis (Atmospheric Impact)

Water Network Cost (MM$/yr)	27.06
Onsite Desalination(tons/d)	0
Total Water Reuse (tons/d)	2200
Water Export (tons/d)	0

Table 7.12 Energy Network aggregate analysis (Atmospheric Impact)

Energy Network Cost (MM$/yr)	1352.81
Total Power Generation (Mw)	3028.56
Total Fuel (Gj/yr)	270.31×10^6
Power Export (Mw)	0

Atmospheric Impact (Objective-Global Warming Minimization): 31.31×10^6 kg CO2-eq

Atmospheric Impact (Objective-Cost Minimization): 32.89×10^6 kg CO2-eq

Deviation from Minimum Cost Structure: -1.58×10^6 kg CO2-eq

Deviation in cost from Minimum Cost Structure: 195.98 MM$

The above-mentioned analysis gives the optimal structure for minimum global warming. To study the variation of cost with the relaxation of constraint on global warming, a Pareto curve is mapped. An extra constraint on the emission parameters was added and the objective of the problem is to minimize the total cost. Figure 7.4 shows the variation of cost with atmospheric impact. Table 7.13 presents the cost and optimal cooling system.

Table 7.13 Cost & Cooling Options for atmospheric impact constraint

Scenario (% decrease)	Cost (MM$/p a)	Cooling System
10	1337.79	OTSW
20	1304.41	OTSW
40	1255.8	OTSW
50	1231.5	OTSW
60	1207.2	OTSW
80	1185.48	OTSW +AC
95	1182.35	OTSW + CT+AC

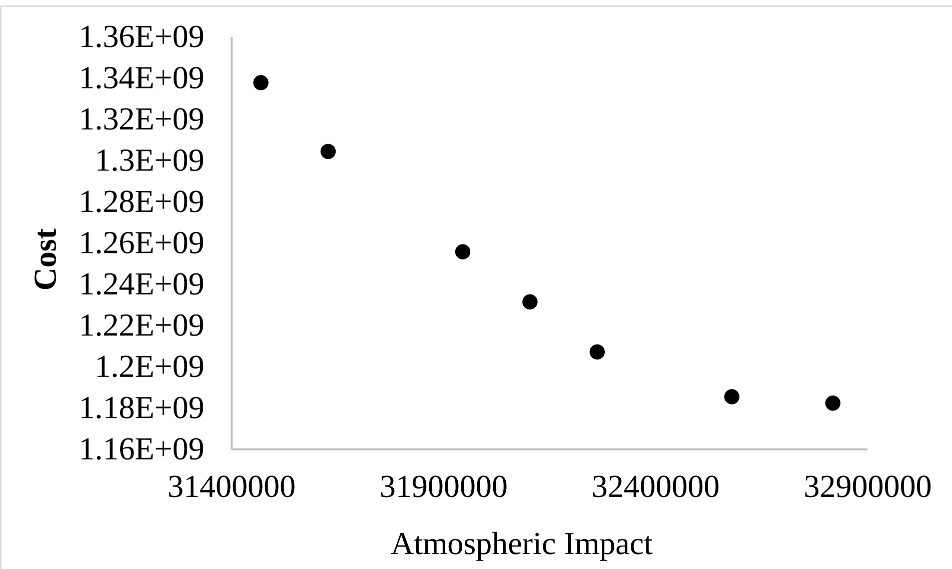


Figure 7.4 Variation of Cost with Atmospheric Impact

The water-energy network for minimum atmospheric impact shows a decrease of -1.58 x 10^6 kg CO2-eq when compared to the most cost-effective structure. This reduction corresponds to reduced energy footprint as desalination is not selected for producing freshwater and air coolers are not used for discharging waste heat as they have a higher energy footprint compared to the cooling tower and once-through seawater discharge. It is however more expensive and costs188.87 MM$ more than the cost-efficient structure. Export or internal use of desalinated water is not seen the structure as this enhances the fuel usage. The water requirements are satisfied by the purchase of freshwater from external agency and water from sources is mostly discharged into the environment. Useful waste heat is converted to both steam and power. Waste heat which can neither be converted into steam or power is discharged through the once-through seawater. We also see duel usage of water when water in the form of steam is transported to a refinery and then used as raw material for process sinks.

The cost shows a downward trend as global warming constraints are relaxed. As the constraint is relaxed, the structure is allowed to desalinate more water for purposes of internal use and export. This increases the fuel footprint and hence global warming. It also leads to a change in the type of cooling system being used. From only seawater cooling, the system transforms into a predominantly Air Cooler arrangement with seawater cooling linked to export and cooling tower option where fresh water comes from the steam exchange condensate.

7.5.2. Aquatic Impact

The second objective function for evaluating the environmental footprint of the combined water-energy network is the aquatic impact. The objective of the problem is changed into the minimization of aquatic impact. We analyze two scenarios:

- Scenario 1: Exchange of only Power allowed.
- Scenario 2: Exchange of both power and steam allowed.

Figure 7.5 presents the optimal structure for aquatic impact minimization for scenario 1.

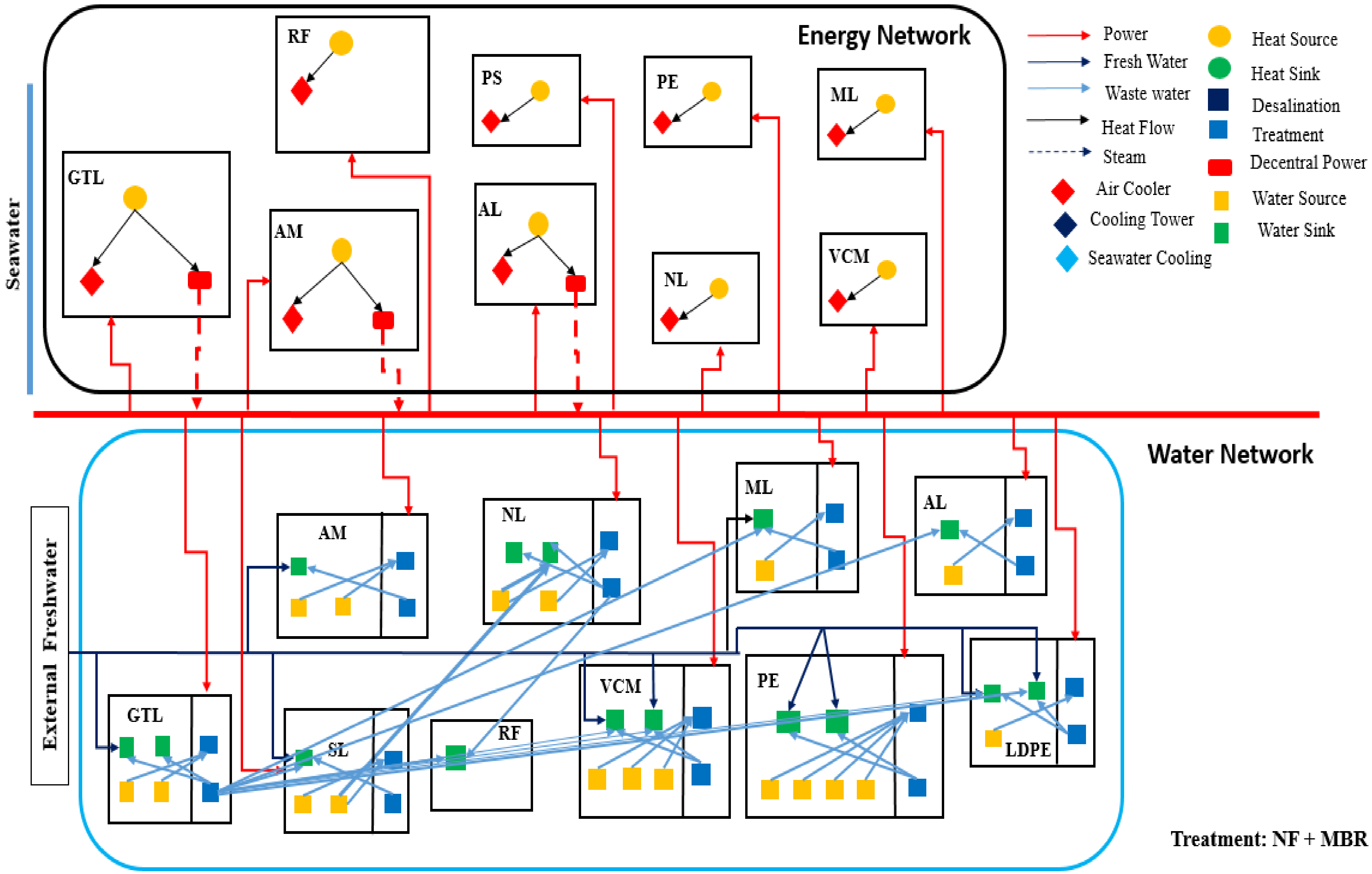


Figure 7.5 Water – Energy Network (Aquatic Impact 1)

Table 7.14 Freshwater usage across plants (Aquatic Impact -1)

Plant	Flowrate (tons/d)
VCM	756
Steel	338.537
LDPE	2460.44
FA	111.22
Ammonia	2250
PE	3850.4
Refinery	4886.35

Table 7.15 Treatment to Sinks (Aquatic Impact -1)

Plant	Flowrate (tons/d)
VCM to VCM	1528.2
Steel to Steel	766.863
LDPE to LDPE	2734.56
Methanol to Methanol	785.08
Ammonia to Ammonia	3150
Aluminum to Aluminum	121.5
GTL to Aluminum	718.5
PE to PE	1263.6
NGL to NGL	365
GTL to GTL	6167
GTL to Steel	3543.6
GTL to VCM	565.8
GTL to LDPE	2156.6
GTL to Methanol	2785.7
GTL to Refinery	839.45
NGL to Refinery	678.65

Table 7.16 Sources to Sinks (Aquatic Impact -1)

Connection	Flowrate (tons/d)
NGL to NGL	516.35
Steel to NGL	1683.93

Freshwater Cost: 6.58 MM$

Desalination Cost: 0 MM$

Treatment Cost: 17.64 MM$

Piping Cost: 4.67 MM$

Total Cost: 28.9 MM$

Treatment technology selected: Nano-Filtration + Membrane Bio-Reactor

The energy network consists of the following connections: Only AC

Table 7.17 Waste Heat to Cooling Systems (Aquatic Impact 1)

	AC (Mw)	CT (Mw)	OTSW (Mw)
GTL	769.25	0	0
Ammonia	413.66	0	0
Methanol	427	0	0
Refinery	113.6	0	0
Aluminum	70.8	0	0
Power Plant	41.67	0	0
NGL	22.7	0	0
PE	46	0	0
VCM	26.4	0	0

Table 7.18 Decentral Power Generation (Aquatic Impact -1)

Steam Levels	Plants				
	Refinery	Ammonia	GTL	Methanol	Aluminum
MP(GTL)	0	21.245	12.345	0	9.388
LP(GTL)	7.536	0	0	32.689	0
MP(Ammonia)	0	0	0	0	0
LP(Ammonia)	2.456	0	5.935769	0	3.99
GTL (LG)	0	19.697	0	5.85	0
Ammonia (LG)	0	0	0	0	0
Aluminum	0	0	0	7.6538	0

Table 7.19 Water network aggregate analysis (Aquatic Impact -1)

Water Network Cost (MM$/yr)	28.9
Onsite Desalination(tons/d)	0
Total Water Reuse (tons/d)	26384.35
Water Export (tons/d)	0

Table 7.20 Energy Network aggregate analysis (Aquatic Impact -1)

Energy Network Cost (MM$/yr)	1381.1
Total Power Generation (Mw)	3145
Total Fuel (Gj/yr)	281.34×10^{6}
Power Export (Mw)	0

Eco- Toxicity (Objective: Aquatic Impact Minimization): 8.61×10^{11}

Eco- Toxicity (Objective: Aquatic Impact Minimization): 5.98×10^{14}

Deviation in cost from Minimum Cost Structure: 224.41 MM$

Following scenario 1, scenario 2 is analyzed in which the exchange of both steam and power is allowed. Figure 7.6 represents a schematic of an optimal structure for scenario 2.

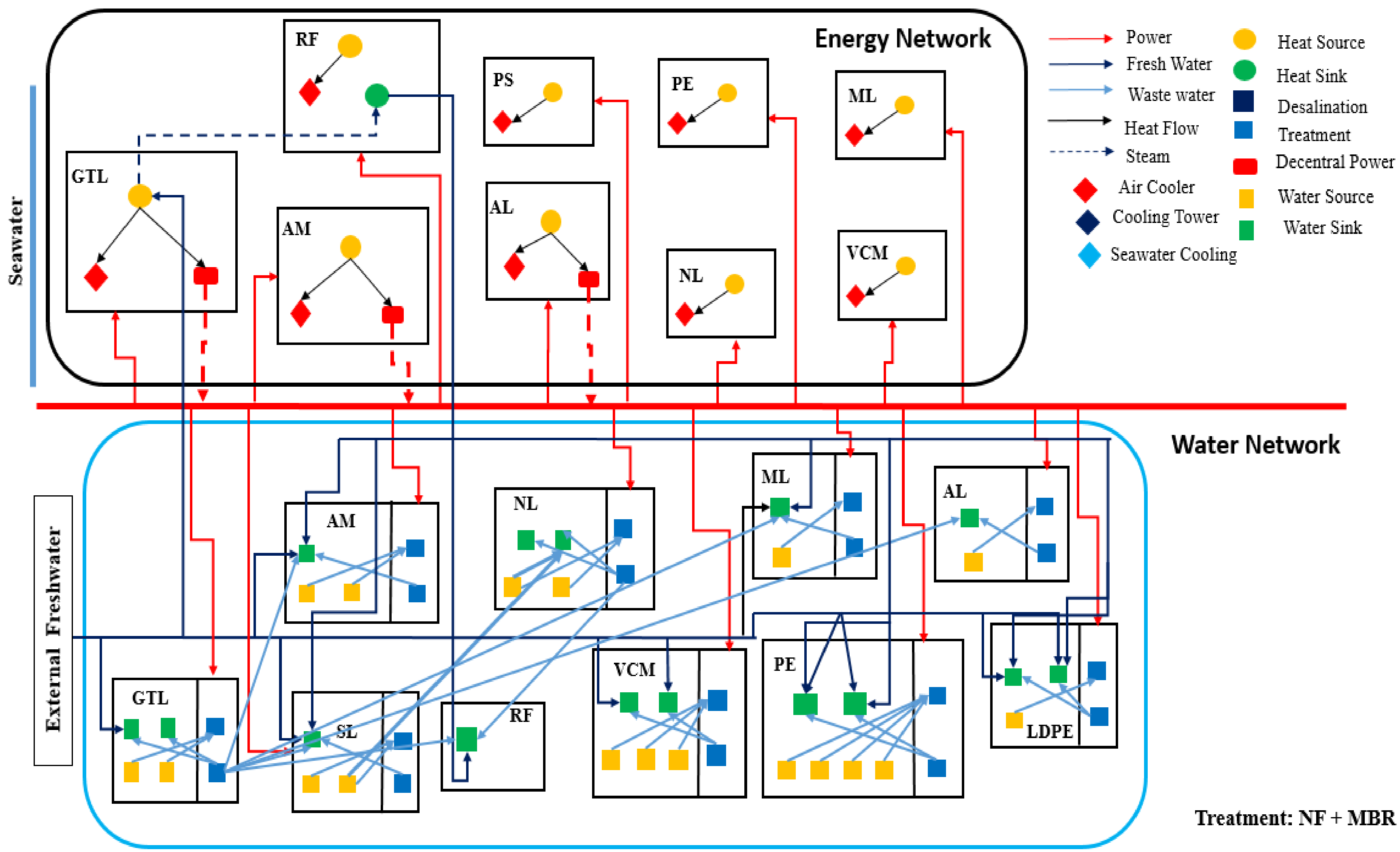


Figure 7.6 Water – Energy Network (Aquatic Impact - 2)

Table 7.21 Freshwater usage across plants (Aquatic Impact - 2)

Plant	Flowrate (tons/d)	Condensate (Refinery) to Plants
VCM	89.87	1231.933
Steel	259.27	582.73
LDPE	2227.61	232.83
FA	550.36	846.47
Ammonia	194.54	298.53
PE	1115.95	2734.45
Refinery	0	2139.19

Table 7.22 Treatment to Sinks (Aquatic Impact – 2)

Plant	Flowrate (tons/d)
VCM to VCM	1528.2
Steel to Steel	766.863
LDPE to LDPE	2734.56
Methanol to Methanol	785.08
Ammonia to Ammonia	3150
Aluminum to Aluminum	121.5
GTL to Aluminum	718.5
PE to PE	1263.6
NGL to NGL	365
GTL to GTL	6167
GTL to Ammonia	1756.94
GTL to Steel	3040.2
GTL to Methanol	1500.09
GTL to Refinery	3594.48
NGL to Refinery	671.34

Table 7.23 Sources to Sinks (Aquatic Impact – 2)

Connection	Flowrate (tons/d)
NGL to NGL	483.3
Steel to NGL	1723.14

Freshwater Cost: 1.28 MM$

Desalination Cost: 0 MM$

Treatment Cost: 17.64 MM$

Piping Cost: 4.43 MM$

Total Cost: 23.36 MM$

Table 7.24 Waste Heat to Cooling Systems (Aquatic Impact – 2)

	AC (Mw)	CT (Mw)	OTSW (Mw)
GTL	617.228	0	0
Ammonia	413.66	0	0
Methanol	427	0	0
Refinery	113.6	0	0
Aluminum	70.8	0	0
Power Plant	41.67	0	0
NGL	22.7	0	0
PE	46	0	0
VCM	26.4	0	0

195 Mw of medium pressure steam produced from excess heat from GTL plant is transferred for heating purposes in Refinery.

Table 7.25 Decentral Power Generation (Aquatic Impact – 2)

Steam Levels	Plants				
	Refinery	**Ammonia**	**GTL**	**Methanol**	**Aluminum**
MP(GTL)	0	0	0	0	0
LP(GTL)	0	0	0	34.419	0
MP(Ammonia)	0	0	0	0	0
LP(Ammonia)	0	9.4531	0	0	2.93
GTL (LG)		0	20.216	0	0
Ammonia (LG)	0	0	0	0	0
Aluminum	4.54	0	0	0	3.32

Table 7.26 Water network aggregate analysis (Aquatic Impact – 2)

Water Network Cost (MM$/yr)	23.36
Onsite Desalination(tons/d)	0
Total Water Reuse (tons/d)	26376.3
Water Export (tons/d)	0

Table 7.27 Energy Network aggregate analysis (Aquatic Impact – 2)

Energy Network Cost (MM$/yr)	1336.44
Total Power Generation (Mw)	3097.34
Total Fuel (Gj/yr)	276.45×10^6
Power Export (Mw)	0

Eco- Toxicity (Objective: Aquatic Impact Minimization): 8.61×10^{11}

Eco- Toxicity (Objective: Aquatic Impact Minimization): 5.98×10^{14}

Deviation in cost from Minimum Cost Structure: 176.16 MM$

Like global warming, the variation of cost with eco-toxicity relaxation is mapped on a Pareto curve. Exchange of steam and power and export of water and power is allowed. Figure

7.7 shows the variation of cost with eco-toxicity. Table 7.28 presents the cost and optimal cooling system.

Table 7.28 Cost & Cooling Options for Aquatic Impact

Scenario (% decrease)	Cost (MM$/p.a)	Cooling System
5	1358.01	OTSW+AC
15	1334.71	OTSW+AC
25	1311.32	OTSW+AC
35	1292.79	OTSW+AC
55	1259.78	OTSW+AC
75	1226.76	OTSW+AC
90	1201.9	OTSW+AC

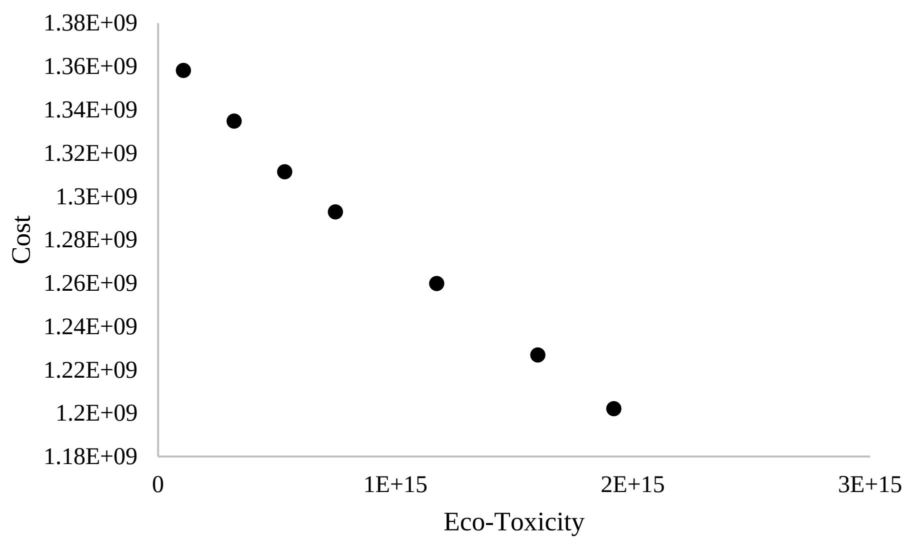


Figure 7.7 Variation of Cost with Aquatic Impact

The water-energy network for minimum eco-toxicity shows a decrease of 5.971 x 10^{14} ecotoxicity when compared to the most cost-effective structure. The huge decrease is because freshwater needs are not met by in-plant desalination but imported from an external source. Also, seawater cooling is not used to discharge waste heat. These two factors play a huge role in this steep decrease. It is however more expensive and costs between 180.52 to 224.41 MM$ more than the cost-efficient structure. Export or internal use of desalinated water is not seen as the structure as there is discharge associated with it.

The water requirements are satisfied by the purchase of freshwater from the external agency and through reuse of water from sources either directly or after treatment. The treatment technology used is nano-filtration in combination with the membrane bioreactor (MBR). Waste heat can either be converted to only power or both steam and power as it doesn't impact the performance of the structure. However, the structure having an exchange of both have a lower price. The cost ranges from 1367.82 to 1411.7 MM$. Useful waste heat is converted into steam and power and lower grade heat is discharged through air coolers. Compared to scenario 1, it is noticed that whether useful waste heat is converted to steam or power, the eco-toxicity remains the same. However, for the same eco-toxicity, we have a spectrum of the solution with a different cost. While analyzing the tradeoffs between cost and eco-toxicity, an improvement in cost is observed as eco-toxicity constraints are relaxed. The cooling system switches from only AC to AC + OTSW as desalination is being allowed for export and to meet the freshwater requirements of the industrial city.

8. FUTURE WORK

A lot of work can be done both on the problem formulation side and on the solver development side as well. Updated utility models can be incorporated which can better represent the real scenario. More objectives related to sustainability and economics can be evaluated to study the impact on the structure. The problem can also be expanded to synthesize a network that just doesn't optimize the cost of running the plant but also accounts for an investment of those savings in relevant avenues to maximize profit.

In the area of solver development, the use of parallel computing resources can be explored which will reduce the duration of solving the problem by several factors. New algorithms can be proposed and tried to solve these problems.

9. CONCLUSIONS

This work analyzes the aspects of water-energy nexus problems in industrial cities with objectives of formulating a new and comprehensive and integrated formulation modeling the links between two networks and including the key building block of utility network into the problem. Apart from providing an enhanced formulation, a novel solution search technique has been proposed and two solvers based on SA and TS and utilizing the search technique have been developed. Past experiences with single resource problem enable us to appreciate the fact that the combined problem will be complex and combinatorically large which led to the development of these solvers. They have robust performance and provide the user with more insight that may not be available with commercially available solvers. An intelligent search framework has been developed which forms the basis of these solvers and has been effective in generating good solutions. The solvers have been developed with a modular architecture and components of the optimization problems have been handled separately which makes them flexible for the user to incorporate changes. The solvers also have a provision of storing multiple solutions which allow the user to understand the tradeoffs across various elements of the problem.

Both Simulated Annealing and Tabu Search have given a robust performance and when compared for speed, Tabu Search is faster than Simulated Annealing. As per observation for the timings, Tabu Search takes around 5-6 hours compared to 6-8 hours for SA runs. However, the solution quality generated by both is almost the same. It takes a lesser number of evaluations for Tabu Search to reach the optimum solution.

Both these solvers have been tested for parameters like Markov chain length, different initial solution. In the case of different Markov chain length, the solution performance increases with increasing chain size. For large chain sizes, the solution performance provided by both the solvers is the same. This fact also in line with the observation that the more the number of states evaluated, the better the performance of the solution obtained. Also with increasing chain size, the solvers become more robust. This fact has been noticed by observing the trend of standard deviation across the chain length. It shows a decreasing trend across both the solvers. If compared between TS and SA, the standard deviation is lesser in TS but for larger chain sizes they are almost the same. The rigorous analysis carried out on the solvers highlights the fact that they are reliable for handling the water-energy nexus problem.

The solutions to our given problem provide insights into the efficient structures that can be obtained if water-energy nexus elements are exploited. Policies on the exchange of steam and power and export of water and excess power have been formulated into constraint and their impact has been studied. If minimization of cost set as the objective of the optimization, the savings across the structure vary from 4% to 12.6% depending upon the scenarios considered.

Converting WH to both steam and power and export of desalinated water provide the biggest savings to the structure. Restricting the conversion only to power and not allowing export provides the least savings. However, the most cost-effective structure requires the generation of more power as the water gets desalinated for export thereby increasing the carbon footprint of the structure. Also, decentral treatment units are observed to be the optimal choice of water treatment framework.

The treatment technology selected across all the scenarios is Nano-filtration as it is the cheapest way to treat the contamination level to environmental discharge levels. No water regeneration and reuse at sinks have been observed for this case study as it would require multiple phases of treatment which is more expensive than desalination.

The choice of cooling option also, vary with the scenarios. If the export is allowed, OTSW is also selected as one of the cooling options. Exchange of steam across GTL and Refinery enables usage of the cooling tower as one of the cost-effective options at Refinery. This is an interesting aspect of the solution because cooling towers have not been selected in Fouladi [93] where the exchange of steam and power has not been considered. The condensed steam provides for as the input water for the cooling tower sink. This feature of the solution shows the dual usage of water. Water in the form of steam carrying energy from GTL to Refinery and then acting as a raw material to a sink in another plant. This nexus couldn't have been harnessed has the problem been looked in isolation and exploiting it provides savings. If the export is not allowed, AC is the predominant cooling option in the structure.

Apart from the cost of the combined structure, sustainability has also been evaluated as an objective. Atmospheric impact and Eco Toxicity have been evaluated and their minimization has been set as optimization target. In the case of atmospheric impact, OTSW has been selected as the preferred choice of cooling option since its power requirement is least across the cooling options. The requirement at process sinks has been met by importing freshwater as in-house desalination will increase the carbon footprint. However, between the conversion of waste heat to power or steam or both are allowed, conversion to steam is preferred as it reduces the amount of heat discharged through the cooling option more than the power option. Exporting water is not an attractive option for this objective as it requires desalination which would mean consumption of more fuel thereby having an enhanced atmospheric impact.

In the case of ecotoxicity, the predominant cooling option used is air cooler as there is no liquid discharge involved. Also, whether steam exchange or power or both take place, it doesn't impact the solution as the generation of power from decentral power generation units do not involve the discharge of water. Also, the dual usage of steam as an energy carrier and then as a raw material for sinks avoids any external discharge.

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APPENDIX A

Delete: Figure A.1 presents the algorithm used in executing the delete move on a matrix.

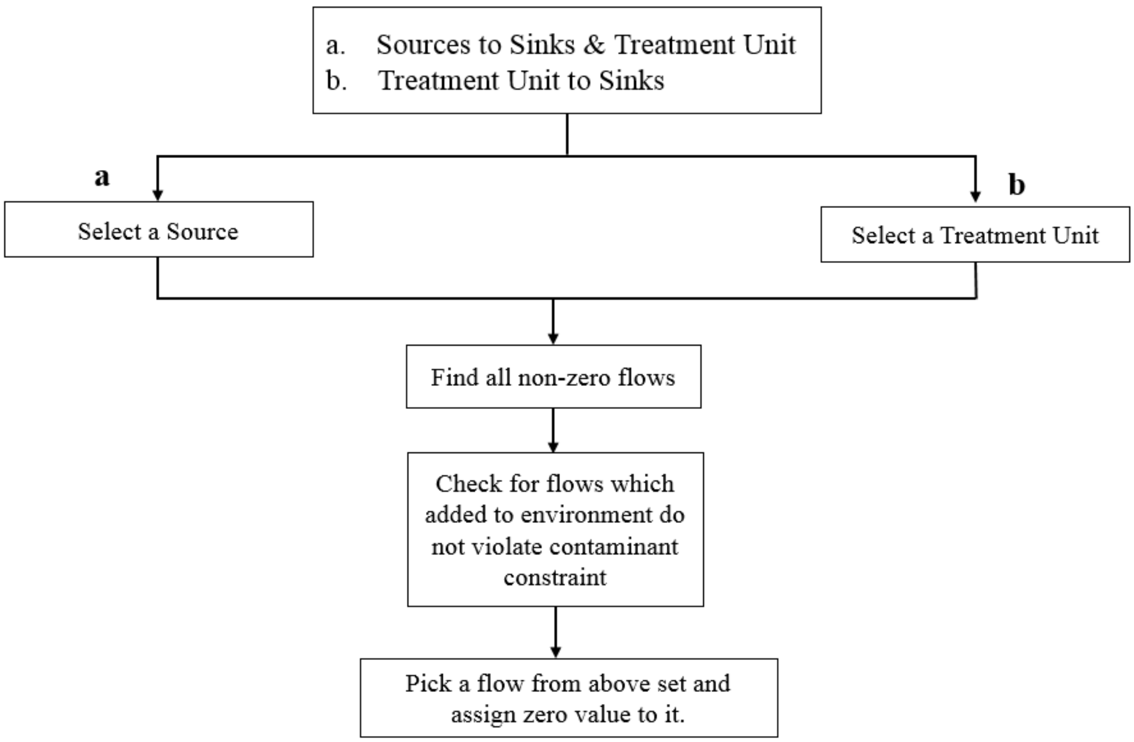

Figure A.1 Delete Transition

The first step is to decide which matrix needs to be altered using this transition. Once a decision is made between a source and treatment units, a set consisting of all non-zero connection is made. Since the deleted connection flow would be discharged into environment in order to maintain the mass balance, a second layer of check for contaminant violation is made and a new set consisting of these flows is made. From the new set, a random selection of the connection is made and its value is set to zero.

Delete with Redistribution: Figure A.2 presents the algorithm used in executing the delete with redistribution move on a matrix.

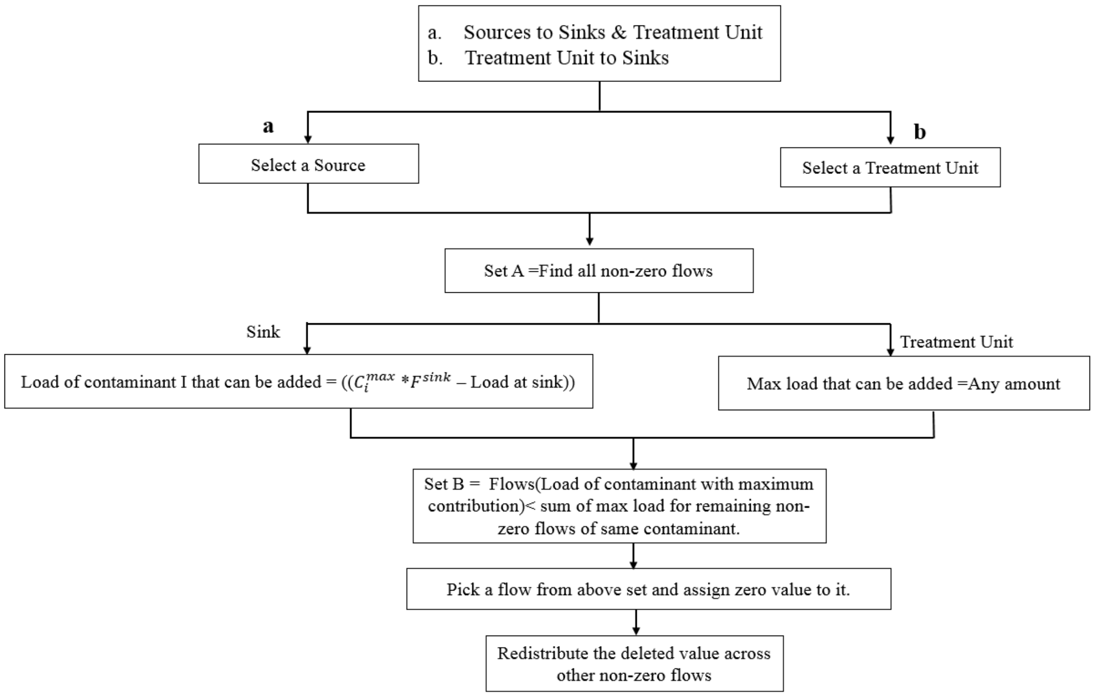

Figure A.2 Delete with Redistribution

This move similar to delete subroutine with the deleted value redistributed across other non-zero flows in the given source or treatment unit. After selection of the source/treatment unit has been done, a set collecting all the non-zero flowrates is formed. For each of the flow in this set, the maximum value of load that can be added to them is calculated. Now a second set is created which contains non-zero flows with load of the contaminant which has highest contribution is less than sum of load of the particular contaminant that can be added to other non-zero flows. From the given set one of the flows is chosen and the flowrate is set to zero. The deleted flowrate is then redistributed across the remaining non-zero flowrate without violating the load constraints at the sink.

Reconnect: Figure A.3 presents the algorithm used for reconnection move.

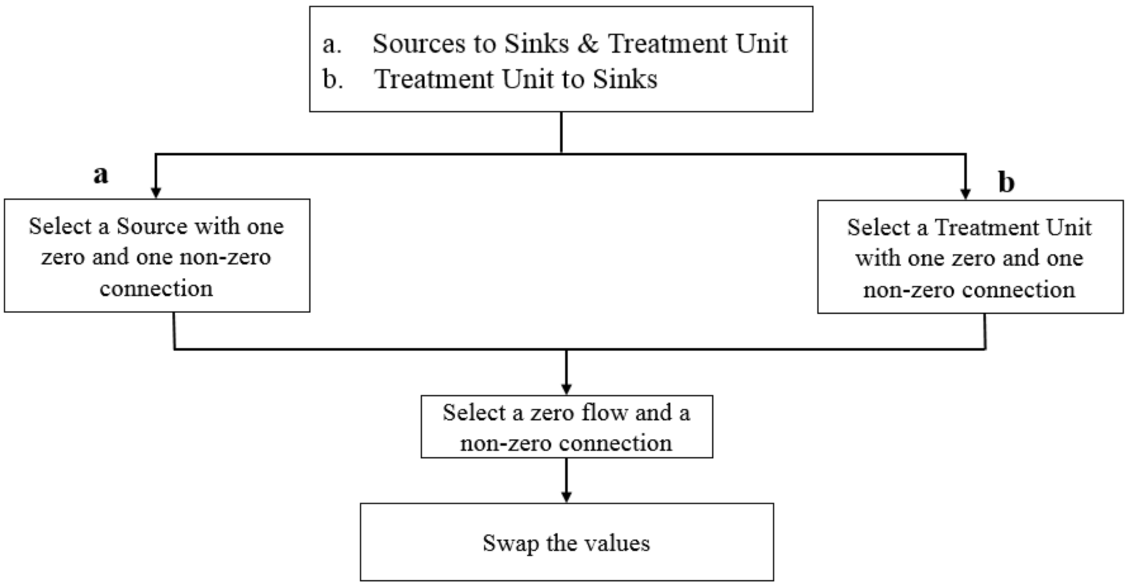

Figure A.3 Reconnection Subroutine

First the matrix on which this move is to be executed is selected. For a given flow which can either be source or treatment unit, select two connection: one with zero flowrate and another with non-zero flowrate. Their values are then swapped.