

**Design and Optimisation of industrial Water
Application Planning (WAP): Modelling multi-
contaminant processes with regeneration
technologies**



**Abertay
University**

**A thesis submitted in partial fulfilment of the requirements
for the degree of Doctor of Philosophy (PhD)**

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Declaration

Candidate's declarations:

I, Sule Abdullahi, hereby certify that this thesis submitted in partial fulfilment of the requirements for the award of Doctor of Philosophy (PhD), Abertay University, is wholly my own work unless otherwise referenced or acknowledged. This work has not been submitted for any other qualification at any other academic institution.

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I certify that this is a true and accurate version of the thesis approved by the examiners, and that all relevant ordinance regulations have been fulfilled.

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Dedication

This is dedicated to my late father to my beloved mother, to my wife and children.

ABSTRACT

In the context of freshwater stress and scarcity, industries use and produce large volume of water with high toxicity. The challenge is to find creative ways to minimise freshwater use with emphasis on protecting the environment. One of such creative ways is Water application Planning (WAP), which employs recycle, regeneration, and reuse to minimise freshwater consumption. In the use of mathematical optimisation methods for solving WAP problems, five major challenges were identified. They are lack of single systematic method to handle reuse/recycle of single and multi-contaminant, a hybrid targeting method which can address multiple local optimal solutions, a single model that provides simultaneous optimisation of the interactions of multiple water-using units and regeneration (wastewater treatment technologies), robust flexible approaches that enables faster numerical solutions and handle single and multi-objective cases of WAP problems. This research developed a framework for WAP optimisation that eliminates all the above challenges without complexity. A Stochastic Optimisation, Genetic Algorithm (GA) improved with a hybrid of the deterministic optimisation, Sequential Quadratic Programming (SQP) algorithm strategy has been used for the analysis of WAP problem in the Matlab software environment to facilitates efficient and effective solution for single objective. It was further developed to handle multi-objective optimisation (MOO) using Multi-objective Genetic Algorithm (MOGA) and improved with the hybrid goal attainment method to increase its performance. Both methods of solution were robust in handling single-contaminant and multi-contaminant WAP problems, with and without regeneration. The time of running WAP model using genetic algorithm (GA) with and without hybrid of deterministic optimisation for different number of industrial processes was investigated. The model runs for the minimum, median and maximum time of 3.0, 5.7 and 16.2 seconds respectively, with the GA population size of 10 for the 2 to 10 number of industrial processes. Furthermore, the result of multi-objective genetic algorithm (MOGA) analysis for WAP problem shows that the model can search for a wide-ranging distribution of Pareto optimal solutions and it has small computational time of 5 seconds for 3 industrial processes. Moreover, a case study of Kaduna Refining and Petrochemical Company Limited (KRPC) refinery was considered in the analysis of minimum freshwater requirement. The challenge of the refinery is to minimise the freshwater use and subsequently the wastewater disposal. The result shows that the sum of freshwater flow rates required by six major water using processes in the refinery can be reduced by 11.3% by reusing wastewater and it can be further reduced by 17.3% through regeneration reuse method. The wastewater produced by the refinery also reduced by the above two percentages. These reductions in water consumption and wastewater production exceed those reported in the literature under similar refinery condition. The superstructure was employed in showing the actual network interconnections of different industrial processes for feasible freshwater minimisation analysed. Finally, the recommendation is to combine two stochastic mathematical optimisation methods with two hybrid functions to improve the optimum solution obtained.

Major Output

1. **Abdullahi, S. A.** (2016): Optimisation of Water Reuse Network Using Water Pinch Technology (WPT) by Considering Single Contaminant for Kaduna Refinery and Petrochemical Company, Nigeria. Journal of Pollution Effects and Control. 4: 173. doi: 10.4173/2375-4397.1000173 2012): (Shown in **Appendix A**)
2. Sule Abdullahi, Ruth Falconer and Joseph Akunna: A Flexible Evolutionary Approach to Minimising Freshwater Use in a Multi-contaminant Water Network.
(Not yet Published)

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List of Symbols and Nomenclatures

C : Concentration of Contaminants, ppm

$C_{i,in}$ is the inlet limiting concentration in process i ; in ppm

$C_{i,out}$ is the outlet limiting concentration in process i ; in ppm

F_i is the freshwater flowrate to process i ; in m³/h

W_i is the wastewater flowrate from process i ; in m³/h

$X_{i,j}$ is the wastewater flow from process i to process j ; in m³/h

$X_{k,j}$ is the water flow from treatment k to process j ; in m³/h

$X_{j,k}$ is the water flow from process j to treatment k ; in m³/h

i is the index representing process i ;

j is the index representing process j ;

k is the index representing treatment process k ;

Δm is the Mass load of contaminant for each process i ; in kg/hr

N is the total number of processes in the network;

CHAPTER ONE

1.0 INTRODUCTION AND PROBLEM STATEMENT

1.1 Introduction

The industrial revolution inspired many industrial processes that utilize water, this make it a key element for the normal functioning of many industries. It is intensively utilised in food, pulp or paper, pharmaceutical, petrochemical and chemical industries. Conventionally, freshwater has been the only source of water for processes used in many industries due to the quality standard required for most of the processes, but it is scarce. This (scarcity of freshwater) and the stringent environmental regulatory specifications for the disposal of their wastewater containing some pollutants, force the industries to look for ways to minimise their freshwater use and wastewater generation and disposal. This leads to different research in water-reuse, recycling, and regeneration-reuse/recycle in the industries.

1.2 Problem statements

Industries consume more than half of the water available for human use. Freshwater withdrawals have tripled over the last 50 years because it is the only source of water for processes used in the industries. In the context of this water stress and scarcity, the challenge will be to find creative ways to minimise water use with emphasis on protecting the environment.

Furthermore, the United States Environmental Protection Agency (USEPA) Guidelines for water reuse (2012) indicate that many industries are under pressure to find ways to minimise the total volume of water used in production. This indicates the need to secure adequate, predictable, and sustainable supplies of water for all uses at reasonable costs, and with efficient usage to maximise product output. This will

allow for greater production of products and less waste, as well as realizing possible economic advantages, and possibly better relations with local citizens and governments.

Furthermore, the world is experiencing unprecedented population growth and climate change which will lead to stress on freshwater and aggravate its scarcity. Fresh water is only 3% of the earth`s total water and only 31.3 % of this is available as surface (0.3%), groundwater (confined and unconfined aquifer) (30.1%), and others (like vapour in the cloud, root zone and unsaturated zone of the soil) (0.9%) (Figure: 1). Freshwater demands of manufacturing and industries are expected to increase by 400% between 2017 and 2050, while, domestic water demands are also expected to rise by 130%, particularly in cities and countries undergoing rapid economic growth.

The present weather conditions attributed to climate change causes high evaporation and evapotranspiration which is coupled with the increase in flooding in some regions, drought in other regions of the world, and subsequent freshwater pollution. On top of that, the Intergovernmental Panel on Climate Change has highlighted adverse negative impacts of climate change on global water resources with repercussions for end users, including industries (IPCC, 2007).

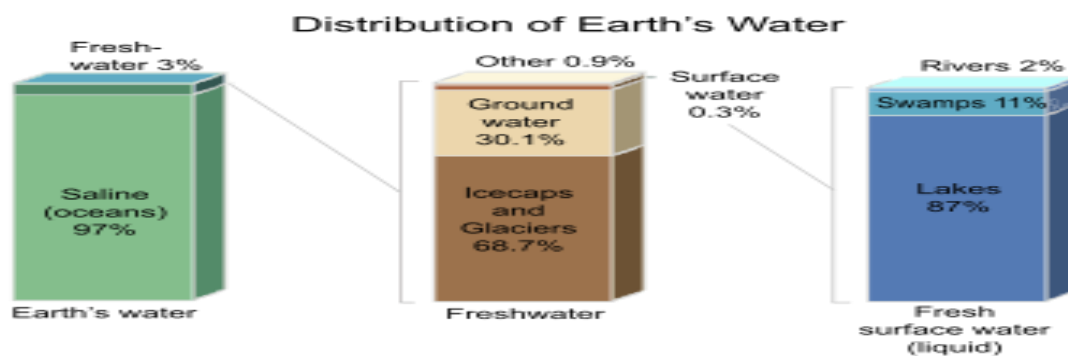


Figure 1-1: Distribution of Earth water

(Source: URL: <http://water.usgs.gov/edu/watercyclesummary.html>, assessed on 11th January, 2017)

Moreover, industries produce large volume of wastewater with contaminants which are detrimental to the environment. The wastewater produced by the industries may

contain different contaminants at different level of concentrations. The contaminants include Total Suspended Solids (TSS), Total Dissolved Solids (TDS), Total Organic Carbon (TOC), Biochemical Oxygen Demand (BOD), Chemical Oxygen Demand (COD), and pH (degree of alkalinity or acidity).

Industrial Scientist and Engineers are working to come up with the various water treatment methods as a solution. These methods can be broadly divided in to physical, chemical, and biological as well as advanced waste treatment. They are used by different industries utilising water in manufacturing and processing to manage the real challenges they face in ensuring that effluent water meets the required discharge levels before being discharged to the environment. However, these methods can account for significant financial investment in a plant (industry), as the cost of the treatment units is dependent on the volume of wastewater that requires treatment. For example, an industrial applications that have 150,000GPD (gallon per day) capacity, will require wastewater treatment systems (WWTS) that cost an estimated value of \$500,000 to \$1.5 million. This cost includes all necessary design, engineering, equipment, installation, and start-up. Furthermore, in certain instances the level of treatment required is quite substantial. Hence, it would be favourable if the volume of water that requires treatment were reduced (Gouws *et al*; 2010).

1.3 Water-Reuse, Regeneration Reuse and Regeneration Recycling

To reduce the volume of water that requires treatment leads to different research in water-reuse, recycling, and regeneration-reuse/recycle as illustrated in figure 1.2 to 1.4.

Water Reuse: this means wastewater from some processes can be directly re-use in other processes. The different process lines are designed based on the quality of wastewater they produced.

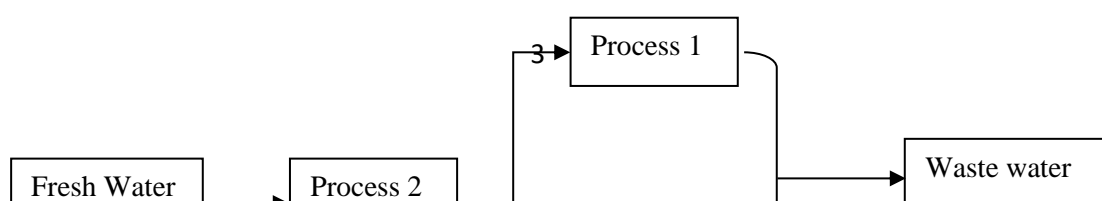


Figure 1-2: Water Reuse Minimisation Method (Feng *et al*, 2006)

Regeneration Reuse: This means wastewater can be regenerated by partial treatment (PH adjustment, filtration and ion exchange) to remove the contaminants and then re-used in other processes.

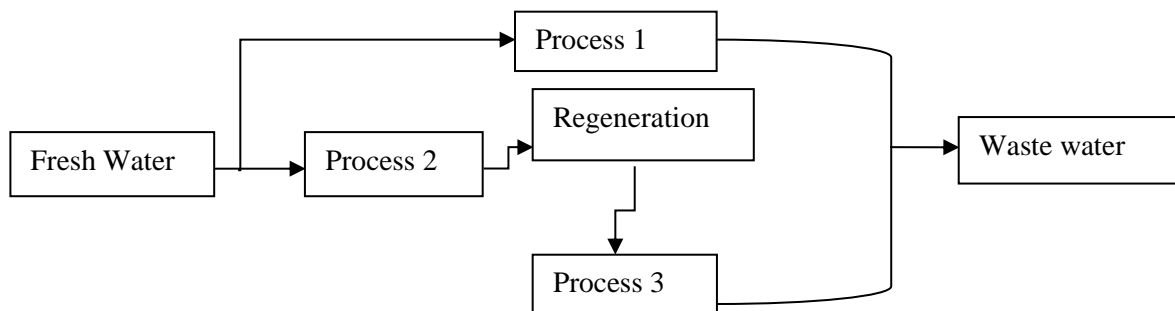


Figure 1-3: Regeneration Reuse Minimisation Method (Feng *et al*, 2006)

Regeneration Recycling: This means that the used water from some processes is recycled back to those same processes after regeneration or treatment.

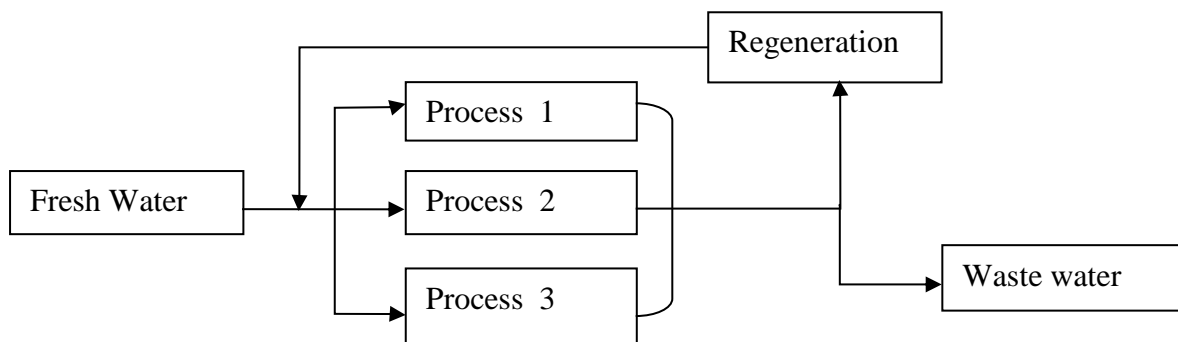


Figure 1-4: Regeneration Recycling Minimisation Method (Feng *et al*, 2006)

Regeneration involves partial treatment by using water treatment and purification technologies such as membrane and steam stripping prior to reuse or recycle. These

different options to minimise the volume of water used by industries combined together is termed Water Application Planning (WAP).

1.4 Approaches to Addressing Water Application Planning (WAP)

Problems

In general, two major approaches to addressing water application planning (WAP) problem can be categorised as insight-based techniques and model-based optimisation methods. The former (insight-based technique) typically involves a water pinch analysis (WPA) technique that offers good insights with low computational burden, yet often at the expense of requiring significant problem simplification as demonstrated in Wang and Smith (1994), El-hawagi *et al.* (2003) and Foo (2009).

On the other hand, model-based optimisation approach allows handling of WAP problems in their full complexity by considering different objective functions. Some of the objective functions are: minimising the quantity of freshwater use, minimising the quantity of wastewater produced, minimising the quantity of wastewater reused by other processes by considering their level of contaminants and the possible interconnections of the processes in the given industry. Model-based optimisation handles multiple contaminants, various constraints and integrates different types of processes involved in any given industry in selecting reasonable re-use or regeneration re-use option. The, major challenges of model based optimisation are high computational burden to achieve optimality, and it does not guarantee global optimum which is the required best result and the lowest value (the global minimum), based on the objective function (Bagajewicz and Savelski; 2001, Chaturvedi *et al*; 2016).

The mathematical programming based approach mainly requires constructing a superstructure of all or many possible interconnections of water network elements that

lead to a mixed-integer linear programming (MILP) or mixed-integer nonlinear programming (MINLP) model formulation. The formulations often incorporate physical insights derived from water pinch analysis as well as concepts from mass integration and property integration (Khor *et al.*; 2014).

The design of Water Application Planning (WAP) is a complex task, especially when multiple contaminants are treated in the same plant with the decision about the use of many regeneration units. This problem has been identified in previous works (e.g. Gunaratnam *et. al.*; 2005, Feng *et. al.*; 2007, and Boix *et. al.*; 2011). The analysis of the literature shows that there is need for formulating a generic framework that consider one or several objective functions and have a robust approach in solving large WAP problems. The mathematical representation of WAP with multiple contaminants is in the class of nonlinear programming (NLP) (Liu *et. al.*; 2015), and the use of mathematical stochastic optimisation was verified to be effective in solving the NLP formulation problems. Doyle, and Smith, (1997), describe linear and non-linear formulations of targeting water reuse problem with multiple contaminants which was combined with the previous method of Wang and Smith (1994) to provide a graphical representation of the problem. However, they use solution from the linear model to provide an initialization for non-linear optimisation solution. Tsai and Chang (2001) developed mathematical programming model for a modified water usage and treatment networks (WUTNs) design problem and solve it using genetic algorithms (GA) that identify the optimal-cost and least-consumption. Tan and Cruz (2004) apply stochastic optimisation based technique in water network synthesis problems, and Tan *et al.* (2009) consider membrane separation based water regenerators for total water network synthesis. Prakotpol and Srinophakun (2004) developed a genetic algorithm (GA) with WPA based program (GA Pinch) to solve the wastewater minimisation problem. Lavric *et al.*, (2005) applied GA optimisation to water systems

with multiple contaminants and several contaminated sources. They generate an overall optimal water network topology with respect to the minimum source water usage that considers all constraints. Moreover, Tudor and Lavric (2010) solved a detailed model of an integrated water/wastewater network (IWWN) using genetic algorithms to obtain the best topology. Moreover, Karuppiah and Grossmann (2006) proposed a piecewise-affine relaxation of non-convex terms in the solution of water network analysis, and Bagajewicz and Savelski (2001) proposed a planning model and way of obtaining global optimum result with piecewise-affine relaxation enhanced with bound contraction and also consider pre-treatment for water network synthesis. Sujak *et al.* (2015) created a model for the design of optimal total water network (OTWN). Sharma and Rangaiah, (2016) proposed designing, retrofitting, and revamping water networks in petroleum refineries using multi-objective optimisation. Boix *et al.* (2011) described multiobjective optimisation of industrial water networks with multiple contaminants. Chaturvedi, *et al.*, (2016) demonstrate the analysis of effect of multiple water sources in a flexible-schedule batch water network.

However, despite all the above mentioned significant achievements in water network analysis research that utilizes optimisation-based modelling techniques and computational strategies there are some challenges in the issues of non-convexity (which leads to the presence of multiple local optimal solutions), nonlinearity (which is due to considering multi-contaminant and regeneration technologies as nonlinear mixed with linear objective function), simultaneous optimisation of the interactions of rigorous design models for wastewater treatment technologies and multiple water-using units, enabling faster numerical solutions, development of easy to understand optimisation-based formulations, uncertainty (posed by the data obtained from the industry), the parameters involved in the analysis of the problems and obtaining the

best result, alternative methods for optimisation under uncertainty such as hybrid stochastic optimisation and extension of the solution to resource recovery systems.

However, the use of stochastic mathematical optimisation algorithm improves the potential future directions in water network analysis and assist in developing feasible, cleaner and more economic industrial water networks (IWN) that drastically reduced freshwater consumption as well as wastewater, and ensure reasonable costs and efficient productivity (Prakotpol, and Srinophakun; 2004). As such, challenges and uncertainties highlighted above can be handled by using stochastic mathematical algorithm optimisation method known as Genetic Algorithm (GA), which is robust stochastic optimisation method.

In consideration of the above developments, this research aim to develop a framework for water (fresh and waste) application planning (WAP) that can be applied to different water allocation contexts. The single contaminants and multiple contaminants WAP problem will be solved using efficient methods of optimisation and multiple objectives will be considered as objective functions with and without regeneration. The WAP problem solution can be further improved using a combination of stochastic GA and hybrid function optimisation method. Hybrid evolutionary algorithms also known as memetic algorithms use local search techniques which are traditionally faster than a typical evolutionary algorithm. The proposed hybrid function is a deterministic optimisation which is gradient-based local optimiser obtained from the Sequential Quadratic Programming (SQP) algorithm. SQP is one of the most popular and robust algorithms for constrained nonlinear single objective optimisation (Tiwari et al., 2009).

Considering the fact that, hybrid functionality in multiobjective function 'gamultiobj' is slightly different from that of the single objective function GA, the hybrid 'fgoalattain' will be applied to the GA-multiobjective to improve its performance in obtaining the optimum result of multi-objective WAP problem. The non-convexity and nonlinearity

challenges will be overcome by using reproduction parameters of GA, which includes Elite Count, Crossover fraction and mutation to obtain possible solutions, by the use of Population creation function that is constraint dependent. The optimisation method handles interactions of rigorous design models for regeneration (wastewater treatment technologies) and multiple water-using units simultaneously.

1.5 Significance of the Study

This research proposes an optimal design methodology for WAP that is very simple and easy to use in minimizing freshwater use in industrial operations and processes. It was developed by analysing the feasibilities of freshwater reuse and recycling of wastewater to minimise freshwater use in industries. This leads to an optimum design of water reuse network for different industries while considering single-contaminant and multi-contaminant wastewater. The methodology is based on a technique that combines Genetic Algorithm (GA) Mathematical Optimization method with hybrid algorithm to obtain an optimum result.

An objective function (model) was developed for minimising the freshwater use of the different processes in the industries and was used to find the optimum solution of WAP problem. The optimisation procedure has been executed by the standard evolutionary method (Genetic Algorithm) with a hybrid in the Matlab 2016a software environment. The Matlab (Mathematical Laboratory) software was used for solving the developed model using single-objective GA (SOGA), Multi-objective GA (MOGA), and two hybrids to find an optimum solution for SOGA and optimum pareto front solution for the multi-objective WAP problems. The proposed method differs from those of previous researchers who have applied genetic algorithms in that the strings used in the genetic algorithm model are coded using real variables, and this avoids the problem of redundant states often found when using binary (and Gray) coding

schemes. This method shows a significant advantage compared with previously published techniques in terms of computational efficiency. The method has been tested on several examples found in the literature and has been shown to be very efficient and robust. The analysis indicates the significant possibility of reducing the freshwater use. It also looks at the sensitivity and scalability of the developed model. The solutions and parametric values so obtained from a case study of different processes were compared with the existing literature values. The developed model handles the NLP functions and obtains optimum solutions within reasonable computational times with the selected GA parameters.

1.6 Research Aim and Objectives

The potential future directions in water application planning (WAP) are towards enabling faster numerical solutions, development of more meaningful (easy to understand) optimisation-based formulations, alternative methods for optimisation under uncertainty and extension to resource recovery systems. As such this research aim is to design a framework for industrial water application planning (WAP) that handle multi-contaminant processes with regeneration technologies.

The optimisation technique of the framework will consider single and multiple contaminants and the type of wastewater and pollutants produced by different industries. An improvement to the optimum design of water reuse network for any industry will be identified by using a stochastic optimisation (evolutionary algorithm) with a hybrid of deterministic optimisation which is gradient-based local optimiser obtained from the Sequential Quadratic Programming (SQP) algorithm in order to facilitate efficient water usage planning and management for single objective WAP problem. While, the hybrid 'fgoalattain' will be applied to the multi-objective GA

(MOGA) to improve its performance in obtaining the optimum pareto front result of multi-objective WAP problem.

However, the specific objectives of the research are:

- i. To identify optimisation methods/strategies that can be applied to single and multi-contaminant water re-use industrial processes.
- ii. To design a solution strategy for optimising water reuse network capable of handling single, multi-contaminants and regeneration.
- iii. To develop a robust solution method for the optimisation of 'Water Application Planning' (WAP) problem considering both single and multi-objectives (MO).
- iv. To assess the application of developed 'Water Application Planning' (WAP) framework for water reuse networks in a refinery.

This will eventually lead to providing a means of minimising the potential dangers facing the aquatic ecosystem as a result of the discharge of industrial effluents containing harmful contaminants in concentrations above the maximum permissible levels.

1.7 Thesis Layout

The thesis is presented in eight chapters, the purpose and content of chapter 2 to 8 is described below.

Chapter 2: Literature review: (Water application planning (WAP)).

This chapter provides a general overview of the literature involved in the Graphical optimisation (Water pinch Technology (WPT)) and Mathematical optimisation (Deterministic and Stochastic) optimisation used as Water Application Planning (WAP) methods, and indicates the strength and weaknesses of this methods. It also includes

general overview of the literature involved in the water-reuse, recycling, and regeneration-reuse/recycle for single contaminant, single contaminant with regeneration, multiple contaminant and multiple contaminant with regeneration as the types of WAP problems that can be modelled.

Chapter 3: Methodology: (Genetic Algorithm (GA) applied to WAP using MATLAB software):

This chapter provides a general overview of the selected method for solving the different Water Application Planning (WAP) problems mentioned in chapter 2. It includes data consideration and description of the software used and its capabilities on the WAP models. It also present the sensitivity analysis of the Genetic Algorithm parameters applied on the WAP model. The aim of the analysis was to determine and select the best GA parameters that provide best solution of the WAP problem. The analysis indicates the best selection of GA parameters using the data obtained from literature.

Chapter 4: Improvement of the Genetic Algorithm (GA) for the solution of Water Application Planning (WAP) model.

This chapter described the hybrid function used with the GA to increase its efficiency in obtaining the solution for WAP problems. The modelling approach used was presented and the results obtained were compared with and without hybrid function. The aim of the analysis was to determine the behaviour of GA with and without hybrid function and the computer time for obtaining the WAP solution. The analysis shows the increase in efficiency of the GA and the statistics of the computer time for different number of industrial processes using the data obtained from literature.

Chapter 5: WAP model for Single contaminant water reuse without regeneration:

This chapter describe the mathematical application of WAP models used in optimisation of Single contaminant water reuse without regeneration and their data set-up requirements. It also described the procedure involved in the general equations that presents the different steps used based on the number of processes involved. This includes use of the problems described in literature to show the steps and the values obtained in this research. The challenges of simultaneous optimisation of the multiple water-using units and non-convexity (which leads to the presence of multiple solutions in mathematical representation of WAP model with single contaminant was handled efficiently with the nonlinear programming (NLP) approach.

Chapter 6: WAP model for Multi-contaminant water reuse with and without regeneration:

This chapter describe the mathematical application of WAP models used in optimisation of multi-contaminant water reuse network with and without regeneration and their data set-up requirements. It also described the procedure involved in the general equations that presents the model based on some selected number of processes involved. This includes use 3 industrial process WAP problem described in the literature to show the steps and the values obtained using this research methodology.

Chapter 7: WAP model for multi-objective water reuse: Multi-objective GA with Hybrid.

This chapter describe the mathematical application of WAP model used in optimisation of different objectives (multi-objective) involved in water reuse network and their data set-up requirements. It also described the procedure involved in the general equations that presents the model based on some selected number of processes involved. This includes use of the problems described in the literature to show the steps and the values obtained using this research methodology. Furthermore, the values of the

solution obtained from the WAP model using multi-objective GA with 'fgoalattain' hybrid function were presented.

Chapter 8: Case Study: Application of the model to a refinery:

This chapter described application of the developed methodology in the previous chapters to real world case of a refinery. The different processes involved in the solution of WAP models were used in the mathematical optimisation of Kaduna refinery. It described the data requirements at each step of the solution. It also described the solutions obtained by the method and compare with the present situation in the refinery. This includes a short review of the present state of the industry.

Chapter 9: Conclusion and recommendations

This chapter presents a summary of the research work carried out and discussion on the WAP results obtained. It also contains an analysis of the objectives of the research that leads achieving the main aim with suggestions for future work.

CHAPTER TWO

2.0 LITERATURE REVIEW

2.1 Introduction

This chapter provides a general overview of the literature involved in the different Water Application Planning (WAP) methods and indicates the strength and weaknesses of the different methods. It also includes information on the most common types of WAP models and their data consideration in design:

Water application planning (WAP) is the design technique of the planning and retrofit of water network for both continuous and batch operations. It covers both water using units and wastewater treatment operations. The goal is to plan a network that combine water using and water regeneration operations by using optimisation technique in minimising cost and negative environmental impacts, while complying with constraints. The industries consider the concept of wastewater treatment, recycling, and reuse in processing facilities for the past four decades due to their potential in saving opportunities foreseen as a result of wastewater reuse that can partially replace freshwater consumption.

2.2 The WAP Superstructure

The way to model an integrated water application planning (WAP) problem is based on the concept of superstructure (Yeomans and Grossmann (1999), Savelski and Bagajewicz (2000)). Ramos et al (2014) explained that from a given number of regeneration units and processes, all possible connections between them may exist, except recycling to the same unit. This constraint forbids self-recycles on process and regeneration units, although the latter is often relevant in some chemical processes. Considering each process within an industry to have a certain freshwater flow rate, output water from other process and or regenerated water, the output from the process

will have effluent with certain level of pollutants which can be discharged, recycled or regenerated for reuse. The regeneration units can interchange effluent for efficient treatment. This system can be represented as the superstructure of the company without detail explanation of physical and chemical phenomena that occur in each process. Ramos et al (2014) presented the super structure as shown in the figure 2.1.

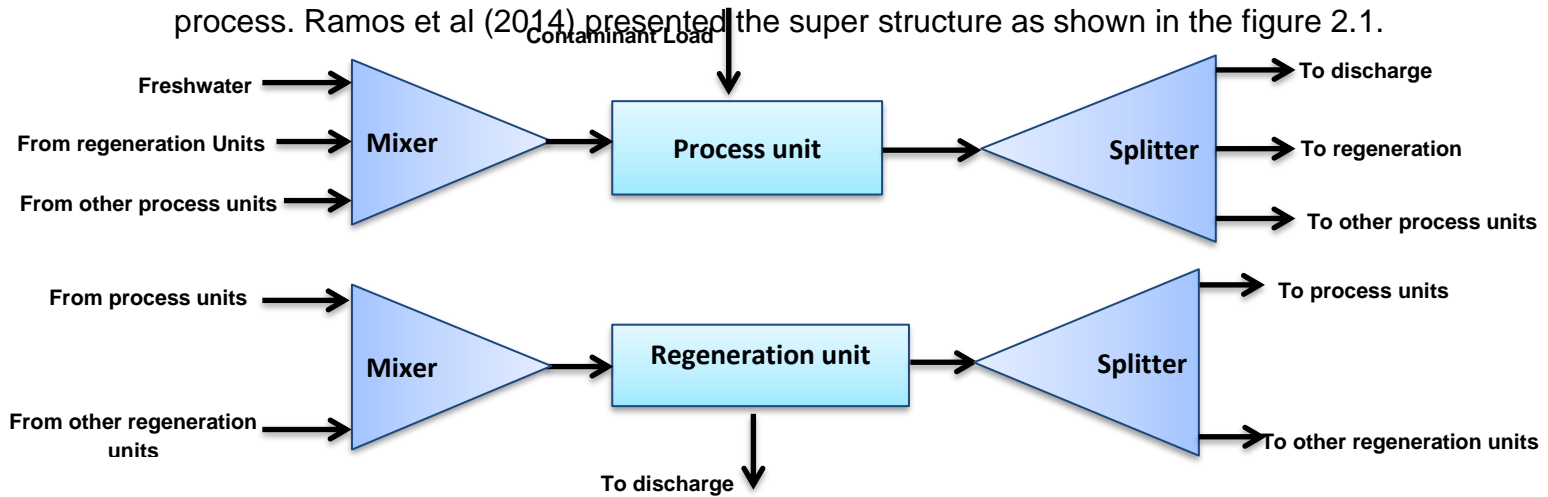


Figure 2.1: General view of the superstructure for WAP problem (Ramos *et al.*, 2014)

The values of superstructure variables for a given process condition is determined so as to minimise the total cost, subject to constraints derived from material balances and interrelationships among water-using units and wastewater-treating units. The optimisation problem was solved by using the Complex method, which was illustrated by its application to the WAP in a petroleum refinery. Mann and Liu (1999) introduced another superstructure method to formulate the water network as linear (LP) and nonlinear programming (NLP) for multiple contaminants systems. This superstructure models present serious numerical difficulties in solving nonlinear programming (NLP) and non-convex mixed integer nonlinear programming (MINLP), due to non-guarantee of their optimum result. But the procedure can be used efficiently for single component problems, and if the concentration of the contaminant is low. The examples from Wang

and Smith, (1994) and Olesen and Polley (1997) were used to substantiate the above claim. The detail of the adopted procedure was from Savelski and Bagajewicz (2001). Savelski and Bagajewicz (2003) developed a MILP model where the objective function is no longer the fresh water consumption but the summation of the number of possible connections among processes. The numbers of interconnections are also reduced in order to obtain a cost-effective design. However, the networks obtained from previous models do not only minimise cost but also minimise number of connections. The rest of subjective constraints for the analysis of interconnections remain the same with that of water allocation problem discussed previously. The integer variables are usually chosen as the interconnections among processes, between processes and the wastewater treatment plant.

However, it is quite often found that connections between certain processes are not allowed or must be imposed due to design or retrofit strategies. For example: heating and cooling limitations may render certain connections beneficial or undesirable; very low flowrate interconnections, may also be discarded due to economic or controllability reasons; finally, distance and space limitations may become decision variables as well. When imposing such restrictions to any of the previous cases we can expect either feasible or infeasible solutions. The infeasibility may arise if no network can be found for the fresh water flowrate fixed at its minimum target.

Limits on inlet and an outlet concentration of pollutant are imposed a-priori on each process and a fixed load of contaminants is used. These inlet and outlet concentrations limit account for corrosion, fouling, maximum solubility etc.

2.3 Existing WAP Research

Water Application Planning (WAP) refers to the technique of designing a network of interconnections of water streams among a set of water-using or water-disposing

processes, so that the overall freshwater consumption is minimised while the processes receiving water of adequate quality (Savelski and Bagajewicz, 2003). However, developing feasible, cleaner and more economic industrial water networks (IWN), that dramatically reduced freshwater consumption as well as wastewater, must ensure reasonable costs and efficient productivity (Ramos et al; 2014).

Much work has been done in the area of research on water minimisation in continuous and batch processes as evidenced by the detailed reviews of Bagajewicz (2000), Foo (2009), Khor et al (2014) and Gouws et al (2010). The previous work that involves wastewater recycle, treatment and reuse within (industrial) consuming processes dates back to 1970's. The critical need in reducing both contaminants and consumption of water and energy necessitate most of them, due to the fact that twenty percent of the world's total water consumption (this widely exceeds 50% in many industrialised countries) has been recently attributed to industries by UNESCO.

The problem of wastewater reuse has received attention from several researchers. The methods used can be classified as mathematical, graphical, heuristic, or algorithmic methods. The practice was analysed first by Prof. Umeda in 1980 (Takama et al., 1980), but the field owes more formal existence to the pioneering work of El-Halwagi and Manousiouthakis (1989) in mass exchange networks. Wang and Smith (1994a) use the concept of mass transfer unit model for water-using processes in the analysis of WAP problem. They developed a new approach using Water Pinch analysis (WPA) that was embedded in wastewater minimisation techniques. Their method offers simple approach and beneficial results when applied to water using industries, but it has a lot of limitations in obtaining the optimum results and the approach is difficult to extend for the analysis of multi-contaminant system.

Methods provided for wastewater minimisation were basically integration techniques. These techniques can include graphical approaches proposed by Wang and Smith,

(1995) as an extension of the above mentioned method. They applied it by considering fixed flow rate through process and multiple freshwater sources. This is not the case in most of the WAP problems. The mathematical programming proposed by Bagajewicz and Savelski (2001) is a robust model for freshwater minimisation and minimise water through the treatment unit, using the two-step procedure; first, the minimum freshwater is determined and then the minimum water via regeneration at the condition of minimum freshwater is determined; conditions on regeneration without recycles were also formulated . However, their method can only handle single contaminant and single objective. El-Halwagi *et.al.*, (2002) propose a rigorous graphical procedure derived from the rules of dynamic programming targeting for resource conservation for single contaminant via material recycle/reuse networks. However, their method uses non-mass-transfer water-using processes and does not include regeneration process.

Karuppiah and Grossmann,(2006) in their work titled `Global optimization for the synthesis of integrated water systems in chemical processes` use the mathematical approach of involving spatial branch and contract algorithms for NLP with piecewise under-estimators and over-estimators (to approximate non-convex terms and branch-and-bound schemes for binary variables. But their method cannot handle multi-objective and the CPU time required for the NLP version for the example with five processes, three treatment operations, and three contaminants is of the order of 231s. Gomes *et. al.* (2006) used a water source diagram (WSD) method based on the outlet flow rate to investigate a petroleum refinery with six operations which consume water, where four contaminants are present with different permissible input values for each operation. However, the contaminants cannot be handled simultaneously. Alva-Argaez et al. (2007) introduced a systematic methodology that empowers conceptual

engineering and water pinch with mathematical programming methods, but the complexity involved in its implementation limits its application.

Ulson de Souza *et.al.* (2009) use Graphical method WSD in a petroleum refinery with six operations which consume water, where four contaminants are present with different permissible input values for each operation. with the aim of reducing the consumption of treated water, the generation of effluents and the costs involved in the treatment of effluents, through the reuse of aqueous effluent streams within the process. However, this method cannot handle multi-contaminant streams efficiently as the analysis is carried out for one contaminant which is taken as the reference and must be the most restrictive component. Mughees and Al-ahmad (2015) combined the water pinch technology (graphical) and mathematical method to minimise the freshwater consumption of Tehran oil refinery by considering single-contaminant. However, this method is difficult to be used under multicontaminant WAP problem.

Therefore, the proposed methodology in this research will provide robust and flexible optimisation technique that can handle single and multi-contaminant with and without regeneration/treatment in WAP problem. The proposed model will handle the nonlinearity interactions of wastewater treatment and multiple water-using units simultaneously. The single and multiple objectives of minimising freshwater use are considered in obtaining the faster optimal solutions.

2. 4. Water Pinch Technology (WPT)

Water pinch technology (WPT) originates from the concept of heat pinch technique. WPT is a systematic technique for reducing water consumption and wastewater generation through integration of water-using activities or processes. WPT was first introduced by Wang and Smith (1994). Since then, it has been widely used as a tool for water conservation in industrial process plants. Manan et al (2006) applied it in

urban/domestic buildings. It was extended in 1998 by Nick Hallale at the University of Cape Town, who developed it as a special case of mass exchange networks for capital cost targeting.

Moreover, WPT can be described as a techniques for setting targets for maximum water recovery capable of handling any type of water-using operation including mass-transfer-based and non-mass-transfer based systems include the source and sink composite curves (Hallale; 2002).

Sorin and Be´dard (1999) presented a two-step procedure to generate a selection of alternative water reuse networks handling single contaminants and having the same raw water consumption and wastewater generation. In the first step, a special Evolutionary Table was used to set raw water and wastewater targets without resorting to graphical solutions. It was also used to identify a point, herein called the ‘Global Pinch Point’, which separates the design problem into two independent parts. In the second step, some special guidelines on mixing strategies for water sources above and below the Global Pinch Point are applied in order to design multiple water reuse networks for the same targets.

The application of water pinch technology in industrial water consumption management in aluminium anodizing industry shows that selection of different operations existing in an industry has an important role in correctness of application of pinch technology. There are various water usages in anodizing industry, but researches have shown that, it has the best efficiency on the selection of rinsing chambers to pinch technology. There are different methods in pinch technology mostly based on mass transfer of single or multiple contaminants. However, a method of selecting effective contaminant to be applied to pinch analysis based on Mann and Liu’s method in single contaminant can be employed. But "the guide for classification of raw water, wastewater and recycled water for industrial and recreation" may be

adopted to use a complex of index contaminants as a single contaminant. This method is very simple and applicable for various industrial processes. By an index contaminant like total dissolved solids, the water usage reduced about 6.7 %. Using pinch technology and this new approach in three rinsing chambers, water usage reduced about 14.4 % (Khezri; 2010)

The historical perspective on important achievements in water application planning using optimisation modelling techniques can be itemised as follows:

1. The inspirational work by Takama et al (1980a and b) of applying an optimisation approach to water network synthesis, which presents a nonconvex, nonlinear programming (NLP) formulation of the most basic level of the WAP design problems. This addresses the problem of optimal water allocation in a petroleum refinery by integrating the water using and wastewater treatment process to account for many possible water reuse and regeneration opportunities.
2. The sequential optimisation approach proposed by Doyle and Smith (1997) which present sequential procedure based on superstructure optimisation approach that utilizes a linear programming (LP) approximation as an initial point to solve an NLP for water network synthesis involving direct reuse or recycle.

The WPA using single contaminant method is done by constructing limiting composite curve (LCC). To construct the LCC, limiting water profiles of individual processes are plotted on an impurity concentration with mass load graph.

The pinch point is established by referring to the water consuming units as sink and water generating units as source, the obtained values are used to construct the limiting composite curves which indicate the pinch point for the particular contaminant considered as a single contaminant to all the processes using mass load calculated as shown in equation 2.1 (Prakotpol, and Srinophakun, 2004).

$$\Delta m_i = \frac{(C_{out} - C_{in})f_i}{1000} \dots\dots\dots (2.1)$$

Where Δm_i is the mass-load for process i, C_{out} and C_{in} are the outlet and inlet contaminant concentrations respectively, and f_i is the fresh water flowrate.

The pinch point indicates the minimum water requirement for the whole system of processes. This value can be used in calculating water requirement for each process.

A basic flow from mass balance equation can be written as:

$$F = \frac{\Delta M}{C_{out} - C_{in}} \dots\dots\dots (2.2)$$

The equation 2.2 is based on the assumption that the rate of mass exchange will be constant:

For multiple contaminant problems, equations 2.3 and 2.4 can be solved for each contaminant, the limiting flow being defined as the maximum value across all contaminants.

:

$$F_{lim} = \frac{\Delta M}{C_{out,Max} - C_{in,Max}} \dots\dots\dots (2.3) \quad \text{and}$$

$$F_{fw} = \frac{\Delta M}{C_{out,Max} - 0} \dots\dots\dots (2.4)$$

The efficient optimisation-based methods for WAP were presented by Li and Chang (2007) and Teles et al. (2008).

Savelski and Bagajewicz (2003) adopted mathematical modelling and presented necessary condition of optimality in solving WAP with non-linear and linear approaches for multiple contaminants.

The graphical (pinch) method is easy to understand but has difficulty in dealing with several contaminants and complex water networks connecting different processes in an industry; While, mathematical programming methods continue to improve by coming up with many algorithms and solutions due to the improvement of modern

computers and their capabilities in solving different complex algorithms (Ramos et al; 2014).

Mathematical programming represent WAP as mass exchange network (MEN) and characterized it by two operators, namely: a distribution network where stream mixing and splitting occurs and a process operator where mass transfer takes place. This approach was used to tackle the problem of minimising the total annual cost (TAC) of mass exchange networks and it was claimed that it guarantees a global optimum; however, this this is not always true (Hallale and Fraser; 2000).

Different researchers applied these concepts to tackled WAP problems involving single and multiple contaminants and single and multi-objective optimisation.

2.5 Mathematical Optimisation

Mathematical programming consists of models that describe complex real world problems and algorithms to find optimal solutions to the problems represented by the models. Optimisation theory is the science of finding the best possible solution for a given problem; it can be implemented through several approaches, such as simulation and marginal analysis, but in the last four decade mathematical programming has become the key approach to implementing optimisation theory for real wold problems (Avriel. et al; 1996). Borraz-Sanchez, (2010) described optimisation as a science in constant development, with a narrow link between computer science and applied mathematics. It involves selecting the initial design variables of a concept, and analysing the system based on the objective function; if the objectives are met then an optimal design has been achieved, otherwise the design variables are changed and put in to the system again (Figure 2.2).

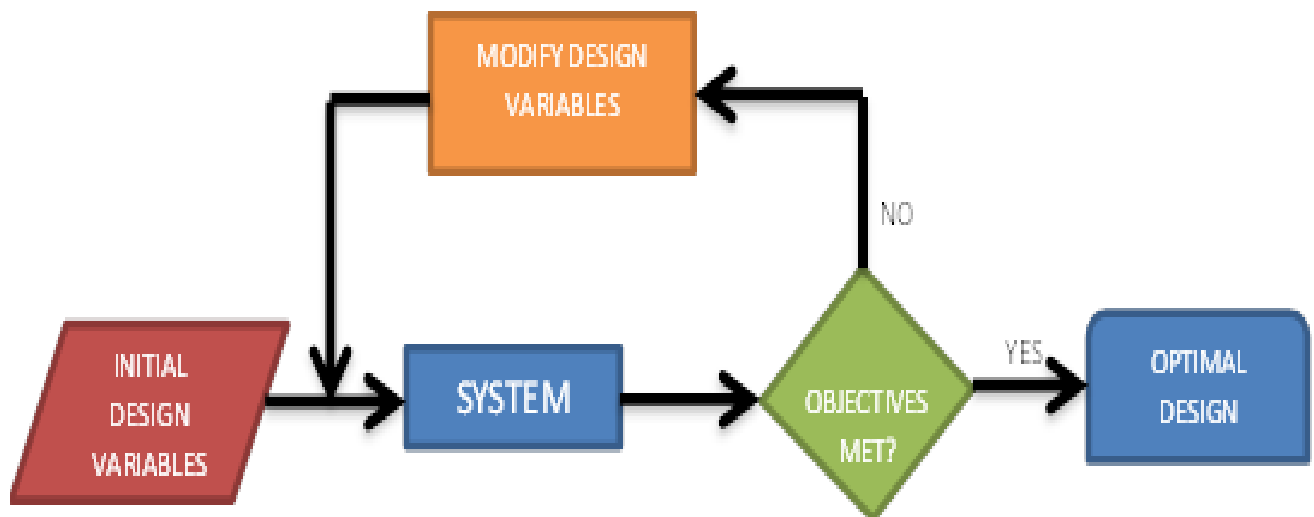


Figure 2. 2: Mathematical Optimisation Technique

2.6 Single Contaminant problems

Some industries can be considered to produce wastewater that has single component pollutant such as: pulp and paper industry, and the washing procedure in the semiconductor industry. The necessary conditions of optimality in water allocation problems were presented by (Savelski, Bagajewicz 2000). It was called optimal water application planning (WAP) which considered wastewater reuse on the basis of single contaminant. The method was used as part of a design procedure (water save) and mixed integer linear programming (MILP) approach in solving the WAP problem.

Takama *et. al.* (1980b) used mathematical programming by considering single contaminant to solve a refinery example. This method can be used efficiently in the pulp and paper industry, the washing procedure in the semiconductor industry and for any washing process even based on solvents other than water as long as the concentration of the contaminants is low. Other researchers such as: Olesen and Polley (1997), Feng *et. al.* (2007), and Deng *et. al.* (2008) presented different methods of minimising water reuse with single contaminant.

To address the minimisation of freshwater use and wastewater production in the process industries, considering single contaminant, the individual processes and their constraints relating to minimum mass transfer driving force, fouling, and corrosion

limitations, a linear and non-linear relationship of water streams and contaminants was considered. This research work proposed superstructure of the model that handle all the relationships between different industrial processes using water as shown in Figure 2.3 The freshwater (F_i), wastewater (W_i) and Reused-water (X_{ij}) flowrate streams were considered as the variables. The number of freshwater and wastewater variables streams are equal to the number of processes. If an industry has N number of processes using water, then the number of variables for both freshwater and wastewater streams will be $2N$. They can be represented as follows:

$$F_i \text{ (freshwater streams)} = [F_1, F_2, F_3 \dots F_N]$$

$$W_i \text{ (Wastewater streams)} = [W_1, W_2, W_3 \dots W_N]$$

While the reused-water streams can be represented by N^2-N variables as shown in matrices below:

$$X_{ij} \text{ (Reused-water streams)} = \begin{bmatrix} 0 & X_{1,2} & X_{1,3} & \dots & X_{1,N} \\ X_{2,1} & 0 & X_{2,3} & \dots & X_{2,N} \\ X_{3,1} & X_{3,2} & 0 & \dots & X_{3,N} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ X_{N,1} & X_{N,2} & X_{N,3} & \dots & 0 \end{bmatrix}$$

The superstructure of the model that handle all the relationships between different industrial processes using water can be represented as shown in Figure 2.3.

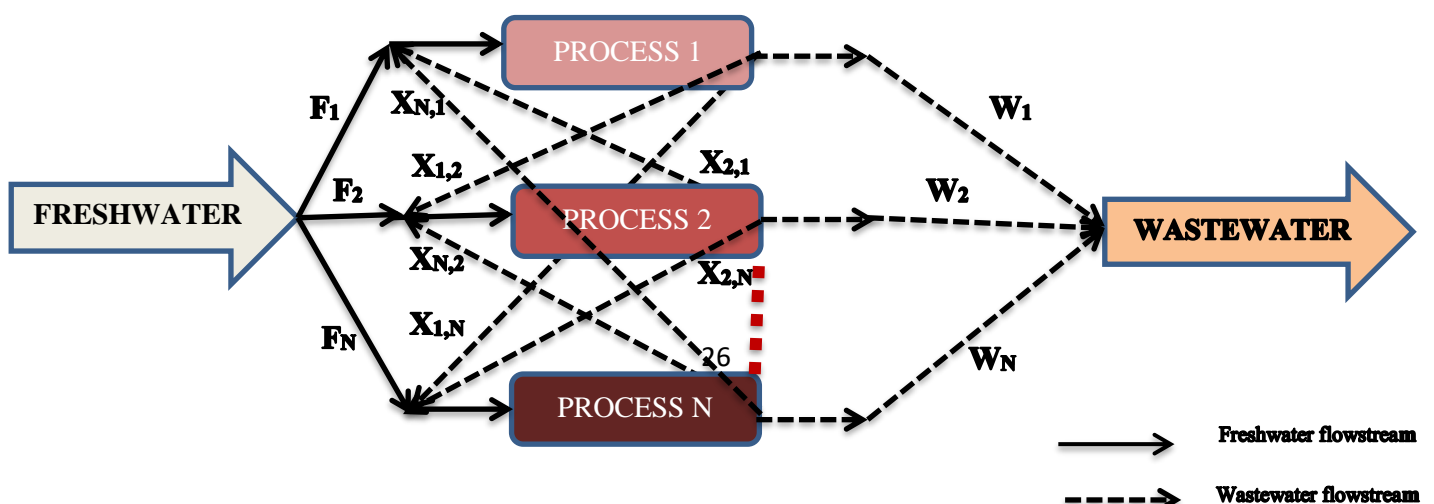


Figure 2. 3: Superstructure of the models

Therefore, for the analysis of single contaminant WAP problem, the total number of variables can be calculated as $2N + N^2 - N = N^2 + N$.

The objective function for the sum of freshwater flow rates at the entrance of all the processes can be expressed as equation 2.5.

$$F = \text{Min} \sum_{i=1}^n F_i \dots \dots \dots (2.5)$$

Where, **F** is the total freshwater flowrate, F_i is the freshwater flow for each process i to n (the number of processes).

The Linear Constraints functions are:

- a. The constraint of the water mass balance of all processes (equation 2.6):

$$F_i + \sum_{j \neq i} X_{i,j} - W_i - \sum_{j \neq i} X_{j,i} = 0 \dots \dots \dots (2.6)$$

- b. The constraint of the contaminant mass balance of all processes (equation 2,7):

$$\sum_{j \neq i} C_{j,out} X_{i,j} + \Delta M_i - C_{i,out} \left(W_i + \sum_{j \neq i} X_{j,i} \right) = 0 \dots \dots \dots (2.7)$$

- c. The Non-Linear Constraint function for Maximum Contaminant inlet concentration is (equation 2.8):

$$C_{j,in} = \frac{\sum_{j \neq i} C_{j,out} X_{i,j}}{\sum_{j \neq i} X_{i,j} + F_i} \leq C_{i,in}^{max} \dots \dots \dots (2.8)$$

Where X_{ij} , is the wastewater flow from process i to j , $C_{i,out}$ and $C_{j,out}$ are the maximum outlet contaminant concentrations limits for the processes i and j , and W_i is the wastewater flowrate out of the system.

The above system of equations 2.5 and 2.6 are derived to be simultaneously solved using mathematical programming by demanding the minimisation of equation 2.5 subject to the constraints 2.6 to 2.8. The obtained minimum freshwater use can then be used to determine the total cost of obtaining freshwater by multiplying the value with the unit cost of freshwater.

2.6.1 Single Contaminant problems With Regeneration

Regeneration is the treatment of the wastewater after it has been used. It is the next possibility of minimising water reuse after exploiting all avenues of direct re-use. It will further reduce freshwater intake and wastewater discharge. The used water is send to regeneration unit after the level of concentration of the contaminants in them cannot be re-used in any other process within the industry. There are, however, lower bounds of the concentration $C_{t,out}^T$ given by the treatment technology limitations. Savelski and Bagajewicz (2001) prove that, this is actually the value that should be used in order to minimise the freshwater used.

If water loss within the regeneration unit is ignored, equation 2.5 and equations 2.9 to 2.11 can be used in solving the WAP problem for single contaminant with regeneration.

The variables for this case are freshwater flow, Wastewater flow to the discharge, Wastewater flow to other processes, flow to the regeneration units and flow from the regeneration units. This can be estimated to be equal to n^2+3n , where n is the number of processes involved in the analysis. The difference in the number of variables from the case without generation is $2n$, which accounts for the flow into and out of

regeneration units. While, the difference between the constraint of single contaminant with and without regeneration is the terms $X_{i,r}$ and $X_{r,i}$ that represents the regeneration.

The fitness function is the sum of freshwater flow rates at the entrance of each water using process, given by equation 1, as described earlier.

The linear constraints functions for the model are:

- a. The constraint of the water mass balance of all process given by equation 2.9.

$$F_i + \sum_{j \neq i} X_{i,j} + X_{i,r} - W_i - \sum_{j \neq i} X_{j,i} - X_{r,i} = 0 \dots \dots \dots (2.9)$$

- b. The constraint of the contaminant mass balance of all processes given by equation 2.10:

$$\sum_{j \neq i} C_{j,out} X_{i,j} + C_o X_{i,r} + \Delta M_i - C_{i,out} \left(W_i + \sum_{j \neq i} X_{j,i} + X_{r,i} \right) = 0 \dots \dots \dots (2.10)$$

The nonlinear Constraints function for the model is:

- c. The maximum contaminant inlet concentration of all processes given by equation 2.11:

$$C_{j,in} = \frac{\sum_{j \neq i} C_{j,out} X_{i,j} + C_o X_{i,r}}{\sum_{j \neq i} X_{i,j} + F_i + X_{i,r}} \leq C_{i,in}^{max} \dots \dots \dots (2.11)$$

The above system of equations 2.9 to 2.11 are derived to describe the inclusion of contaminants constraint for the purpose of procedure required in optimisation. These equations are solved simultaneously by using mathematical programming by d the minimisation of equation 2.5 subject to the constraints 2.9 to 2.11. The obtained minimum freshwater use can then be used to determine the total cost of obtaining freshwater by multiplying the value with the unit cost.

2.7 Multiple contaminant problems

Most of the industries produce wastewater with different kind of pollutants, some in solution and others as suspended solids; as such, they require different treatment before reuse.

Wang et al (2002) describe the design methodology for water networks of multiple contaminants with single internal water main, and proposed a new concept of 'water-saving factor', which emphasized on the location of the first internal water main that relate to the maximum water-saving potential. The proposed design steps are as follows:

1. Determine the concentration of the first internal water main.
2. Calculate the water-saving factor of each unit process.
3. Create a general diagram of water network.
4. Allocate flowrates from freshwater and the internal water main to each unit process.

When flowrates from freshwater and internal water mains to each unit process are determined, the construction for the network is finished. This indicate that water networks with internal water mains provide simpler water networks, which is easy to design, operate and control, for plants involving many unit processes, such as those in petrochemical and chemical complexes.

Key steps in Waste Water Minimisation for Multiple Contaminant problems

A number of key steps are to be followed for implementing a Wastewater minimisation project (Dakwala et al., 2009).

Step 1: The need of waste water minimisation identified based on limited availability of freshwater, economic and environmental regulation consideration.

Step 2: Data related to plant/industry is collected which include fresh water use by a particular unit, process quality requirement, cost and capability of treating water for initial input to the process and the wastewater generated in the end by the process.

Step 3: Drawing a flow sheet of the processes, which shows water balance diagram of the processes.

Step 4: Identification of the key contaminants for the processes; these are the contaminants that are to be reduced so that the discharged waste water can be reused or disposed under the specified control standards for an industry.

Step 5: The two major types of approaches is applied for solving the wastewater minimisation problems.

1. Insight-based techniques which can also be termed as Heuristics approach: It typically involves water pinch analysis (WPA) techniques, and it consists of following steps:

- Analysis of the problem by considering individual contaminants and constraints
- Determination of Reuse and Regeneration opportunities based on the existing contaminants and constraints
- Selection of the final treatment operations based on constraints and environmental regulations

2. Mathematical programming approach: It has following steps:

- Definition of superstructure by considering each process within an industry to have a certain freshwater flow rate, output water from other process and or regenerated water, the output from the process will have effluent with certain level of pollutants concentration which can be discharged, recycled or regenerated for reuse.
- Mathematical optimisation
- Analysis of solution

Step 6: After carrying out various analysis and calculations a Wastewater minimisation project can be implemented.

The variables for the case of multi-contaminant water re-use analysis are freshwater flow, Wastewater flow to the discharge, Wastewater flow to other processes and the concentration of different contaminants in different processes. These can be estimated to be equal to $n^2 + n + nm$, where n is the number of processes and m is the number of contaminants involved in the analysis. The difference between the constraint of single contaminant and multi-contaminant are the terms $C_{i,k,out}$ and $C_{j,k,out}$ that represent the multi-contaminant in to and out of each process.

The fitness function is the sum of freshwater flow rates at the entrance of each water using process, as described earlier in equation 2.5.

The linear constraints functions for the model are:

- a. The constraint of the water mass balance of all process given by equation 2.12.

$$F_i + \sum_{j \neq i} X_{i,j} - W_i - \sum_{j \neq i} X_{j,i} = 0 \dots \dots \dots (2.12)$$

- b. The constraint of the contaminant mass balance of all processes given by equation 2.13:

$$\sum_{j \neq i} C_{j,k,out} X_{i,j} + \Delta M_{i,k} - C_{i,k,out} \left(W_i + \sum_{j \neq i} X_{j,i} \right) = 0 \dots \dots \dots (2.13)$$

The nonlinear Constraints function for the model is:

- c. The maximum contaminant inlet concentration of all processes given by equation 2.14:

$$C_{j,in} = \frac{\sum_{j \neq i} C_{j,k,out} X_{i,j}}{\sum_{j \neq i} X_{i,j} + F_i} \leq C_{i,in}^{max} \dots \dots \dots (2.14)$$

The above system of equations 2.12 to 2.14 are derived to describe the inclusion of multi-contaminants constraint for the purpose of process required in optimisation.

These equations are simultaneously solved by using mathematical programming by minimisation of equation 2.5 subject to the constraints 2.12 to 2.14. The obtained minimum freshwater use can then be used to determine the total cost of obtaining freshwater by multiplying the value with the unit cost.

However, the internal structure of the model is based on the sum of all the different contaminants concentrations inlet and outlet of each industrial process.

2.7.1 Multiple contaminant problems With Regeneration

Savelski and Bagajewicz (2003) presented necessary conditions of optimality for multicomponent water allocation systems in refineries and process plants. They extend the necessary conditions of optimality proved for single component by Savelski and Bagajewicz (2000). They prove the necessary condition of monotonicity and show that at least one component reaches the maximum concentration at the outlet of a freshwater user process. These conditions establish that if a system is optimum, freshwater user processes have at least one component reaching its maximum concentration. The monotonicity conditions was derived which correspond to special components called key components, and these necessary conditions can be used in future works to develop an algorithmic procedure to design multicomponent water allocation systems.

The variables for this case are freshwater flow, wastewater flow to the discharge, Wastewater flow to other processes and the concentration of different contaminants in different processes. This can be estimated to be equal to $n^2 + 3n + nm$.

Where, n is the number of processes and m is the number of contaminants involved in the analysis.

The fitness function is the sum of freshwater flow rates at the entrance of each water using process, given by equation 5, as described earlier.

The linear constraints functions for the model are:

- a. The constraint of the water mass balance of all process given by equation 2.15.

$$F_i + \sum_{j \neq i} X_{i,j} + X_{i,r} - W_i - \sum_{j \neq i} X_{j,i} - X_{r,i} = 0 \dots \dots \dots (2.15)$$

- b. The constraint of the contaminant mass balance of all processes given by equation 2,16:

$$\sum_{j \neq i} C_{j,k,out} X_{i,j} + C_o X_{i,r} + \Delta M_i - C_{i,k,out} \left(W_i + \sum_{j \neq i} X_{j,i} + X_{r,i} \right) = 0 \dots \dots \dots (2.16)$$

The nonlinear Constraints function for the model is:

- c. The maximum contaminant inlet concentration of all processes given by equation 2.17:

$$C_{j,in} = \frac{\sum_{j \neq i} C_{j,k,out} X_{i,j} + C_o X_{i,r}}{\sum_{j \neq i} X_{i,j} + F_i + X_{i,r}} \leq C_{i,in}^{max} \dots \dots \dots (2.17)$$

The above system of equations 2.15 to 2.17 are derived to describe the inclusion of multiple contaminants with regeneration for the purpose of procedure required in optimisation. These equations are simultaneously solved by using mathematical programming by minimisation of equation 5 subject to the constraints 2.15 to 2.17.

The obtained minimum freshwater use can then be used to determine the total cost of obtaining freshwater by multiplying the value with the unit cost.

However, the internal structure of this regeneration part of the model is based on the sum of all the different contaminants concentrations inlet and outlet of each regeneration process.

2.8 Optimisation

2.8.1 Single objective mathematical programming

Single objective mathematical programming is usually used as an effective method for the analysis, synthesis and retrofit of water-using networks for industrial water reuse

and wastewater minimisation and of distributed effluent treatment system for minimising the water treatment flowrate. The single objective function that is usually considered in WAP problem is the sum of fresh water flow rates at the entrance of each water using process as presented in equation 5. However, other objectives can also be handled efficiently if considered separately and a single “optimal” solution can be achieved.

2.8.2 Multi-objective Optimisation

Multi-objective Optimisation (MOO) is concerned with the minimisation of multiple objective functions that are subject to a set of constraints. MOO enables optimisation of the process with respect to two or more objectives simultaneously, to provide a set of non-dominated solutions.

Walter (2011) in his review article explains that in many areas where decisions under uncertainty have to be made, different objectives that cannot be reduced to each other occur (which leads to the formation of) multi-objective consideration of decision problems. Formally, such decision problems can often be represented as multi-objective stochastic optimisation problems, and many of them are of combinatorial type. There are several solution concepts for multi-objective optimisation models, such as lexicographic optimisation, multi-attribute utility theory (MAUT), and determining Pareto-optimal (or: efficient) solutions.

The MAUT uses the concept of representing the preferences of the decision maker numerically on the set of all multiple objectives using a numerical function called a utility function. However this method is applicable only when all the data are expressed in exactly the same unit and the final result will be based on the quantification of the data and the decision maker’s expertise. Furthermore, the method is purely based on

normative value of an item approach (Shanmuganathan *et. al*; 2018). These constraints limit its application in the WAP problem.

The solution methods for the multi-objective optimisation problems are classified in accordance to the number of solutions generated (Generating Methods) and the role of the decisions maker (DM) inside the problem solution (preference based methods) as indicated in Figure 2.3 (Ramos *et al*; 2014).

The computation of the set of Pareto-optimal solutions (short: Pareto set) allows obtaining information on the trade-off between the different objectives before being forced to weigh them against each other. Instead of delivering a single “optimal” solution, the system provides the decision maker with a set of reasonable alternatives, among which a final choice can be made. By a Pareto-optimal solution, one understands a solution that is not dominated by any other solution in the search space, where a solution y dominates a solution x if y is at least as good as x in all objectives and better than x in at least one objective.

Caballero *et al.* (2004) investigated stochastic multi-objective continuous optimisation problems and outline the two essential alternative paths to tackle it as follows:

- (i) Multi-objective approach: The problem is first reduced to a deterministic multi-objective problem, which is then solved by techniques of multi-objective optimisation.
- (ii) Stochastic approach: The problem is first reduced to a single-objective stochastic problem, which is then solved by techniques of stochastic optimisation.

The same two paths can also be followed when solving a multi-objective stochastic combinatorial optimisation problem (SCOP).

For the multi-objective approach, the simplest way is to draw a fixed sample of random scenarios in order to reduce the stochastic problem to a deterministic (still multi-objective) problem, and then to apply a metaheuristic technique to obtain the set of Pareto-optimal solutions with respect to the average objective function values over the

sample. However, relying on a fixed sample has the disadvantage that the probability model specified by the drawn sample scenarios is only an approximation to the original probability model, such that even if the applied multi-objective metaheuristic should provide the exact Pareto set of the deterministic problem, it needs not to be the Pareto set of the original problem. Therefore, several articles on multi-objective SCO work with variable samples or with the execution of simulation modules as sub-procedures.

Boix; et al (2011) provide set of potential network solutions in the form of a Pareto front. He presented a strategy for choosing the best network solution among those given by Pareto fronts using two approaches for the Multiple Criteria Decision Making (MCDM) problem. The problem was solved by means of implementing a classical TOPSIS analysis and then an innovative strategy based on the global equivalent cost (GEC) in freshwater. The later turns out to be more efficient for choosing a good network according to a practical point of view.

Doyle and Smith (1997) presented a new method for targeting maximum water reuse in processing systems, by considering two cases. In the first case, the mass transfer was modelled in terms of a fixed mass load. This leads to a problem that can be solved as a non-linear optimisation problem. In the second case, the mass transfer was modelled in terms of a fixed outlet concentration. This leads to a problem which can be solved as a linear optimisation problem.

However, in practice, many water-using operations will call for the mass exchange characteristics of some contaminants to be modelled by fixed mass load and others to be modelled by fixed outlet concentration, leading overall to a non-linear problem. To overcome the difficulties associated with non-linear optimisation, a combined approach is employed, in which the linear model is used to provide an initialization for non-linear optimisation. This method can also be combined with graphical approach

to provide a representation which incorporates all constraints, not only concentration, but also flowrate constraints and forbidden matches.

Furthermore, another solution method of multi-objective optimisation proposed by Ramos *et al.*, (2014) is by using a priori solution methods (specifically goal programming) and specifying decision making (DM) priorities inside the optimisation problem (Figure 2.4).

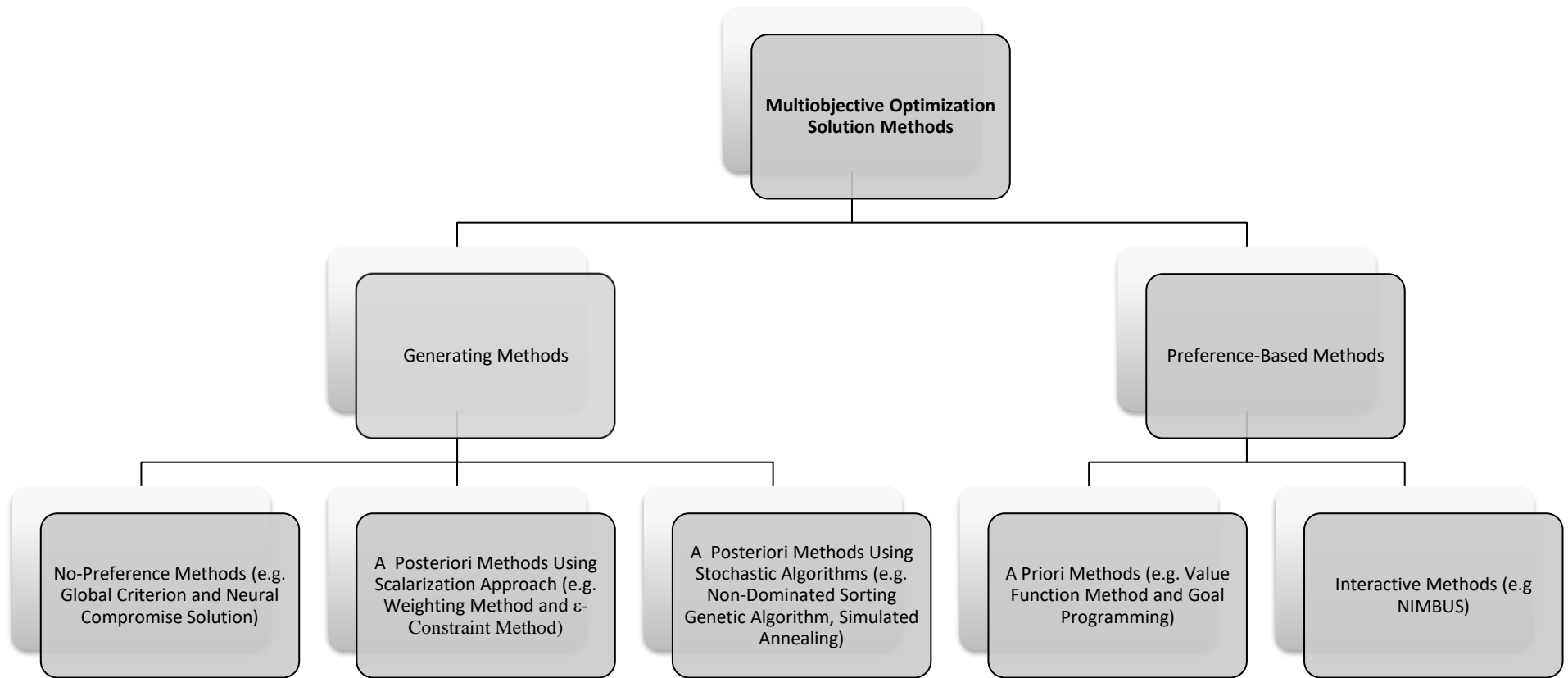


Figure 2.4: Classification of Multi-objective Optimisation (Solution) Methods, Ramos *et. al.*, (2014)

Therefore, in this research a Posteriori Methods Using Stochastic Algorithms (Multi-objective Genetic Algorithm) is considered as the right option for the analysis of the multi-objective considered.

The multi-objective Functions considered are:

1. Sum of freshwater flow rates at the entrance of all water using processes (equation 2.18):

$$FRW = \sum_{i=1}^n F_i \dots \dots \dots (2.18)$$

2. The sum of wastewater produced by all water using processes. The amount of wastewater minimisation will lead to environmental protection and reduction in the cost of treatment equation 2.19):.

$$WWR = \sum_{i=1}^n X_{i,j} \dots \dots \dots (2.19)$$

3. The sum of all the values of Reuse Wastewater. This will limit the reuse to only such processes that accept the level of contaminant in the wastewater and reduce the disposal cost (equation 2.20).

$$RWR = \sum_{i=1}^n X_{2n+1,j} \dots \dots \dots (2.20)$$

4. The sums of all the nodes of wastewater reuse interconnections. This will lead to reducing the complexity, represented by the number of interconnections of the network of wastewater reuse. Furthermore, Chew et al., 2008; shows that pipes and associated infrastructure significantly contribute to the network investment cost (equation 2.22).

$$CWWR = \text{if } \sum_{i=1}^n X_{2n+1,j} \geq 1,1 \text{ else } 0 \dots \dots \dots (2.21)$$

5. The regenerated water flow-rate expressed as the sum of the water flow-rates going from a process to a regeneration unit and from a one regeneration unit to another. The amount of regenerated water will logically increase if the freshwater is minimized. Subsequently, this criterion is related to economical insight because if the amount of regenerated water is high, the cost will increase for the user, as the cost of the treatment units is dependent on the volume of wastewater that requires treatment (Boix, *et. al.* 2011). Hence, it would be favourable if the volume of water that requires treatment were reduced (equation 2.22).

$$RWR = \sum_{i=1}^n \left(\sum_{i=1}^n X_{i,r} + \sum_{i=1}^n X_{r,i} \right) \dots \dots \dots (2.22)$$

The above system of equations 2.18 to 2.22 are used as the main fitness functions in minimising the constraints. The obtained minimum quantity of freshwater, wastewater and regenerated water can then be used to determine the total cost of obtaining freshwater by multiplying the value with the unit cost.

2.9 Conclusion

This chapter provides a general overview of the literature involved in the different Water Application Planning (WAP) methods. It described the way to model an integrated water application planning (WAP) problem based on the concept of superstructure. The superstructure was employed in showing the actual network interconnections of different industrial processes of feasible fresh water minimisation. The existing WAP research section presents the attention received by the problem of wastewater reuse from several researchers. The basic concepts of Water pinch technology (WPT) or Water pinch Analysis (WPA) and mathematical programming as applied to WAP problems was presented. It assists in the identification of different

methods of water reuse optimisation. This leads to coming up with a proposed way to model an integrated water application planning (WAP) problem based on the concept of superstructure and the feasibility of the solution.

The existing WAP researches and their shortcomings were analysed and the proposed methodology that will handle all those shortcomings were described.

The branches of analysis of WAP problem were identified as single contaminant problems with and without Regeneration, multi-contaminant problems with and without Regeneration. It also assist in identification of data requirement and the procedure involved in finding the solution for each method.

In the computational strategy that utilizes optimisation-based modelling techniques for industrial WAP the challenges were identified. They are: multiple local optimal solutions, nonlinearity (due to multi-contaminant), simultaneous optimisation of the interactions of models (for wastewater treatment technologies and multiple water-using units), enabling faster numerical solutions, and alternative methods for optimisation under uncertainty. For these reasons, this research developed a framework for industrial WAP that handle multi-contaminant industrial processes with regeneration technologies that minimised the above challenges without complexity. Literature described the stochastic optimisation as tough method to use in solving uncertainty problems. Therefore, the above challenges and uncertainties can be handled by using stochastic mathematical algorithm optimisation method. The selected algorithm is known as Genetic Algorithm (GA), which is robust stochastic optimisation method.

The multi-objective Optimisation (MOO) application is concerned with the minimisation of multiple objective functions that are subject to a set of constraints. MOO Stochastic

Algorithms (Multi-objective Genetic Algorithm) is considered as the right option for the analysis of the multi-objective optimisation of the WAP problem to provide a set of non-dominated solutions.

The next chapter will provide a general overview of the selected method for solving the different Water Application Planning (WAP) problems.

CHAPTER THREE

3.0 METHODOLOGY

This chapter provides a general overview of the selected method for solving the different Water Application Planning (WAP) problems. It includes data consideration and description of the number of variables for different number of Industrial Processes. The key steps followed in using Genetic Algorithm (GA) optimisation in matlab software for solving WAP models are presented. This is needed for the fact that having knowledge on how the algorithms work is important in order to understand the way GA should be applied, The sensitivity analysis of the GA parameters applied on the WAP model and the scalability of the WAP model were presented. The aim of the analysis is to determine and select the best GA parameters that provide optimum result at the shortest possible computational time. The analysis indicates the best selection of GA parameters that are supposed to be used in solving the WAP model.

3.1 Introduction

The water distribution network in any given industry is affected by the sequence of processes and meeting the process's water requirement is extremely difficult task under the condition of minimal freshwater supply. The optimal design of WAP was developed to minimise freshwater use, wastewater production and protect the environment by using mathematical optimization modelling method. An appropriate number of options for this problem were managed by using a non-linear programming (NLP) model. The solutions in the design of such a model are reached with very low requirements as regards to employed computer time and without the difficulties of the non-convexity that arises when dealing with detailed models for representing the involved units operations that prevents its efficient performance.

To solve WAP problem the required data from any given industry will be:

- (a) Sources of water used for running the processes and their quality parameters.
- (b) The number of processes that use water in the whole industry.
- (c) The quantity of water used, and wastewater produced by each process.
- (d) The maximum contaminants produced by each process.
- (e) The maximum acceptable contaminants for each process.
- (f) The structural pattern of water distribution in the industry.
- (g) Wastewater treatment or regeneration, and recycle that exist in the industry.

After getting the data, the most important step in WAP analysis is the selection of the optimisation method that handles the problem efficiently. Table 3.1 presents the different number of variables involved in the solution of the model for 2 to 10 industrial processes, depending on whether it is a single contaminant or multi-contaminant analysis with or without regeneration.

Table 3 1: Number of Variables for Industrial Processes in WAP problem.

Number of Industrial Process (n)	Single Contaminant WAP problems		Multi-Contaminant (m) WAP problems (Assuming m=3)	
	Number of variables without regeneration (n ² +n)	Number of variables with regeneration (n ² +3n)	Number of variables without regeneration (n ² +n+nm)	Number of variables with regeneration (n ² +3n+nm)
2	6	10	12	16
3	12	18	21	27
4	20	28	32	40
5	30	40	45	55
6	42	54	60	72
7	56	70	77	91
8	72	88	96	112
9	90	108	117	135
10	110	130	140	160

The GAs is adaptive meta-heuristic search algorithm premised on the evolutionary ideas of natural selection and genetics. They represent an intelligent exploitation of a

random search within a defined search space to provide solution to a problem that consistently outperforms other methods (Srinivasa *et. al.* 2014). Davis (1991) has identified three main advantages of GAs in optimization: “First, they generally find nearly global optima in complex spaces. Second, genetic algorithms do not require any form of smoothness, that is, they can handle nonlinearity and discontinuity and third, considering their ability to find global optima, GAs are fast, especially when tuned to the domain on which they are operating. Advantageous features of GAs in solving large scale, nonlinear optimization problems are that they can be used with continuous or discrete parameters, require no simplifying assumptions about the problem and they do not require computation of derivative information during the optimization (Haupt and Haupt, 2004). Therefore, it is considered in this research to be the most appropriate method for the solution to WAP problem.

GA mimics the natural selection process that drives biological evolution in solving both constrained and unconstrained optimisation problems. The GA repeatedly modifies a population of individual solutions. At each step, it selects individuals at random from the current population to be parents and uses them to produce the children for the next generation. Over successive generations, the population "evolves" toward an optimal solution. The GA can be applied to solve a variety of optimisation problems that are not well suited for standard optimisation algorithms, including problems in which the objective function is discontinuous, non-differentiable, stochastic, or highly nonlinear. It can address problems of mixed integer programming, where some components are restricted to be integer-valued. It works with a coding of the parameter set, not the parameters themselves. It searches from a population of points, not a single point. It uses objective function information, not derivatives or other auxiliary knowledge and it use probabilistic transition rules not deterministic rules. Therefore, it is considered as

the best option for optimisation of WAP problem in this research. Other operations parameters and their variations for the GA are shown in the Table 3.2.

The GA uses Selection, Crossover and Mutation rules at each step to create the next generation from the current population. Selection rules select the individuals, called parents that contribute to the population at the next generation. Crossover rules combine two parents to form children for the next generation, and mutation rules apply random changes to individual parents to form children.

The GA differs from a classical, derivative-based, optimisation algorithm in that it generates a population of points at the end of each computational procedure, selects the next population by computation which uses random number generators, while, the best point in the population approaches an optimal solution. This makes it a renowned technique for avoiding local optima in improving search space of any mathematical problem.

Table 3 2: Operations and parameters of genetic algorithm.

S/No.	Genetic Algorithm Process	Genetic Algorithm Parameters	Parameters Variation
1.	POPULATION	Population Type	Double vector Bit String
		Population Size	Number of variables to Infinity
		Creation Function	Constraint Dependant
			Uniform
			Feasible population
		Initial Population	Number of variables and population size
		Initial Scores	Only non-integer problems
Initial Range	Only non-integer Problems		
2.	FITNESS SCALING	Scaling Function	Rank
			Proportional
			Top
			Shift Linear
3.	SELECTION	Selection Function	Stochastic Uniform
			Remainder
			Uniform
			Roulette
			Tournament
4.	REPRODUCTION	Elite Count	$0.05 * \min(\max(10 * \text{No. of variables}, 40), 100)$ (for I-problem)
		Crossover Fraction	Fraction between 0 and 1
5.	MUTATION	Mutation Function	Constraint dependent
			Gaussian
			Uniform
			Adaptive Feasible
6.	CROSSOVER	Crossover Function	Scattered
			Single Point
			Two Point
			Intermediate
			Heuristic
			Arithmetic
7.	MIGRATION	Direction	Forward Both directions
		Fraction	0 to 1
		Interval	Number of generations
8.	CONSTRAINT PARAMETERS	Initial Penalty	Non-linear only, 1 to infinity
		Penalty Factor	1 to infinity
9.	HYBRID FUNCTIONS	Hybrid Functions	fminsearch
			patternsearch
			fminunc
			fmincon
10.	FUNCTION EVALUATION	Evaluation of Fitness and Constraint Functions	In serial
			Vectorised
			In parallel
		Number of Iterations	

3.2 Solving the WAP problem using GA Optimisation method

3.2.1 Algorithm Implementation

The basic flow chart for the implementation of Genetic Algorithm (GA) is shown in Figure 3.1. However, depending on the optimisation software used in finding the solution, the steps may require a little adjustment in execution. The steps involve initial generation of chromosomes, using the objectives function and constraints functions for water reuse. The GA will use these functions, generate initial random population, and provide offspring values for the subsequent crossover and mutation. After attaining the optimum result from GA, the hybrid optimisation function switches on to find the final result within the optimum region of the GA. It starts by defining decision variables and objective function and terminates by testing for convergence of the objective function.

The GA process begins with a population of chromosomes, which is the set of possible solutions for the decision variables of an optimization problem, and moves toward achieving better solutions through evolution. The decision variables are encoded as real-valued strings (genes) for a given search space. A chromosome is the set of these substrings (genes). The evolution starts from a population of completely random chromosomes and occurs in generations. In each generation, the fitness of the whole population is evaluated, and multiple chromosomes are stochastically selected from the current population (based on their fitness) and modified using genetic operators such as crossover and mutation to form a new population. The new population is then used in the next iteration (generation) of the algorithm (Davis, 1991). Population size depends on the nature of the problem, but typically there are hundreds or thousands of possible solutions. This algorithm is repeated sequentially until the desired stopping criterion is achieved.

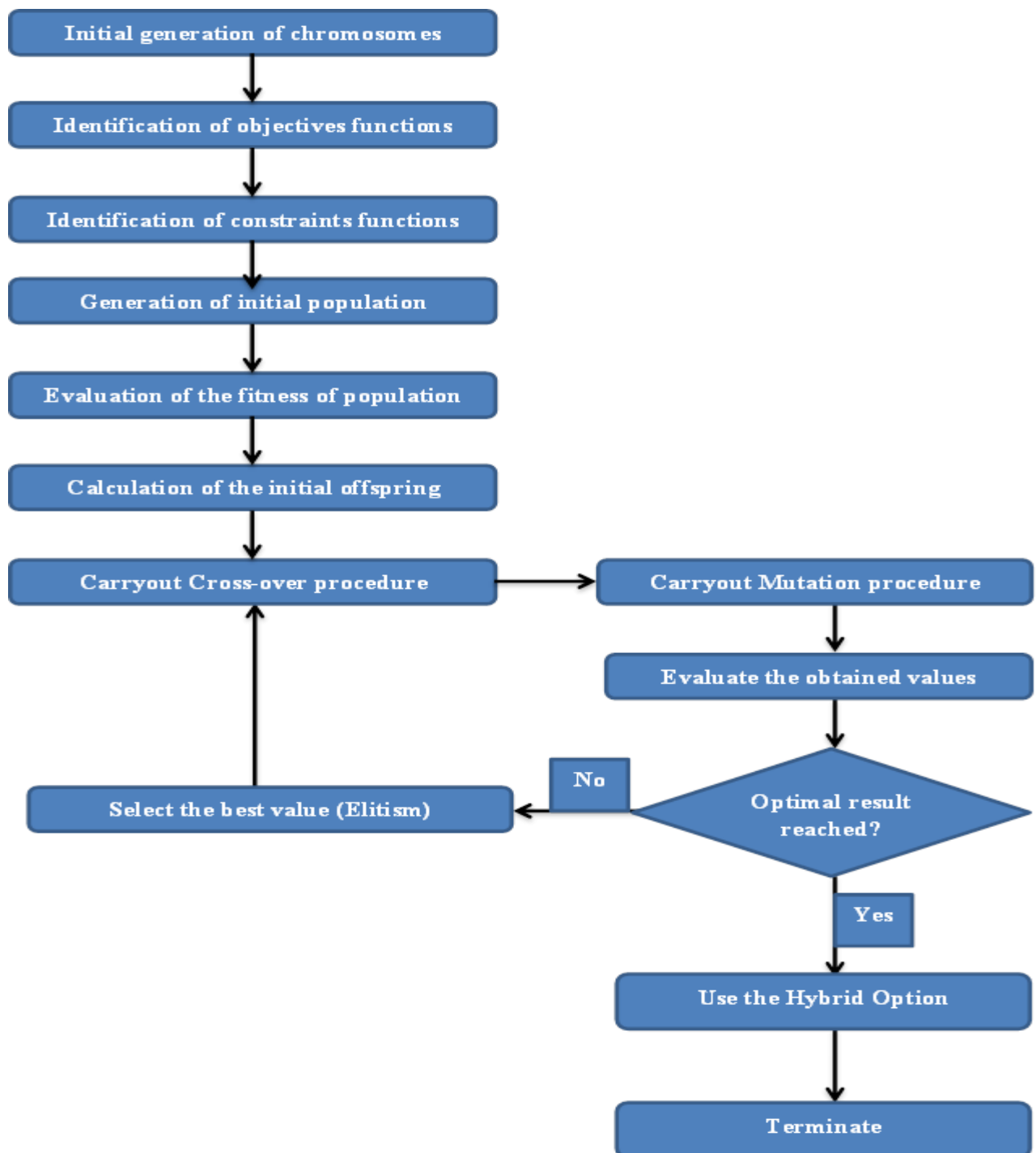


Figure 3. 1: Key steps for Genetic Algorithm (GA) solution

3.2.2 Initial Generation of Chromosomes

The term chromosomes is used in biological systems to refer to the thread-like structure found in the nuclei of both animal and plant cells that carry hereditary information passed down from parents. It combined to form the total genetic prescription for the construction and operation of everything that's shows the organism

as the replica of the parents. But in the artificial genetic system this are represented or coded as strings or variables. In this research real value coding was adopted to increase the accuracy and efficiency of the search space of the GA and decrease the burden of additional calculation. The number of variables in a given WAP problem represents the chromosomes.

The chromosomes for each industrial process are derived from freshwater, wastewater and wastewater for reuse, represented as follows: F_i , W_i , and $X_{i,j}$ respectively. A chromosome representing search space will be:

$$C_j = (F_1 \dots F_N, W_1 \dots W_N, X_{1,2} \dots X_{N,N-1})$$

Each gene within the chromosome represents freshwater, wastewater and wastewater for reuse for any given industrial process. They can take up any value between the upper and lower bounds of supply within the system. The entire search space for the problem is represented by the number of chromosomes generated within the upper and lower limits of the decision variables (i.e. freshwater F_i , wastewater W_i and wastewater for reuse $X_{i,j}$). The population is generated using real value coding in the matlab software. The software generates initial chromosomes or strings randomly by using boundary limits of all positive real values i.e. $X_{i,j} \geq 0$. This creates a matrix that represents all the variables in the linear and nonlinear constraints. The values of contaminants were directly used in the equations either as the coefficient of the variable or as a constant. The rows and columns of the matrix represent the number of chromosomes and constraints in the problem, respectively. The number of chromosomes generated will depend on the number of variables in the problem.

For example, a single contaminant without regeneration WAP problem of 2 industrial process ($n = 2$) have 6 variables as described in Table 3.1. The chromosomes for each

industrial process are derived from freshwater, wastewater and wastewater for reuse, represented as: $F_1, F_2, W_1, W_2, X_{1,2}$ and $X_{2,1}$ respectively. A chromosome representing search space will be: $(F_1, F_2, W_1, W_2, X_{1,2}, X_{2,1})$ and the objective is to minimise the value of freshwater $F(x)$, where $F(x) = (F_1 + F_2)$. Since there are six variables in the objective and constrain equations, namely $F_1, F_2, W_1, W_2, X_{1,2}$ and $X_{2,1}$,

The chromosomes are composed as follows:

Initialization

For example we define the number of chromosomes in population for 2 industrial processes as 6, and then we generate random value of gene $F_1 + F_2$ for 6 chromosomes

Chromosome [1] = $[F_1 ; F_2] = [12; 08]$

Chromosome [2] = $[F_1 ; F_2] = [02; 03]$

Chromosome [3] = $[F_1 ; F_2] = [10; 14]$

Chromosome [4] = $[F_1 ; F_2] = [20; 06]$

Chromosome [5] = $[F_1 ; F_2] = [02; 19]$

Chromosome [6] = $[F_1 ; F_2] = [20; 01]$

Evaluation

We compute the objective function value for each chromosome produced in initialization step:

$$F_obj[1] = (12 + 08) = 20$$

$$F_obj[2] = (02 + 03) = 05$$

$$F_obj[3] = (10 + 14) = 24$$

$$F_obj[4] = (20 + 06) = 26$$

$$F_obj[5] = (02 + 19) = 21$$

$$F_obj[6] = (20 + 03) = 23$$

Selection

1. The fittest chromosomes have higher probability to be selected for the next generation. To compute fitness probability we must compute the fitness of each chromosome. To avoid divide by zero problem, the value of F_obj is added by 1.

$$\text{Fitness}[1] = 1 / (1 + F_obj[1]) = 1 / 21 = 0.0476$$

$$\text{Fitness}[2] = 1 / (1 + F_obj[2]) = 1 / 6 = 0.1667$$

$$\text{Fitness}[3] = 1 / (1 + F_obj[3]) = 1 / 25 = 0.040$$

$$\text{Fitness}[4] = 1 / (1 + F_obj[4]) = 1 / 27 = 0.0370$$

$$\text{Fitness}[5] = 1 / (1 + F_obj[5]) = 1 / 22 = 0.0455$$

$$\text{Fitness}[6] = 1 / (1 + F_obj[6]) = 1 / 24 = 0.0417$$

$$\text{Total} = 0.0476 + 0.1667 + 0.040 + 0.0370 + 0.0455 + 0.0417 = 0.3415$$

The probability for each chromosomes is formulated by: $P[i] = \text{Fitness}[i] / \text{Total}$

$$P[1] = 0.0476 / 0.3415 = 0.1394$$

$$P[2] = 0.1667 / 0.3415 = 0.4881$$

$$P[3] = 0.040 / 0.3415 = 0.1171$$

$$P[4] = 0.0370 / 0.3415 = 0.1083$$

$$P[5] = 0.0455 / 0.3415 = 0.1332$$

$$P[6] = 0.0417 / 0.3415 = 0.1221$$

From the above probabilities we can see that Chromosome 2 has the highest fitness, this chromosome has highest probability to be selected for next generation chromosomes.

For the selection process we use uniform selection by taking the fitness probabilities values that are slightly less than Chromosome 2 values. The new set of chromosomes is:

New Chromosome [1] = Chromosome [2]

New Chromosome [2] = Chromosome [1]

New Chromosome [3] = Chromosome [5]

New Chromosome [4] = Chromosome [6]

New Chromosome [5] = Chromosome [3]

New Chromosome [6] = Chromosome [4]

Chromosomes in the population thus became:

Chromosome [1] = [02; 03]

Chromosome [2] = [10; 14]

Chromosome [3] = [12; 08]

Chromosome [4] = [20; 01]

Chromosome [5] = [10; 14]

Chromosome [6] = [20; 06]

The Parent chromosome which will mate is randomly selected and the number of mate Chromosomes is controlled using crossover rate (0.8) parameters.

3.3 Genetic Algorithm (GA) in Matlab

MATLAB is a technical computing environment that provide framework to develop tailored algorithms for advanced analyses and data visualisation. Its language provides Interfaces to other programming languages, including FORTRAN and C that enables the sharing of ideas and the development of solutions.

MATLAB gives immediate access to high-performance numerical computing with more than 600 mathematical, statistical, and engineering functions. This functionality is extended with add-on and Signal Processing toolboxes and interactive graphical capabilities for creating plots, images, surfaces, and volumetric representations.

Matlab software (MATLAB R2016a) was used for implementing the steps used in the solution of GA; as such, some adjustments were adopted in obtaining the best result. The collections of routines, written mostly in m-files, which implement the most important functions in genetic algorithms, are used for solving the optimisation model in Matlab. Tarek *et.al.* (2006) observed that incorporating a search method within a genetic algorithm can improve the search performance on the condition that their roles cooperate to achieve the optimisation goal. Therefore, to further improve the diversity and convergence of the solutions of the WAP obtained by MATLAB, a hybrid function was incorporated. The crossover and mutation operator combine to improve the search ability of the algorithm and produce the best solution, which further provide optimum solution with hybrid function.

3.3.1 Steps in Genetic Algorithm implementation in Matlab

The following steps are followed in using Matlab software for the minimisation of WAP problem in MATLAB.

1. Combining all variables in one vector.
2. Writing vector for lower and upper bounds (lb and ub).
3. Writing matrix and vector of inequalities (A and b).
4. Writing matrix and vector of equalities (Aeq and beq).
5. Writing nonlinear constraint function.
6. Calling the solver: $[x \text{ fval}] = \text{ga}(\text{fitnessfcn}, \text{nvars}, \text{A}, \text{b}, \text{Aeq}, \text{beq}, \text{lb}, \text{ub})$
7. Calling the hybrid solver as an option function.

The hybrid function is called to improve the convergence of the GA to optimum solution. It is described in detail in chapter 4.

3.4 Genetic Algorithm (GA) Sensitivity analysis

This section presents the study on parametric sensitivity analysis carried out on the GA applied to Water reuse Optimisation Model. The aim of the study was to evaluate the relative influence of the GA parameters based on the values of the solution of the WAP fitness function used in the analysis, to the minimum of the desired model output. Sensitivity analysis of the parameters of the GA approach was applied to identify the combination of the parameters that produce minimum and acceptable solution as presented in the literatures. Examples from literature of industrial processes were used to determine the variation of GA parameters with the WAP problem to reach the solution that is indicated by the literature as the accepted solution based on the problem analysed. This analysis is practically important in the application of the model to real-world problem.

Most of the researches done on optimization of WAP problem pay much attention to obtaining a global optimum result, without paying the required attention for parameters sensitivity analysis. Some authors compare their solution with the previous research that preceded their methods and claim a better result outcome (e.g. Jie Bai *et al.* 2009). Therefore, the study reported in this chapter used sensitivity analysis techniques reported by Srinivasa *et al.* (2014). The technique involves evaluation of the fitness function value based on the interaction of different GA's parametric condition. However, the discovery of an optimal setting for the parameters or even the existence of one can be determined only with a detailed trial and error approach (Sundaram, 1998).

3.4.1 Algorithm Testing

The GA parameters setting that is excellent for one problem may not be suitable for another one, therefore sensitivity analysis of the key GA parameters of the approach was done to identify the parameters that produce quality solutions (Yuan and Gallagher, 2005; Srinivasa et al. 2014). Sensitivity analysis is done by comparing the fitness objective function value based on different combination of the four key parameters. The selected key parameters are: Population size, Crossover functions, Crossover Fraction and Mutation Functions. This will enable the determination of a subset of GA parameters that make the identification of an optimum solution more likely.

In this research the selected parameters related to the implementation of the genetic algorithm were tuned before the algorithm is confirmed. These parameters are Population, Fitness Scaling, Selection, Reproduction, Crossover, Mutation, Migration, Constraint Parameters, Hybrid Function and Function Evaluation. Obviously, by the stochastic nature of Genetic Algorithm (GA), multiple runs on the same problem are necessary to get a good estimate of performance. Therefore, the algorithm was run more than 1000 times to observe the average result. The runs took several weeks on a desktop computer that is versatile with powerful processing and Graphics Card. The hardware platform has simple scalability that can handle a wide variety of functions with Hard Drive of 465GB ROM, 3.3GH RAM built on high-performing 7th Generation Intel® Core™ vPro™ processor device with 23" widescreen LCD Monitor and Display Ports. The software platform has Window XP Professional editions Operating System with variable file system support and different device drivers.

3.4.2 Population Size

The size of population is one of the significant parameters of genetic algorithm since it has direct influence on its search abilities (Yuri, 2003). Its diversity is one of the most important factors that determine the performance of the genetic algorithm. If the average distance between individuals is large, the diversity is high; if the average distance is small, the diversity is low. Getting the right amount of diversity is a matter of start and error. If the diversity is too high or too low, the genetic algorithm might not perform well. The Population size field in Population options determines the size of the population at each generation. Increasing the population size enables the genetic algorithm to search more points and thereby obtain a better result. However, the larger the population size, the longer the genetic algorithm takes to compute each generation.

Yuri (2003) shows in his research on GA that in most cases increase in population size tends to give better solution accompanied by greater time for search even with less number of generations. However, Matlab software recommend use of 50 population size for five or fewer variables in GA analysis and 200 otherwise (MATLAB, 2017)

In this research the population size was varied from 10 to 1000 to analyse and obtain the size that provides answer to the WAP problem with the lowest value. The analyses indicates that the population size of 10 give the lowest fitness function value of WAP problem, followed by 20 model as shown in Figure 3.2.

The observed result shows that the optimal population size is 10 for accurate and minimum model values and this may leads to obtaining result in a reasonable computational time.

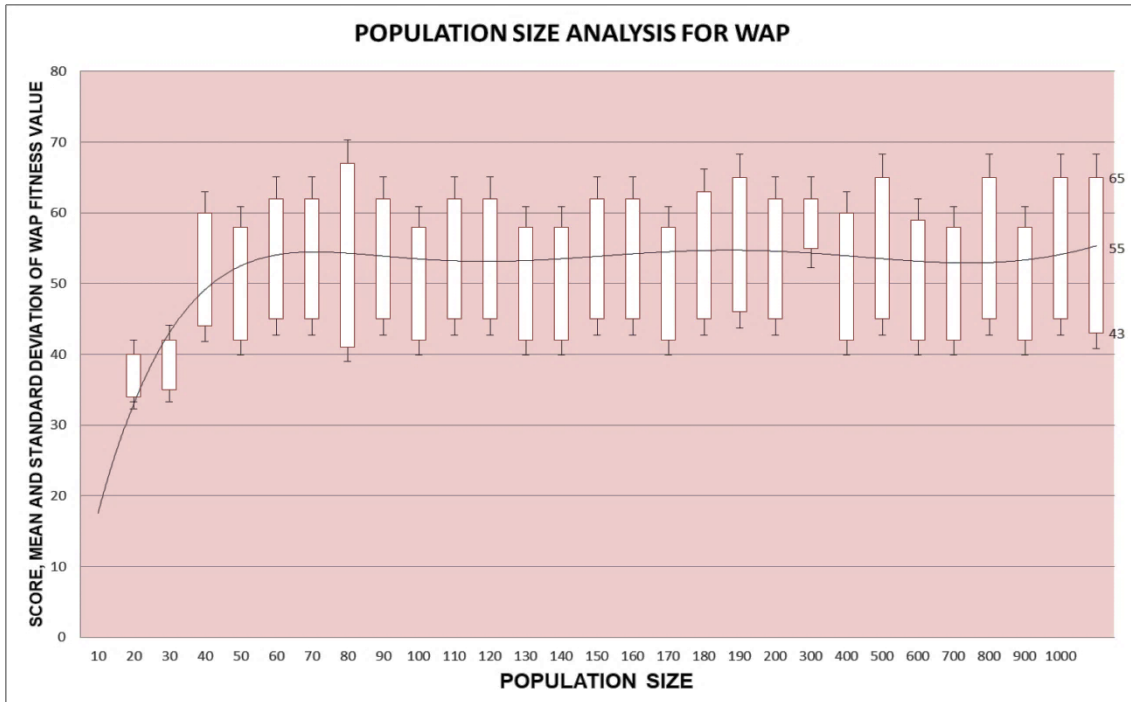


Figure 3. 2: Population Size analysis for Genetic Algorithm (GA) solution

3.4.3 Crossover Function

Crossover is the process in GA that interchange information between randomly selected parent chromosomes by recombining parts of their corresponding strings. It recombines genetic material of two parent chromosomes to produce offspring for the next generation (Bandyopadhyay and Saha, 2013).

Matlab have the following crossover functions: Constraint dependent, Scattered, Single Point, Two Point, Intermediate, Heuristic and Arithmetic as shown in Table 3.2.

The analysis of the crossover functions indicate that Constraint dependent and Intermediate functions gives the lowest fitness function values for WAP problem model as shown in Figure 3.3.

The two functions perform crossover using the constraint. However, Intermediate creates offsprings by a weighted average of the parents. It is also controlled by a scaling factor chosen uniformly at random over an interval defined by the size of the

area for possible offspring and it is limited by a deficiency of managing non-linear constraints. While, the Constraint dependent crossover function chooses the crossover points based on the constraints of the objective function and produce “viable” offspring based on the constraints. Therefore the constraint dependent crossover function was selected for this research.

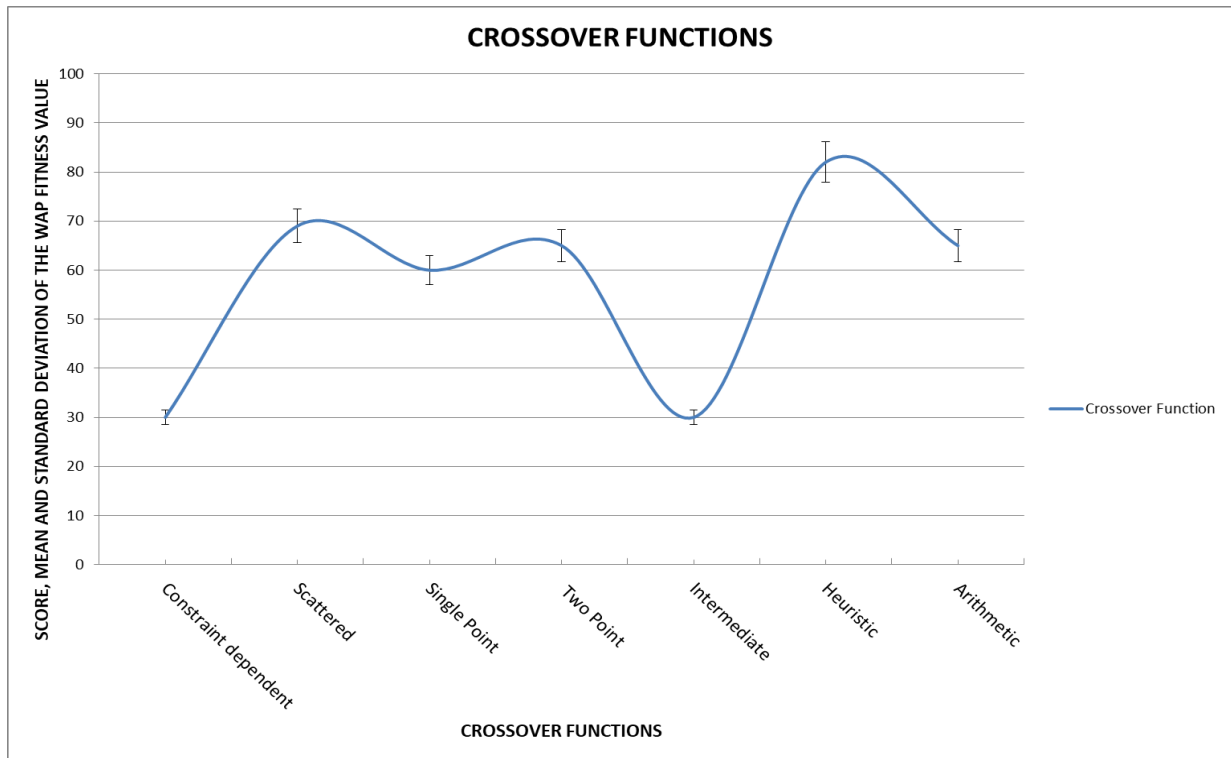


Figure 3.3: Crossover Functions analysis for Genetic Algorithm (GA) solution

3.4.4 Crossover Fraction

Many researchers use the value of Crossover Fraction between 0.6 and 1.0 and it also depends on the type of crossover function used. The result of using the GA for the solution of WAP problem (for single contaminant without regeneration) with crossover fraction between 0 and 1 is shown in Figure 3.4. The plot presents the means and standard deviations of the best fitness values for each value of the Crossover fraction.

The analysis indicates that the value of 0.8 crossover fraction is the best value for the minimisation of WAP problem model.

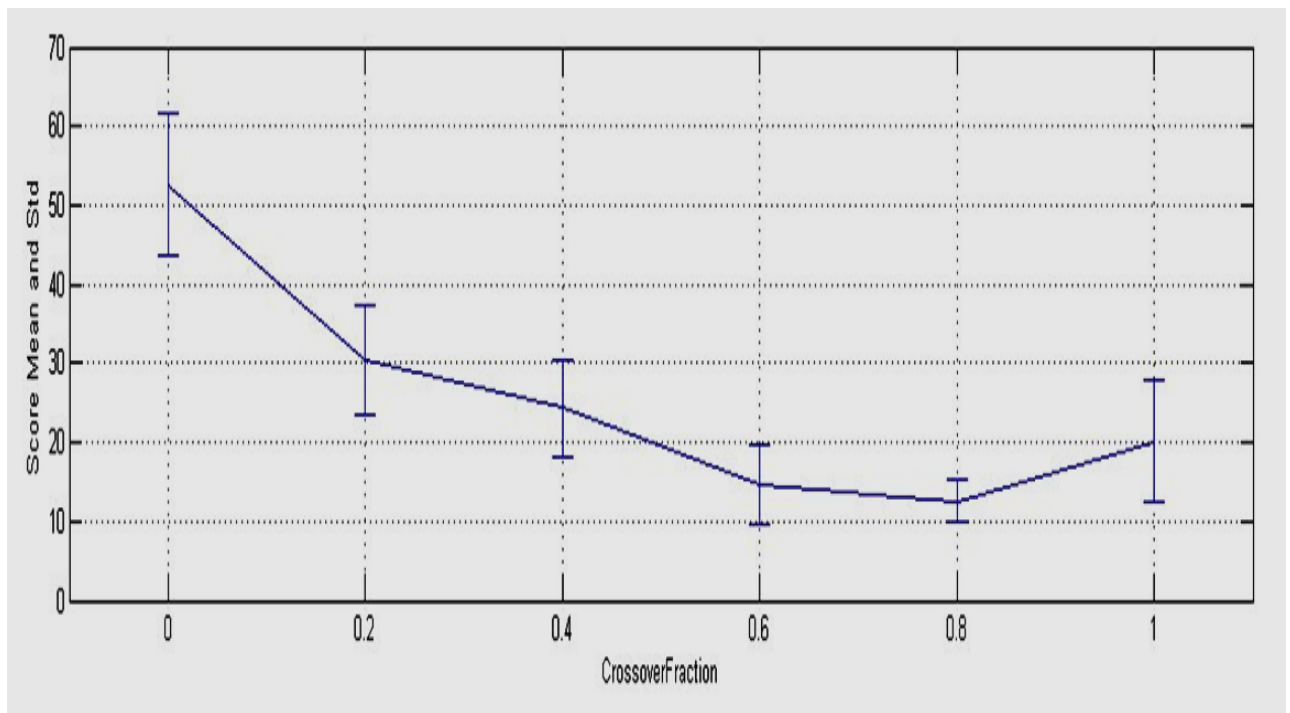


Figure 3. 4: Reproduction for Genetic Algorithm (GA) solution.

Therefore, GA optimisation of WAP model (for single contaminant without regeneration) solution was found to perform better with Constraint dependent Crossover function and Crossover Fraction of 0.8. This agrees with the results of Ayad, *et. al.*, (2013) on parametric analysis of GA for the solution of water distribution networks.

3.4.5 Mutation

Mutation Function assists the GA to make small random changes in the individuals obtained as the solution in the population to create new solution. Mutation provides genetic diversity and enables the GA to search a broader space (Matlab, 2017). According to Thomas Back (1993 and 1996) analyses of mutation rate for the simple

counting problem the optimal mutation rate is inversely proportional to the number of variables.

Matlab have the following mutation functions: Constraint dependent, Gaussian, Uniform and Adaptive Feasible as shown in Table 3.2. The amount of mutation is proportional to the standard deviation of the distribution of the variables and it decreases at each new generation. The Scale and Shrink options was used with the Gaussian function to control the average amount of mutation that the algorithm applies to a parent in each generation.

Scale controls the standard deviation of the mutation at the first generation, which is Scale multiplied by the range of the initial population, which is specified with the Initial range option. While, Shrink controls the rate at which the average amount of mutation decreases. The standard deviation decreases linearly so that its final value equals 1 – Shrink times its initial value at the first generation. The effect of mutation of each analyses was presented by running the genetic algorithm on a problem and using the plot options ‘Distance and Range’. The formula for the standard deviation used to perform the analyses is shown in equation 3.1:

$$\sigma_k = \sigma_{k-1} \left(1 - SHRINK \frac{k}{Generation} \right) \dots \dots \dots (3.1)$$

The Gaussian Mutation is not suitable for the solution of WAP problem due to the consideration of the constraint, as it is used only for unconstraint problems.

Uniform mutation is a two-step process. First, the algorithm selects a fraction of the vector entries of an individual for mutation, where each entry has a probability Rate of being mutated. The default value of Rate is 0.01. In the second step, the algorithm replaces each selected entry by a random number selected uniformly from the range for that entry (MATLAB, 2017). Figure 3.5 shows the plot of uniform mutation for the

three processes WAP problem. The plot terminates at low regeneration value of less than 200.

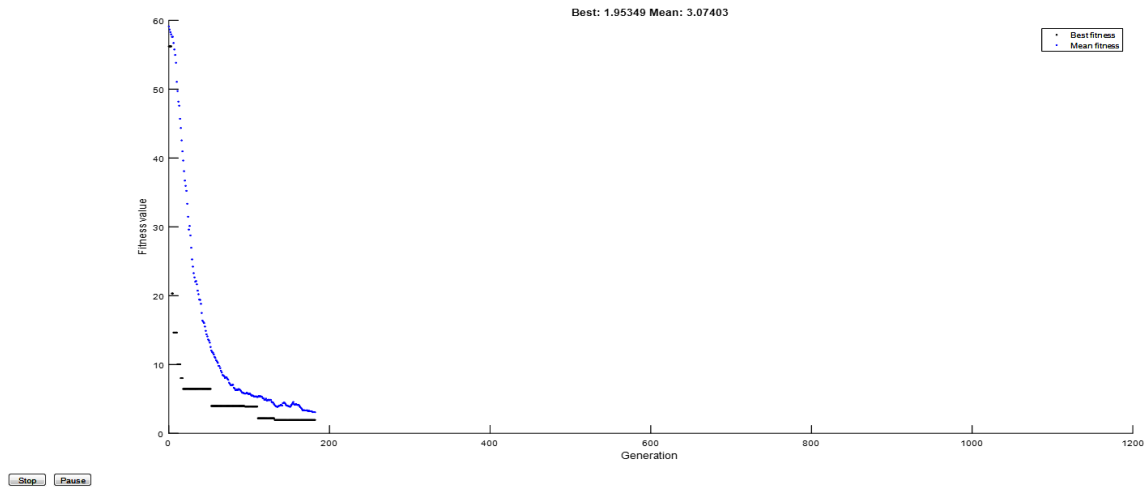


Figure 3.5: Uniform Mutation for Genetic Algorithm (GA) solution.

Adaptive Feasible is the mutation function that allows the use of constraints on the optimisation problem. It randomly generates directions that are adaptive with respect to the last generation and goes to the direction that satisfies bounds and linear constraints. Figure 3.6 shows the plot of uniform mutation for the 3 industrial processes WAP problem. The plot terminates at regeneration value of 205. Therefore, Adaptive Feasible is the best mutation function for the GA optimisation of WAP model.

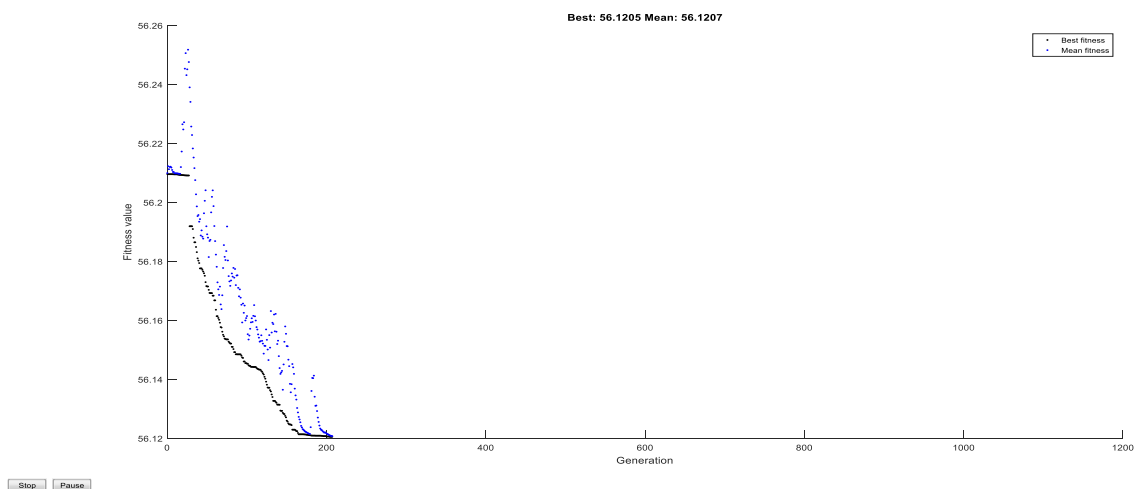


Figure 3.6: Adaptive Feasible Mutation for Genetic Algorithm (GA) solution.

3.5 Conclusion

The description of the data required for solving WAP problem from any given water using industry is presented. The data can be used to determine the number of variables involved in setting up the WAP model. Matlab software (MATLAB R2016a) was used for implementing the steps used in the solution of WAP problem using GA. However, a major concern in genetic algorithm design is efficiency in terms of the time needed to reach a solution of desired quality and selection of the appropriate parameters for running it. GA uses Population size as one of the parameters to search for the optimum solution of WAP model. Other parameters are crossover probability and mutation probability. It was established that GA optimisation of WAP model solution will perform better with the population size of 10, and Constraint dependent Crossover functions. The result of the analysis of the Crossover fraction indicates that the best value for GA on the WAP problem model is 0.8. The mutation rate depends on the number of variable in any given WAP problem set up as described in Table 3.1. However, the Crossover Fraction of 0.8; with 'mutation Adapt-Feasible' as the mutation probability function gives the result with less regeneration, this will ultimately leads to shorter computational time.

The next chapter will analyse the improvement on the GA method for solving the different WAP problems and the different population sizes to solve the different WAP model problems and the computational time taken by the computer.

CHAPTER FOUR

4.0 IMPROVEMENT OF THE GENETIC ALGORITHM (GA) FOR THE SOLUTION OF WATER APPLICATION PLANNING (WAP) MODEL

4.1 Introduction

This chapter provides analysis of the improvement on the Genetic Algorithm (GA) method for solving the different Water Application Planning (WAP) problems. It described the hybrid function used with the GA to increase its efficiency in obtaining the solution for WAP problems. The modelling approach used was presented and the results obtained were compared with and without hybrid function. The aim of the analysis is to determine the behaviour of GA with and without hybrid function and the computer time for obtaining the WAP solution. The objective function is to minimise the total water supply consumption of the industrial processes. The result shows that there is a high efficiency in using the GA for solving the WAP problem and in obtaining the optimum result with hybrid function. This motivates the research to propose using hybrid function with GA to improve its performance.

4.1.1 Method for the Hybrid Approach of Single-Objective

Incorporating a hybrid within a genetic algorithm can improve the search performance on the condition that their roles cooperate to achieve the optimisation goal (Tarek *et al.*, 2006). The gradient-based local deterministic optimisation function, known as the Sequential Quadratic Programming (SQP) algorithm was used as hybrid function for single objective WAP problem. In single objective GA the hybrid function starts at the best point returned by the GA.

The method involves combining principles of Genetic Algorithms (GA) and SQP algorithm that performs the computation of the Hessian of the objective function and

its non-linear constraints. The hybrid function prevents the GA from being stuck in the local minimum solution of the WAP problem.

The Hessian for an unconstrained problem is the matrix of second derivatives of the objective function f , as shown in equation 4.1.

$$\text{Hessian } H_{ij} = \frac{d^2 f}{dx_i dx_j} \dots \dots \dots (4.1)$$

The Hessian for a constrained problem is the Hessian of the Lagrangian. For an objective function f , non-linear inequality constraint vector c , and nonlinear equality constraint vector c_{eq} , the Lagrangian is given by equation 4.2

$$L = f + \sum_i \lambda_i c_i + \sum_j \lambda_j c_{eq_j} \dots \dots \dots (4.2)$$

The λ_i are Lagrange multipliers.

The Hessian of the Lagrangian is shown in equation 4.3.

$$H = \nabla^2 L = \nabla^2 f + \sum_i \lambda_i \nabla^2 c_i + \sum_j \lambda_j \nabla^2 c_{eq_j} \dots \dots \dots (4.3)$$

Matlab software provides SQP as “fmincon” which minimise constraint function based on a powerful concept in optimisation known as trust regions. “Fmincon” uses a Hessian as an input function. The Hessian in this case is the matrix of second derivatives of the nonlinear constraints functions of the WAP model.

4.2 Population Size Analysis of Single Contaminant Water Reuse without Regeneration for 2 to 10 Industrial processes

The population size parameter of the genetic algorithm (GA) and the time taken by the single contaminant water reuse model that does not include regeneration was analysed for two to ten industrial processes, using different examples from the

literature. Increasing the population size enables the GA to search more points and thereby obtain a better result. However, the larger the population size, the longer the GA takes to compute each generation. The number of variables for single contaminant water reuse without regeneration as described in the previous chapter (Chapter 3) is equal to n^2+n , where n is the number of industrial processes involved in the analysis. To compare the time for achieving the optimum result for the solution of Water Application Planning (WAP) model using the genetic algorithm (GA) with and without hybrid, different population sizes from 3 to 1000 were used.

However, we intend to experiment with different settings for Population size to determine the value that return optimal results without taking a prohibitive amount of time for the algorithm to execute.

The hybrid function “fmincon” was added to the GA analysis to improve its performance in obtaining the final result. The population size used was categorised into three groups. The first group is the range of 3 to 10, in step of 1. The second group is the range of 10 to 100 in step of 10, while the third group is 100 to 1000 in step of 100. The three groups were used for the model containing 2 to 10 industrial processes. The maximum, minimum and median time taken for running the model using GA without hybrid function for all the three population size groups were determined (Table 4.1). The time-based performance measures of algorithms are not normally distributed; therefore, median is used as a measure of central tendency.

The Pearson's correlation coefficient (equation 4.4) was used to measure the linear correlation between the time taken with and without hybrid function as y and x , respectively.

$$R_{xy} = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{\sqrt{n \sum x_i^2 - (\sum x_i)^2} \sqrt{n \sum y_i^2 - (\sum y_i)^2}} \dots \dots \dots (4.4)$$

Where R_{xy} is the Pearson's correlation coefficient, n is number of runs, x_i are the individual average time taken (Without Hybrid Function) points indexed with i ; and y_i are the individual average time taken (With Hybrid Function) points indexed with i .

Each set of the population size was used to run the model for 2 to 10 number of industrial processes. The analysis leads to getting an estimate of the running time as a function of the population size used in solving the GA, as shown in Table 4.1.

Table 4.1: Categorisation of Population Size groups and the time of the model runs

Group	Population Range	Time of run for 2 to 10 number of industrial processes (s)		
		Minimum	Median	Maximum
First	3 to 10	3.0	5.7	16.2
Second	10 to 60	3.6	8.5	18.7
	70 to 100	7.2	15.9	25.3
Third	100	11.2	19.5	25.3
	200	53.2	70.0	90.1
	300	141.0	176.8	218.0
	400	354.1	369.8	548.0
	500	806.6	879.7	1151.3
	600	1570.7	1932.1	2286.5
	700	2871.2	3175.8	3534.9
	800	6468.2	6805.2	7292.3
	900	10632.0	11236.1	11719.8
	1000	16141.2	16180.7	16978.3

For the first group, the time taken for running the model using GA is similar with hybrid function incorporated in to the GA for analysis. For the second group the time is different by 2 seconds, when the Hybrid function is included in the running of the GA for all the industrial processes. However, for the third group, each population category exhibit different time range with clear difference. The population size of 100 have median of 19.6 seconds with hybrid function. The population size of 200, 300, 400 and

500 have median of 63.6, 190.0, 399.8 and 908.7 seconds with hybrid function, respectively.

The median time taken for the population size range of 1 to 100 with and without hybrid function included in running the GA for the solution of 2 to 10 industrial processes WAP problem are shown in Figures 4.1 and 4.2, respectively. The trend lines of the two graphs indicate a similar exponential relationship as shown in equation 4.5 and 4.6.

$$Y = 0.08x^2 - 0.6x + 6.4 \dots \dots \dots (4.5)$$

$$Y = 0.085x^2 - 0.7x + 6.6 \dots \dots \dots (4.6)$$

The Pearson's correlation coefficient of the two variations of time, with and without Hybrid function is 0.95. This indicates a strong correlation of the two data.

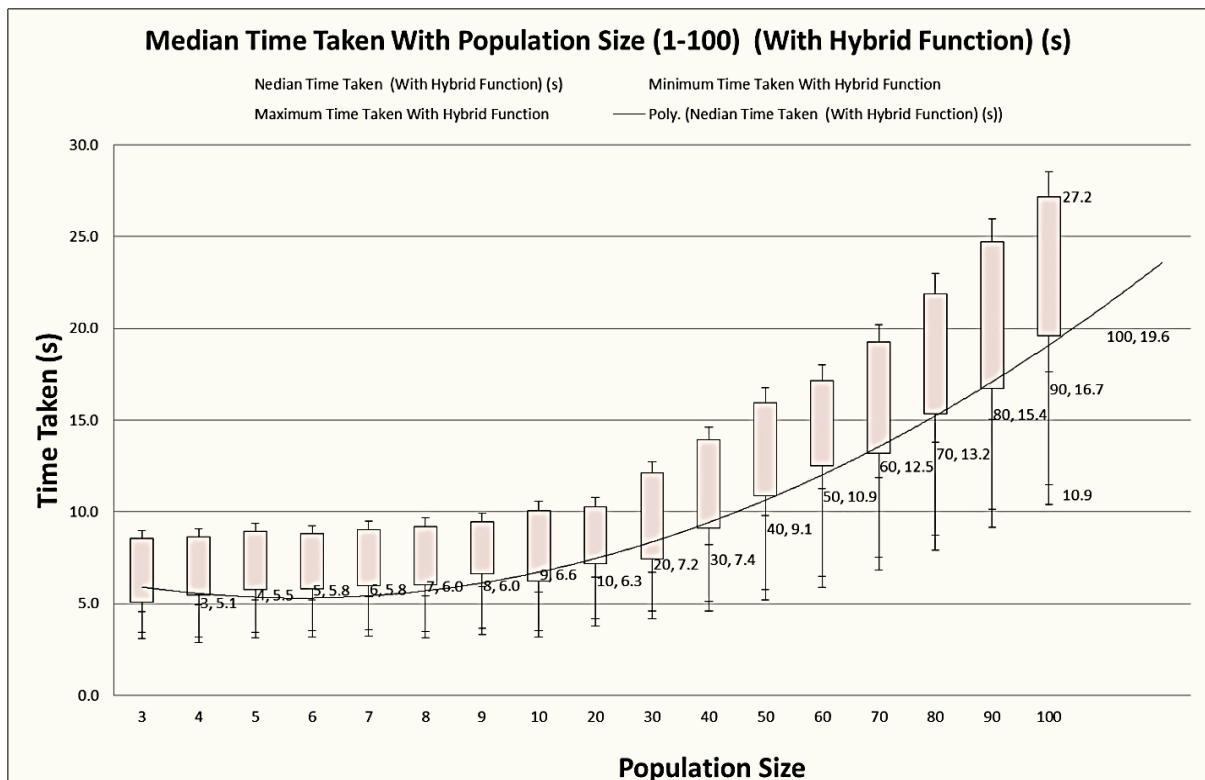


Figure 4. 1: Median Time for Population 1-100 without hybrid function included in running the GA for the solution of 2 to 10 industrial processes WAP problem.

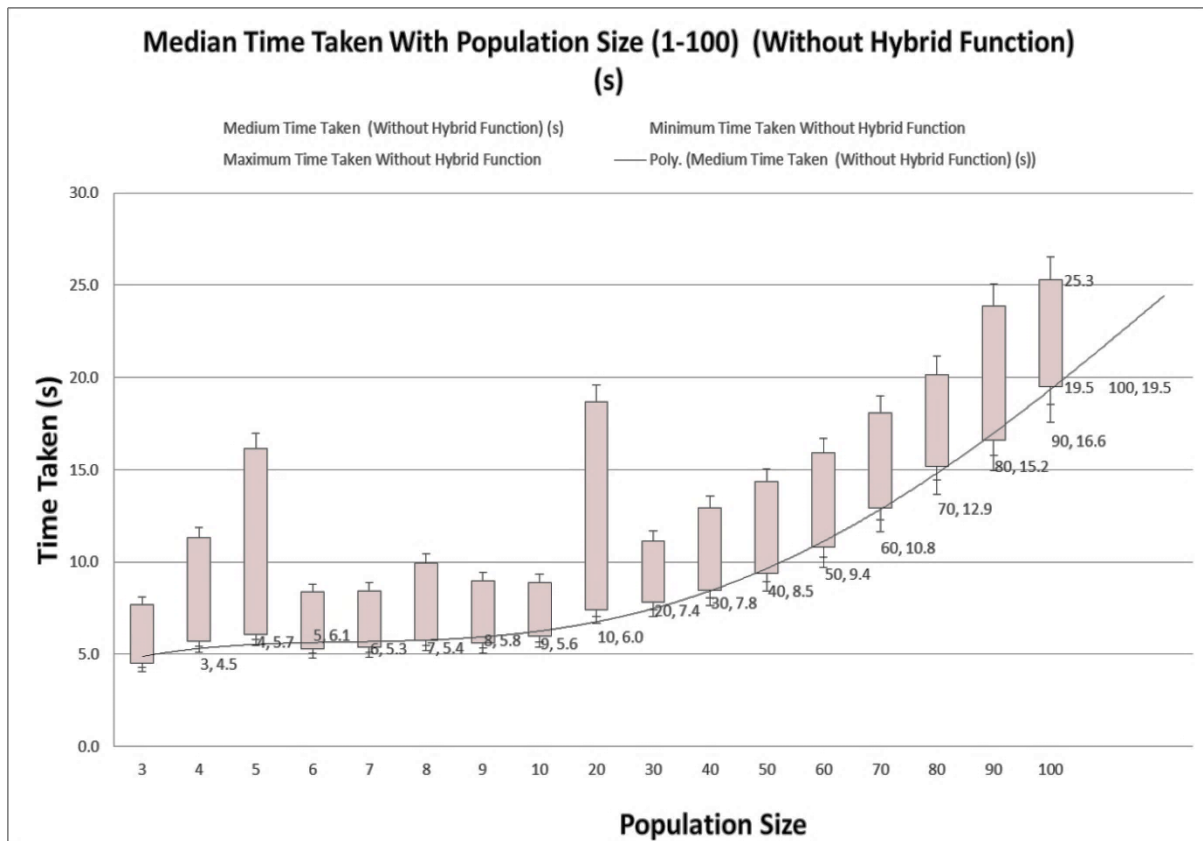


Figure 4.2: Median Time for Population 1-100 with hybrid function included in running the GA for the solution of 2 to 10 industrial processes WAP problem.

Figure 4.3 shows the percentage of the optimum Result obtained for the solution of 2 to 10 industrial processes WAP problem using the Population Size 3-1000 with and without hybrid function included in running the GA. Observation of the objective function results for the different industrial processes from 2 to 10 obtained indicates that population size of 10 gives the highest percentage (90%) of the optimum result, which is 90%. However, running the GA with and without hybrid function takes almost the same time, but analysis of the population size of 3 to 1000 indicates a median difference of 50% in the number of times GA with hybrid gives the optimum result.

Running the model for two industrial processes indicates that, once the population size is more than the number of variables which is in this case 6, the GA with hybrid

achieved optimum result. However, the model gets stuck in the local optimum for up to the population size of 40 without hybrid function.

Running the model for three, five, six and seven industrial processes indicates that the GA with hybrid achieved optimum result for almost all population sizes, but get stuck in the local optimum for all the population sizes without hybrid function. Running the model for four industrial processes indicates that, once the population size is more than 3 the GA with hybrid achieved optimum result for the population size range from 4 to 20 and 200 to 1000, but gets stuck in the local optimum for the remaining population sizes and for all without hybrid function. This also indicates that the population size of less than 3 cannot be used in the solution of WAP problem.

Running the model for eight industrial processes indicates that, only the population sizes of 4, 5, 6, 10, 50, 60, 100, 600 and 800 for the GA with hybrid achieved optimum result, but get stuck in the local optimum for all the population sizes of GA without hybrid function.

Running the model for nine industrial processes indicates that, only the population size of 10 for the GA with hybrid achieved optimum result, and the population sizes of 5 and 80 of GA without hybrid function, but gets stuck in the local optimum for all the remaining population sizes of GA with and without hybrid function. Running the model for ten industrial processes indicates that, there is no difference in the results obtained with or without hybrid.

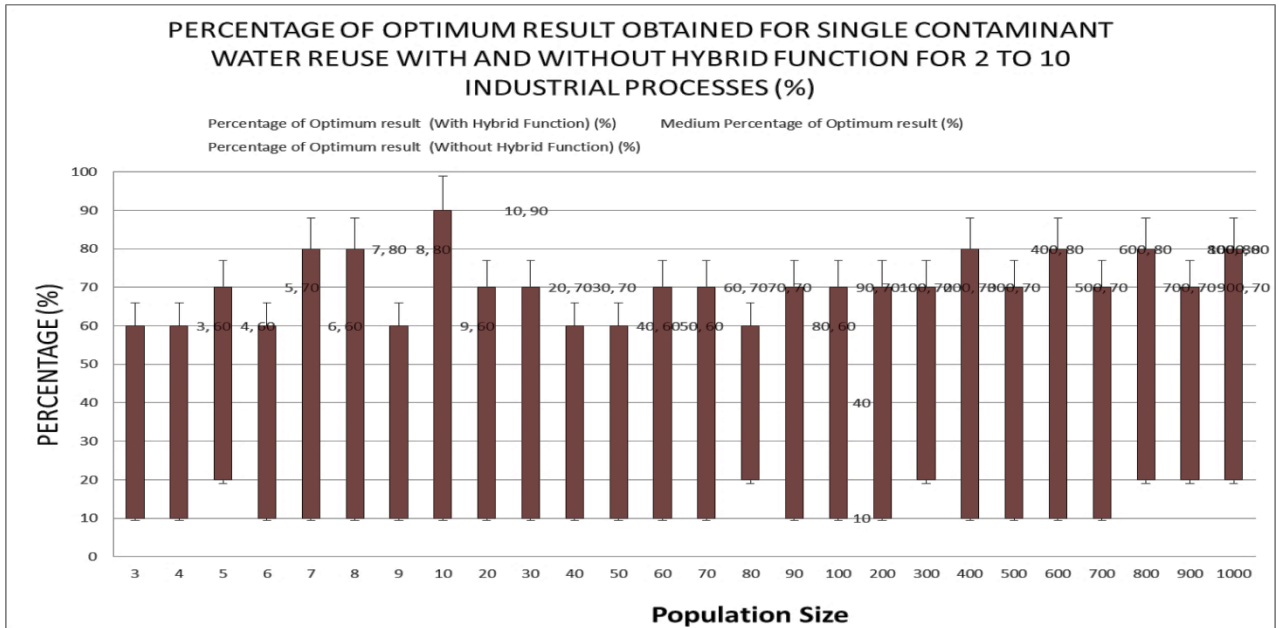


Figure 4.3: Percentage of the optimum result obtained for the solution of 2 to 10 industrial processes WAP problem using the Population Size 3-1000 with and without hybrid function included in running the GA.

The raw data of the figure 4.3 is shown in Appendix G.

The time scalability of the GA for the solution of 2 to 10 industrial processes WAP problem for Population size of 10 is shown in Figure 4.4.

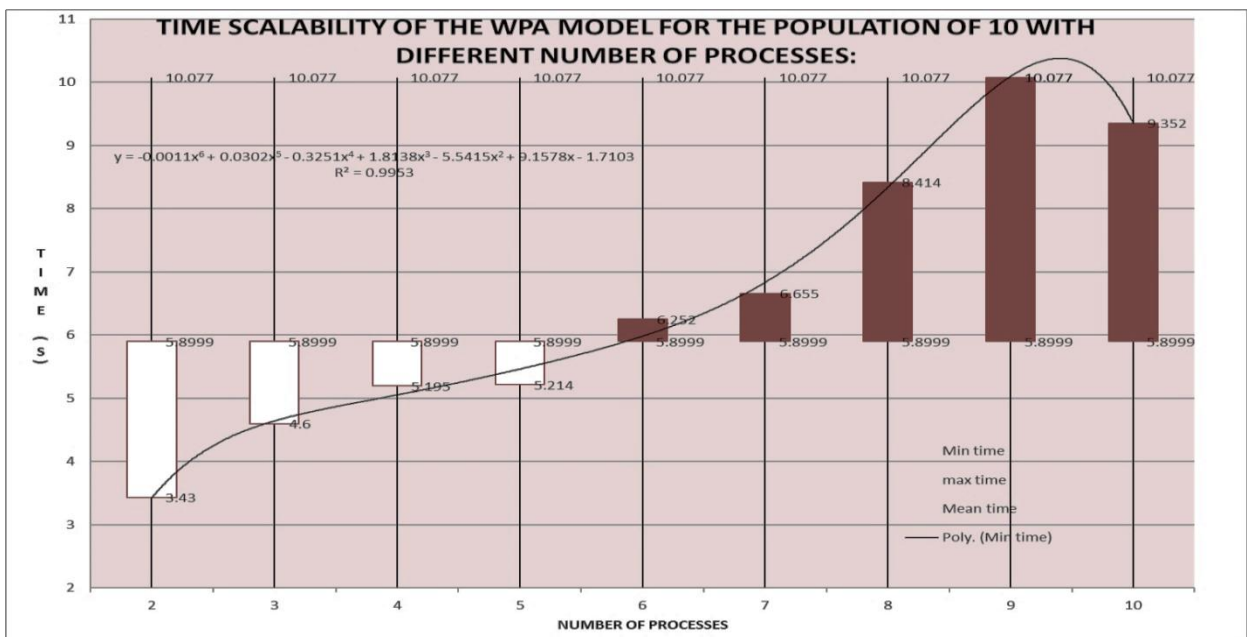


Figure 4.4: Time Scalability the GA for the solution of 2 to 10 industrial processes WAP problem for Population size of 10.

The population size of 10 produce algorithm results of the WAP problem in a short time of 3.4 to 10.1 seconds for the 2 to 10 industrial processes and 90% of the trial time the optimum result is achieved.

4.2.1 In-depth Population Size Analysis for Single Contaminant Water Reuse without Regeneration for 2 Industrial Processes

In this analysis, the population size was grouped in to the ranges of 3 to 10 instep of 1, 10 to 100 in steps of 10 and 100 to 500 in step of 100. Each population size group was re-run 10 times with different stochastic GA seeding generated automatically by the computer for 2 industrial processes WAP problem. Therefore, the algorithm was re-run 420 times for the 3 groups and the median optimum fitness function result and time taken by the computer for each population size was observed. The time taken in seconds for each run was recorded, with and without hybrid function. The statistical analysis and the Pearson's correlation coefficient of the time taken by each population size for running the model to find solution for 2 industrial processes, while considering single contaminant without regeneration with and without hybrid function was determined.

The median time taken using the population size of 3 to 10 is 3 seconds, 20 and 100 population sizes take between 4 to 12 seconds, while 200 to 500 population sizes takes around 1 to 15 minutes without hybrid function. While, with hybrid function, the median time taken using the population size of 3 to 10 is 3.5 seconds, 20 and 100 population sizes take between 4 to 13 seconds, while 200 to 500 population sizes takes around 1 to 15 minutes also.

The time Scalability of the GA for the solution of 2 industrial processes WAP problem for Population size of 3 to 100 with and without hybrid function included in running the

GA are shown in Figure 4.5 and 4.6, respectively. This shows that there is no much time variation in solving the WAP problem with or without hybrid function.

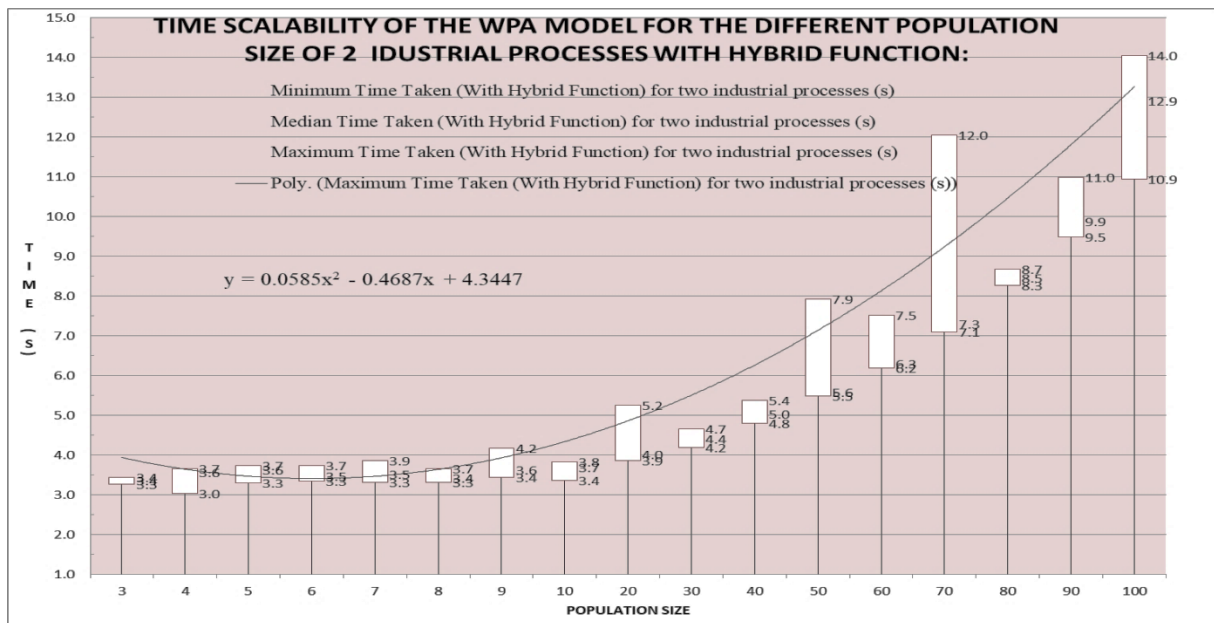


Figure 4.5: Time Scalability of the GA for the solution of 2 industrial processes WAP problem for Population size of 3 to 100 with hybrid function.

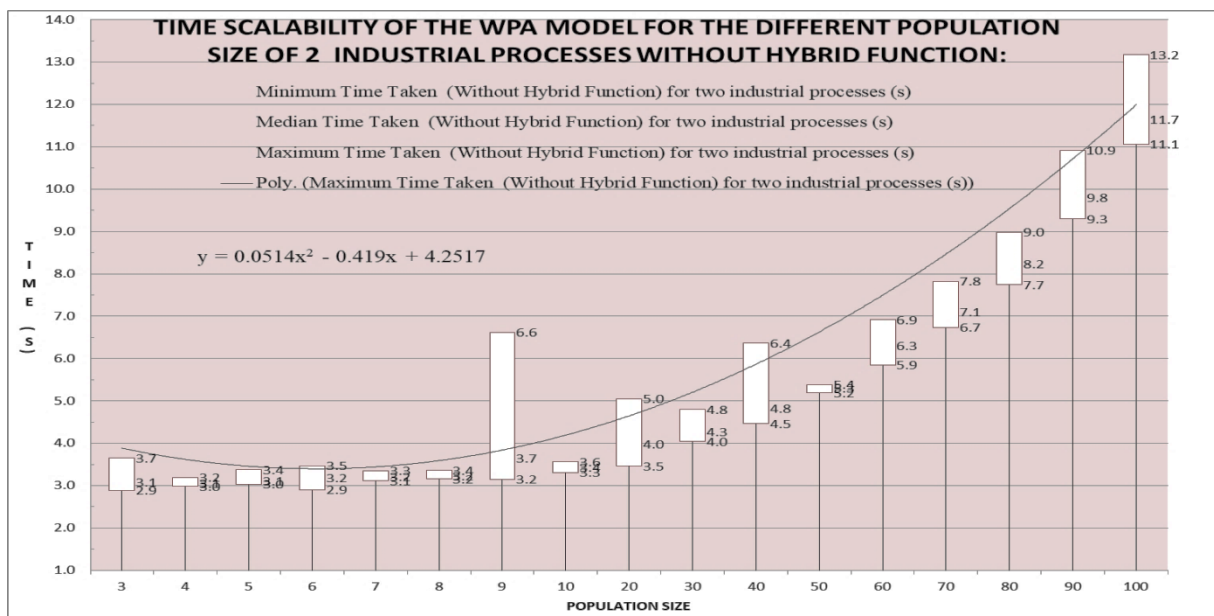


Figure 4. 6: Time Scalability of the GA for the solution of 2 industrial processes WAP problem for Population size of 3 to 100 without hybrid function.

The trend lines of the two graphs indicate a similar exponential relationship as shown in equations 4.7 and 4.8, with the Pearson's correlation coefficient of 0.98.

$$y = 0.059x^2 - 0.47x + 4.34 \dots \dots \dots (4.7)$$

$$y = 0.051x^2 - 0.42x + 4.25 \dots \dots \dots (4.8)$$

Furthermore, for the population size of 100 to 500 in step of 100 group variations used for analysis with and without hybrid function included in running the GA are shown in Figure 4.7 and 4.8, respectively. These indicate that, the median time taken for the population size range of 100 to 500 with and without hybrid function included in running the GA are similar. The trend lines of the two graphs indicate similar exponential relationship as shown in equations 4.9 and 4.10. The Pearson's correlation coefficient of the two sets of data is 0.99.

$$Y = 90.6x^2 - 300.9x + 250.5 \dots \dots \dots (4.9)$$

$$Y = 91.2x^2 - 290.3x + 236.5 \dots \dots \dots (4.10)$$

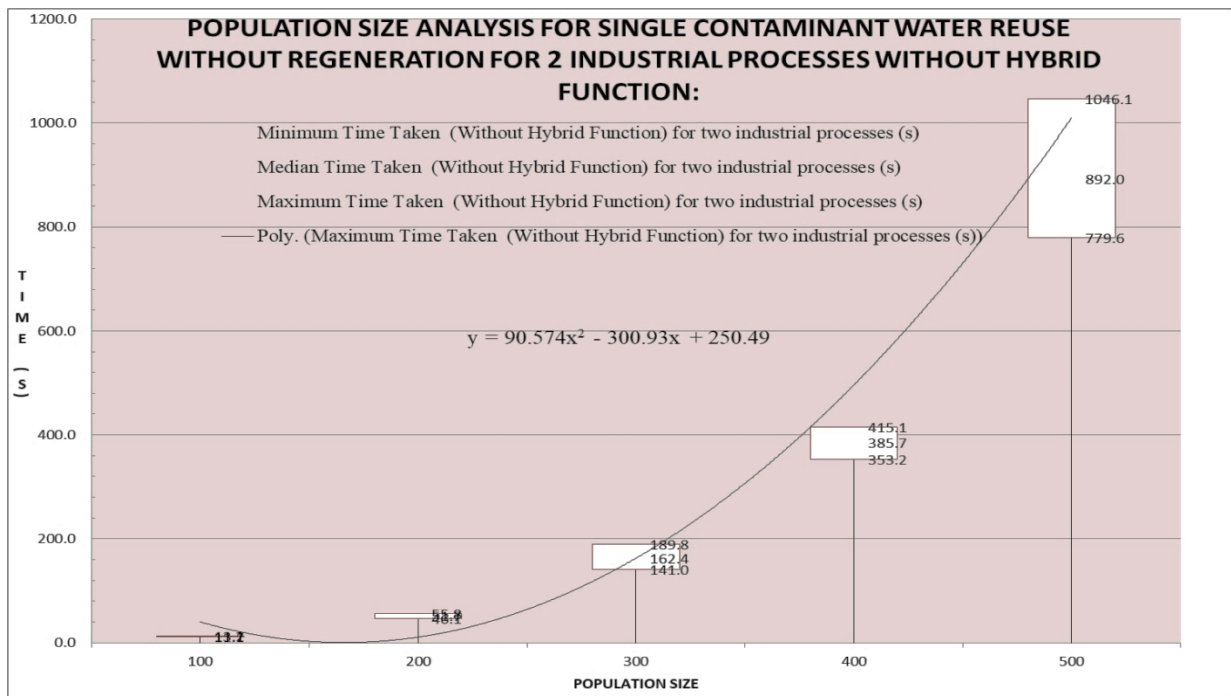


Figure 4. 7: The Median Time taken in running GA for 2 industrial processes with Population size of 100 to 500 without hybrid function.

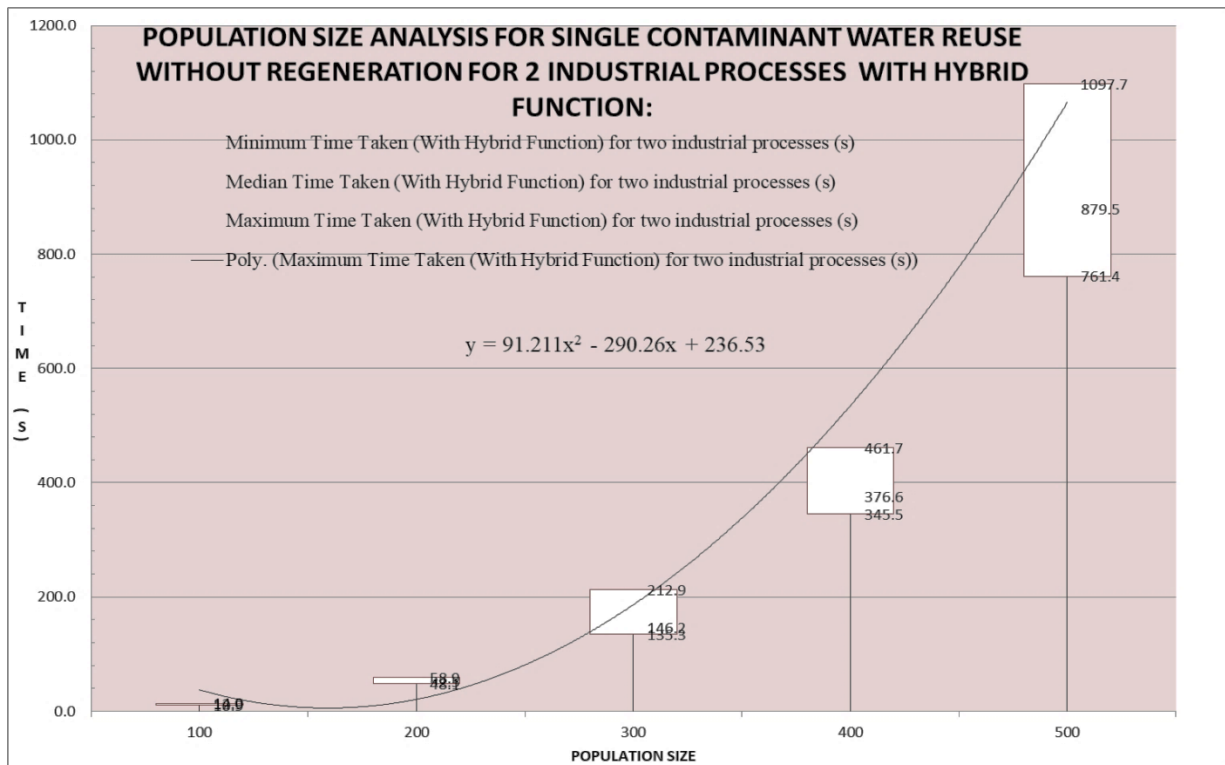


Figure 4.8: The Median Time taken in running GA for 2 industrial processes with Population size of 100 to 500 with hybrid function.

Moreover, for the comparison of getting an optimum result as reported by the literature, the percentage of number of times optimum result was obtained for two industrial process with and without hybrid function are shown in Figure 4.9. This indicates that using hybrid function assist in obtaining the optimum result for almost all the population sizes. However, running the GA for WAP model solution without hybrid function usually gets stuck in the local minimum or non-optimum result. The analysis indicates that the optimum result can be achieved in all running (100%) for the population sizes of 20, 30, 60, 70, 80, 90, 100, 300, 400 and 500 with the hybrid function. While these population sizes have 40% or less chance of achieving optimum results without hybrid function.

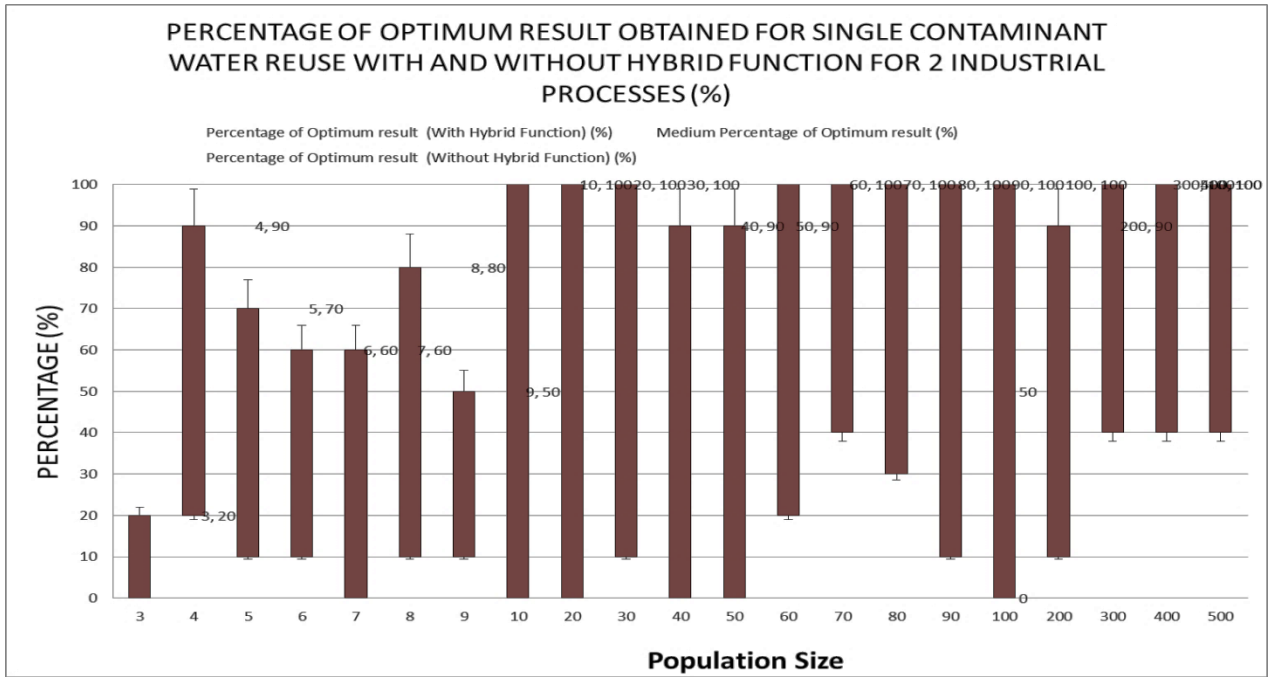


Figure 4.9: Percentage of the optimum result obtained and Population size for two industrial processes.

4.2.2 In-depth Population Size Analysis for Single Contaminant Water Reuse without Regeneration for 3 Industrial Processes

In the analysis for single contaminant water reuse without regeneration for 3 industrial processes, the population size was varied also from 3 to 10 in step of 1, 10 to 100 in steps of 10 and 100 to 500 in step of 100 as done in section 4.2.1. Each population size was re-run 10 times with different stochastic GA seeding generated automatically by the computer. Therefore, the algorithm was re-run 420 times to observe the optimum fitness function result and time taken by the computer for each population size. The time taken for each run was recorded in seconds, with and without hybrid function. The statistical analysis was conducted for the data of time taken by all the groups of population sizes. The minimum, maximum, mean, standard deviation, and variance of the time taken by different population sizes for running the model with 3 industrial processes, while considering single contaminant without regeneration was

examined. Figure 4.10 shows the Scalability of the time taken by the computer in running the GA for the solution of 3 industrial processes WAP problem with Population sizes of 3 to 100 variations without hybrid function, while Figure 4.11 shows the variations of the time taken by the computer in running the GA solution with hybrid function. The median time taken using the population size of 3 to 10 is 4 seconds, 20 to 100 population sizes take between 6 to 14 seconds, while 200 to 500 population sizes takes around 1 to 16 minutes.

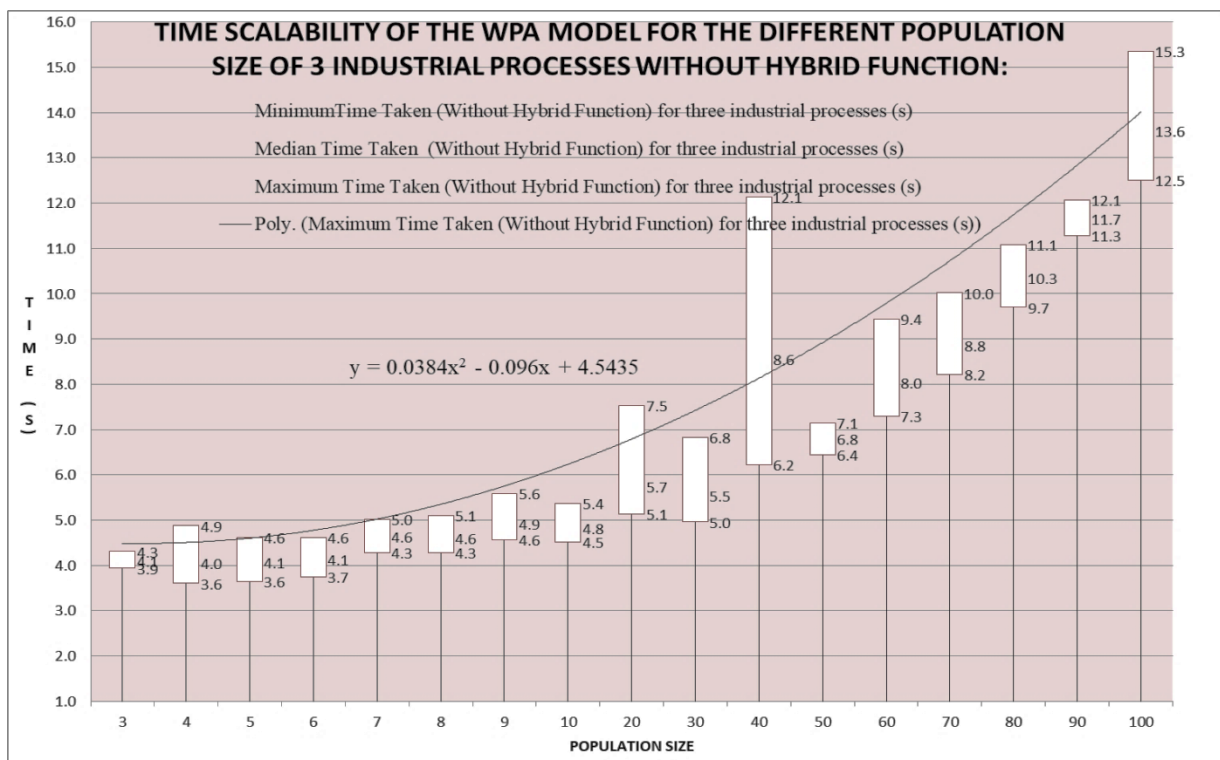


Figure 4. 10: Time Scalability of the GA for the solution of 3 industrial processes WAP problem for Population size of 3 to 100 without hybrid function.

Figure 4.10 show that there is significant difference in the median time of running the GA with WAP model for the population sizes of 3 to 100 without hybrid function. The median time taken using the population size of 3 to 10 is 5 seconds, 20 to 100 population sizes take between 6 to 15 seconds. However, there are no significant differences between the population sizes of 40, 50, 60, and 70.

Figure 4.11 also show that there is similar difference in the median time of running the GA with WAP model for the population sizes of 3 to 100 with hybrid function. However, there is no significant difference in the median time of running the GA with WAP model for the population sizes of 3 to 30 with hybrid function. But, there are little differences between the population sizes of 40 to 100. This shows that there is no time variation in solving the WAP problem with or without hybrid function for 3 industrial processes as indicated in Figure 4.10 and 4.11.

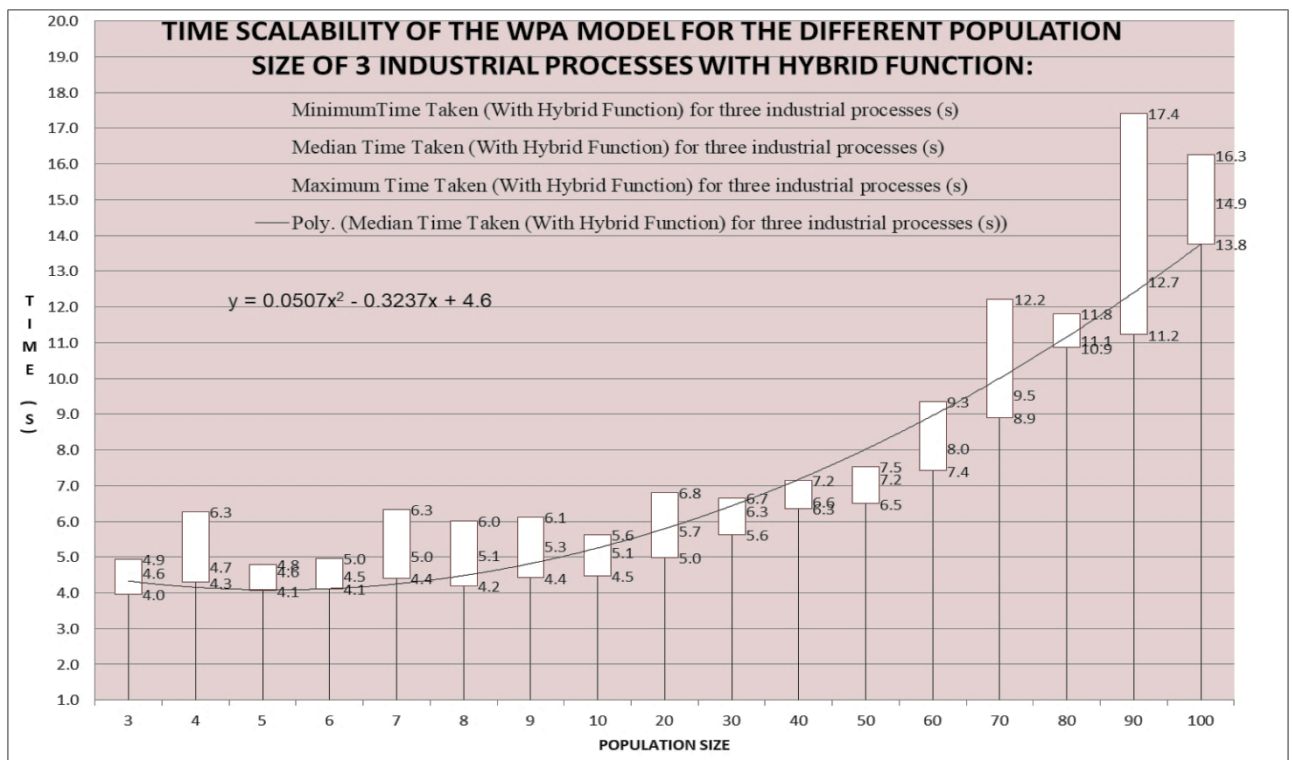


Figure 4.11: Time Scalability of the GA for the solution of 3 industrial processes WAP problem for Population size of 3 to 100 with hybrid function.

The trend line of the two graphs indicates a similar exponential relationship as shown in equation 4.11 and 4.12. The Pearson's correlation coefficient of the two sets of data is 0.98.

$$y = 0.04x^2 - 0.1x + 4.5 \dots \dots \dots (4.11)$$

$$y = 0.05x^2 - 0.3x + 4.6 \dots \dots \dots (4.12)$$

Furthermore, the median time taken for the population size range of 100 to 500 with and without hybrid function included in running the GA for the 3 industrial process are shown in Figure 4.12 and 4.13, respectively.

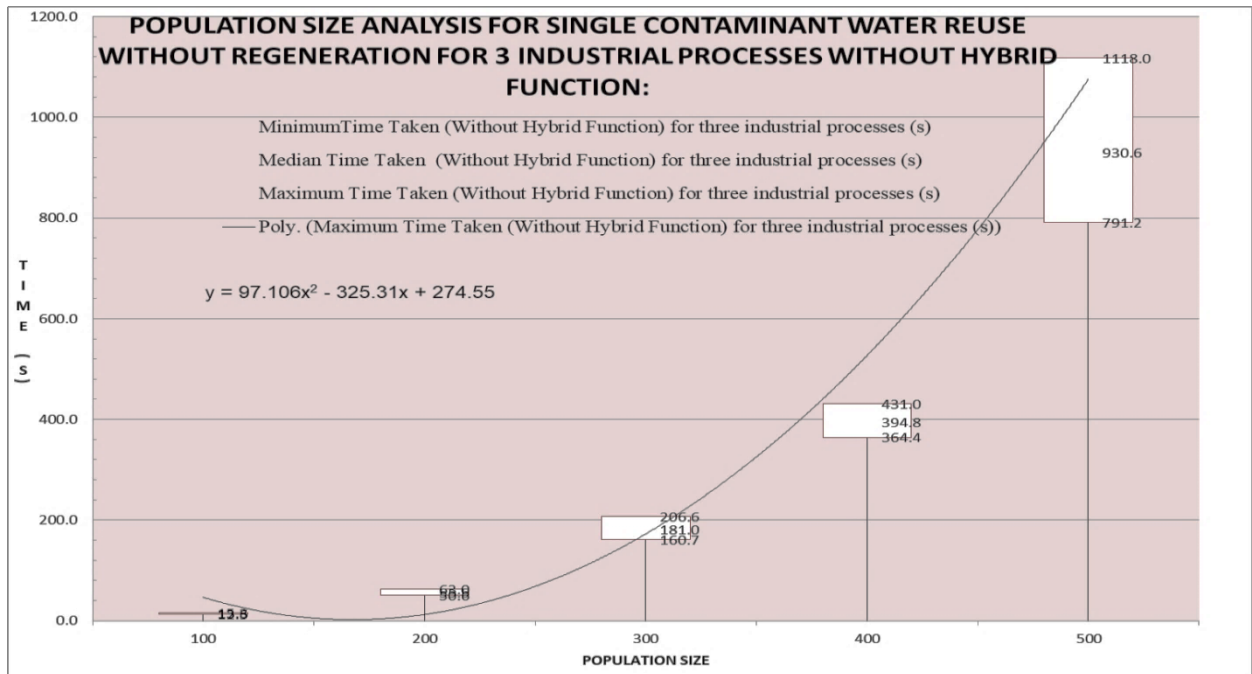


Figure 4. 12: The Median Time taken in running GA for 3 industrial processes with Population size of 100 to 500 without hybrid function.

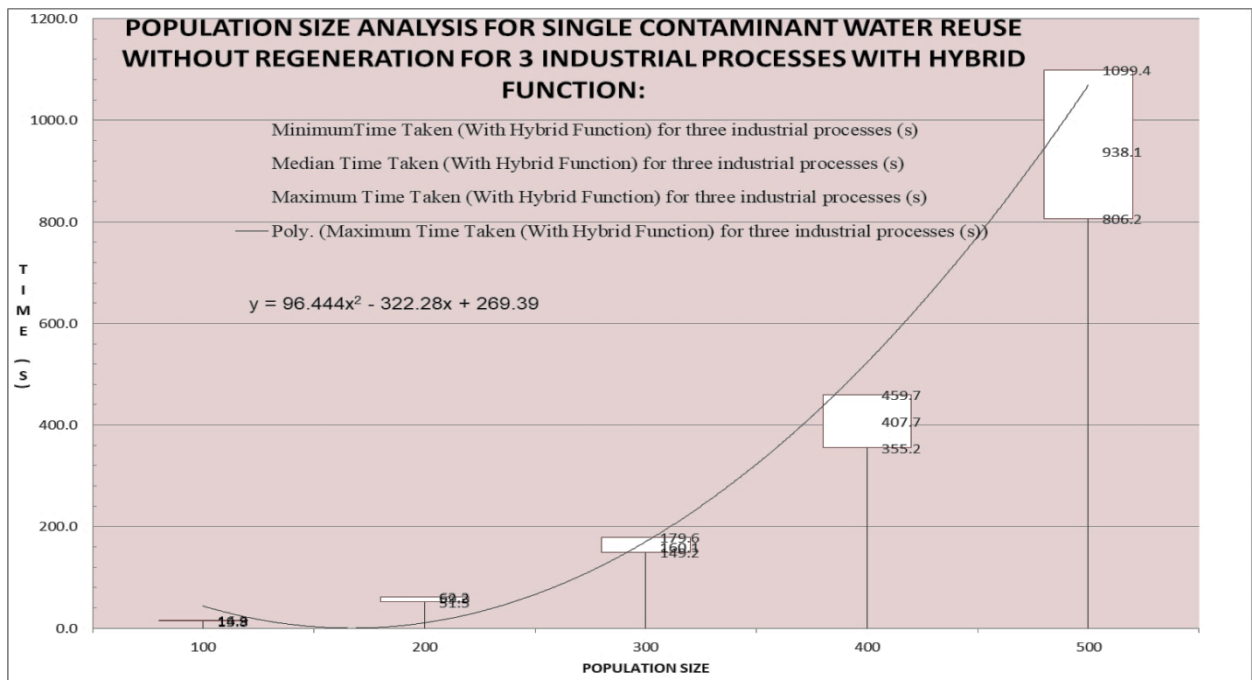


Figure 4.13: The Median Time taken in running GA for 3 industrial processes with Population size of 100 to 500 with hybrid function.

The population size of 100 to 500 in step of 100 group variations indicate that,

The trend line of the two graphs indicate a similar exponential relationship as shown in equation 4.13 and 4.14, with the Pearson's correlation coefficient of 0.99 for the median time value of with and without hybrid function.

$$y = 97.1x^2 - 325.3x + 274.6 \dots\dots\dots(4.13)$$

$$y = 96.4x^2 - 322.3x + 269.4 \dots\dots\dots(4.14)$$

The percentages of optimum result obtained for the 3 industrial processes with and without hybrid function for different population sizes are shown in Figure 4.14. This indicates that using hybrid function assist in obtaining the optimum result for almost all the population sizes. However, running the GA for WAP model solution without hybrid function usually gets stuck in the local minimum (non-optimum) result. The analysis indicates that the optimum result can be achieved in all running (100%) for all the population sizes except for the population size of 3 which has 60% with the hybrid function. While no population sizes does achieved best (optimum) result without hybrid function.

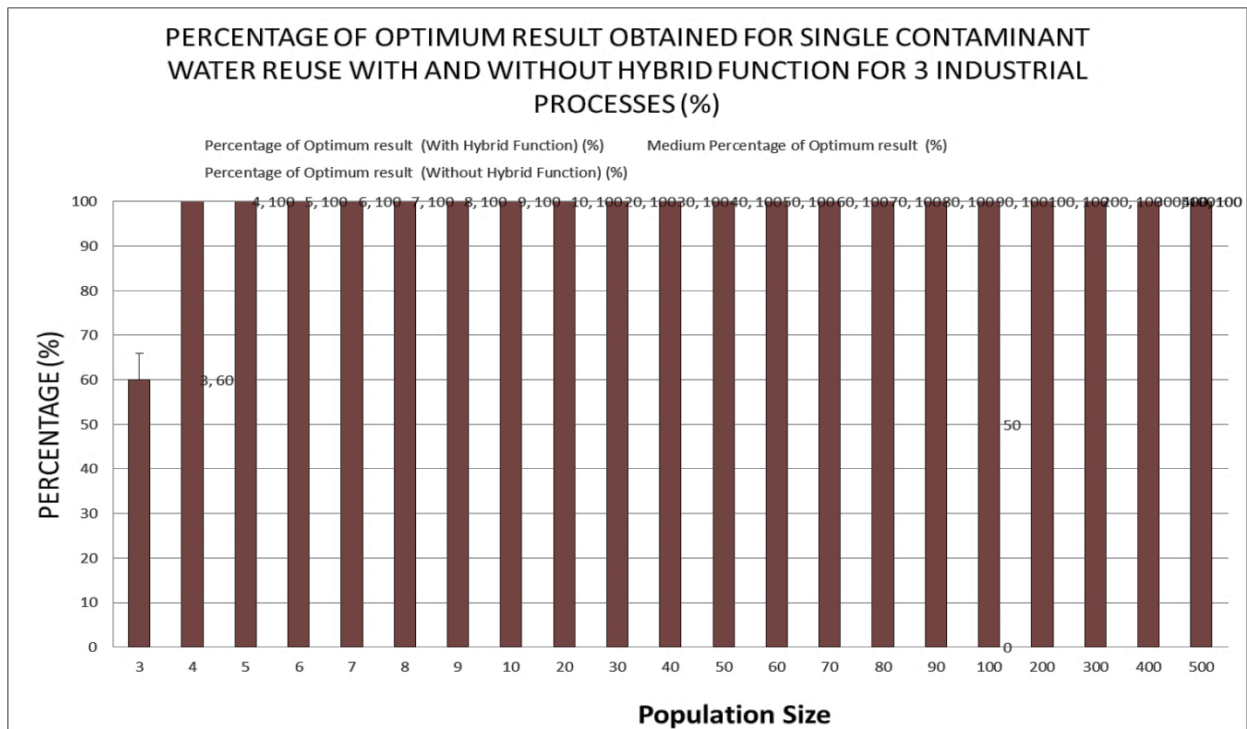


Figure 4.14: Percentage of the optimum result obtained and Population size for 3 industrial processes.

Furthermore, to make sure that the results obtained are specific to the WAP model we tried the same procedure for the different cases of water minimisation problem of different number of industrial processes from two (2) to ten (10) for single-contaminant without regeneration, each with and without hybrid function. This is to ensure that all aspects of the model results were analysed efficiently.

4.3 Conclusion

The analysis of the hybrid on the Genetic Algorithm (GA) method for solving the different Water Application Planning (WAP) problems to improve its performance in obtaining the final result was presented. The hybrid used for single-objective GA optimisation is 'fmincon'. The hybrid function was used for the analysis of the time taken for running the WAP model for different population sizes of the GA. The population sizes were varied from 3 to 1000 for the single contaminant water reuse

model that does not include regeneration for 2 to 10 industrial processes, using different examples from the literature. The median time taken for the first population size group of 3 to 10 the model runs for 6 seconds for the different number of industrial processes. For the second group 10 to 100 the model runs for the median time of 10 seconds for the population size of 10 to 60, and it runs for the median time of 15 seconds for the population size of 70 to 100. For the third group 100 to 1000, each population category exhibit different time range with clear difference.

Furthermore, an in-depth analysis of two and three industrial processes was done to ascertain the gap left in the initial analysis by considering the population sizes from 3 to 10 instep of 1, 10 to 100 in steps of 10 and 100 to 500 in step of 100 with and without hybrid function. In the analysis the trend line equations of the graphs were presented to assist in describing the time taken by the model based on the specific population size. The equations give the detail of the median time values obtained in running the algorithm.

Observation of the fitness function results for different industrial processes from 2 to 10 obtained with and without hybrid function indicates that population size of 10 gives the highest percentage of the optimum result, which is 90%. In-depth analysis of single contaminant water reuse without regeneration for 2 industrial processes fitness function results indicates that the optimum result can be achieved in all running (100%) for the population sizes of 20, 30, 60, 70, 80, 90, 100, 300,400 and 500 with the hybrid function. While these population sizes have 40% or less chance of achieving optimum results without hybrid function. While in-depth analysis of single contaminant water reuse without regeneration for 3 industrial processes fitness function results indicates that the optimum result can only be achieved with the hybrid function in all running (100%) for all the population sizes except 3 which has 60% chance.

The next chapter will analyse the mathematical application of WAP models used in optimisation of single contaminant water reuse network and the data set-up requirements for different number of industrial processes. It will also describe the procedure involved in the general equations that presents the model based on the number of processes.

CHAPTER FIVE

5.0 WATER APPLICATION PLANNING (WAP) MODEL FOR SINGLE CONTAMINANT WATER REUSE WITHOUT REGENERATION

This chapter describe the mathematical optimisation method and the data set-up requirements used in solving WAP model of single contaminant water reuse network. It also described the procedure involved in the general equation that presents the model based on the number of processes. This includes use of the problems described in the literature to show the steps and the values obtained using this research methodology. This is to guide the reader through the process of setting up WAP model optimization. Furthermore, the values of the solution obtained from the WAP model using GA with and without hybrid function were compared and the percentage errors of the values obtained without hybrid function were presented.

5.1 Introduction

The WAP model developed in this research was used to find solution for different WAP problems for Single contaminant water reuse without regeneration using GA and 'fmincon' hybrid in Matlab software. The problems were selected from the literature to validate the selected method for the solution of the WAP model. Table 5.1 shows the referenced literatures where those problems were obtained. The table shows the number of industrial processes, process type (single-contaminant), the method used by the literature in obtaining the solution and the result obtained. This will be used as a basis for the validation of the efficiency of GA with hybrid of deterministic mathematical optimization method as the selected method for the solution of WAP problem model in this research.

Table 5.1: Literature (referenced) WAP problems.

Literature (Reference)	Number of Industrial Processes	Process Type.	Method Used	Result Obtained (m ³ /h.)
Wang and Smith (1995)	2	Single Contaminant/Reuse	Mathematical programming	29.82
Mann and Liu (1999); Prakotpol and Srinophakun (2004)	3	Single Contaminant/Reuse	Mathematical programming	56.67
Wang and Smith (1994a).	4	Single Contaminant/Reuse	graphical approach	90
Mann and Liu (1999); Prakotpol and Srinophakun (2004)	5	Single Contaminant/Reuse	Mathematical programming	30
Olesen and Polley (1997)	6	Single Contaminant/Reuse	Mathematical programming	157.14
Bagajewicz <i>et al.</i> , (2002), Feng <i>et al.</i> , (2009) and Liang, and Hui, (2016)	7	Single Contaminant/Reuse	Mathematical Programming	131.2
Bagajewicz <i>et. al.</i> (2002)	8	Single Contaminant/Reuse	Mathematical programming	138.2
Bagajewic and Savelski (2001)	9	Single Contaminant/Reuse	Mathematical programming	158.1
Bagajewic and Savelski (2001); Trigueros et al. (2012)	10	Single Contaminant/Reuse	Mathematical programming	252.42

All the variables used below were defined in the list of symbols and nomenclature section of this thesis.

5.2 Single Contaminant Water Reuse without Regeneration for 2 Industrial Processes

The number of variables for 2 industrial processes can be calculated using $n^2 + n = 6$ as described in chapter two. Where n is the number of industrial processes. The variables are: freshwater, wastewater and wastewater for reuse, represented as follows: $F_1, F_2; W_1, W_2; X_{12}, X_{21}$ respectively.

The fitness function is the sum of fresh water flow rates at the entrance of all water using processes as shown in equation 5.1.

$$F = \text{Min} \sum_{i=1}^3 F_i \dots \dots \dots (5.1a)$$

$$F = F_1 + F_2 \dots \dots \dots (5.1b)$$

Equation 5.2 and 5.3 present the Linear Constraints functions of the water and contaminant mass balance as follows:

1. The constraint of the water mass balance of all process

$$F_i + \sum_{j \neq i} X_{i,j} - W_i - \sum_{j \neq i} X_{j,i} = 0 \dots \dots \dots (5.2a)$$

$$F_1 + X_{1,2} - W_1 - X_{2,1} = 0 \dots \dots \dots (5.2b)$$

$$F_2 + X_{2,1} - W_2 - X_{1,2} = 0 \dots \dots \dots (5.2c)$$

2. The constraint of the contaminant mass balance of all processes:

$$\sum_{j \neq i} C_{j,out} X_{i,j} + \Delta M_i - C_{i,out} \left(W_i + \sum_{j \neq i} X_{j,i} \right) = 0 \dots \dots \dots (5.3a)$$

$$C_{2,out} X_{1,2} + \Delta M_1 - C_{1,out} (W_1 + X_{2,1}) = 0 \dots \dots \dots (5.3b)$$

$$C_{1,out} X_{2,1} + \Delta M_2 - C_{2,out} (W_2 + X_{1,2}) = 0 \dots \dots \dots (5.3c)$$

3. The nonlinear constraint function of the maximum contaminant inlet concentration are represented in equation 5.4 as follows:

$$C_{j,in} = \frac{\sum_{j \neq i} C_{j,out} X_{i,j}}{\sum_{j \neq i} X_{i,j} + F_i} \leq C_{i,in}^{max} \dots \dots \dots (5.4a)$$

$$C_{2,out} = \frac{C_{2,out} X_{1,2}}{F_1 + X_{1,2}} \leq C_{1,in}^{max} \dots \dots \dots (5.4b)$$

$$C_{1,out} = \frac{C_{1,out} X_{2,1}}{F_2 + X_{2,1}} \leq C_{2,in}^{max} \dots \dots \dots (5.4c)$$

The process of expansion of fitness functions for the number of industrial processes.

5.2.1 Test Problem: Input Rough Limiting Process Data for 2 industrial processes

The rough limiting process data refers to maximum contaminant concentration allowed in and minimum contaminant concentration produced out in ppm and mass load in kg/hr produced by a given industrial process. These are the values used in constraint equations to determine the minimum fresh water requirement of a given industrial process.

The rough limiting process data for water minimisation of a specialty chemical production industry having 2 industrial processes that requires freshwater, obtained from Wang and Smith (1995) are shown in Table 5.2. The industry will require 30.0m³/h of fresh water to operate without optimization.

The expected freshwater to be used in the analysis is assumed to have zero impurity. The consequence of this assumption is that there is need for treating water for initial input to the processes. The rough limiting process data have mass load, concentration allowed in and produced out for each industrial process. This data is used to optimise the freshwater requirement of the industry. To determine the minimum flowrate of freshwater for all the industrial processes to run efficiently.

Table 5.2: Rough Limiting Process Data for 2 industrial processes

Rough Limiting Process Data			
Operation	Mass Load ΔM (kg/hr)	Contaminant Concentration (Allowed in) C^{lim}_{in} (ppm)	Contaminant Concentration (Produced out) C^{lim}_{out} (ppm)
1	0.5	50	100
2	1	0	50

5.2.2 Representation of Single Contaminant Water Reuse without Regeneration

in Matlab for 2 industrial processes

The fitness function in equation 5.1b is vectorised and represented in Matlab as

follows:

```
Function f=FRW(x)
% return the sum of all the values of fresh water x
f = x(:,1) + x(:,2);
End
```

In matlab software the linear equalities have the form $A_{eq} \cdot x = beq$, which represents m equations with n -component vector x , while, linear inequality constraints have the form $A \cdot x \leq b$. Where, A is m -by- n , matrix with m constraints on a variable x with n components. The linear equality constraints are represented in the A_{eq} and beq arguments. The linear constraints equations in equations 5.2a to 5.3c are represented in Matlab software as the matrix and vector of equalities (A_{eq} and beq) using the coefficient of the variables as follows:

```
Aeq = [1    0    -1    0    1    -1; 0    1    0    -1    -1    1;
       0    0   -100    0    50   -100; 0    0    0   -50   -50   100]
beq = [0;0;-500;-1000]
```

The matrix and vector of inequalities are not available in the constraints of WAP problem, therefore (A and b) are represented as empty set as follows: $A = []$, $b = []$,

The vector for lower and upper bounds (LB and UB) are represented with the set of lowest and highest value of outcome of each point as follows:

```
Lower bounds: LB = [0, 0, 0, 0, 0, 0]
Upper bounds: UB = [inf,inf,inf,inf,inf,inf]
```

Where inf , in the upper bound represent an assumption of infinity limit, The consequence of this assumption is that it allows the search space for the GA to be relatively imprecise and limitless about initial result. This will lead to obtaining an optimum result within the shortest time possible.

The Nonlinear Constraints functions are vectorised and represented in Matlab as follows:

```
Function [c,ceq] = Constraints_FRW0(x)
% return the values of the nonlinear constraints
C1out=0; C2out=50; C1in=0; C2in=0;
C = [(( C2out*x(:,5))/(x(:,1)+x(:,6)))-C1in;
      (( C1out*x(:,6))/(x(:,2)+x(:,5)))-C2in)];
Ceq = [];
End
```

The syntax for obtaining the solution in Matlab is as follows:

x = ga(fitnessfcn,nvars,A,b,Aeq,beq,LB,UB,nonlcon,options)

Where x is the local minimum values of the fitness function, ga is the protocol of the genetic algorithm code, fitnessfcn is the fitness function to be minimised, nvars is the dimension or number of variables in the WAP problem, A, b are inequality constraint equations of the problem, Aeq, beq, are equality constraint of the problem, LB is the lower bounds of the search space, UB is the upper bounds of the search space, nonlcon is the nonlinear constraints functions of the problem, options refers to different options used in the GA process like crossover , mutation and plot functions for displaying the graphs.

This will search for the possible solution of the problem and display the result as vector when the stopping criterion is met.

5.2.3 The result of Single Contaminant Water Reuse without Regeneration in Matlab for 2 industrial processes

The set of functions, genetic parameters and genetic operators used by GA for diagnostic analysis of the problem are shown in Table 5.3.

Table 5.3: Set of functions, Genetic parameters and Operators for GA to solve 2 industrial processes WAP problem

S/No.	Genetic Parameters/ Operators	Value /method
1.	Fitness function	@FRW0
2.	Number of variables	6
3.	Inequality constraints	0
4.	Equality constraints	4
5.	nonlinear constraint	@Constraints_FRW0'
6.	Population Size	10
7.	Crossover Fraction	0.8
8.	Selection Function	@selection uniform
9.	Crossover Function	@crossover heuristic 1.2
10.	Mutation Function	@ mutation adaptfeasible [] []
11.	Hybrid Function	@fmincon []
12.	Display	'diagnose'
13.	graphical display (Plot Function)	@gaplotbestindiv

Optimization come to termination when the average change in the fitness value is less than Function Tolerance (which is the difference between the function value at the previous best point and function value at the current best point of the fitness function) $1e-3$ (0.001), and constraint violation is less than Constraint Tolerance (which is the maximum of the values of all constraint functions at the current point). This result is shown in Table 5.4. The generation indicate the number of times the genetic algorithm solver performs some intermediate calculations that eventually lead to the local minimum. The f-count is the number of function evaluations that the GA solver took to converge to a local solution. The obtained result is $30.0\text{m}^3/\text{h}$ which is indicated in column 3 as the best-f(x) for the first 3 generations. The maximum constraints value in column 4 indicates the values that satisfy the constraints and the stall-generation gives the number of times the minimum of generations are computed regardless of the convergence criteria.

Table 5.4: End of diagnostic information for the solution of 2 processes

Generation	f-count	Best - f(x)	Max - constraint	Stall - Generations
1	570	30	0	0
2	1090	30	0	1
3	1610	30	0	2
4	10600	25.0032	8.28e 05	3
5	21000	25.0118	1.536e 08	4
6	31400	25.0118	2.02e 11	5

Switching to the hybrid optimisation algorithm (fmincon) at regeneration 4 leads to Local minimum within the last region, which is the optimum result of the minimum fresh water with constraints satisfied. The final result of $25,0\text{m}^3/\text{h}$ is displayed as shown in the generation 5 and 6 of Table 5.4.

Table 5.5 shows the solution of the individual variables in the problem after running the GA analysis. This indicates that the variable number 1 (F_1) has the value of $5\text{ m}^3/\text{h}$,

number 2 (F_2) has value of 20.0 m³/h, number 3 (W_1) has value of 10 m³/h, number 4 (W_2) has the value of 15.0 m³/h, number 5 (X_{12}) has value of 0.0 m³/h and number 6 (X_{21}) has value of 5.0 m³/h, The variable number 6 (X_{21}) means that 5.0 m³/h of wastewater can be reused from process number 1 by process number 2.

Table 5. 5: Solution of Single Contaminant Water Reuse without Regeneration for 2 industrial processes in Matlab.

F_1	F_2	W_1	W_2	X_{12}	X_{21}
5.0	20.0	10.0	15.0	0.0	5.0

Table 5.6 described the obtained result, indicating that the minimum total freshwater required by the industry is 25m³/h, 5m³/h for process 1 and 20m³/h for process 2. There is reuse of 5.0 m³/h of wastewater by process number 1 from process number 2 in the industry. Moreover, the maximum contaminant level of 50ppm produced by process 2 is allowed to be reused by process 1 as indicated on Table 5.2.

Table 5.6: End of diagnostic solution of the problem corresponding to Figure solution of 2 industrial processes.

Process Number	Type of water used by the process	Fresh water intake(m ³ /h)	Wastewater reuse (m ³ /h)	Contaminant Concentration (Allowed in) C_{in}^{lim} (ppm)	Contaminant Concentration (Produced out) C_{out}^{lim} (ppm)
1	Freshwater and wastewater	5.0	5.0	50	100
2	Freshwater only	20.0	0.0	0	50
Total Flowrate (m ³ /h)		25.0	5.0		

Superstructure Schematic Network:

The superstructure representation of the solution is shown in Figure 5.1, with freshwater value of 25.0m³/h as the input and the same wastewater value as the output.

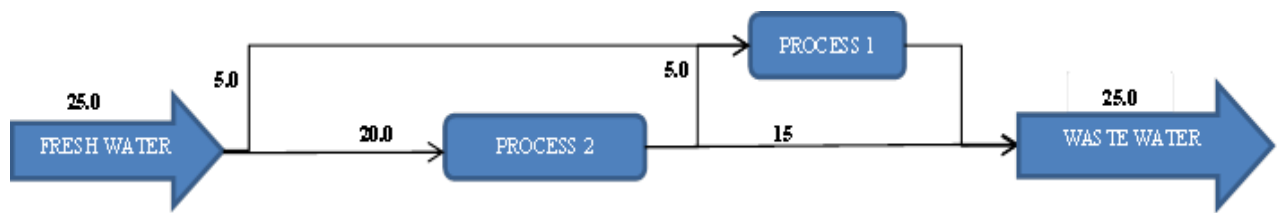


Figure 5.1: The diagrammatical Superstructure representation of the solution of 2 industrial processes.

Wang and Smith (1995), proposed a design rules of loop breaking technique which allow flowrate constraints to be met, which showed how the above problem can be solved with the constraints of the flowrate used for each process. However, the proposed method by Wang and Smith (1995) achieved an optimised value of 29.82m³/h which is higher than the value of 25.0m³/h obtained from this research method. Their method is also difficult and complex to implement for large systems due to their proposed design procedure. The difficulty stems from the fact that at each step the method requires new set of criterion. To overcome this difficulty, the method used in this work proposed a simplified design procedure for single contaminant that addressed the optimal allocation of fresh water in combination with the distribution of quality of the wastewater that is allocated to each process. For the computational time of the above problem, GAs spends a very short time in solving the problem. It takes 3.4 seconds without hybrid function and 3.7 seconds with hybrid function to obtain the optimum result. So, this method is superior to other methods in asphyxiating the deficiency of taking long time to solve WAP problem as observed.

5.2.4 The expansion of the equations of Single Contaminant Water Reuse without Regeneration for different number of industrial processes

The expansion of equation 5.1 to 5.4 for the different number of industrial processes is as follows:

The symbol F in equation 5.1 represents flow rate and the subscript “i” in all the equations denotes the number of processes that takes freshwater and j represents the subsequent processes that accept wastewater from any other process. All the values of i are allocated to the F from 1 to i for equation 5.1 as the number of industrial processes to be analysed.

In equation 5.2 of the constraint of the water mass balance of all process, the additional symbols of X and W represent all the possible combination of wastewater reuse from one process to the other and wastewater produced by each process, respectively. This equation is formed by varying the i and j values depending on all the possible combinations of i and j with the exception of $i = j$ for all the parameters in the equation. This means that the wastewater produced by one operation does not re-enter the operation where it was emitted. This leads to the restriction of reusing wastewater the same industrial process.

The constraint of the contaminant mass balance of all processes presented in equation 5.3 has additional symbols C and M which denote the contaminants concentration and the mass load, respectively. The subscript “out” refers to the outlet condition of the contaminant. This equation is formed by varying the value of i and j for different number of industrial processes as described above.

The nonlinear constraint function of the maximum contaminant inlet concentration presented in equation 5.4 has additional subscript. “in” and superscript max on the symbol C , These denote the inlet condition and maximum allowable limit of the contaminant for each industrial process, respectively. This equation is also formed by varying the value of i and j for different number of industrial processes as described above. The full expansion of all the equations 5.1 to 5.4 for 3 to 10 industrial processes are shown in in Appendix B1 to B8

5.3 Single Contaminant Water Reuse without Regeneration for 3 Industrial Processes

The number of variables for 3 industrial processes can be determined using $n^2 + n = 12$, as described in chapter 2. The variables are freshwater, wastewater and wastewater for reuse, represented as: $F_1, F_2, F_3, W_1, W_2, W_3; X_{1,2}, X_{1,3}, X_{2,3}, X_{2,1}, X_{3,1}, X_{3,2}$ respectively.

5.3.1 Test Problem: Input Limiting Process Data for 3 processes

The limiting data for water minimisation for a specialty chemical production industry having 3 industrial processes was also obtained from Mann and Liu (1999) and Prakotpol and Srinophakun (2004). The rough limiting process data for mass load, contaminant concentration allowed in and produced out are shown in Table 5.7. The expected freshwater to be used in this case was assumed to have zero impurity. This data was used to determine the minimum flowrate of freshwater and wastewater for the 3 industrial processes.

Table 5.7: Rough Limiting Process Data for 3 industrial processes

Rough Limiting Process Data			
Operation	Mass Load ΔM (kg/hr)	Contaminant Concentration (Allowed in) C_{in}^{lim} (ppm)	Contaminant Concentration (Produced out) C_{out}^{lim} (ppm)
1	3.75	0	75
2	1	50	100
3	1	75	125

5.3.2 Representation of Single Contaminant Water Reuse without Regeneration in Matlab for 3 industrial processes

The fitness function is vectorised and the linear constraints equations in equations 5.6a to 5.7d are represented in Matlab software as the matrix and vector of equalities (Aeq and beq) using the coefficient of their variables. The matrix and vector of

inequalities are not available in the constraints, therefore (A and b) are represented as empty set as follows: $A = []$, $b = []$.

The vector for lower and upper bounds (LB and UB) are represented with the set of lowest and highest value of outcome of each point. The nonlinear constraints functions are vectorised and represented in Matlab as described in appendix C1.

The Matlab code for obtaining the solution in Matlab is presented in appendix C1.

This will search for the possible solution of the problem and display the result as vector when the stopping criteria are met.

5.3.3 The result of Single Contaminant Water Reuse without Regeneration in Matlab for 3 industrial processes

The set of functions, genetic parameters and genetic operators used by GA for diagnostic analysis of the problem are as shown in Table 5.3. The differences are Fitness function is @FRW with 12 number of variables, 6 equality constraints and '@Constraints_FRW' as the nonlinear constraint function.

Optimization comes to termination when the average change in the fitness value is less than Function Tolerance and constraint violation is less than Constraint Tolerance. The obtained result at the termination is $59.95\text{m}^3/\text{h}$.

Switching to the hybrid optimization algorithm (fmincon) leads to Local minimum within the last region, which is the optimum result if Constraints are satisfied. The final result is displayed as shown in Table 5.8. The f-count is the number of function evaluations that the GA solver took to converge to a local solution. The obtained result is indicated in column 3 as the best-f(x) for the first 2 generations. The maximum constraints value in column 4 indicates the values that satisfy the constraints and the stall-generation gives the number of times the minimum of generations are computed regardless of the convergence criteria.

Table 5.8: End of diagnostic information for the solution of 3 industrial processes

Generation	f-count	Best - f(x)	Max - constraint	Stall - Generations
1	572	59.9556	2.359e-15	0
2	1092	59.9556	2.359e-15	1
3	1662	56.7324	4.472e-16	0
4	2182	56.7324	4.472e-16	0

Table 5.9 present the individual values of each variable after the analysis.

Table 5.9: End of diagnostic solution of 3 industrial processes

F ₁	F ₂	F ₃	W ₁	W ₂	W ₃	X ₁₂	X ₁₃	X ₂₃	X ₂₁	X ₃₁	X ₃₂
50.0	6.7	0.0	16.7	20.0	20.0	0.0	0.0	0.0	13.3	20.0	0.0

Solution of the problem corresponding to the diagrammatical Superstructure representation of the solution is shown in Table 5.10. The obtained result, indicates that the minimum total freshwater required by the industry is 56.7m³/h, 50m³/h for process 1 (F₁) and 6.7m³/h for process 2 (F₂). While, process 2 reuse 13.3m³/h additional wastewater and process 3 (F₃) reuse 20 m³/h of wastewater all from process 1.

Table 5.10: End of diagnostic solution of the problem corresponding to Figure solution of 3 industrial processes.

Process Number	Type of water used by the process	Fresh water intake (m ³ /h)	Wastewater reuse (m ³ /h)	Contaminant Concentration (Allowed in) C ^{lim} _{in} (ppm)	Contaminant Concentration (Produced out) C ^{lim} _{out} (ppm)
1	Freshwater only	50.0	0.0	0	75
2	Fresh & wastewater	6.7	13.3	50	100
3	Terminal wastewater	0.0	20.0	75	125
Total Flowrate (m ³ /h)		56.7	33.3		

Superstructure Schematic Network

The superstructure schematic MATLAB optimum result for 3 industrial processes WAP problem is shown in figure 5.2

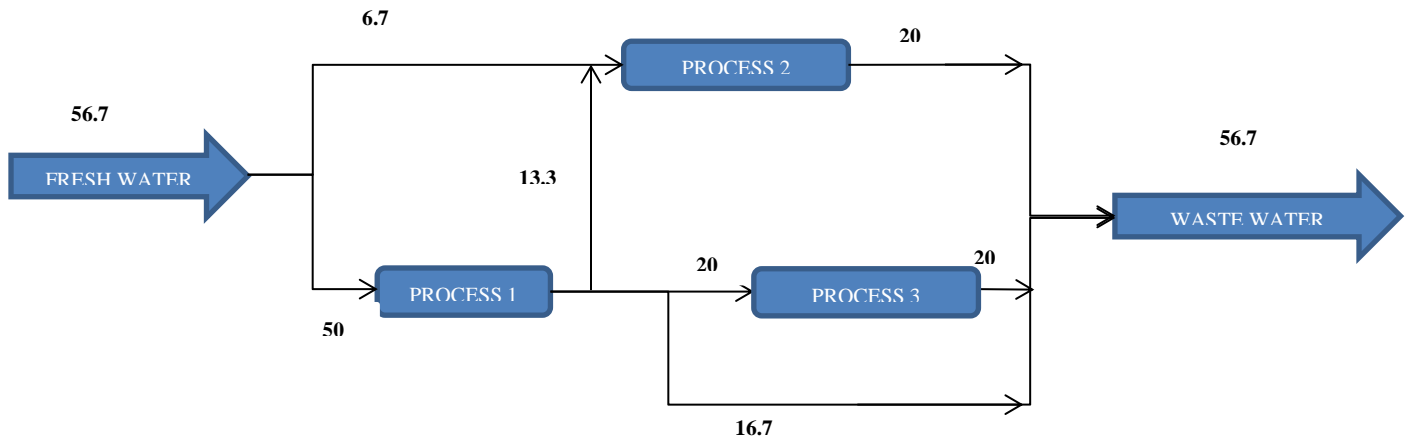


Figure 5.2: The diagrammatical Superstructure representation of the solution of 3 industrial processes.

Mann and Liu (1999) and Prakotpol and Srinophakun (2004) obtained a value of $56.67\text{m}^3/\text{h}$ as the optimum result. However, the value obtained by the method used in this research is approximately equal to their value. However, this research method takes a very short computational time in solving the above problem. It takes 4.8 seconds without hybrid function and 5.1 seconds with hybrid function to obtain the optimum result.

5.4: Single Contaminant Water Reuse without Regeneration for 4 industrial Processes

The number of variables as described in chapter two for 4 industrial processes is $n^2+n=20$. The variables are freshwater, wastewater and wastewater for reuse, represented as follows: $F_1, F_2, F_3, F_4, W_1, W_2, W_3, W_4, X_{12}, X_{13}, X_{14}, X_{23}, X_{24}, X_{34}, X_{21}, X_{31}, X_{32}, X_{41}, X_{42}, X_{43}$, respectively.

5.4.1 Test Problem: Input Limiting Process Data for 4 industrial processes

The limiting data for water minimisation for a specialty chemical production industry having 4 industrial processes was obtained from Savelski and Bagajewicz (2000) in their paper titled 'Algorithmic procedure to design water utilization systems featuring a single contaminant in process plants' also used by Gomes *et. al.*, (2007). The rough limiting process data for mass load, contaminant concentration allowed in and produced out are shown in Table 5.11. The expected freshwater to be used in this case was assumed to have zero impurity. This data was used to determine the minimum flowrate of freshwater and wastewater for the 4 industrial processes.

Table5. 11: Rough Limiting Process Data for 4 Industrial processes

Rough Limiting Process Data			
Operation	Mass Load ΔM (kg/hr)	Contaminant Concentration (Allowed in) $C^{\text{lim}}_{\text{in}}$ (ppm)	Contaminant Concentration (Produced out) $C^{\text{lim}}_{\text{out}}$ (ppm)
1	2	0	100
2	5	50	100
3	30	50	800
4	4	400	800

5.4.2: Representation of Single Contaminant Water Reuse without Regeneration in Matlab for 4 industrial processes

The fitness function is vectorised and represented in Matlab as shown in appendix C2. The linear constraints equations in equations 5.10a to 5.11e are represented in Matlab software as the matrix and vector of equalities (Aeq and beq) using the coefficient of the variables.

The matrix and vector of inequalities are not available in the constraints, therefore (A and b) are represented as empty set as follows: $A = []$, $b = []$. The vector for lower and upper bounds (LB and UB) are represented with the set of lowest and highest value of outcome of each point. The Nonlinear Constraints functions are vectorised and represented in Matlab as shown in appendix C2.

The code for obtaining the solution in Matlab is shown in appendix C2. This will search for the possible solution of the problem and display the result as vector when the stopping criteria are met.

5.4.3 The result of Single Contaminant Water Reuse without Regeneration in Matlab for 4 industrial processes

The set of functions, genetic parameters and genetic operators used by GA for diagnostic analysis of the problem are as shown in Table 5.3. The differences are Fitness function is @FRW2 with 20 number of variables, 8 Equality constraints and '@Constraints_FRW2' as the nonlinear constraint function .

Optimization comes to termination when the average change in the fitness value is less than Function Tolerance and constraint violation is less than Constraint Tolerance. The obtained result was $92.5\text{m}^3/\text{h}$.

Switching to the hybrid optimization algorithm (fmincon) leads to Local minimum within the last region, which is the optimum result if Constraints are satisfied. The final result

is displayed as shown in Table 5.12. The f-count is the number of function evaluations that the GA solver took to converge to a local solution. The obtained result is indicated in column 3 as the best-f(x) for the first 2 generations. The maximum constraints value in column 4 indicates the values that satisfy the constraints and the stall-generation gives the number of times the minimum of generations are computed regardless of the convergence criteria.

Table 5.1: End of diagnostic information for the solution of 4 industrial processes

Generation	f-count	Best - f(x)	Max - constraint	Stall - Generations
1	10732	93.3071	7.568e-06	0
2	21132	92.5071	2.46e-06	0
3	31532	91.3071	2.499e-06	1
4	128532	90.307	9.941e-05	2
5	211732	90.1066	0.000113	3

Table 5.13 present the individual values of each variable after the analysis.

Table 5.2: End of diagnostic solution of four industrial processes.

F ₁	F ₂	F ₃	F ₄	W ₁	W ₂	W ₃	W ₄	X ₂₁	X ₃₁	X ₄₁	X ₃₂	X ₄₂	X ₄₃	X ₁₂	X ₁₃	X ₂₃	X ₁₄	X ₂₄	X ₃₄
20	50.1	20	0	0.0	40.1	40.0	10.0	0	0	0	0	0	0	0	20.0	0	0	10.0	0

Solution of the problem corresponding to the diagrammatical Superstructure representation of the solution is shown in Table 5.14. It described the obtained result, indicating that the minimum total freshwater required by the industry is 90.1m³/h, 20m³/h for process 1 (F₁), 50m³/h for process 2 (F₂) and 20.0m³/h for process 3 (F₃). While, process 3 and 4 reuse 19.9m³/h and 3.7 m³/h of wastewater respectively, from process 1.

Table 5.3: End of diagnostic solution of the problem corresponding to Figure solution of four industrial processes.

Process Number	Type of water used by the process	Fresh water intake (m ³ /h)	Wastewater reuse (m ³ /h)	Contaminant Concentration (Allowed in) C ^{lim} _{in} (ppm)	Contaminant Concentration (Produced out) C ^{lim} _{out} (ppm)
1	Freshwater only	20.0	0.0	0	100
2	Freshwater only	50.1	0.0	50	100
3	Fresh & wastewater	20.0	20.0	50	800
4	Wastewater only	0.0	10.0	400	800
Total Flowrate (m ³ /h)		90.1	30.0		

Superstructure Schematic Network

The superstructure schematic MATLAB result network configuration for 4 industrial processes optimum water-using network of the solution is shown in figure 5.3.

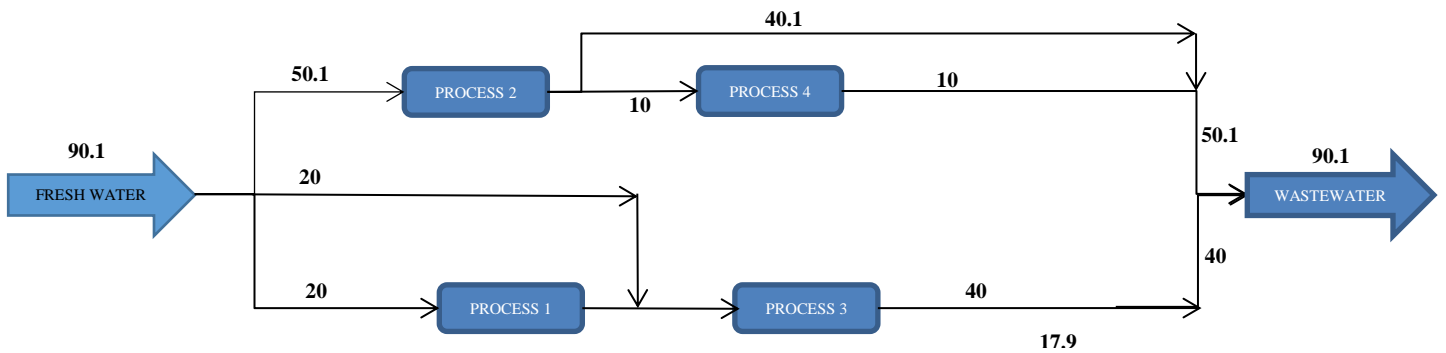


Figure 5.3: The diagrammatical Superstructure representation of the solution of 4 industrial processes.

The minimum flowrate reported in Wang and Smith (1994) is 90.0m³/h obtained using a method of loops breaking with several simplifications that minimises the freshwater use and the number of water sources. The method provides a flowsheet that is rather complex and also introduced several process splittings. It was observed that, even after breaking the loops, the final designs of their solution may be of no practical use. The method for instance, proposed a splitting of process three. If process three were an indivisible unit, such as a desalter or a reflux drum, the network would have no real meaning. However, the method used in this research provides a simple superstructure

representation configuration of the solution that is realistic and gives superior option for practical implementation. Moreover, the value obtained by this method is approximately equal to their value. For the computational time, GAs spends a very short time in solving this problem, it spends 3.5 seconds without hybrid function and 5.2 seconds with hybrid function to obtain the optimum. So, the algorithm is improved to overcome the deficiency of taking long time to solve WAP problem as explained by other researchers like Prakotpol and Srinophakun (2004).

5.5: Single Contaminant Water Reuse without Regeneration for 5 industrial Processes

The number of variables as described in chapter 2 for five industrial processes are $n^2+n = 30$. The variables are freshwater, wastewater and wastewater for reuse, represented as follows: $F_1, F_2, F_3, F_4, F_5, W_1, W_2, W_3, W_4, W_5, X_{12}, X_{13}, X_{14}, X_{15}, X_{21}, X_{23}, X_{24}, X_{25}, X_{31}, X_{32}, X_{34}, X_{35}, X_{41}, X_{42}, X_{43}, X_{45}, X_{51}, X_{52}, X_{53}, X_{54}$ respectively.

5.5.1 Test Problem: Input Limiting Process Data for 5 industrial processes

Considering limiting data for water minimization for a specialty chemical production process used by Mann and Liu (1999); Prakotpol and Srinophakun (2004) and Feng, *et. al.*, (2008) is shown in Table 5.15. The freshwater in this case is assumed to have zero impurity. This data will be used to determine the minimum flowrate of freshwater and wastewater for the processes. This data will be used to determine the minimum flowrate of freshwater and wastewater for the processes.

Table 5.4: Rough Limiting Process Data for 5 Industrial processes

Rough Limiting Process Data			
Operation	Mass Load ΔM (kg/hr)	Contaminant Concentration (Allowed in) C_{in}^{lim} (ppm)	Contaminant Concentration (Produced out) C_{out}^{lim} (ppm)
1	1	0	100
2	1	0	50
3	0.5	50	100
4	0.625	75	200
5	4	100	300

5.5.2 Representation of Single Contaminant Water Reuse without Regeneration in Matlab for 5 industrial processes

The fitness function is vectorised and represented in Matlab as shown in appendix C3. The linear constraints equations in equations 5.14b to 5.15f are represented in Matlab software as the matrix and vector of equalities (Aeq and beq) using the coefficient of the variables. The matrix and vector of inequalities are not available in the constraints, therefore (A and b) are represented as empty set as follows: $A = []$, $b = []$. The vector

for lower and upper bounds (LB and UB) are represented with the set of lowest and highest value of outcome of each point. The Nonlinear Constraints functions are vectorised and represented in Matlab as shown in appendix C3. The code for obtaining the solution in Matlab is shown in appendix C3. This will search for the possible solution of the problem and display the result as vector when the stopping criteria are met.

5.5.3 The result of Single Contaminant Water Reuse without Regeneration in Matlab for 5 industrial processes

The set of functions, genetic parameters and genetic operators used by GA for diagnostic analysis of the problem are as shown in Table 5.3. The differences are Fitness function is @FRW3 with 30 number of variables, 10 Equality constraints and '@Constraints_FRW3' as the nonlinear constraint function.

Optimisation comes to termination when the average change in the fitness value is less than Function Tolerance and constraint violation is less than Constraint Tolerance. The obtained result at termination is 36.3m³/h.

Switching to the hybrid optimisation algorithm (fmincon) leads to Local minimum within the last region, which is the optimum result after satisfying the constraints. The final result is displayed as shown in Table 5.16.

The f-count is the number of function evaluations that the GA solver took to converge to a local solution. The obtained result is indicated in column 3 as the best-f(x) for the first 4 generations. The maximum constraints value in column 4 indicates the values that satisfy the constraints and the stall-generation gives the number of times the minimum of generations are computed regardless of the convergence criteria.

Table 5.5: End of diagnostic information for the solution of five industrial process

Generation	f- count	Best - f(x)	max - constraint	Stall- Generations
1	10760	36.3018	1.109e-16	0
2	21160	36.3018	1.109e-16	1
3	31560	36.3018	1.109e-16	2
4	41960	36.3018	1.109e-16	3
5	658	30.2	3.257e-06	0
6	1178	30.2	3.257e-06	1
7	1698	30.0	3.257e-06	2
8	2218	30.0	3.257e-06	3

Table 5.6: End of diagnostic solution of the problem corresponding to Figure solution of five industrial processes.

Process Number	Type of water used by the process	Fresh water intake (m ³ /h)	Wastewater reuse (m ³ /h)	Contaminant Concentration (Allowed in) C ^{lim} _{in} (ppm)	Contaminant Concentration (Produced out) C ^{lim} _{out} (ppm)
1	Freshwater only	10.0	0.0	0	100
2	Freshwater only	20.0	0.0	0	50
3	Wastewater only	0.0	10.0	50	100
4	Wastewater only	0.0	(Second reuse) 5.0	75	200
5	Wastewater only	0.0	20.0	100	300
Total Flowrate (m ³ /h)		30.0	25.0		

Superstructure Schematic Network:

The superstructure schematic MATLAB result network configuration for 5 industrial processes optimum water-using network of the solution is shown in Figure 5.4.

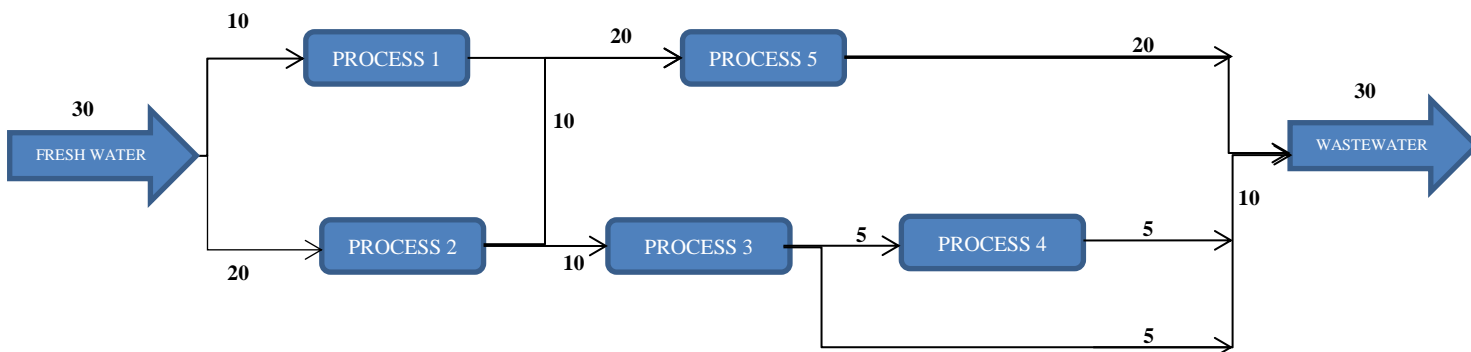


Figure 5.4: The diagrammatical Superstructure representation of the solution of 5 industrial processes.

Solution of the problem corresponding to the diagrammatical Superstructure representation of the solution is shown in Table 5.17. It present the obtained result, indicating that the minimum total freshwater required by the industry is 30.0m³/h, 10.0m³/h for process 1 (F₁) and 20.0m³/h for process 2 (F₂). Process 3 (F₃) and 5 (F₅) reuse 10.0m³/h of wastewater each from process 2 (F₂), while process 4 (F₄) re-reuse (use again) the 5.0m³/h of wastewater from process 3 (F₃).

The results from this analysis reach the same value of minimum freshwater consumption for single contaminant as presented by Mann and Liu (1999); Prakotpol and Srinophakun (2004) and Feng, *et. al.*, (2008), but they present different configurations. However, this research gives the superstructure representation configuration of the solution that is simpler and gives better option for practical implementation than when compared to that of other researchers. Wastewater from process 2 (20.0m³/h) reused by process 3 (10.0m³/h) is also reused by process 4 (5.0m³/h). For the computational time of the above problem, this method takes a very short time in solving this problem, it spends 5.2 seconds without hybrid function and 6.0 seconds with hybrid function to obtain the optimum. So, the algorithm is improved to overcome the deficiency of taking long time to solve WAP problem as observed by other researchers.

5.6: Single contaminant Water Reuse without Regeneration for 6

Industrial Processes

The number of variables as described in chapter two for 6 industrial processes is $n^2+n = 42$. The variables are freshwater, wastewater and wastewater for reuse, represented as follows: $F_1, F_2, F_3, F_4, F_5, F_6, W_1, W_2, W_3, W_4, W_5, W_6, X_{12}, X_{13}, X_{14}, X_{15}, X_{16}, X_{21}, X_{23}, X_{24}, X_{25}, X_{26}, X_{31}, X_{32}, X_{34}, X_{35}, X_{36}, X_{41}, X_{42}, X_{43}, X_{45}, X_{46}, X_{51}, X_{52}, X_{53}, X_{54}, X_{56}, X_{61}, X_{62}, X_{63}, X_{64}, X_{65}$ respectively.

5.6.1 Test Problem: Input Limiting Process Data for 6 industrial processes

The rough limiting process data for 6 Industrial processes is shown in Table 5.18 This example of WAP problem is taken from Olesen and Polley (1997) in their paper titled 'A simple methodology for the design of water networks handling single contaminants'. The same data also used by Savelski and Bagajewicz (2000) in their paper titled 'Design of water utilization systems in process plants with a single contaminant'.

Table 5.7: Rough Limiting Process Data for 6 Industrial processes

Rough Limiting Process Data			
Operation	Mass Load ΔM (kg/hr)	Contaminant Concentration (Allowed in) C^{lim}_{in} (ppm)	Contaminant Concentration (Produced out) C^{lim}_{out} (ppm)
1	2	25	80
2	5	25	100
3	4	25	200
4	5	50	100
5	30	50	800
6	4	400	800

5.6.2 Representation of Single Contaminant Water Reuse without Regeneration in Matlab for 6 industrial processes

The fitness function is vectorised and represented in Matlab as shown in appendix C4. The linear constraints equations in equations 5.18b to 5.19g are represented in Matlab software as the matrix and vector of equalities (Aeq and beq) using the coefficient of the variables.

The matrix and vector of inequalities are not available in the constraints, therefore (A and b) are represented as empty set as follows: $A = []$, $b = []$. The vector for lower and upper bounds (LB and UB) are represented with the set of lowest and highest value of outcome of each point. The Nonlinear Constraints functions are vectorised and represented in Matlab as shown in appendix C4. The code for obtaining the solution in Matlab is shown in appendix C4. This will search for the possible solution of the problem and display the result as vector when the stopping criteria are met.

5.6.3 The result of Single Contaminant Water Reuse without Regeneration in Matlab for 6 industrial processes

The set of functions, genetic parameters and genetic operators used by GA for diagnostic analysis of the problem are as shown in Table 5.3. The differences are Fitness function is @FRW4 with 42 number of variables, 12 Equality constraints and '@Constraints_FRW4' as the nonlinear constraint function.

Optimisation comes to termination when the average change in the fitness value is less than Function Tolerance and constraint violation is less than Constraint Tolerance. The obtained result at termination is 166.30m³/h.

Switching to the hybrid optimisation algorithm (fmincon) leads to Local minimum within the last region, which is the optimum result of 156.0m³/h after the constraints are satisfied. The final result is displayed as shown in Table 5.19.

The f-count is the number of function evaluations that the GA solver took to converge to a local solution. The obtained result is indicated in column 3 as the best-f(x) for the first 5 generations. The maximum constraints value in column 4 indicates the values that satisfy the constraints and the stall-generation gives the number of times the minimum of generations are computed regardless of the convergence criteria.

Table 5.8: End of diagnostic information for the solution of 6 industrial processes

Generation	f-count	Best- f(x)	Max - constraint	Stall - Generations
1	11172	166.25	0.2956	0
2	21704	166.475	0	0
3	32104	166.475	0	1
4	42504	166.475	0	2
5	71704	166.309	0	0
6	1058	165.225	0	1
7	1578	160.225	0	2
8	2098	158.225	0	0
9	2618	157.225	0	0
10	3138	156.225	0	0
11	1058	156.025	0	0

Solution of the problem corresponding to the diagrammatical Superstructure representation is shown in Table 5.20.

Table 5.20: End of diagnostic solution of the problem corresponding to Figure solution of 6 industrial processes.

F ₁	F ₂	F ₃	F ₄	F ₅	F ₆	W ₁	W ₂	W ₃	W ₄	W ₅	W ₆
28.2	48.0	16.0	46.4	17.4	0.0	0.0	48.0	22.0	39.3	38.0	8.0
X ₁₂	X ₁₃	X ₁₄	X ₁₅	X ₁₆		X ₂₁	X ₂₃	X ₂₄	X ₂₅	X ₂₆	
1.5	0.0	2.5	0.0	0.0		6.7	0.0	5.7	0.0	0.0	
X ₃₁	X ₃₂	X ₃₄	X ₃₅	X ₃₆		X ₄₁	X ₄₂	X ₄₃	X ₄₅	X ₄₆	
0.0	8.0	0.0	0.0	0.0		22.1	1.0	0.0	0.0	0.0	
						X ₆₁	X ₆₂	X ₆₃	X ₆₄	X ₆₅	
						0.0	2.1	1.7	2.2	2.0	
X ₅₁	X ₅₂	X ₅₃	X ₅₄	X ₅₆							
14.6	3.4	0.0	4.9	0.0							

Table 5.21: End of diagnostic solution of the problem corresponding to Figure solution of 6 industrial processes.

Process Number	Type of water used by the process	Fresh water intake (m ³ /h)	Wastewater reuse (m ³ /h)	Contaminant Concentration (Allowed in) C ^{lim} _{in} (ppm)	Contaminant Concentration (Produced out) C ^{lim} _{out} (ppm)
1	Freshwater only	28.2	0.0	25	80
2	Freshwater only	48.0	0.0	25	100
3	Fresh & wastewater	16.0	28.2	25	200
4	Freshwater only	46.4	0.0	50	100
5	Fresh & wastewater	17.4	0.0	50	800
6	Wastewater only	0.0	67.0	400	800
Total Flowrate (m ³ /h)		156	47.2		

Superstructure Schematic Network

The superstructure schematic MATLAB result network configuration for 6 industrial processes optimum water-using network of the solution is shown in figure 5.5.

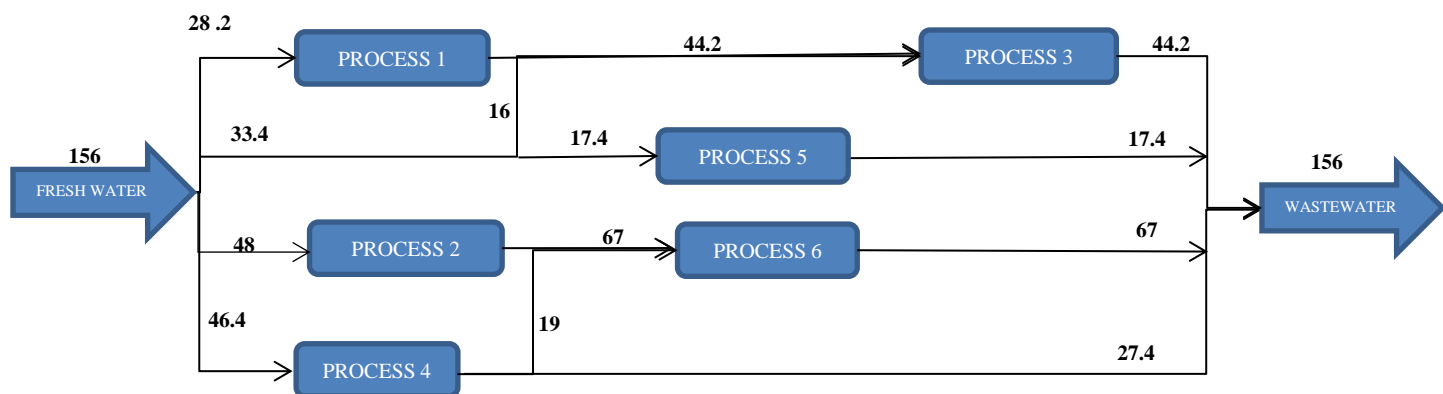


Figure 5.5: The diagrammatical Superstructure representation of the solution of 6 industrial processes.

The description of the final solution represented in superstructure of Figure 5.5 is shown in Table 5.21. It present the obtained result, indicating that the minimum total freshwater required by the industry is 156.0m³/h. That is 28.2m³/h for process 1 (F₁), 48m³/h for process 2 (F₂), 16m³/h for process 3 (F₃), 46.4m³/h for process 4 (F₄), and 17.4m³/h for process 5 (F₅). Process 3 reuse additional 28.2m³/h of wastewater from

processes 1. Process 6 (F_6) reuse $48.0\text{m}^3/\text{h}$ and $19.0\text{ m}^3/\text{h}$ of wastewater from processes 2 and 4, respectively.

The results from this analysis reach an optimal value of $156.0\text{m}^3/\text{h}$ minimum freshwater consumption for this 6 industrial processes single contaminant WAP problem. This is lower than $157.14\text{ m}^3/\text{h}$ as the solution presented by Olesen and Polley (1997) and Savelski and Bagajewicz (2000), and they present different configurations. However, this research gives the superstructure representation configuration of the solution that is simpler and gives better option for practical implementation than when compared to that of other researchers.

For the computational time of the above problem, this method takes very short time in solving this problem. It spends 5.4 seconds without hybrid function and 6.2 seconds with hybrid function to obtain the optimum result. So, the algorithm is improved to overcome the deficiency of taking long time to solve WAP problem as observed by other researchers.

5.7: Single Contaminant Water Reuse without Regeneration for 7

Processes

The number of variables as described in chapter two for 7 industrial processes is $n^2+n = 56$. The variables are freshwater, wastewater and wastewater for reuse, represented as follows: $F_1, F_2, F_3, F_4, F_5, F_6, F_7, W_1, W_2, W_3, W_4, W_5, W_6, W_7, X_{12}, X_{13}, X_{14}, X_{15}, X_{16}, X_{17}, X_{21}, X_{23}, X_{24}, X_{25}, X_{26}, X_{27}, X_{31}, X_{32}, X_{34}, X_{35}, X_{36}, X_{37}, X_{41}, X_{42}, X_{43}, X_{45}, X_{46}, X_{47}, X_{51}, X_{52}, X_{53}, X_{54}, X_{56}, X_{57}, X_{61}, X_{62}, X_{63}, X_{64}, X_{65}, X_{67}, X_{71}, X_{72}, X_{73}, X_{74}, X_{75}, X_{76}$, respectively.

5.7.1 Test Problem: Input Limiting Process Data for 7 industrial processes

Table 5.22 shows rough limiting process data for seven industrial processes, which was taken from Bagajewicz *et al.*, (2002), Feng *et al.*, (2009) and Liang, and Hui, (2016).

Table 5. 9: Rough Limiting Process Data for 7 Industrial processes

Rough Limiting Water using Data			
Process	Mass Load ΔM (kg/hr)	Contaminant Concentration (Allowed in) C^{lim}_{in} (ppm)	Contaminant Concentration (Produced out) C^{lim}_{out} (ppm)
1	2	25	80
2	2.88	25	90
3	4	25	200
4	3	50	100
5	30	50	800
6	5	400	800
7	2	400	600

5.7.2 Representation of Linear Constraint functions in Matlab for 7 industrial processes

The fitness function is vectorised and represented in Matlab as shown in appendix C5. The linear constraints equations in equations 5.22 to 5.23 are represented in Matlab software as the matrix and vector of equalities (Aeq and beq) using the coefficient of the variables. The matrix and vector of inequalities are not available in the constraints,

therefore (A and b) are represented as empty set as follows: $A = []$, $b = []$. The vector for lower and upper bounds (LB and UB) are represented with the set of lowest and highest value of outcome of each point. The Nonlinear Constraints functions are vectorised and represented in Matlab as shown in appendix C5. The code for obtaining the solution in Matlab is also shown in appendix C5. This will search for the possible solution of the problem and display the result as vector when the stopping criteria are met.

5.7.3 The result of Single Contaminant Water Reuse without Regeneration in Matlab for 7 industrial processes

The set of functions, genetic parameters and genetic operators used by GA for diagnostic analysis of the problem are as shown in Table 5.3. The differences are Fitness function is @FRW5 with 56 number of variables, 14 Equality constraints and '@Constraints_FRW5' as the nonlinear constraint function.

Optimisation comes to termination when the average change in the fitness value is less than Function Tolerance and constraint violation is less than Constraint Tolerance. The obtained result was 131.2m³/h.

Switching to the hybrid optimisation algorithm (FMINCON) leads to Local minimum within the last region, which is the optimum result if Constraints are satisfied. The final result is displayed as shown in Table 5.23.

The f-count is the number of function evaluations that the GA solver took to converge to a local solution. The obtained result is indicated in column 3 as the best-f(x) for the first 3 generations. The maximum constraints value in column 4 indicates the values that satisfy the constraints and the stall-generation gives the number of times the minimum of generations are computed regardless of the convergence criteria.

Table5. 10: End of diagnostic information for the solution of 7 industrial processes

Generation	f-count	Best - f(x)	Max - constraint	Stall - Generations
1	10890	132.702	0	0
2	21290	131.702	0	1
3	31690	131.202	0	2
4	46490	121.408	0	0
5	85690	115.997	0	0

Table 5.24 present the individual values of each variable after the analysis.

Table 5. 11: End of diagnostic solution of 7 industrial processes.

F ₁	F ₂	F ₃	F ₄	F ₅	F ₆	F ₇	W ₁	W ₂	W ₃	W ₄	W ₅	W ₆	W ₇
25.8	31.8	16.3	25.2	16.9	0.0	0.0	0.0	0.0	20.2	43.5	36.5	8.2	7.8
X ₁₂	X ₁₃	X ₁₄	X ₁₅	X ₁₆	X ₁₇	X ₂₁	X ₂₃	X ₂₄	X ₂₅	X ₂₆	X ₂₇		
4.1	0.0	1.0	0.0	0.0	0.0	3.4	0.0	1.0	0.0	0.0	0.0		
X ₃₁	X ₃₂	X ₃₄	X ₃₅	X ₃₆	X ₃₇	X ₄₁	X ₄₂	X ₄₃	X ₄₅	X ₄₆	X ₄₇		
2.5	2.7	1.3	0.0	0.0	0.0	14.6	17.9	0.0	0.0	0.0	0.0		
X ₅₁	X ₅₂	X ₅₃	X ₅₄	X ₅₆	X ₅₇	X ₆₁	X ₆₂	X ₆₃	X ₆₄	X ₆₅	X ₆₇		
9.0	12.9	0.0	1.2	0.0	0.0	0.0	0.0	0.9	6.3	1.6	0.2		
X ₇₁	X ₇₂	X ₇₃	X ₇₄	X ₇₅	X ₇₆								
0.0	0.0	1.8	3.6	1.4	1.7								

Table 5. 12: End of diagnostic solution of the problem corresponding to Figure solution of 7 industrial processes.

Process Number	Type of water used by the process	Freshwater intake (m ³ /h)	Wastewater reuse (m ³ /h)	Contaminant Concentration (Allowed in) C ^{lim} _{in} (ppm)	Contaminant Concentration (Produced out) C ^{lim} _{out} (ppm)
1	Freshwater only	25.8	0.0	25	80
2	Freshwater only	31.8	0.0	25	100
3	Fresh & wastewater	16.3	3.9	25	200
4	Fresh & wastewater	25.2	18.3	50	100
5	Fresh & wastewater	16.9	19.6	50	800

6	Wastewater only	0.0	8.2	400	800
7	Wastewater only	0.0	7.8	400	800
Total Flowrate (m ³ /h)		116	53.9		

Superstructure Schematic Network

The superstructure schematic MATLAB result network configuration for 7 industrial processes Optimum water-using network of the solution is shown in figure 5.6.

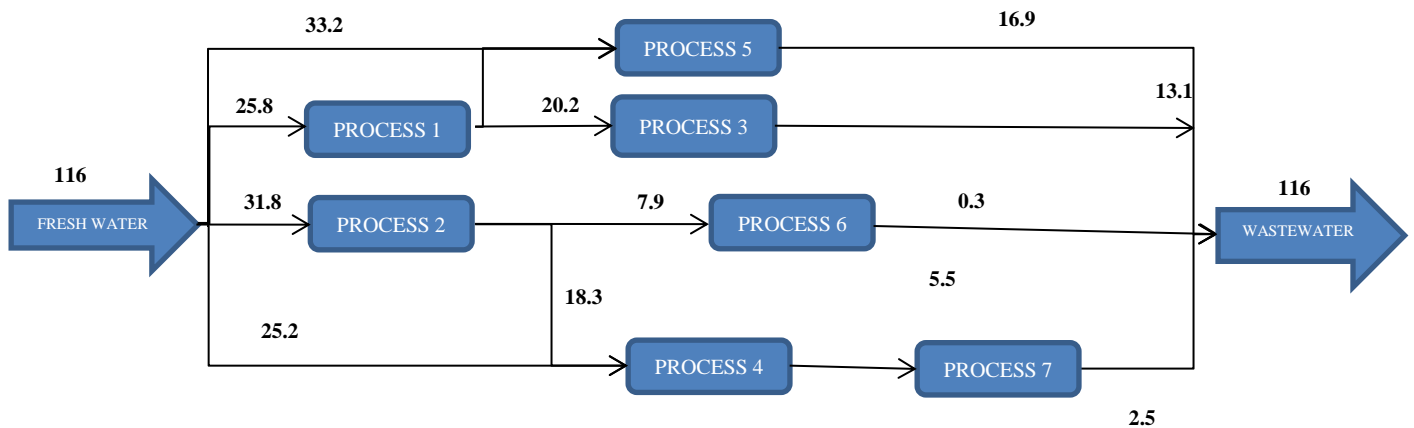


Figure 5.6: The diagrammatical Superstructure representation of the solution of 7 industrial processes.

The solution of the problem corresponding to the diagrammatical Superstructure representation of the solution is shown in Table 5.25. It present the obtained result, indicating that the minimum total freshwater required by the industry is 116.0m³/h, 25.8 m³/h for process 1, 31.8 m³/h for process 2, 16.3 m³/h for process 3, 25.2 m³/h for process 4, and 16.9 m³/h for process 5. Process 3, 4 and 5 reuse additional 3.9m³/h, 18.3m³/h and 19.6 m³/h of wastewater respectively. While, process 6 and 7 reuse 8.2m³/h and 7.8 m³/h of wastewater, respectively. This result is lower than the result obtained by Bagajewicz *et al.*, (2002), and Feng *et al.*, (2009), which is 131.2m³/h. However, the computational time of the above problem, using this research method takes a very short time. The computer takes 6.7 seconds without hybrid function and 7.0 seconds with hybrid function to obtain the optimum result. So, this method is also improved to overcome the deficiency of taking long time to solve WAP problem as observed by other researchers.

5.8: Single Contaminant Water Reuse without Regeneration for 8

Industrial Processes

The number of variables as described in chapter 2 for eight industrial processes is $n^2+n = 72$. The variables are freshwater, wastewater and wastewater for reuse, represented as follows: $F_1, F_2, F_3, F_4, F_5, F_6, F_7, F_8, W_1, W_2, W_3, W_4, W_5, W_6, W_7, W_8, X_{12}, X_{13}, X_{14}, X_{15}, X_{16}, X_{17}, X_{18}, X_{21}, X_{23}, X_{24}, X_{25}, X_{26}, X_{27}, X_{28}, X_{31}, X_{32}, X_{34}, X_{35}, X_{36}, X_{37}, X_{38}, X_{41}, X_{42}, X_{43}, X_{45}, X_{46}, X_{47}, X_{48}, X_{51}, X_{52}, X_{53}, X_{54}, X_{56}, X_{57}, X_{58}, X_{61}, X_{62}, X_{63}, X_{64}, X_{65}, X_{67}, X_{68}, X_{71}, X_{72}, X_{73}, X_{74}, X_{75}, X_{76}, X_{78}, X_{81}, X_{82}, X_{83}, X_{84}, X_{85}, X_{86}, X_{87}$ respectively.

5.8.1 Test Problem: Input Limiting Process Data for 8 industrial processes

Test Problem: Input Limiting Process Data

The rough limiting process data for 8 Industrial processes Taken from Bagajewicz *et al.*, (2002), Feng *et al.*, (2009) and Liang, and Hui, (2016) is shown in Table 5.26.

Table 5. 13: Rough Limiting Process Data for 8 Industrial processes

Rough Limiting Water using Data			
Process	Mass Load ΔM (kg/hr)	Contaminant Concentration (Allowed in) $C^{\text{lim}}_{\text{in}}$ (ppm)	Contaminant Concentration (Produced out) $C^{\text{lim}}_{\text{out}}$ (ppm)
1	2	25	80
2	2.88	25	90
3	4	25	200
4	3	50	100
5	30	50	800
6	5	400	800
7	2	400	600
8	1	0	100

5.8.2 Representation of Single Contaminant Water Reuse without Regeneration in Matlab for 8 industrial processes

The fitness function is vectorised and represented in Matlab as shown in appendix C6. The linear constraints equations in equations 5.2a to 5.3c are represented in Matlab software as the matrix and vector of equalities (Aeq and beq) using the coefficient of the variables. The matrix and vector of inequalities are not available in the constraints, therefore (A and b) are represented as empty set as follows: A= [], b= []. The vector for lower and upper bounds (LB and UB) are represented with the set of lowest and highest value of outcome of each point as shown in appendix C6. The Nonlinear Constraints functions are vectorised and represented in Matlab as shown in appendix C6. The code for obtaining the solution in Matlab is shown in appendix C6. This will search for the possible solution of the problem and display the result as vector when the stopping criteria are met.

5.8.3 The result of Single Contaminant Water Reuse without Regeneration in Matlab for 8 industrial processes

The set of functions, genetic parameters and genetic operators used by GA for diagnostic analysis of the problem are as shown in Table 5.3. The differences are Fitness function is @FRW6 with 72 number of variables, 16 Equality constraints and '@Constraints_FRW6' as the nonlinear constraint function.

Optimisation comes to termination when the average change in the fitness value is less than Function Tolerance and constraint violation is less than Constraint Tolerance. The obtained result was 138.9m³/h.

Switching to the hybrid optimisation algorithm (fmincon) leads to Local minimum within the last region, which is the optimum result if Constraints are satisfied. The final result is displayed as shown in Table 5.27.

The f-count is the number of function evaluations that the GA solver took to converge to a local solution. The obtained result is indicated in column 3 as the best-f(x) for the first 2 generations. The maximum constraints value in column 4 indicates the values that satisfy the constraints and the stall-generation gives the number of times the minimum of generations are computed regardless of the convergence criteria.

Table 5. 14: End of diagnostic information for the solution of 8 industrial processes

Generation	f-count	Best - f(x)	Max - constraint	Stall - Generations
1	572	139.9556	2.359e-15	0
2	1092	138.9056	2.359e-15	1
3	1662	138.6324	4.472e-06	0
4	2182	138.2324	4.472e-06	0

Table 5.28 present the individual values of each variable after the analysis.

Table 5. 15: End of diagnostic solution of 8 industrial processes.

F ₁	F ₂	F ₃	F ₄	F ₅	F ₆	F ₇	F ₈
36.4	44.3	10.0	27.5	10.0	0.0	0.0	10.0

W ₁	W ₂	W ₃	W ₄	W ₅	W ₆	W ₇	W ₈
0.0	14.3	22.9	38.5	40.0	12.5	10.0	0.0

X ₁₂	X ₁₃	X ₁₄	X ₁₅	X ₁₆	X ₁₇	X ₁₈
0.0	12.9	23.5	0.0	0.0	0.0	0.0

X ₂₁	X ₂₃	X ₂₄	X ₂₅	X ₂₆	X ₂₇	X ₂₈
0.0	0.0	0.0	30.0	0.0	0.0	0.0

X ₃₁	X ₃₂	X ₃₄	X ₃₅	X ₃₆	X ₃₇	X ₃₈
0.0	0.0	0.0	0.0	0.0	0.0	0.0

X ₄₁	X ₄₂	X ₄₃	X ₄₅	X ₄₆	X ₄₇	X ₄₈
0.0	0.0	0.0	0.0	12.5	0.0	0.0

X ₅₁	X ₅₂	X ₅₃	X ₅₄	X ₅₆	X ₅₇	X ₅₈
11.2	12.1	0.0	0.0	0.0	0.0	0.2

X ₆₁	X ₆₂	X ₆₃	X ₆₄	X ₆₅	X ₆₇	X ₆₈
0.0	0.0	2.3	1.7	0.8	0.9	3.2

X ₇₁	X ₇₂	X ₇₃	X ₇₄	X ₇₅	X ₇₆	X ₇₈
0.0	0.0	0.3	0.7	0.8	0.0	10.0

X ₈₁	X ₈₂	X ₈₃	X ₈₄	X ₈₅	X ₈₆	X ₈₇
0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 5. 16: End of diagnostic solution of the problem corresponding to Figure solution of 8 industrial processes

Process Number	Type of water used by the process	Fresh water intake (m ³ /h)	Wastewater reuse (m ³ /h)	Contaminant Concentration (Allowed in) C ^{lim} _{in} (ppm)	Contaminant Concentration (Produced out) C ^{lim} _{out} (ppm)
1	Freshwater only	36.4	0.0	25	80
2	Freshwater only	44.3	0.0	25	100
3	Fresh & wastewater	10.0	12.9	25	200
4	Fresh & wastewater	27.5	32.5	50	100
5	Fresh & wastewater	10.0	30.0	50	800
6	Wastewater only	0.0	12.5	400	800
7	Wastewater only	0.0	10.0	400	600
8	Fresh & wastewater	10.0	0.0	0	100
Total Flowrate (m ³ /h)		138.2	97.9		

Superstructure Schematic Network

The superstructure schematic MATLAB result network configuration for 8 processes

Optimum water-using network of the solution is shown in figure 5.7.

Matlab result for 8 industrial processes optimum water-using network for an example problem of single contaminant-water reuse.

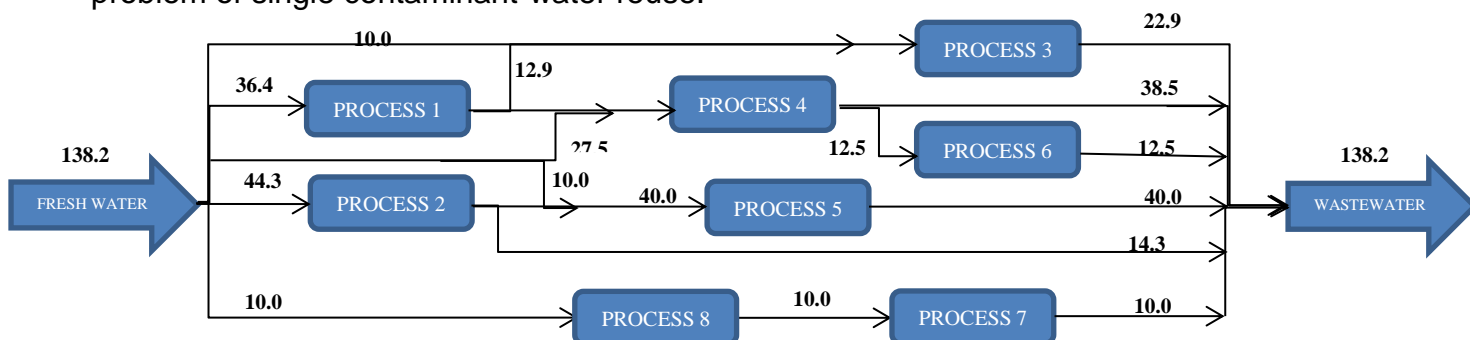


Figure 5.7: The diagrammatical Superstructure representation of the solution of 8 industrial processes.

The solution of the problem corresponding to the diagrammatical Superstructure representation of the solution is shown in Table 5.29. It present the obtained result, indicating that the minimum total freshwater required by the industry is 138.2 m³/h, 36.4m³/h for process 1 (F₁), 44.3m³/h for process 2 (F₂), 16.3m³/h for process 3 (F₃), 10.0m³/h for process 4 (F₄), 10.0m³/h for process 5 (F₅), and 10.0m³/h for process 8 (F₈). Processes 3, 4, and 5 reuse additional 12.9m³/h, 23.5m³/h, and 30.0m³/h of wastewater respectively. While, processes 6 (F₆) and 7 (F₇) reuse 12.5m³/h and 10.0m³/h of wastewater from processes 4 and 8, respectively. This result is exactly equal to the result obtained by Bagajewicz et al., (2002); Feng et al., (2009) and Liang, and Hui, (2016) which is 138.2m³/h as shown in Table 5.1.

For the computational time of the above problem, the method used in this research takes a very short time in solving the problem. It spends 7.1 seconds without hybrid function and 8.4 seconds with hybrid function to obtain the optimum result. So, the algorithm is improved to overcome the deficiency of taking long time to solve WAP problem as observed by other researchers.

5.9: Single Contaminant Water Reuse without Regeneration for 9 Processes

The number of variables as described in chapter 2 for nine industrial processes is $n^2+n = 90$. The variables are freshwater, wastewater and wastewater for reuse, represented as follows: $F_1, F_2, F_3, F_4, F_5, F_6, F_7, F_8, F_9, W_1, W_2, W_3, W_4, W_5, W_6, W_7, W_8, W_9, X_{12}, X_{13}, X_{14}, X_{15}, X_{16}, X_{17}, X_{18}, X_{19}, X_{21}, X_{23}, X_{24}, X_{25}, X_{26}, X_{27}, X_{28}, X_{29}, X_{31}, X_{32}, X_{34}, X_{35}, X_{36}, X_{37}, X_{38}, X_{39}, X_{41}, X_{42}, X_{43}, X_{45}, X_{46}, X_{47}, X_{48}, X_{49}, X_{51}, X_{52}, X_{53}, X_{54}, X_{56}, X_{57}, X_{58}, X_{59}, X_{61}, X_{62}, X_{63}, X_{64}, X_{65}, X_{67}, X_{68}, X_{69}, X_{71}, X_{72}, X_{73}, X_{74}, X_{75}, X_{76}, X_{78}, X_{79}, X_{81}, X_{82}, X_{83}, X_{84}, X_{85}, X_{86}, X_{87}, X_{89}, X_{91}, X_{92}, X_{93}, X_{94}, X_{95}, X_{96}, X_{97}, X_{98}$ respectively.

5.9.1 Test Problem: Input Limiting Process Data for 9 industrial processes

Table 5.30 shows rough limiting process data for 9 Industrial processes, taken from Bagajewicz *et al.*, (2002), Feng *et al.*, (2009) (Feng, X.; Li, Y.; and Shen, R. (2009).A new approach to design energy efficient water allocation networks. *Appl. Therm. Eng.*, 29 (11–12), pp. 2302–2307), and Liang, and Hui, (2016).

Table 5. 30: Rough Limiting Process Data for 9 Industrial processes

Rough Limiting Water using Data			
Process	Mass Load ΔM (kg/hr)	Contaminant Concentration (Allowed in) $C^{\text{lim}}_{\text{in}}$ (ppm)	Contaminant Concentration (Produced out) $C^{\text{lim}}_{\text{out}}$ (ppm)
1	2	25	80
2	2.88	25	90
3	4	25	200
4	3	50	100
5	30	50	800
6	5	400	800
7	2	400	600
8	1	0	100
9	1	0	100

5.9.2 Representation of Single Contaminant Water Reuse without Regeneration in Matlab for 9 industrial processes

The fitness function is vectorised and represented in Matlab as shown in appendix C7. The linear constraints equations in equations 5.30 to 5.31i are represented in Matlab software as the matrix and vector of equalities (Aeq and beq) using the coefficient of the variables. The matrix and vector of inequalities are not available in the constraints, therefore (A and b) are represented as empty set as follows: A= [], b= []. The vector for lower and upper bounds (LB and UB) are represented with the set of lowest and highest value of outcome of each point as shown in appendix B7. The Nonlinear Constraints functions are vectorised and represented in Matlab as shown in appendix C7. The code for obtaining the solution in Matlab is shown in appendix C7. This will search for the possible solution of the problem and display the result as vector when the stopping criteria are met.

5.9.3 The result of Single Contaminant Water Reuse without Regeneration in Matlab for 9 industrial processes

The set of functions, genetic parameters and genetic operators used by GA for diagnostic analysis of the problem are as shown in Table 5.3. The differences are Fitness function is @FRW7 with 90 number of variables, 18 Equality constraints and '@Constraints_FRW7' as the nonlinear constraint function.

Optimisation comes to termination when the average change in the fitness value is less than Function Tolerance and constraint violation is less than Constraint Tolerance. The obtained result at termination of GA is 167.71m³/h.

However, switching to the hybrid optimisation algorithm (fmincon) leads to Local minimum within the last region, which is the optimum result at the satisfaction of all constraints. The final result is displayed as shown in Table 5.31.

The f-count is the number of function evaluations that the GA solver took to converge to a local solution. The obtained result is indicated in column 3 as the best-f(x) for the first 3 generations. The maximum constraints value in column 4 indicates the values that satisfy the constraints and the stall-generation gives the number of times the minimum of generations are computed regardless of the convergence criteria.

Table 5.31: End of diagnostic information for the solution of 9 industrial processes

Table 5.32 present the individual values of each variable after the analysis.

Generation	f-count	Best - f(x)	Max - constraint	Stall - Generations
1	11520	167.96	0.1979	0
2	22196	167.809	0.001871	0
3	32872	167.709	0	0
4	43272	158.809	0	1
5	53672	158.109	0	2

Table5. 17: End of diagnostic solution of 9 industrial processes.

W_1	W_2	W_3	W_4	W_5	W_6	W_7	W_8	W_9
3.8 ^{F1}	24.3 ^{F2}	10.0 ^{F3}	47.5 ^{F4}	40.0 ^{F5}	12.5 ^{F6}	10.5 ^{F7}	0.0 ^{F8}	10.0 ^{F9}
25.5	31.9	17.0	28.9	18.1	0.0	0.0	11.3	13.0
X_{12}	X_{13}	X_{14}	X_{15}	X_{16}	X_{17}	X_{18}	X_{19}	
0.3695	0.1979	0.3659	0.0000	0.0027	0.0000	0.0000	0.0000	

X_{21}	X_{23}	X_{24}	X_{25}	X_{26}	X_{27}	X_{28}	X_{29}
1.5797	0.0356	0.2135	0.0000	0.0037	0.0000	0.0000	0.0000

X_{31}	X_{32}	X_{34}	X_{35}	X_{36}	X_{37}	X_{38}	X_{39}
1.0674	1.6761	2.8311	0.0000	0.0039	0.0000	0.0262	0.0000
X_{41}	X_{42}	X_{43}	X_{45}	X_{46}	X_{47}	X_{48}	X_{49}
4.5107	3.6808	0.1042	0.0000	0.0027	0.0000	0.0000	0.0000

X_{51}	X_{52}	X_{53}	X_{54}	X_{56}	X_{57}	X_{58}	X_{59}
6.1622	6.8862	0.0000	4.5408	0.0000	0.0000	3.0047	1.3273

X_{61}	X_{62}	X_{63}	X_{64}	X_{65}	X_{67}	X_{68}	X_{69}
0.2669	0.8707	1.4441	4.5810	3.2252	0.0000	0.0736	0.0594

X ₇₁	X ₇₂	X ₇₃	X ₇₄	X ₇₅	X ₇₆	X ₇₈	X ₇₉
0.2107	1.5244	0.0441	3.2095	2.7434	0.0	0.0464	0.0322
X ₈₁	X ₈₂	X ₈₃	X ₈₄	X ₈₅	X ₈₆	X ₈₇	X ₈₉
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

X ₉₁	X ₉₂	X ₉₃	X ₉₄	X ₉₅	X ₉₆	X ₉₇	X ₉₈
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

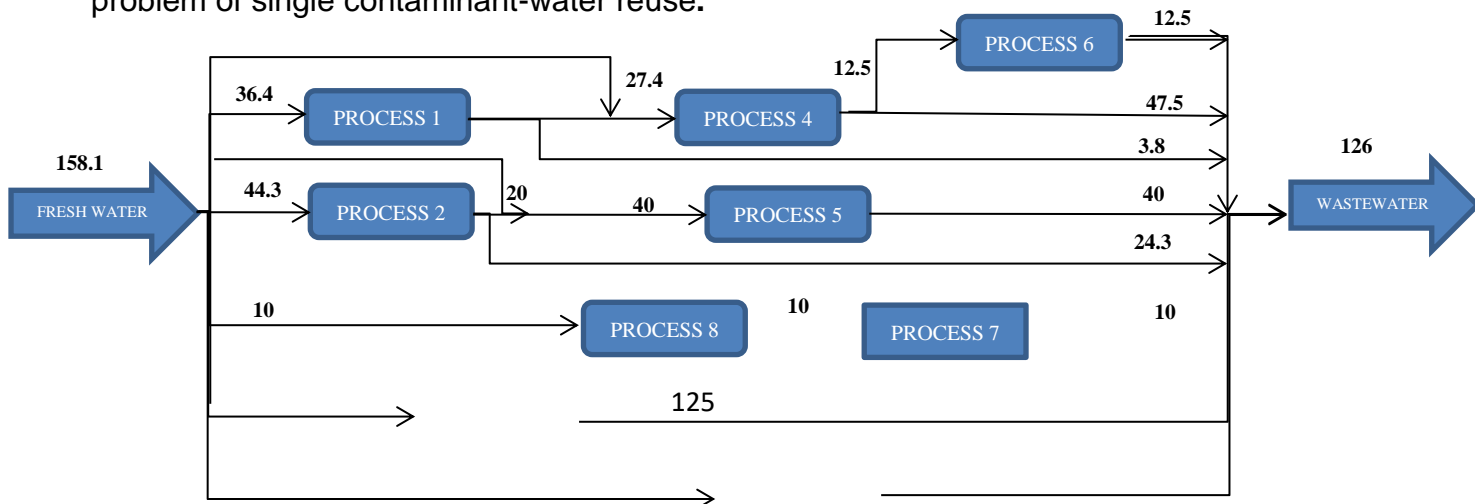
Table 5.18: End of diagnostic solution of the problem corresponding to Figure solution of 9 industrial processes.

Process Number	Type of water used by the process	Freshwater intake (m ³ /h)	Wastewater reuse (m ³ /h)	Contaminant Concentration (Allowed in) C ^{lim} _{in} (ppm)	Contaminant Concentration (Produced out) C ^{lim} _{out} (ppm)
1	Freshwater only	36.4	0.0	25	80
2	Freshwater only	44.3	0.0	25	100
3	Fresh & wastewater	10.0	12.9	25	200
4	Fresh & wastewater	27.4	32.6	50	100
5	Fresh & wastewater	20.0	20.0	50	800
6	Wastewater only	0.0	12.5	400	800
7	Wastewater only	0.0	10.0	400	800
8	Freshwater only	10.0	0.0	0	100
9	Freshwater only	10.0	0.0	0	100
Total Flowrate (m ³ /h)		158.1	88.0		

Superstructure Schematic Network:

The superstructure schematic matlab result network configuration for 9 industrial processes optimum water-using network of the solution is shown in figure 5.8.

MATLAB results for 9 processes optimum water-using network for an example problem of single contaminant-water reuse.



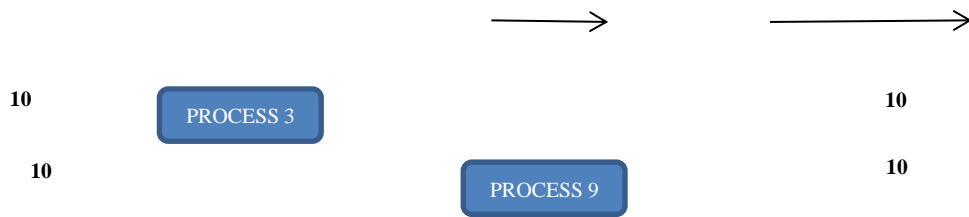


Figure 5.8: The diagrammatical superstructure representation of the solution of 9 industrial processes.

The solution of the problem corresponding to the diagrammatical Superstructure representation of the solution is shown in Table 5.33. It present the obtained result, indicating that the minimum total freshwater required by the industry is 145.7 m³/h, 25.4 m³/h for process 1, 31.9 m³/h for process 2, 17.0 m³/h for process 3, 28.9 m³/h for process 4, 18.1 m³/h for process 5, 11.3 m³/h for process 8 and 13.0 m³/h for process 9. Process 3 and 5 reuse additional 3.8 m³/h and 15.9 m³/h of wastewater respectively. While, process 6 and 7 reuse 10.5 m³/h and 7.8 m³/h of wastewater respectively. This result is exactly equal to the result obtained by Bagajewicz *et al.*, (2002), Feng *et al.*, (2009) and Liang, and Hui, (2016). However the superstructure obtained from this method is much easier to implement practically in any given industry with 9 water using processes and similar levels of contaminant.

For the computational time of the above problem, GA takes a very short time in solving this problem, it spends 7.5 seconds without hybrid function and 10.1 seconds with hybrid function to obtain the optimum result. So, the algorithm is improved to overcome the deficiency of taking long time to solve WAP problem as observed by other researchers.

5.10: Single Contaminant Water Reuse without Regeneration for 10 (ten)

Processes:

The number of variables as described in chapter 2 for ten industrial processes is $n^2+n=110$. The variables are freshwater, wastewater and wastewater for reuse, represented as follows: $F_1, F_2, F_3, F_4, F_5, F_6, F_7, F_8, F_9, F_{10}, W_1, W_2, W_3, W_4, W_5, W_6, W_7, W_8, W_9, W_{10}, X_{12}, X_{13}, X_{14}, X_{15}, X_{16}, X_{17}, X_{18}, X_{19}, X_{110}, X_{21}, X_{23}, X_{24}, X_{25}, X_{26}, X_{27}, X_{28}, X_{29}, X_{210}, X_{31}, X_{32}, X_{34}, X_{35}, X_{36}, X_{37}, X_{38}, X_{39}, X_{310}, X_{41}, X_{42}, X_{43}, X_{45}, X_{46}, X_{47}, X_{48}, X_{49}, X_{410}, X_{51}, X_{52}, X_{53}, X_{54}, X_{56}, X_{57}, X_{58}, X_{59}, X_{510}, X_{61}, X_{62}, X_{63}, X_{64}, X_{65}, X_{67}, X_{68}, X_{69}, X_{610}, X_{71}, X_{72}, X_{73}, X_{74}, X_{75}, X_{76}, X_{78}, X_{79}, X_{710}, X_{81}, X_{82}, X_{83}, X_{84}, X_{85}, X_{86}, X_{87}, X_{89}, X_{810}, X_{91}, X_{92}, X_{93}, X_{94}, X_{95}, X_{96}, X_{97}, X_{98}, X_{910}, X_{101}, X_{102}, X_{103}, X_{104}, X_{105}, X_{106}, X_{107}, X_{108}, X_{109}$, respectively.

5.10.1 Test Problem: Input Limiting Process Data for Ten industrial process:

Test Problem: Input Limiting Process Data:

It comprises a system of 10 processes. This example is taken from the literature Bagajewicz and Savelski (2001); Poplewski et al. (2011) and Trigueros et al. (2012)

The problem is based on the consideration of salt as a contaminant in a refinery wastewater data.

Table 5.19: Rough Limiting Process Data for Ten Industrial processes

Rough Limiting Process Data			
Operation	Mass Load ΔM (kg/hr)	Contaminant Concentration (Allowed in) C_{in}^{lim} (ppm)	Contaminant Concentration (Produced out) C_{out}^{lim} (ppm)
1	2	25	80
2	2.88	25	90
3	4	25	200
4	3	50	100
5	30	50	800
6	5	400	800
7	2	400	600
8	1	0	100
9	20	50	300
10	6.5	150	300

5.10.2 Representation of Single Contaminant Water Reuse without Regeneration in Matlab for 10 industrial processes

The fitness function is vectorised and represented in Matlab as shown in appendix C8. The linear constraints equations in equations 5.2a to 5.3c are represented in Matlab software as the matrix and vector of equalities (Aeq and beq) using the coefficient of the variables. The Nonlinear Constraints functions are vectorised and represented in Matlab as shown in appendix C8. The code for obtaining the solution in Matlab is shown in appendix C8. This will search for the possible solution of the problem and display the result as vector when the stopping criteria are met.

5.10.3 The result of Single Contaminant Water Reuse without Regeneration in Matlab for 10 industrial processes

The set of functions, genetic parameters and genetic operators used by GA for diagnostic analysis of the problem are as shown in Table 5.3. The differences are Fitness function is @FRW8 with 110 number of variables, 20 Equality constraints and '@Constraints_FRW8' as the nonlinear constraint function.

Optimisation comes to termination when the average change in the fitness value is less than Function Tolerance and constraint violation is less than Constraint Tolerance. The obtained result at termination is 169.4m³/h.

Switching to the hybrid optimisation algorithm (fmincon) leads to Local minimum within the last region, which is the optimum result if Constraints are satisfied. The final result is displayed as shown in Table 5.34.

The f-count is the number of function evaluations that the GA solver took to converge to a local solution. The obtained result is indicated in column 3 as the best-f(x) for the first 2 generations. The maximum constraints value in column 4 indicates the values

that satisfy the constraints and the stall-generation gives the number of times the minimum of generations are computed regardless of the convergence criteria.

Table 5.20: End of diagnostic information for the solution of 10 industrial processes/

Generation	f-count	Best - f(x)	Max - constraint	Stall - Generations
1	572	169.9556	2.359e-15	0
2	1092	169.4056	2.359e-15	1
3	1662	165.9324	4.472e-16	0
4	2182	165.9024	4.472e-16	0

Table 5.35 present the individual values of each variable after the analysis.

Table 5.21: End of diagnostic solution of Ten industrial processes.

F ₁	F ₂	F ₃	F ₄	F ₅	F ₆	F ₇	F ₈	F ₉	F ₁₀
25.3	31.9	16.4	28.9	17.9	0.0	0.0	10.0	35.5	0.0
W ₁	W ₂	W ₃	W ₄	W ₅	W ₆	W ₇	W ₈	W ₉	W ₁₀
0.0	0.0	0.0	0.0	40.0	10.0	10.0	0.0	64.4	41.5

X ₁₂	X ₁₃	X ₁₄	X ₁₅	X ₁₆	X ₁₇	X ₁₈	X ₁₉	X ₁₁₀
1.8895	0	0.3209	0	0	0	0	0.0000	0
X ₂₁	X ₂₃	X ₂₄	X ₂₅	X ₂₆	X ₂₇	X ₂₈	X ₂₉	X ₂₁₀
0.9415	0.0000	0.0000	0	0	0	0	0.0000	0
X ₃₁	X ₃₂	X ₃₄	X ₃₅	X ₃₆	X ₃₇	X ₃₈	X ₃₉	X ₃₁₀
2.2077	3.1651	1.0995	0	0.0000	0	0.0000	0.0000	0.0000
X ₄₁	X ₄₂	X ₄₃	X ₄₅	X ₄₆	X ₄₇	X ₄₈	X ₄₉	X ₄₁₀
3.6812	3.4551	0	0.0000	0	0.0000	0.0959	0	0
X ₅₁	X ₅₂	X ₅₃	X ₅₄	X ₅₆	X ₅₇	X ₅₈	X ₅₉	X ₅₁₀
6.1645	8.6897	0.0000	7.2477	0.0000	0	0.0000	0	0.0000
X ₆₁	X ₆₂	X ₆₃	X ₆₄	X ₆₅	X ₆₇	X ₆₈	X ₆₉	X ₆₁₀
0.0000	0	0.1914	0.0000	0.6371	0.7563	0.0000	9.3153	0.1525

X ₇₁	X ₇₂	X ₇₃	X ₇₄	X ₇₅	X ₇₆	X ₇₈	X ₇₉	X ₇₁₀
0	0	0.4113	0.0045	0.6666	1.4163	0	7.0141	0.4853

X ₈₁	X ₈₂	X ₈₃	X ₈₄	X ₈₅	X ₈₆	X ₈₇	X ₈₉	X ₈₁₀
0.0000	0.0000	0	0.0000	0.0000	0	0	0.0000	0.0000

X ₉₁	X ₉₂	X ₉₃	X ₉₄	X ₉₅	X ₉₆	X ₉₇	X ₉₈	X ₉₁₀
14.5318	15.6375	0	12.0738	0.0000	0.0000	0	2.2270	0.0000

X ₁₀₁	X ₁₀₂	X ₁₀₃	X ₁₀₄	X ₁₀₅	X ₁₀₆	X ₁₀₇	X ₁₀₈	X ₁₀₉
0.0000	0.0000	21.6667	13.9901	0	0	0.0000	7.6766	0.0000

Table 5. 22: End of diagnostic solution of the problem corresponding to Figure solution of ten industrial processes.

Process Number	Type of water used by the process	Fresh water intake (m ³ /h)	Wastewater reuse (m ³ /h)	Contaminant Concentration (Allowed in) C ^{lim} _{in} (ppm)	Contaminant Concentration (Produced out) C ^{lim} _{out} (ppm)
1	Freshwater only	25.3	0.0	25	80
2	Freshwater only	31.9	0.0	25	100
3	Freshwater only	16.4	0.0	25	200
4	Freshwater only	28.9	0.0	50	100
5	Fresh & wastewater	17.9	22,1	50	800
6	Wastewater only	0.0	10.0	400	800
7	Wastewater only	0.0	10.0	400	600
8	Freshwater only	10.0	0.0	0	100
9	Fresh & wastewater	35.5	28.9	50	300
10	Wastewater only	0.0	41.5	150	300
Total Flowrate (m ³ /h)		165.9	113.7		

Superstructure Schematic Network

The superstructure schematic MATLAB result network configuration for 10 industrial processes Optimum water-using network of the solution is shown in figure 5.9.

Matlab results for 10 industrial processes optimum water-using network for an example problem of single contaminant-water reuse.

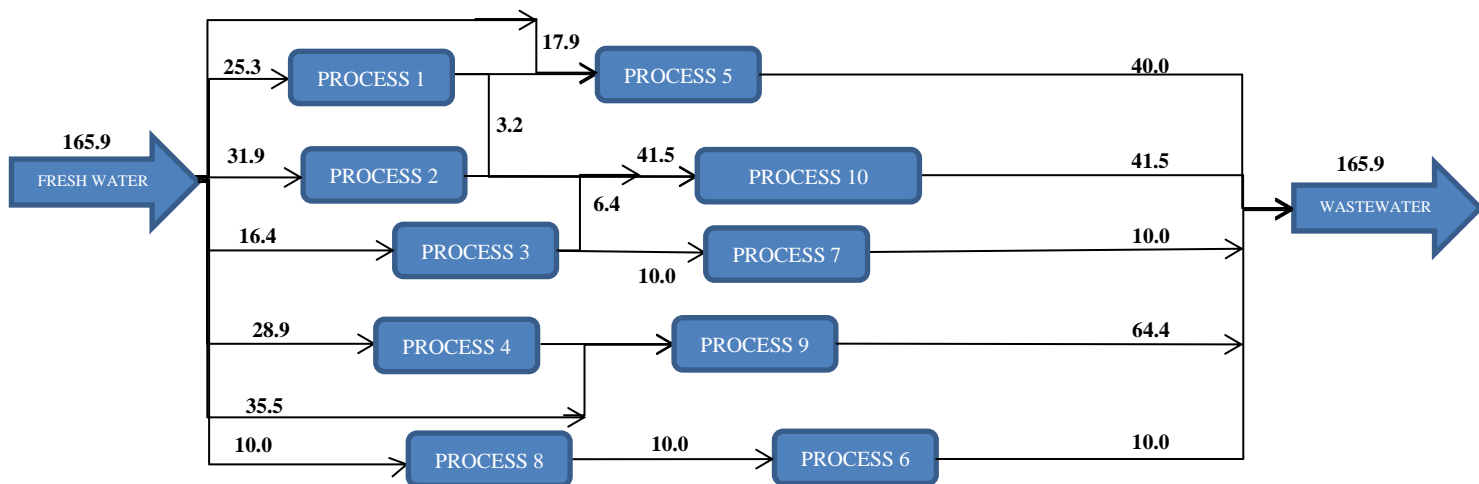


Figure 5.9: The diagrammatical Superstructure representation of the solution of 10 industrial processes.

Solution of the problem corresponding to the diagrammatical Superstructure representation of the solution is shown in Table 5.36. It present the obtained result, indicating that the minimum total freshwater required by the industry is 165.9 m³/h, 25.3 m³/h for process 1, 31.9 m³/h for process 2, 16.4 m³/h for process 3, 28.9 m³/h for process 4, 17.9 m³/h for process 5, 10.0 m³/h for process 8 and 35.5 m³/h for process 9. Process 5 and 9 reuse additional 20.8 m³/h and 28.2 m³/h of wastewater respectively. While, process 6, 7 and 10 reuse 9.6 m³/h, 9.2m³/h and 42.7 m³/h of wastewater respectively. This result is exactly equal to the result obtained by Bagajewicz and Savelski (2001); Poplewski et al. (2011) and **Trigueros et al. (2012)**

For the computational time of the above problem, GA takes a very short time in solving this problem. It takes 8.9 seconds without hybrid function and 9.4 seconds with hybrid function to obtain the optimum result. So, the algorithm is improved to overcome the deficiency of taking long time to solve WAP problem as observed by other researchers.

5.11 Values obtained for Single Contaminant Water Reuse without Regeneration for all Processes With and without Hybrid function

The above examples were selected from literature to show the mathematical application of WAP models used in optimisation for Single contaminant and their data set-up requirements. It also described the procedure involved in the general equations that presents the model based on the number of processes. Table 5.37 shows the values of the solution obtained from the WAP model using GA with and without hybrid function and the percentage error of the value obtained without hybrid function.

Table 5.23: Comparison of End of diagnostic solution of the problems for 1 to 10 industrial processes with and without using hybrid function.

Number of Industrial Process	Solution of WAP using GA without hybrid function (A)	Solution of WAP using GA with hybrid function (B)	Percentage Error without Hybrid (A-B)/B
2	30.0	25.0	20.0%
3	60.0	56.7	5.8%
4	92.5	90	2.8%
5	40.8	30	36.0%
6	187	156	19.9%
7	131.2	116.0	13.1%
8	138.9	138.2	0.5%
9	167.7	158.1	6.1%
10	169.4	165.9	2.1%

The solution indicates the advantage of using hybrid function for GA hybrid function, which is preventing the GA from being stuck in the local minimum as described in the last chapter. From the above problems obtained from the literature it can be observed that inclusion of the hybrid function in finding the solution of WAP problem using GA prevents up to 36% error for five industrial processes, 20% for two and six industrial process as shown in Table 5.37.

5.12 Conclusion

This chapter has presented all the necessary mathematical steps required in solving the WAP problem for single contaminant water reuse of 2 to 10 industrial processes using GA. The WAP problems analysed were obtained from the literature. They were used here to validate the selected method for the solution of the WAP model. The total minimum freshwater needs of those problems were determined subject to contaminant mass balance and maximum inlet concentration constraints. All the equality constraints were satisfied before accepting the final value as the optimum solution. The hybrid function in each case goes further to obtain the optimum solution which is better than that in the literature as indicated. This also indicates the advantage of adding 'fmincon' hybrid function in finding the optimum result of the GA analysis for single objective of freshwater minimisation. The superstructure diagram of the solution for possible practical application of the result is also presented. The solution for each number of processes has efficiency ranging from 2.8% to 36% compared with the solution using GA without hybrid function. The solution was also compared with result in the literature. The computational time of all the problems analysed is very short compared to what was reported in the literature. The reader can easily follow the steps to obtain the optimum result of any WAP problem as demonstrated.

The next chapter will analyse the mathematical application for solving WAP model in the optimisation of multi-contaminant water reuse network with and without regeneration of the wastewater.

CHAPTER SIX

6.0 WATER APPLICATION PLANNING (WAP) MODEL FOR MULTI-CONTAMINANT WATER REUSE WITH AND WITHOUT REGENERATION

This chapter describe the mathematical application of WAP model in the optimisation of multi-contaminant water reuse network and their data set-up requirements. It also described the procedure involved in the general equations that presents the model based on the selected 3 industrial processes WAP problems. The 3 industrial processes WAP problems are obtained from the literature to describe the required steps in solving the multi-contaminant WAP problem with and without regeneration. The 3 processes were selected for easy and clear demonstration of the capabilities of the selected method. Furthermore, the values obtained using GA with hybrid function as proposed by this research methodology was compared with that of literature.

6.1 Introduction

The model developed in this research was used to find solution for 3 industrial processes multi-contaminant WAP problems for water reuse with and without regeneration using GA and 'Fmincon' hybrid in MATLAB software. The problems were obtained from the literature as described in each section.

Regeneration here refers to the processes of treatment of wastewater to be reused or disposed in to the environment. The model will consider the removal efficiency of various technologies (e.g. Reverse osmosis, sedimentation, ultrafiltration, ion exchange, activated sludge, and trickling filter, Electro-dialysis reversal (EDR), etc) capable of removing different types of contaminants. All the variables were defined in the list of symbols and nomenclature section of this thesis.

6.2 Multi-Contaminant Water Reuse without Regeneration for 3 Industrial Processes

The number of variables as described in chapter 3 for three processes with three (3) Multi-Contaminants (m) in WAP problem without regeneration is $n^2+n+nm = 21$. The variable are freshwater, produced wastewater, wastewater for reuse and contaminants concentrations represented as follows: $F_1, F_2, F_3, W_1, W_2, W_3; X_{1,2}, X_{1,3}, X_{2,1}, X_{2,3}, X_{3,1}, X_{3,2}, C_{11}, C_{12}, C_{13}, C_{21}, C_{22}, C_{23}, C_{31}, C_{32}, C_{33}$, respectively.

The fitness function is the Sum of fresh water flow rates at the entrance of each water using process as shown in equation 6.1a and b:

$$F = \text{Min} \sum_{i=1}^3 F_i \dots \dots \dots (6.1a)$$

$$F = F_1 + F_2 + F_3 \dots \dots \dots (6.1b)$$

The Linear Constraints functions of the water mass balance are the same with single contaminant WAP problem, the differences are in the linear constraints of the contaminant mass balance and maximum contaminant inlet concentrations, the subscript k was added to the initial subscripts i and j. The constraints are represented in equation 6.2 and 6.3 as follows:

4. The constraint of the contaminant mass balance of all processes:

$$\sum_{j \neq i} C_{j,k,out} X_{i,j} + \Delta M_{i,k} - C_{i,k,out} \left(W_i + \sum_{j \neq i} X_{j,i} \right) = 0 \dots \dots \dots (6.2a)$$

$$C_{2,1,out} X_{1,2} + C_{3,1,out} X_{1,3} + \Delta M_{1,1} - C_{1,1,out} (W_1 + X_{2,1} + X_{3,1}) = 0 \dots \dots \dots (6.2b)$$

$$C_{2,2,out} X_{1,2} + C_{3,2,out} X_{1,3} + \Delta M_{1,2} - C_{1,2,out} (W_1 + X_{2,1} + X_{3,1}) = 0 \dots \dots \dots (6.2c)$$

$$C_{2,3,out} X_{1,2} + C_{3,3,out} X_{1,3} + \Delta M_{1,1} - C_{1,3,out} (W_1 + X_{2,1} + X_{3,1}) = 0 \dots \dots \dots (6.2d)$$

$$C_{1,1,out} X_{2,1} + C_{3,1,out} X_{2,3} + \Delta M_{2,1} - C_{2,1,out} (W_2 + X_{1,2} + X_{3,2}) = 0 \dots \dots \dots (6.2e)$$

$$C_{1,2,out}X_{2,1} + C_{3,2,out}X_{2,3} + \Delta M_{2,2} - C_{2,2,out}(W_2 + X_{1,2} + X_{3,2}) = 0 \dots \dots \dots (6.2f)$$

$$C_{1,3,out}X_{2,1} + C_{3,3,out}X_{2,3} + \Delta M_{2,3} - C_{2,3,out}(W_2 + X_{1,2} + X_{3,2}) = 0 \dots \dots \dots (6.2g)$$

$$C_{1,1,out}X_{3,1} + C_{2,1,out}X_{3,2} + \Delta M_{3,1} - C_{3,1,out}(W_3 + X_{1,3} + X_{2,3}) = 0 \dots \dots \dots (6.2h)$$

$$C_{1,2,out}X_{3,1} + C_{2,2,out}X_{3,2} + \Delta M_{3,2} - C_{3,2,out}(W_3 + X_{1,3} + X_{2,3}) = 0 \dots \dots \dots (6.2i)$$

$$C_{1,3,out}X_{3,1} + C_{2,3,out}X_{3,2} + \Delta M_{3,3} - C_{3,3,out}(W_3 + X_{1,3} + X_{2,3}) = 0 \dots \dots \dots (6.2j)$$

3. The Constraints of Maximum Contaminant inlet concentration:

$$C_{j,in} = \frac{\sum_{j \neq i} C_{j,k,out} X_{i,j}}{\sum_{j \neq i} X_{i,j} + F_i} \leq C_{i,in}^{max} \dots \dots \dots (6.3a)$$

$$C_{2,1,out} = \frac{C_{2,1,out} X_{1,2} + C_{3,1,out} X_{1,3}}{F_1 + X_{1,2} + X_{1,3}} \leq C_{1,1,in}^{max} \dots \dots \dots (6.3b)$$

$$C_{2,2,out} = \frac{C_{2,2,out} X_{1,2} + C_{3,2,out} X_{1,3}}{F_1 + X_{1,2} + X_{1,3}} \leq C_{1,2,in}^{max} \dots \dots \dots (6.3c)$$

$$C_{2,3,out} = \frac{C_{2,3,out} X_{1,2} + C_{3,3,out} X_{1,3}}{F_1 + X_{1,2} + X_{1,3}} \leq C_{1,3,in}^{max} \dots \dots \dots (6.3d)$$

$$C_{1,1,out} = \frac{C_{1,1,out} X_{2,1} + C_{3,1,out} X_{2,3}}{F_2 + X_{2,1} + X_{2,3}} \leq C_{2,1,in}^{max} \dots \dots \dots (6.3e)$$

$$C_{1,2,out} = \frac{C_{1,2,out} X_{2,1} + C_{3,2,out} X_{2,3}}{F_2 + X_{2,1} + X_{2,3}} \leq C_{2,2,in}^{max} \dots \dots \dots (6.3f)$$

$$C_{1,3,out} = \frac{C_{1,3,out} X_{2,1} + C_{3,3,out} X_{2,3}}{F_2 + X_{2,1} + X_{2,3}} \leq C_{2,3,in}^{max} \dots \dots \dots (6.3g)$$

$$C_{1,1,out} = \frac{C_{1,1,out} X_{3,1} + C_{2,1,out} X_{3,2}}{F_3 + X_{3,1} + X_{3,2}} \leq C_{3,in}^{max} \dots \dots \dots (6.3h)$$

$$C_{1,2,out} = \frac{C_{1,2,out} X_{3,1} + C_{2,2,out} X_{3,2}}{F_3 + X_{3,1} + X_{3,2}} \leq C_{3,in}^{max} \dots \dots \dots (6.3i)$$

$$C_{1,3,out} = \frac{C_{1,3,out} X_{3,1} + C_{2,3,out} X_{3,2}}{F_3 + X_{3,1} + X_{3,2}} \leq C_{3,in}^{max} \dots \dots \dots (6.3j)$$

6.2.1 Test Problem: Input Limiting Process Data for 3 industrial processes with 3 contaminants

The limiting data for water minimisation for a specialty chemical production industry having 3 industrial processes units and three contaminants was obtained from Mann and Liu (1999), Prakotpol and Srinophakun (2004), and Cao et al (2007) with the limiting water data for the process units shown in Table 6.1 below: The rough limiting process data for mass load, contaminant concentration allowed in and produced out are shown. The expected freshwater to be used in this case was assumed to have zero impurity. This data was used to determine the minimum flowrate of freshwater and wastewater for the 3 (three) industrial processes with three different contaminants.

Table 6.1: Rough Limiting Process Data for three processes with three contaminants

Rough Limiting Process Data				
Process unit	Contaminant	Mass Load M (g/h)	Contaminant Concentration (Allowed in) $C_{in,max}$ (ppm)	Contaminant Concentration (Produced out) $C_{out,max}$ (ppm)
1	A	3000	0	100
	B	2400	0	80
	C	1800	0	60
2	A	4000	50	150
	B	3000	40	115
	C	3600	15	105
3	A	1500	50	125
	B	600	50	80
	C	2000	30	130

6.2.2 Representation of Multi-Contaminant Water Reuse without Regeneration in Matlab for three industrial processes:

The fitness function is vectorised and represented in Matlab as shown in appendix D1. The linear constraints equations in equations 5.14 (a-f) and 5.15 (a-f) in appendix B3

are used to solve this problem and are represented in Matlab software as the matrix and vector of equalities (Aeq and beq) using the coefficient of the variables. The matrix and vector of inequalities are not available in the constraints, therefore (A and b) are represented as empty set as follows: A= [], b= [].

The vector for lower and upper bounds (LB and UB) are represented with the set of lowest and highest value of outcome of each point as shown in appendix D1. The Nonlinear Constraints functions in equation 6.2 and 6.3 are vectorised and represented in Matlab as shown in appendix D1. The code for obtaining the solution in Matlab is shown in appendix D1. This will search for the possible solution of the problem and display the result as vector when the stopping criteria are met.

6.2.3 The result of Multi-Contaminant Water Reuse without Regeneration in Matlab for 3 industrial processes

The set of functions, genetic parameters and genetic operators used by GA for diagnostic analysis of the problem are as shown in Table 5.3 of chapter five. The differences are Fitness function is @FRW with 21 number of variables, 12 Equality constraints and '@ConstraintsMULT_FRW' as the nonlinear constraint function.

Optimisation comes to termination when the average change in the fitness value is less than Function Tolerance and constraint violation is less than Constraint Tolerance.

Switching to the hybrid optimisation algorithm (FMINCON) leads to Local minimum within the last region, which is the optimum result if Constraints are satisfied. The final result is displayed as shown in Table 6.2.

Table 6. 2: End of diagnostic information for the solution of three process

Generation	f-count	Best - f(x)	Max - constraint	Stall - Generations
1	572	72.9556	2.359e-15	0

2	1092	72.9556	2.359e-15	1
3	1662	72.7324	4.472e-06	0
4	2182	72.7324	4.472e-06	0

Table 6.3 present the individual values of each variable after the analysis.

Table 6. 3: End of diagnostic solution of three process

F₁	F₂	F₃	W₁	W₂	W₃
30	34	7	7	36	28

X₁₂	X₁₃	X₂₁	X₂₃	X₃₁	X₃₂
0	0	1	1	20	0

X₁₁₁	X₁₁₂	X₁₁₃	X₁₂₁	X₁₂₂	X₁₂₃	X₁₃₁	X₁₃₂	X₁₃₃
24	19	14	116	96	0	42	61	50

Solution of the problem corresponding to the diagrammatical Superstructure representation of the solution is shown in Table 6.4. The obtained result, indicates that the minimum total freshwater required by the industry is 71.0 m³/h, 30m³/h for process 1 and 34.0 m³/h for process 2 and 7.0 m³/h for process 3. While, process 2 and 3 reuse 2.0m³/h and 21.0 m³/h of wastewater respectively, from process 1.

Table 6. 4: End of diagnostic solution of the problem corresponding to the solution of 3 industrial processes.

Process Number	Type of water used by the process	Fresh water intake (m ³ /h)	Wastewater reuse (m ³ /h)
1	Freshwater only	30.0	0.0
2	Fresh & wastewater	34.0	2.0
3	Fresh & wastewater	7.0	21.0
Total Flowrate (m ³ /h)		71.0	23.0

Superstructure Schematic Network:

The superstructure schematic matlab result network configuration for 3 processes optimum water-using network of the solution is shown in Figure 6.1

MATLAB results for 3 industrial processes Optimum water-using network for an example problem of Multi-contaminant-water reuse.

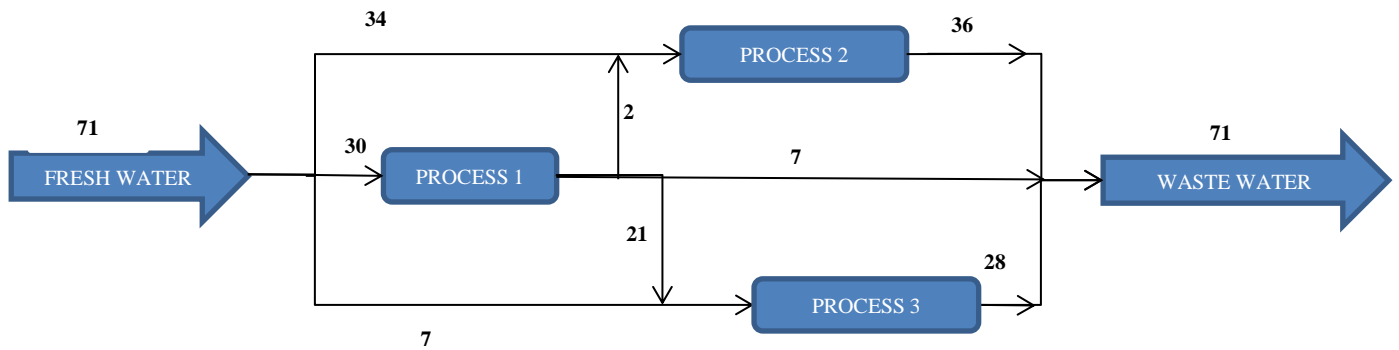


Figure 6.1: The diagrammatical Superstructure representation of the solution of multi-contaminant water reuse without regeneration for 3 industrial processes.

The minimum fresh water consumption reported by the literature in the work of Mann and Liu (1999), Prakotpol and Srinophakun (2004) and Cao *et. al.*, (2007) is 70m³/h. Process 1 is a head process and the mass loads are such that all the three contaminants A, B and C exit at the maximum possible concentrations. Also both processes 2 and 3 have contaminants B and C at their maximum possible outlet concentrations.. The realizing superstructure representation of the solution of multi-contaminant water reuse without regeneration for 3 industrial processes is shown in Figure 6.1.

6.3 Multi-Contaminant Water Reuse with Regeneration for 3 Industrial Processes

The number of variables as described in chapter three for 3 industrial processes with 3 multi-contaminants (m) in WAP problem with regeneration is $n^2+3n+nm = 27$. The variable are freshwater, produced wastewater, wastewater for reuse, contaminants concentrations and regeneration process used as treatment, represented as: $F_1, F_2, F_3; W_1, W_2, W_3; X_{1,2}, X_{1,3}, X_{2,1}, X_{2,3}, X_{3,1}, X_{3,2}; C_{11}, C_{12}, C_{13}, C_{21}, C_{22}, C_{23}, C_{31}, C_{32}, C_{33}; R_{1r}, R_{2r}, R_{3r}, R_{r1}, R_{r2}, R_{r3}$; respectively.

The fitness function is the Sum of fresh water flow rates at the entrance of each water using process as shown in equation 6.4:

$$F = \text{Min} \sum_{i=1}^3 F_i \dots \dots \dots (6.4a)$$

$$F = F_1 + F_2 + F_3 \dots \dots \dots (6.4b)$$

The Linear Constraints functions of the water mass balance and contaminant mass balance and maximum contaminant inlet concentrations are different from the case of WAP problem without regeneration in that, the term $X_{i,r}$ was added to the initial terms as the regeneration variable. The linear constraints are represented in equation 6.5 and 6.6, while nonlinear constraint of maximum contaminant inlet concentration is represented in equation 6.7 as follows:

CONSTRAINTS:

Linear Constraint functions:

1. The constraint of the water mass balance of all process

$$F_i + \sum_{j \neq i} X_{i,j} + X_{i,r} - W_i - \sum_{j \neq i} X_{j,i} - X_{r,i} = 0 \dots \dots \dots (6.5a)$$

$$F_1 + X_{1,2} + X_{1,3} + X_{1,r} - W_1 - X_{2,1} - X_{3,1} - X_{r,1} = 0 \dots \dots \dots (6.5b)$$

$$F_2 + X_{2,1} + X_{2,3} + X_{2,r} - W_2 - X_{1,2} - X_{3,2} - X_{r,2} = 0 \dots \dots \dots (6.5c)$$

$$F_3 + X_{3,1} + X_{3,2} + X_{3,r} - W_3 - X_{1,3} - X_{2,3} - X_{r,3} = 0 \dots \dots \dots (6.5d)$$

2. The constraint of the contaminant mass balance of all processes:

$$\sum_{j \neq i} C_{j,k,out} X_{i,j} + C_o X_{i,r} + \Delta M_{i,k} - C_{i,k,out} \left(W_i + \sum_{j \neq i} X_{j,i} + X_{r,i} \right) = 0 \dots \dots \dots (6.6a)$$

$$C_{2,1,out} X_{1,2} + C_{3,1,out} X_{1,3} + C_{o,1} X_{1,r} + \Delta M_{1,1} - C_{1,1,out} (W_1 + X_{2,1} + X_{3,1} + X_{r,1}) = 0 \dots \dots (6.6b)$$

$$C_{2,2,out} X_{1,2} + C_{3,2,out} X_{1,3} + C_{o,2} X_{1,r} + \Delta M_{1,2} - C_{1,2,out} (W_1 + X_{2,1} + X_{3,1} + X_{r,1}) = 0 \dots \dots (6.6c)$$

$$C_{2,3,out} X_{1,2} + C_{3,3,out} X_{1,3} + C_{o,3} X_{1,r} + \Delta M_{1,3} - C_{1,3,out} (W_1 + X_{2,1} + X_{3,1} + X_{r,1}) = 0 \dots \dots (6.6d)$$

$$C_{1,1,out} X_{2,1} + C_{3,1,out} X_{2,3} + C_{o,1} X_{2,r} + \Delta M_{2,1} - C_{2,1,out} (W_2 + X_{1,2} + X_{3,2} + X_{r,2}) = 0 \dots \dots (6.6e)$$

$$C_{1,2,out} X_{2,1} + C_{3,2,out} X_{2,3} + C_{o,2} X_{2,r} + \Delta M_{2,2} - C_{2,2,out} (W_2 + X_{1,2} + X_{3,2} + X_{r,2}) = 0 \dots \dots (6.6f)$$

$$C_{1,3,out} X_{2,1} + C_{3,3,out} X_{2,3} + C_{o,3} X_{2,r} + \Delta M_{2,3} - C_{2,3,out} (W_2 + X_{1,2} + X_{3,2} + X_{r,2}) = 0 \dots \dots (6.6g)$$

$$C_{1,1,out} X_{3,1} + C_{2,1,out} X_{2,3} + C_{o,1} X_{3,r} + \Delta M_{3,1} - C_{3,1,out} (W_3 + X_{1,3} + X_{2,3} + X_{r,3}) = 0 \dots \dots (6.6h)$$

$$C_{1,2,out} X_{3,1} + C_{2,2,out} X_{3,2} + C_{o,2} X_{3,r} + \Delta M_{3,2} - C_{3,2,out} (W_3 + X_{1,3} + X_{2,3} + X_{r,3}) = 0 \dots \dots (6.6i)$$

$$C_{1,3,out} X_{3,1} + C_{2,3,out} X_{3,2} + C_{o,3} X_{3,r} + \Delta M_{3,3} - C_{3,3,out} (W_3 + X_{1,3} + X_{2,3} + X_{r,3}) = 0 \dots \dots (6.6j)$$

3. Maximum Contaminant inlet concentration:

$$C_{j,in} = \frac{\sum_{j \neq i} C_{j,k,out} X_{i,j} + C_{o,k} X_{i,r}}{\sum_{j \neq i} X_{i,j} + F_i + X_{i,r}} \leq C_{i,in}^{max} \dots \dots \dots (6.7a)$$

$$C_{2,1,out} = \frac{C_{2,1,out} X_{1,2} + C_{3,1,out} X_{1,3} + C_{o,1} X_{1,r}}{F_1 + X_{1,2} + X_{1,3} + X_{1,r}} \leq C_{1,1,in}^{max} \dots \dots \dots (6.7b)$$

$$C_{2,2,out} = \frac{C_{2,2,out} X_{1,2} + C_{3,2,out} X_{1,3} + C_{o,2} X_{1,r}}{F_1 + X_{1,2} + X_{1,3} + X_{1,r}} \leq C_{1,2,in}^{max} \dots \dots \dots (6.7c)$$

$$C_{2,3,out} = \frac{C_{2,3,out} X_{1,2} + C_{3,3,out} X_{1,3} + C_{o,3} X_{1,r}}{F_1 + X_{1,2} + X_{1,3} + X_{1,r}} \leq C_{1,3,in}^{max} \dots \dots \dots (6.7d)$$

$$C_{1,1,out} = \frac{C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + C_o X_{2,r}}{F_2 + X_{2,1} + X_{2,3} + X_{2,r}} \leq C_{2,in}^{max} \dots \dots \dots (6.7e)$$

$$C_{1,2,out} = \frac{C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + C_o X_{2,r}}{F_2 + X_{2,1} + X_{2,3} + X_{2,r}} \leq C_{2,in}^{max} \dots \dots \dots (6.7f)$$

$$C_{1,3,out} = \frac{C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + C_o X_{2,r}}{F_2 + X_{2,1} + X_{2,3} + X_{2,r}} \leq C_{2,in}^{max} \dots \dots \dots (6.7g)$$

$$C_{1,1,out} = \frac{C_{1,out} X_{3,1} + C_{2,out} X_{3,2} + C_o X_{3,r}}{F_3 + X_{3,1} + X_{3,2} + X_{3,r}} \leq C_{3,in}^{max} \dots \dots \dots (6.7h)$$

$$C_{1,2,out} = \frac{C_{1,out} X_{3,1} + C_{2,out} X_{3,2} + C_o X_{3,r}}{F_3 + X_{3,1} + X_{3,2} + X_{3,r}} \leq C_{3,in}^{max} \dots \dots \dots (6.7i)$$

$$C_{1,3,out} = \frac{C_{1,out} X_{3,1} + C_{2,out} X_{3,2} + C_o X_{3,r}}{F_3 + X_{3,1} + X_{3,2} + X_{3,r}} \leq C_{3,in}^{max} \dots \dots \dots (6.7j)$$

6.3.1 Test Problem (Input Limiting Process Data for 3 industrial processes)

The limiting data for water minimisation used in this section is the same as the data in section 5.1.1, as obtained from Mann and Liu (1999), also used by Cao et al (2007) with the limiting water data for the process units shown in Table 5.1. However, here the regeneration units were assumed to have efficiency of treating all the contaminants to the new concentration level of 25 ppm. While, the expected freshwater to be used in this case was assumed to have zero impurity (i.e. 0 ppm). This data was used to determine the minimum flowrate of freshwater and wastewater for the 3 industrial processes with regeneration.

6.3.2 Representation of Multi-Contaminant Water Reuse with Regeneration in Matlab for 3 Industrial Processes.

The fitness function is vectorised and represented in Matlab as shown in appendix D2. The linear constraints equations in equations 5.5a to 5.6j are represented in Matlab software as the matrix and vector of equalities (Aeq and beq) using the coefficient of the variables. The matrix and vector of inequalities are not available in the constraints, therefore (A and b) are represented as empty set as follows: A= [], b= []. The vector for lower and upper bounds (LB and UB) are represented with the set of lowest and highest value of outcome of each point as shown in appendix D2.

The Nonlinear Constraints functions are vectorised and represented in Matlab as shown in appendix D2. The code for obtaining the solution in Matlab is shown in appendix D2. The syntax for obtaining the solution in Matlab is as follows:

$x = \text{ga}(\text{fitnessfcn}, \text{nvars}, \text{A}, \text{b}, \text{Aeq}, \text{beq}, \text{LB}, \text{UB}, \text{nonlcon}, \text{options})$

This will search for the possible solution of the problem and display the result as vector when the stopping criteria are met.

6.3.3 The result of Multi-Contaminant Water Reuse with Regeneration in Matlab for 3 industrial processes

The set of functions, genetic parameters and genetic operators used by GA for diagnostic analysis of the problem are as shown in Table 5.3. The differences are Fitness function is @FRW with 27 number of variables due to increase in number of contaminants, 12 Equality constraints and '@ConstraintsMULT_REG_FRW2' as the nonlinear constraint function.

Optimisation comes to termination when the average change in the fitness value is less than Function Tolerance and constraint violation is less than Constraint Tolerance.

Switching to the hybrid optimisation algorithm (Fmincon) leads to Local minimum within the last region, which is the optimum result after the satisfaction of the constraints conditions. The final result is displayed as shown in Table 6.5 and 6.6.

Table 6. 5: End of diagnostic information for the solution of four industrial process

Generation	f-count	Best - f(x)	Max - constraint	Stall - Generations
1	10732	51.3071	7.568e-06	0
2	21132	51.3071	2.46e-06	0
3	31532	51.3071	2.499e-06	0
4	128532	51.307	9.941e-05	0
5	211732	51.3066	0.000113	0

Table 6.6 present the individual values of each variable after the analysis.

Table 6. 6: End of diagnostic solution of three process

F1	F2	F3	W1	W2	W3	X12	X13	X21	X23	X31	X32
45	6	0	0	25	26	21	0	0	0	0	9

C1A	C1B	C1c	C2A	C2B	C2c	C3A	C3B	C3c
514	514	0	200	0	0	0	41	18

R1r	R2r	R3r	Rr1	Rr2	Rr3
16	10	0	0	0	26

Table 6. 7: End of diagnostic solution of the problem corresponding to Figure solution of three industrial processes with regeneration.

Process Number	Type of water used by the process	Fresh water intake (m ³ /h)	Wastewater reuse (m ³ /h)
1	Freshwater only	45.0	0.0
2	Fresh & wastewater	6.0	19.0
3	Wastewater only	0.0	20.0
Total Flowrate (m ³ /h)		51.0	39.0

Superstructure Schematic Network:

The superstructure schematic MATLAB result network configuration for three (3) processes Optimum water-using network of the solution is shown in Figure 6.2

MATLAB results for 3 processes Optimum water-using network for an example problem of Multi-contaminant-water reuse with regeneration.

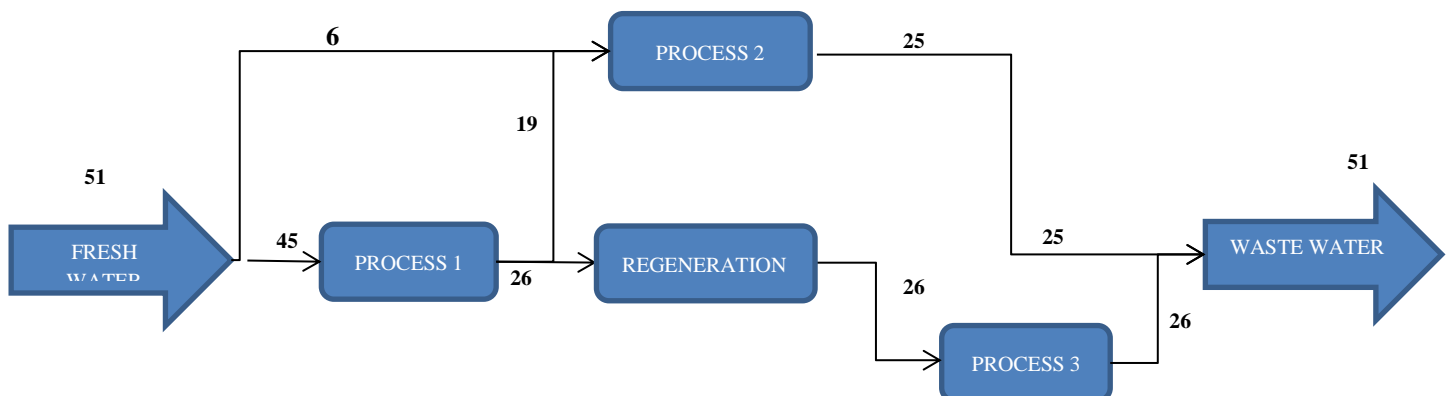


Figure 6 2: The diagrammatical Superstructure representation of the solution for 3 industrial processes with multi-contaminants and regeneration.

Solution of the problem corresponding to the diagrammatical Superstructure representation of the solution is shown in Table 6.7. The obtained result, indicates that the minimum total freshwater required by the industry with regeneration of 25 ppm is 51.0 m³/h, 45 m³/h for process 1 and 6.0 m³/h for process 2. Process 2 use additional 19.0 m³/h of wastewater. While, process 3 reuse 20.0 m³/h of wastewater only, from process 1 after regeneration.

6.4: Synthesis of Analysis of 3 industrial processes systems of multi-contaminant (with and without regeneration)

The obtained result of single contaminant water reuse without regeneration for 3 industrial processes from chapter 5, indicates that the minimum total freshwater required by the industry is 56.7m³/h (50m³/h for process 1 and 6.7m³/h for process 2. While, process 2 and 3 reuse 13.3m³/h and 20 m³/h of wastewater respectively, from process 1). Whereas, the result of multi-contaminant water reuse without regeneration for 3 industrial processes, indicates that the minimum total freshwater required by the industry is 71.0 m³/h (30m³/h for process 1 and 34.0 m³/h for process 2 and 7.0 m³/h for process 3. While, process 2 and 3 reuse 2.0m³/h and 21.0 m³/h of wastewater respectively, from process 1). There is an increase in water requirement of 25.2% for the industry due to consideration of different contaminants.

However, using regeneration of 25 ppm the minimum total freshwater required by the same industry (multi-contaminant water reuse) reduced to 51.0 m³/h (45 m³/h for process 1 and 6.0 m³/h for process 2. Process 2 use additional 19.0 m³/h of wastewater, while, process 3 reuse 20.0 m³/h of wastewater from process 1 after regeneration). This is reduction of 28.6% for the industry due to consideration of regeneration of different contaminants.

6.5: Conclusion:

This chapter has presented all the necessary mathematical steps required in solving the WAP problem for multi-contaminant water reuse of 3 industrial processes using GA, with and without regeneration. It also shows the advantage of adding regeneration in finding the optimum minimum freshwater. The required freshwater has reduced from 71.0 m³/h to 51.0 m³/h when regeneration of the wastewater using assumed regeneration unit of 25 ppm was used in the analysis. This is reduction of 28.6% for the industry due to consideration of regeneration of different contaminants. The readers can easily follow the steps to obtain the optimum result for other number of processes as demonstrated.

The next chapter will describe the mathematical application of WAP models used in optimisation of different objectives (multi-objective) involved in water reuse network and their data set-up requirements.

CHAPTER SEVEN

7.0 WATER APPLICATION PLANNING (WAP) MODEL FOR MULTI-OBJECTIVE WATER REUSE

This chapter describes the mathematical application of WAP models used in optimisation of different objectives (multi-objective) involved in water reuse network and their data set-up requirements. It also describes the procedure involved in the general equations that presents the model by using 3 industrial processes WAP problem obtained from literature. The 3 processes were selected for easy and clear demonstration of the capabilities of the selected method. Furthermore, the steps and the values obtained using multi-objective Genetic Algorithm (MOGA) with 'fgoalattain' hybrid function with and without regeneration were presented.

7.1 Introduction

The model developed in this research was used to find solution for different WAP problems for Multi-objective water reuse with MOGA and 'fgoalattain' hybrid in MATLAB software. The problems were obtained from different literature as described in each section.

The research use MATLAB (Mathematical Laboratory) software for solving the developed model using MOGA and a hybrid to accomplish a wider distribution of the Pareto Optimal Solution for the multi-objective WAP problem. The MATLAB software uses the syntax "gamultiobj" for the MOGA.

The "gamultiobj" uses the basis of a controlled selective GA (a variant of NSGA-II). The selective GA always favours a better output solution and the solution that tend to increase the diversity of the population of the fitness function value even if they have a lower fitness value. The diversity of the population of the fitness function value is always preserved to ensure the convergence to an optimal Pareto front. This is achieved by adjusting the elite members of the population as the algorithm progresses,

by using the MATLAB options, 'ParetoFraction' and 'DistanceFcn'. The Pareto fraction option limits the number of individuals on the Pareto front (elite members) and the distance function keep the diversity on a front by giving preference to the fitness function solution that are relatively far-off on the front (Sampreeti *et. al.*, 2013).

All the variables were defined in the list of symbols and nomenclature section of this thesis.

7.1.1 Method for the Hybrid Approach of Multi-Objective:

The hybrid functionality in multi-objective function 'gamultiobj' is slightly different from that of the single objective function GA. Its hybrid solver will start at all the points on the Pareto front returned by 'gamultiobj'. The new individuals returned by the hybrid solver are combined with the existing population and a new Pareto front is obtained.

The 'gamultiobj' can reach the region near an optimal Pareto front relatively quickly, but it can take many function evaluations to achieve convergence. A commonly used technique is to run 'gamultiobj' for a small number of generations to get near an optimum front. Then the solution from 'gamultiobj' is used as an initial point for another optimisation solver that is faster and more efficient for a local search as hybrid. We use 'fgoalattain' as the hybrid solver with 'gamultiobj' to find an optimal Pareto front for the multi-objective WAP problem. 'fgoalattain' solves the goal attainment problem, which is one formulation for minimising a multi-objective optimisation problem.

The goal attainment method of Gembicki (1974) was used for this research. A set of objectives are linked to a set of design goals. This allows the objectives to be under- or overachieved, enabling automatic selection of the goals. The relative degree of under- or overachievement of the goals is controlled by a vector of weighting

coefficients, and is expressed as a standard optimisation problem using the following formulation (equation 7.1).

$$\begin{aligned}
 & \text{Min } Y \\
 & Z(x) - w_i \gamma \leq \text{goal} \\
 & C(x) \leq 0, \text{ceq}(x) = 0, Ax \leq b, \text{Aeq}x = \text{beq}, \dots \dots \dots (7.1)
 \end{aligned}$$

The term $w_i \gamma$ introduces an element of slackness into the problem, which otherwise imposes that the goals be rigidly met. Introducing slack variables replaces each inequality constraint with an equality constraint, and leads to a non-negativity constraint. The weighting vector, w , enables the expression of a measure of the relative trade-offs between the objectives. For instance, setting the weighting vector w equal to the initial goals indicates that the same percentage under- or over attainment of the goals F^* is achieved. The hard constraints can be incorporated into the strategy by setting a particular weighting factor to zero (i.e. $w_i = 0$). The goal attainment method provides a convenient intuitive interpretation of the WAP problem, which is solvable using standard optimisation procedure. Illustrative examples of the use of the goal attainment method in control system design can be found in Fleming (1985 and 1986).

The Goal Attainment method is represented geometrically in Figure 7.1, the Specification of the goals, $[F^*_1, F^*_2]$, defines the goal point, P . The weighting vector defines the direction of search from P to the feasible function space, $\wedge(\gamma)$. During the optimisation γ is varied, which changes the size of the feasible region. The constraint boundaries converge to the unique solution point F_{1s}, F_{2s} .

The 'gamultiobj' estimates the pseudo weights (required input for fgoalattain) for each point on the Pareto front and runs the hybrid solver starting from each point on the Pareto front. If the Pareto fronts obtained by 'gamultiobj' alone and by using the hybrid

$$FRW = \sum_{i=1}^n F_i \dots \dots \dots (7.2)$$

2. The sum of wastewater produced by all water using processes

$$WWR = \sum_{i=1}^n X_{i,j} \dots \dots \dots (7.3)$$

3. The sum of all the values of Reuse Wastewater.

$$RWR = \sum_{i=1}^n X_{2n+1,j} \dots \dots \dots (7.4)$$

4. The sum of all the nodes of Wastewater reuse interconnections:

$$CWWR = if \sum_{i=1}^n X_{2n+1,j} \geq 1,1 \text{ else } 0 \dots \dots \dots (7.5)$$

The above system of equations 7.2 to 7.5 are used as the main fitness functions in minimising the constraints presented in the previous chapters. The obtained minimum quantity of freshwater, wastewater and interconnections can then be used to determine the total cost of obtaining freshwater by multiplying the values obtained with the unit cost.

7.2.1 Test Problem: Input Limiting Process Data for 3 industrial processes

The limiting data for water minimisation for a specialty chemical production industry having 3 industrial processes as used in section 6.2.1, obtained from Mann and Liu (1999), also used by Cao et al (2007) is used in this case. The rough limiting process data for mass load, contaminant concentration allowed in and produced out are shown in Table 6.1 in chapter six. This is multi-contaminant and multi-objective WAP problem.

7.2.2 Setting up Multi-objective WAP Problem for 3 industrial processes

The setting up of the problem is done with Fitness function as @FRW_MULTOBJ having 12 number of variables, 4 Number of objectives, 6 Equality constraints and '@Constraints_FRW' as the nonlinear constraint function . The fitness functions in equations 7.1 to 7.4 are vectorised and represented in Matlab as shown in appendix E1. The linear and nonlinear constraints functions in equations 5.6a to 5.8d are used in Matlab software as the matrix and vector of equalities (Aeq and beq) using the coefficient of the variables and nonlinear function, as presented in chapter five.

The multi-objective genetic algorithm (MOGA) solver in MATLAB run the setup and display the number of solutions found on the Pareto front and the number of generations.

The set of functions, parameters and genetic operators used by the multi-objective genetic algorithm (MOGA) for diagnostic analysis of the problem are shown in Table 7.1.

Table 7. 1: Set of functions, Genetic parameters and Operators for GA to solve 3 industrial processes WAP problem

S/No.	Genetic Parameters/ Operators	Value /method
1.	Fitness function	@FRW_MULTOBJ
2.	Number of variables	27
3.	Number of objectives	4
4.	Equality constraints	15
5.	nonlinear constraint	@Constraints_FRW
6.	Population Size	10
7.	Crossover Fraction	0.8
8.	Migration Interval	6
8.	Creation Function	@gacreationnonlinearfeasible
10.	Selection Function	@selectiontournament 3
11.	Crossover Function	@crossover heuristic 1.3
12.	MutationFcn	@mutationadaptfeasible
13.	Hybrid Function	@fgoalattain

Furthermore, two options 'ParetoFraction' and 'MigrationFraction' are used to control the elitism. The Pareto fraction option limits the number of individuals on the Pareto front (elite members) and the distance function helps to maintain diversity on a front

by favoring individuals that are relatively far away on the front. The Pareto fraction value of 0.35 is used, the solver will try to limit the number of individuals in the current population that are on the Pareto front to 35 percent of the population size. The 'MigrationFraction' of 0.5 is used

7.2.3 The result of Multi-objective Water Reuse for 3 industrial processes without regeneration

Optimisation come to termination when the average change in the spread of pareto solutions is less than function tolerance option and constraint violation is less than Constraint Tolerance.

The generation of the population used for analysis is computed using the non-dominated rank and a distance measure of the individuals in the current generation. The distance measure of an individual is used to compare individuals with equal rank. It is a measure of how far an individual is from the other individuals with the same rank. The average distance between individuals based on generation is shown in Figure 7.2

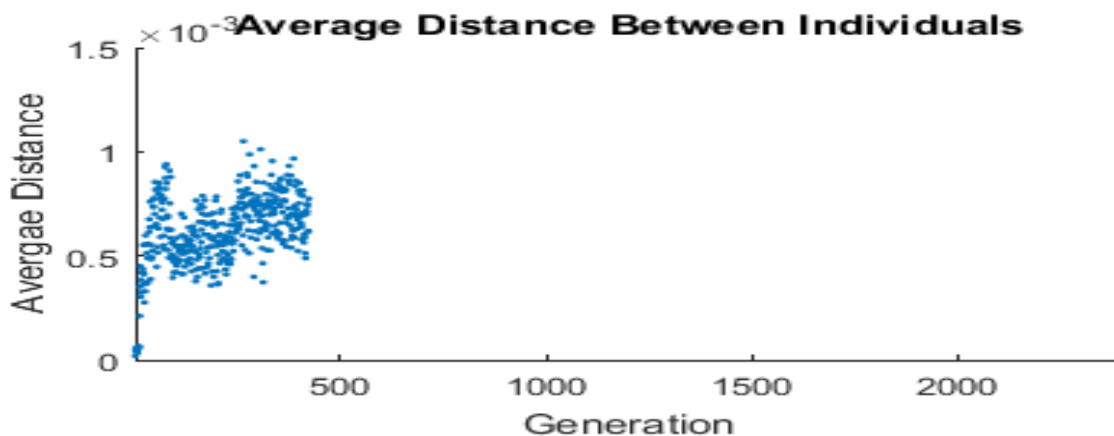


Figure 7.2: Average Distance between Individuals

Switching to the hybrid optimisation solver (fgoalattain) leads to Local minimum within the last region, which is the optimum result if constraints are satisfied. The final end of diagnostic information for the solution is displayed as shown in Table 7.1.

Table 7. 1: End of diagnostic information for the solution of three process

Generation	f-count	Average Pareto distance	Average Pareto spread
1	300	0	0
2	420	3.65501e-06	0.0733204
3	900	0	0
4	1210	0	0

Figure 7.3 shows the graphical Pareto front solution of two competing objectives without hybrid function as the MOGA search for the solution. This gives different possible combination of the objectives as the solution of the problem. The chart is featured by two objectives at several levels of constraints. Objective1 (the sum of freshwater flow rates at the entrance of all water using processes) vs. objective 2 (the sum of wastewater produced by all water using processes), placed on the horizontal and vertical axes of the chart, respectively. The values of third and fourth objective not displayed as this graph is two dimensional only.

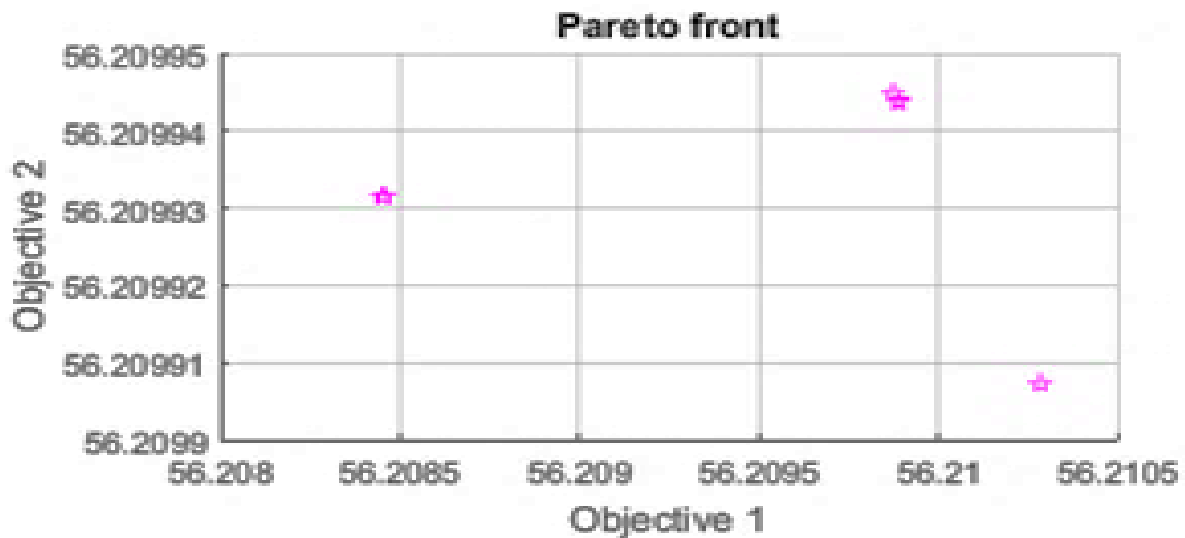


Figure 7. 3: The graphical display of the Pareto front solution without hybrid function for two objectives

Figure 7.4 shows the graphical display of the Pareto front solution with the hybrid function as the MOGA reach the termination of the analysis. This gives one solution as the optimum solution of the objectives for the problem. It is certain that using the hybrid function will result in an optimal Pareto front but we may lose the diversity of

the solution (because `fgoalattain` does not try to preserve the diversity). This can be indicated by a value of the average distance measure and the spread of the front.

This takes only 5 seconds to execute.

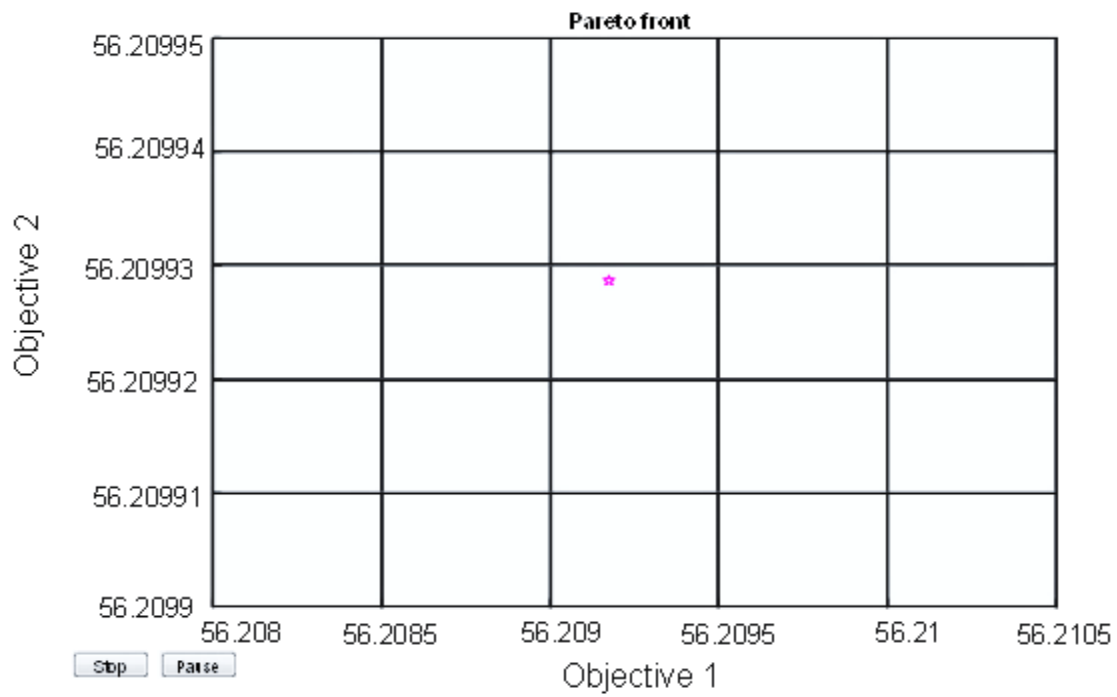


Figure 7.4: The graphical display of the Pareto front solution with hybrid function for two objectives.

Table 7.4 present the individual values of each objective after the analysis.

Table 7. 2: End of diagnostic solution of three process

FRW	WWR	RWR	CWWR
56.2	56.2	41.9	1

The Solution of the problem shown in Table 7.2 indicate that the sum of fresh water flow rates at the entrance of all water using processes (FRW) is 56.2 m³/h, the sum of wastewater produced by all water using processes (WWR) is 56.2 m³/h, the sum of all the values of Reuse Wastewater (RWR) is 41.9 m³/h and the sum of all the nodes of wastewater reuse inter-connections (F4) is 1.

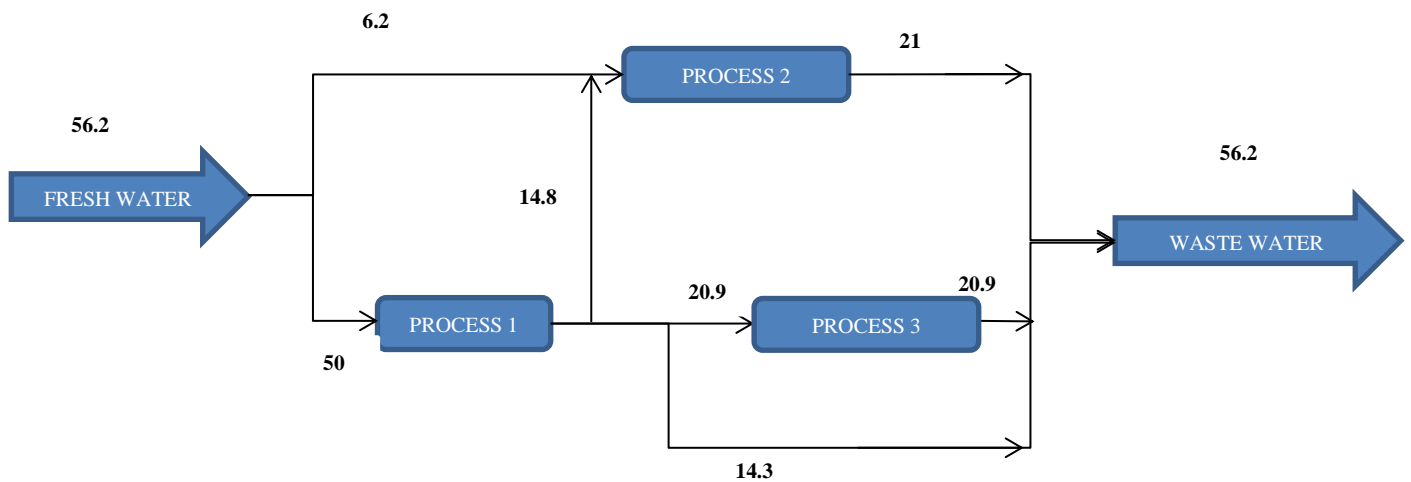


Figure 7. 5: The diagrammatical Superstructure representation of the solution of 3 industrial processes using multi-objective.

7.2.4 The result of Multi-objective Water Reuse for 3 industrial processes with regeneration

If the quantity of regeneration water is included as one of the objective, then the equation that finds the sum of all regenerated water must be included in the set of objective function. Therefore, equation 7.5 will be added as one of the objective:

5. The regenerated water flow-rate expressed as the sum of the water flow-rates going from a process to a regeneration unit and from a regeneration unit to another

$$RWR = \sum_{i=1}^n \left(\sum_{i=1}^n X_{i,r} + \sum_{i=1}^n X_{r,i} \right) \dots \dots \dots (7.5)$$

The five systems of equations 7.1 to 7.5 are used as the fitness function. The fitness functions in equations 7.1 to 7.5 are vectorised and represented in Matlab as shown in appendix E2:

A set of Pareto optimal solution is obtained with the addition of hybrid function 'fgoalattain'. Figure 7.6 shows the graphical display of the pareto front solution without the hybrid function as the MOGA reach the termination of the analysis. This gives different solutions as the optimum solution of the objectives for the problem. It is certain that using the hybrid function will result in an optimal Pareto front but we may lose the diversity of the solution (because 'fgoalattain' does not try to preserve the diversity). This takes only 6 seconds to execute.

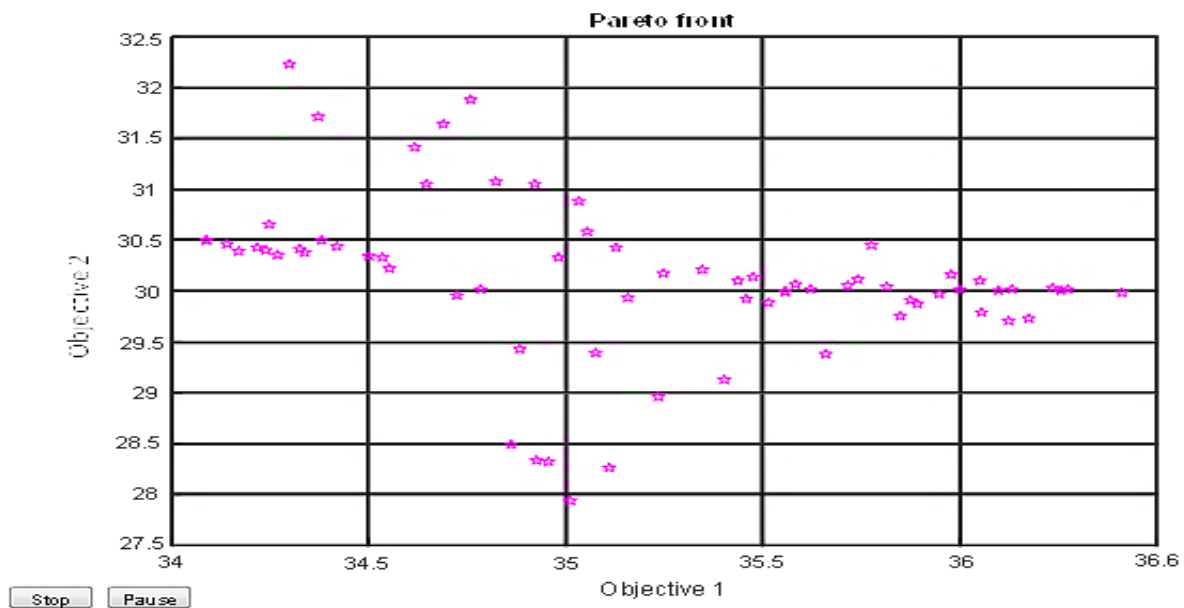


Figure 7.6: The graphical display of the Pareto front solution without hybrid function of WAP with regeneration for two objectives

Table 7.3 present the individual values of each objective after the analysis.

Table 7.3: End of diagnostic solution of three process

FRW	WWR	RWR	CWWR	RWR
35.1	35.1	19.4	1	46.8

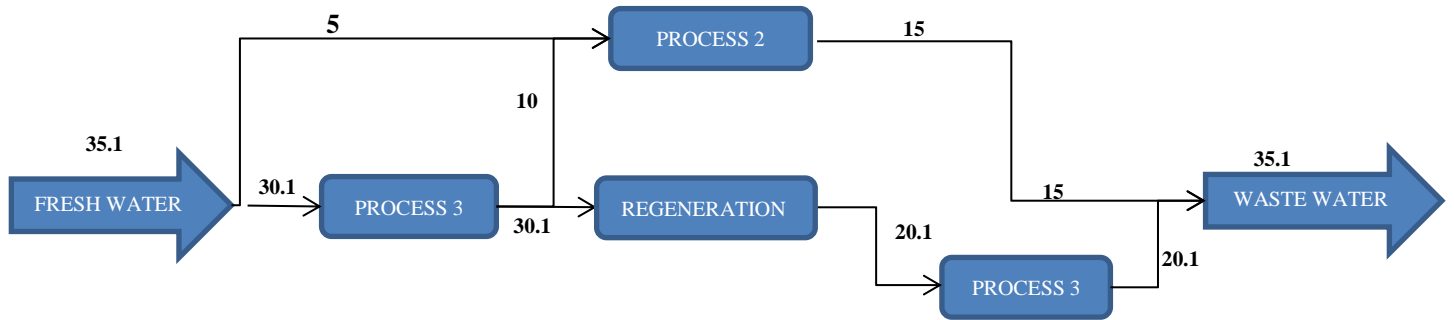


Figure 7.7: The diagrammatical Superstructure representation of the solution with regeneration.

The Solution of the multi-objective problem shown in Table 7.3 as represented in Figure 7.7 indicate that the sum of freshwater flow rates at the entrance of all water using processes (FRW) is 35.1 m³/h. The sum of wastewater produced by all water using processes (WWR) is 35.1m³/h. The sum of all the values of reuse wastewater (RWR) is 10.0 m³/h and the sum of all the nodes of Wastewater reuse inter-connections (CWWR) is 1 and the regenerated water flow-rate expressed as the sum of the water flow-rates going from a process to a regeneration unit and from a regeneration unit to another (RWR) is 20.1 m³/h.

7.3: Synthesis of Analysis of 3 industrial processes water reuse of multi-contaminant (with and without regeneration)

The result of Multi-objective analysis for 3 industrial processes without regeneration: indicate that the sum of freshwater flow rates at the entrance of all water using processes (FRW) is 56.2m³/h. The sum of wastewater produced by all water using processes (WWR) is also 56.2m³/h and the sum of all the values of reuse wastewater (RWR) is 41.9m³/h. The sum of all the nodes of wastewater reuse inter-connections (CWWR) is 1. Whereas, with regeneration, the sum of freshwater flow rates at the entrance of all water using processes (FRW) is 35.1 m³/h, the sum of wastewater produced by all water using processes (WWR) is also 35.1 m³/h. The sum of all the values of reuse wastewater (RWR) is 10.0 m³/h (without regeneration), the sum of all

the nodes of wastewater reuse inter-connections (CWWR) is 1 and the regenerated water flow-rate expressed as the sum of the water flow-rates going from a process to a regeneration unit and from a regeneration unit to another (RWR) is 20.1 m³/h.

This shows that the freshwater consumption of the industry will be reduced from 56.2 m³/h to 35.1 m³/h, by using regeneration, using multi-objective approach. There is a difference of 21.1 m³/h, which is 37.5% reduction in freshwater consumption of the industry. This is due to the different available solution options that can be selected based on the different combination of objectives. The solution obtained using single-objective is also part of the solutions obtained using multi-objective but it is not the Pareto front (or optimum) in this case.

7.4: Conclusion:

This chapter has presented all the necessary mathematical steps required in solving the multi-objective genetic algorithm WAP problem based on Pareto front for a single-contaminant water reuse of 3 industrial processes, with and without regeneration. The result shows that this model can search a wide-ranging distribution of Pareto optimal solution and it has a noble performance and small computational time. The result of single and multi-contaminant water reuse with and without regeneration for 3 industrial processes were compared. The readers can easily follow the steps to obtain the optimum result for other number of processes as demonstrated.

The next chapter will describe the present situation and different data obtained from the Kaduna Refining and Petrochemical Company Limited (KRPC). The data will be used to analyse the minimum freshwater requirement of the KRPC using WAP models of mathematical optimisation as described in previous chapters.

CHAPTER EIGHT

8.0 CASE STUDY: APPLICATION OF THE MODEL TO A REFINERY

This chapter describes the present situation and different data obtained from the Kaduna Refining and Petrochemical Company Limited (KRPC). The data was used to analyse the minimum freshwater requirement of the KRPC using WAP models of mathematical optimisation. It described the solution obtained by the WAP model using Multi-objective Genetic Algorithm (MOGA) and 'fgoalattain' hybrid function under multi-objective consideration. The expected saving of the freshwater with and without regeneration as determined by the research to the refinery was discussed.

8.1 Introduction

This research involves data collection from the relevant industries and literature. One of the companies visited was Kaduna Refining and Petrochemical Company Limited (KRPC), a Subsidiary of Nigerian National Petroleum Corporation (NNPC). The relevant data was obtained and evaluated. The analysis of the data obtained was carried out using multi-contaminant, multi-objective methods presented in the previous chapters.

The Kaduna Refining and Petrochemical Company Limited (KRPC) (Figure 1), is a Subsidiary of Nigerian National Petroleum Corporation (NNPC). From the information obtained during data collection, the refinery project and the Fuels Plant was completed and commissioned in 1980. While the two other subsections of the refinery, the Lubes Plant and Petrochemical Plant were commissioned in 1983 and 1988 respectively. Kaduna Refinery occupies an area of 2.89 Square Kilometres (Km²). The plot plan is designed with safety and ease of maintenance in mind. The design also attempts to minimise operating costs.



Figure 8.1: The picture of Kaduna Refining and Petrochemical Company Limited (KRPC)

The refinery was designed to process both imported paraffinic and Nigerian crude oils into fuels and lubes products and was constructed by Chiyoda Chemical Engineering and Construction Company (now Chiyoda Corporation) of Japan. The total installed capacity of the refinery is 110,000 Barrel per Stream Day (BPSD) (<http://www.nnpcgroup.ng/KRPC.aspx.htm>, 2015).

The raw water intake facilities of the company are located beside River Kaduna, about 13 kilometres from the KRPC complex. The freshwater from the river is the only source of water for the refining and other utilities in the company. The river water is pre-treated at the Intake before being pumped through a 13km water pipeline into two large storage tanks on site. Each of the raw water tanks has a storage capacity of 75,000 cubic meters. The stored water can meet the demands of the refinery and petrochemical complex for a period of 10 days.

The typical characteristics of the raw water from River Kaduna are high suspended solids (with seasonal variation), high dissolved solids (metals), and variable turbidity. The existing water usage network by various units is shown in Figure 8.2.

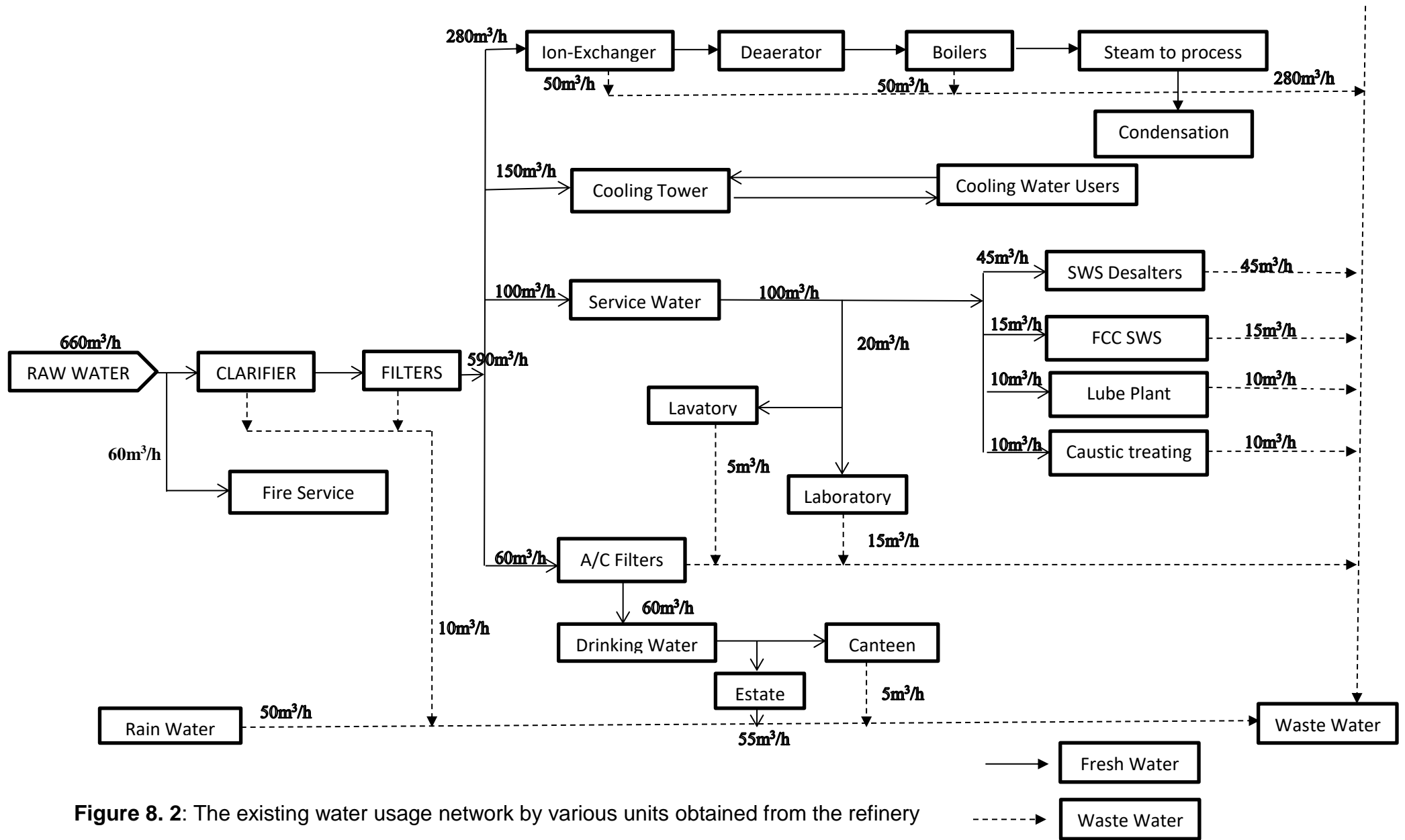


Figure 8. 2: The existing water usage network by various units obtained from the refinery

(This are known values from the case study)

Table 8.1 shows the flow rate and the maximum allowable concentration at inlet (C_{in}) and outlet (C_{out}) of major water using units obtained from the industry. However, the value for fire unit indicated as 60.0m³/h may reach 150.0m³/h during fire fighting and is taken directly from raw water before the treatment.

Table 8. 1:The maximum allowable value of major water using units obtained from the refinery (This are the obtained values from the case study)

Unit No.	Unit Name	Flow rate of Fresh water (m ³ /h)	Suspended Solid (SS)		Hardness (H)		Chemical oxygen demand (COD)		Free hydrocarbons (FH)	
			C_{in} (ppm)	C_{out} (ppm)	C_{in} (ppm)	C_{out} (ppm)	C_{in} (ppm)	C_{out} (ppm)	C_{in} (ppm)	C_{out} (ppm)
1	Cooling Tower	150.0	40	500	5	10	0	150	0	5
2	Ion Exchangers	280.0	10	20	20	100	0	150	0	5
3	Laboratory	20.0	25	250	50	200	400	1000	0	5
4	SWS Desalters	45.0	30	300	20	100	400	1000	0	1000
5	FCC SWS	15.0	15	30	20	100	600	1200	0	10
6	Caustic treating	10.0	15	20	20	100	600	1200	0	10
7	Drinking	60.0	20	150	10	200	0	0.05	0	0
8	Fire	60.0	-	-	-	-	-	-	-	-

The multi-contaminant and multi-objective analysis was carried out on the above data based on the methods described in the previous chapters. However, only 6 (six) processes were considered because of their relevance to the production in the refinery. The processes are Ion Exchangers, Cooling Tower, Laboratory, Sour Water Strippers (SWS) Desalters, Fluid catalytic cracking (FCC) SWS and Caustic treating. The contaminants considered for the solution are Suspended Solid (SS), Hardness (H), Chemical oxygen demand (COD) and free hydrocarbons (FH).

8.2 Multi-Objective, Multi-Contaminant Water Reuse for the Kaduna

Refinery:

The multi-objective Functions described in chapter six were used as the objectives in minimising freshwater use in the Kaduna refinery. First, the model was used to minimise freshwater without using any suggestion for regeneration, as is the present situation in the refinery.

The number of variables as described in chapter 3 for six processes with four (4) multi-contaminants (m) in WAP problem without regeneration is $n^2+n+nm = 66$. The variables are freshwater, produced wastewater, wastewater for reuse and contaminants concentrations represented as follows: $F_1, F_2, F_3, F_4, F_5, F_6, W_1, W_2, W_3, W_4, W_5, W_6, X_{12}, X_{13}, X_{14}, X_{15}, X_{16}, X_{21}, X_{23}, X_{24}, X_{25}, X_{26}, X_{31}, X_{32}, X_{34}, X_{35}, X_{36}, X_{41}, X_{42}, X_{43}, X_{45}, X_{46}, X_{51}, X_{52}, X_{53}, X_{54}, X_{56}, X_{61}, X_{62}, X_{63}, X_{64}, X_{65}, C_{11}, C_{12}, C_{13}, C_{14}, C_{21}, C_{22}, C_{23}, C_{24}, C_{31}, C_{32}, C_{33}, C_{34}, C_{41}, C_{42}, C_{43}, C_{44}, C_{51}, C_{52}, C_{53}, C_{54}, C_{61}, C_{62}, C_{63}, C_{64}$, respectively.

The fitness functions are the Sum of fresh water flow rates at the entrance of all water using processes, the sum of wastewater produced by all water using processes, the sum of all the values of Reuse Wastewater and the sum of all the nodes of Wastewater reuse interconnections as described in chapter seven (equation 7.2 to 7.5).

8.2.1 Representation of Multi- Contaminant, Multi-objective Water Reuse in

Matlab for Kaduna Refinery:

The fitness functions in equations 7.2 to 7.5, the Nonlinear Constraints functions and the code function for obtaining the solution are vectorised and represented in Matlab as shown in appendix F1. The linear constraints equations are represented in Matlab software as the matrix and vector of equalities (Aeq and beq) using the coefficient of

the variables. The matrix and vector of inequalities are not available in the constraints, therefore (A and b) are represented as empty set as follows: A= [], b= []. The vector for lower and upper bounds (LB and UB) are represented with the zero set of lowest and infinity set of highest value of boundary as shown in appendix F1. The syntax for obtaining the solution in Matlab is as follows:

x = gamultiobj(@FRW4KAD_MULTTOBJ,nvars,A,b,Aeq,beq,lb,ub,@Constraints_FRW4KADMULTI,options)

Where x is the local minimum values of the fitness function, `gamultiobj` is the protocol of the multi-objective genetic algorithm code, `@FRW4KAD_MULTTOBJ` is the set of fitness functions to be minimised, `nvars` is the dimension or number of variables in the WAP problem, A, b are inequality constraint equations of the problem, Aeq, beq, are equality constraint of the problem, lb is the lower bounds (LB) of the search space, ub is the upper bounds (UB) of the search space, `@Constraints_FRW4KADMULTI` is the nonlinear constraints functions of the problem, `options` refers to different options used in the GA process like crossover , mutation and plot functions for displaying the graphs. The only known variables are the levels of contaminants in Table 8.1.

This syntax search for the possible solution of the problem and display the result as vector when the stopping criteria is met, which is when the average change in the spread of Pareto solutions is less than Function Tolerance option and constraint violation is less than Constraint Tolerance.

8.2.2 The result of Multi-contaminant, Multi-objective Water Reuse in Matlab for Kaduna Refinery:

The set of functions, parameters and genetic operators used by the multi-objective genetic algorithm (MOGA) for diagnostic analysis of the problem are shown in Table 7.1.

The differences are Fitness function is @FRW4KAD_MULTOBJ with 66 (Sixty six) number of variables, 4 Number of objectives, 30 (thirty) Equality constraints and '@Constraints_FRW4KADMULTI' as the nonlinear constraint function.

Optimization of WAP using MOGA come to termination when the average change in the spread of Pareto solutions is less than Function Tolerance option and constraint violation is less than Constraint Tolerance.

Displaying the graph of the analysis of interactions of the 4 objectives is difficult; due to the limitation of the 3-dimensional display as the highest graphical display in matlab. Therefore the 3-dimensional graphical display of the 3 objectives pareto front spread is shown in Figure 8.3, as the solution search was running. This gives the opportunity of presenting the 3 objectives and their interaction on the same graph.

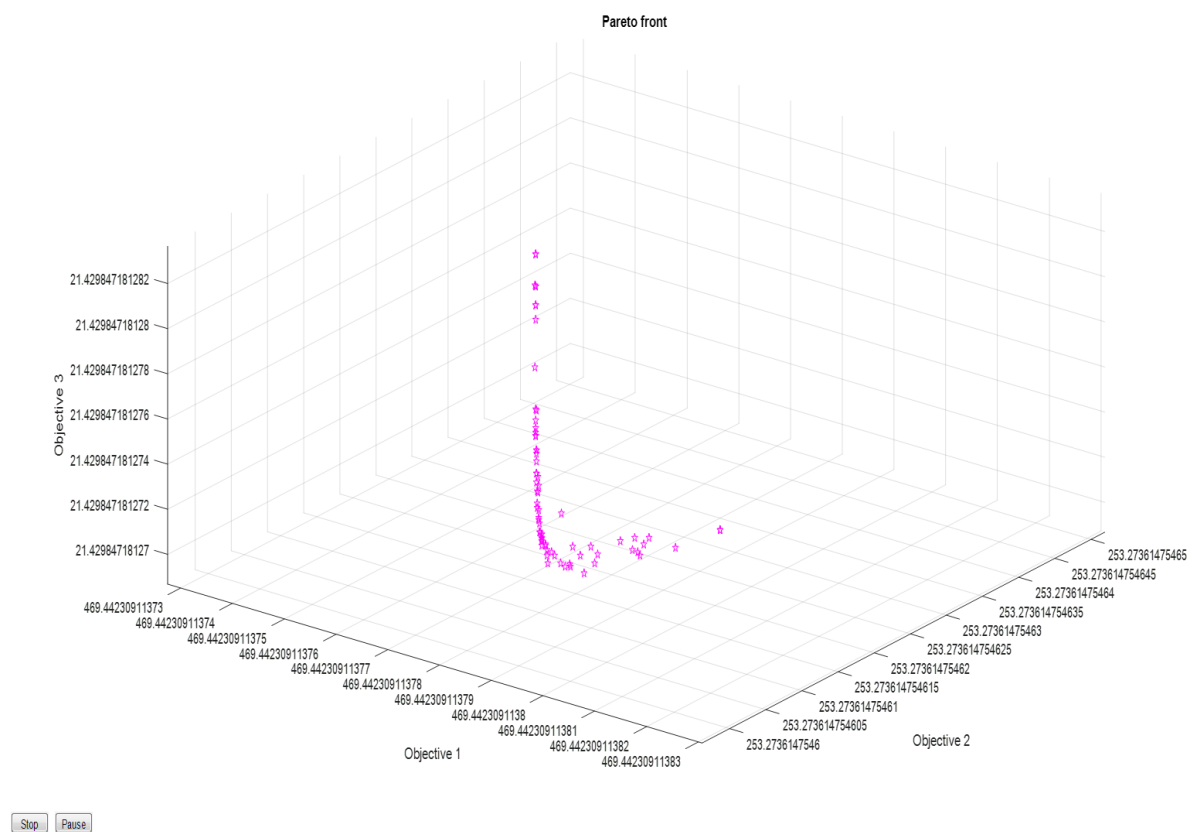


Figure 8.3: The 3-dimension graphical display of the solution.

The final 3-dimensional graphical display of the solution at the termination of the MOGA for the 3 objectives is shown in Figure 8.4. This indicates that the MOGA got stuck at the solution of 469.4 for objective 1, 242.6 for objective 2 and 21.4 for objective 3. Objective 4 is not shown graphically, but it was found as 1 in the solution. At this stage the hybrid function 'fgoalattain' takes over and found the optimum solution as in Table 8.2.

Switching to the hybrid optimisation solver (fgoalattain) leads to Local minimum, which is the optimum result after the satisfaction of the constraints. The final end of diagnostic information for the solution is displayed as shown in Table 8.2.

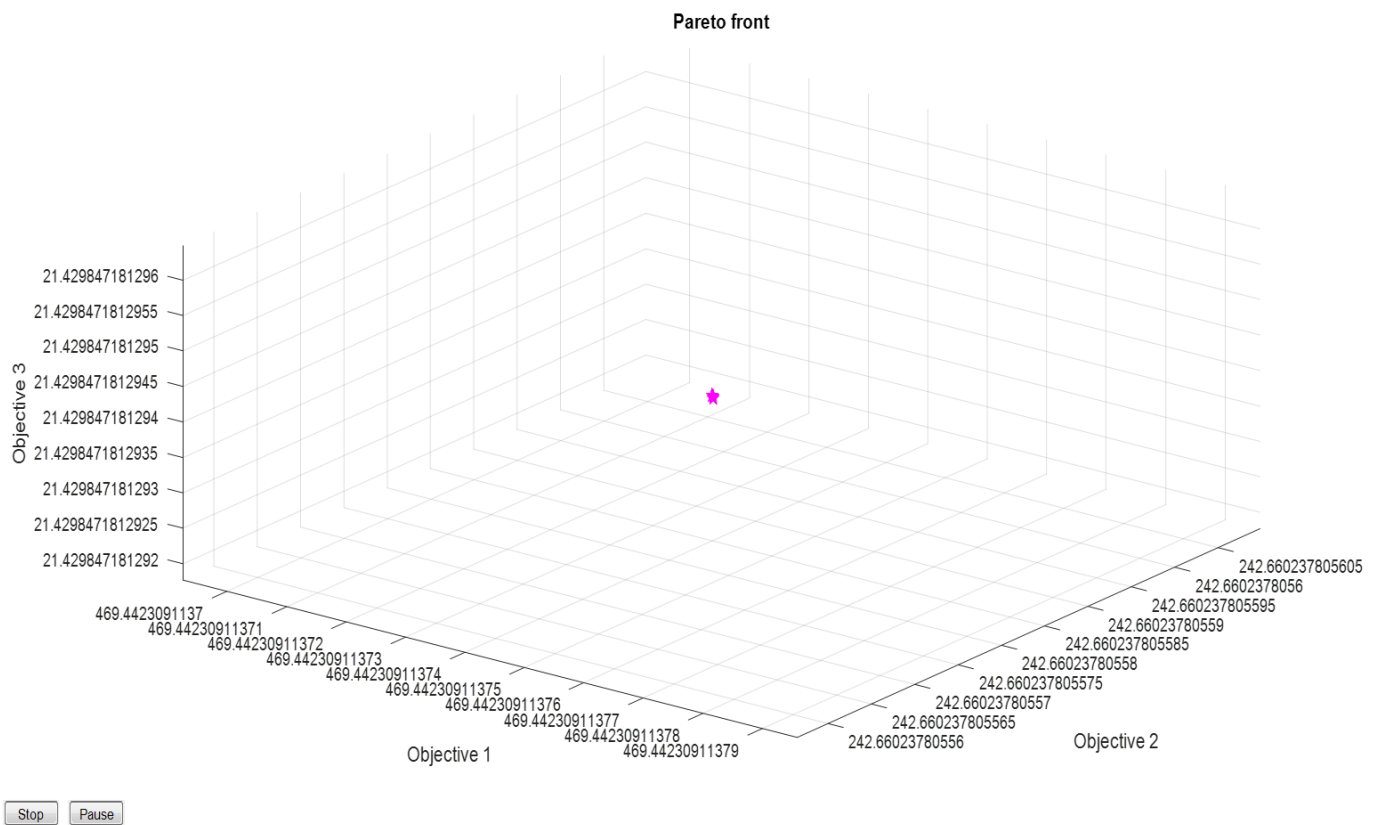


Figure 8. 4: The graphical display of the solution.

Table 8.2 present the generation, function count, average pareto distance and pareto spread after the analysis.

Table 8. 2: End of diagnostic information for the solution of 3 processes

Generation	f-count	Average	Average
------------	---------	---------	---------

		Pareto distance	Pareto spread
1	401	0	0
2	6201	0	0
3	12201	0	0
4	20601	0	1
5	26501	0	2
6	33161	0	0
7	39821	0	0
8	46481	0	0
9	53141	0	1
10	59801	0	2
11	66461	0	0
12	73121	0	0

Table 8.3 present the individual values of each objective after the analysis.

Table 8. 3:End of diagnostic solution of Kaduna Refinery

FRW	WWR	RWR	CWWR
460	460	60.0	2

The Solution of the problem shown in Table 8.3 indicate that the sum of fresh water flow rates at the entrance of all water using processes (FRW) is 460 m³/h, and the sum of wastewater produced by all water using processes (WWR) is 460 m³/h, These are the two values indicated on the superstructure of Figure 8.5. The sum of all the values of Reuse Wastewater (RWR) is 60.0m³/h and the sum of all the nodes of Wastewater reuse inter-connections (CWWR) is 2.

Furthermore, considering the level of contaminant concentration produced out C_{out} (ppm) by Ion exchanger process of Suspended Solid (SS) 20, Hardness (H) 100, Chemical oxygen demand (COD) 150, and Free hydrocarbons (FH) 5 the analysis indicates that the two processes (SWS Desalters and FCC SWS) with C_{out} (ppm) of SS 300 and 30, H 100 and 100, COD 1000 and 1200, FH 1000 and 10 can reuse wastewater from that process. This is possible due to the fact that none of the C_{out} (ppm) produced by the (Ion exchanger) process exceed the C_{out} (ppm) produced by

the two processes (SWS Desalters and FCC SWS). Therefore, this refinery can use only 460.0 m³/h instead of 520.0m³/h as shown in Table 8.4.

Table 8. 4: Solution of the problem corresponding to Figure 8.6

Process Number	Type of process	Type of water	Fresh water intake(m ³ /h)	Wastewater reuse (m ³ /h)
1	Cooling Tower	Freshwater only	150	0.0
2	Ion Exchangers	Freshwater only	280	0.0
3	Laboratory	Freshwater only	20	0.0
4	SWS Desalters	Wastewater only	0.0	45.0
5	FCC SWS	Wastewater only	0.0	15.0
6	Caustic treating	Freshwater only	10	0.0
Total Flowrate (m ³ /h)			460	60.0

Superstructure Schematic Network:

The superstructure schematic MATLAB result network configuration for multi-contaminant and multi-objective optimum water reuse network of the Kaduna refinery solution is shown in Figure 8.6

Matlab result for multi-contaminant and multi-objective optimum water reuse network for Kaduna refinery.

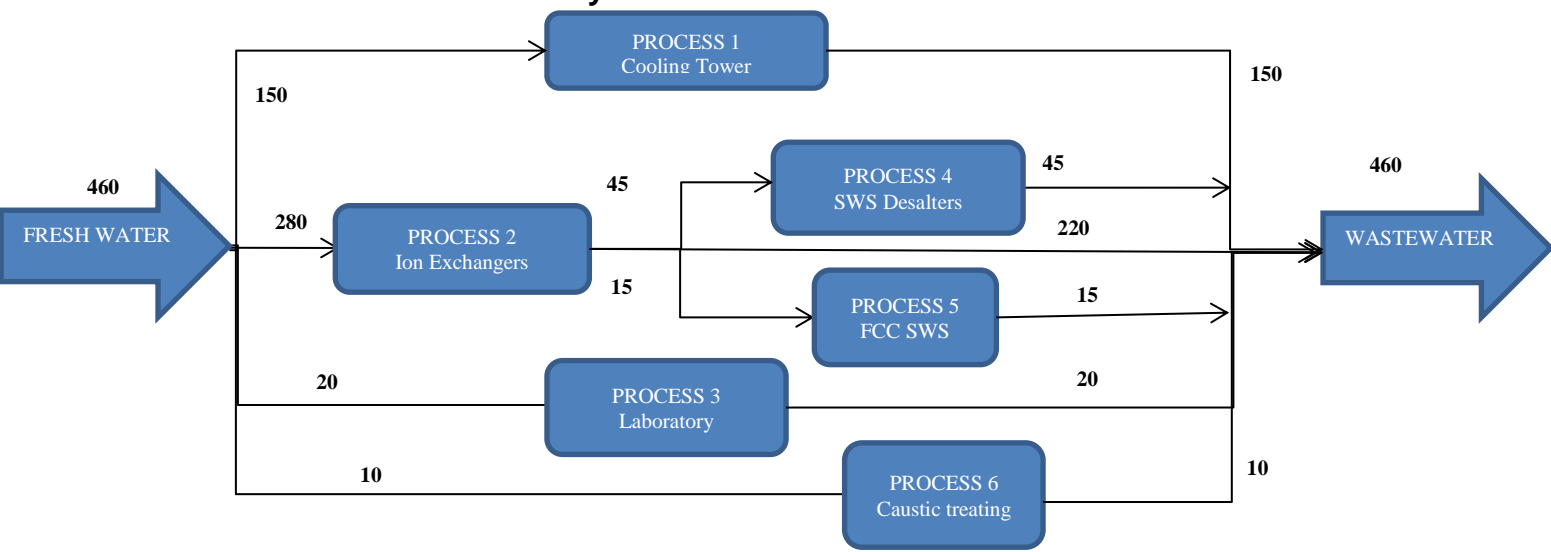


Figure 8.5: The diagrammatical Superstructure representation of the solution of water reuse network for Kaduna Refinery.

Figure 8.6 shows diagnostic solution of wastewater reuse without regeneration for the refinery. The connection modification required for the reuse of wastewater from Ion exchanger process by the SWS Desalters and FCC SWS processes is shown with a bold arrow.

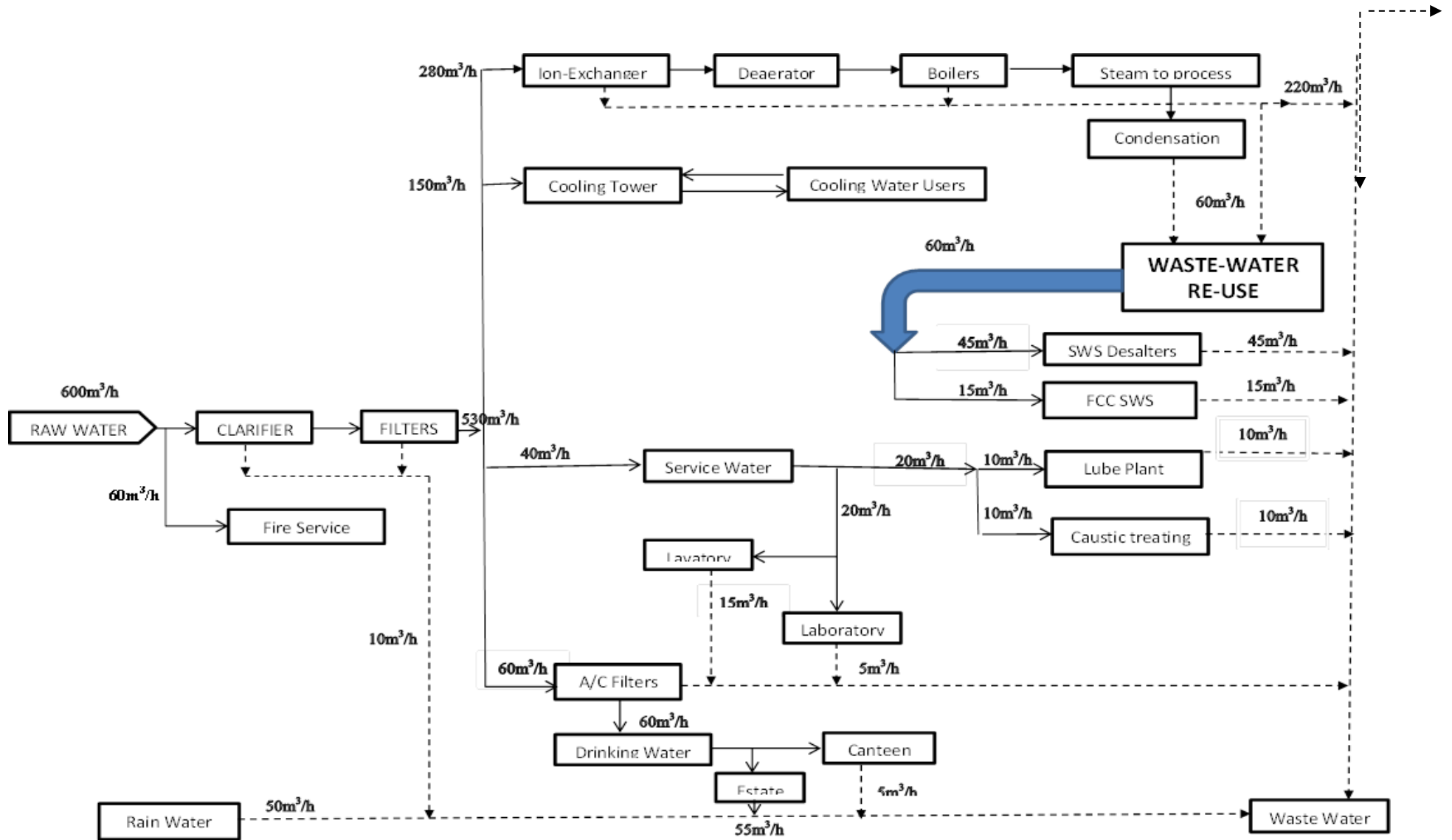


Figure 8. 6: The diagnostic solution of wastewater reuse without regeneration for the refinery.

8.3 Multi-Objective, Multi-Contaminant Water Reuse with regeneration for the Kaduna Refinery:

Considering the quantity of regeneration water as one of the objectives, then the equation that finds the sum of all regenerated water must be included in the set of objective function. Therefore, equation 6.5 will be added to the vectorised system of equations presented in section 8.1.2 as one of the objective.

The number of variables as described in chapter three for 6 industrial processes with 4 multi-contaminants (m) in WAP problem with regeneration is $n^2+3n+nm = 78$. The variables are freshwater, produced wastewater, wastewater for reuse, contaminants concentrations and regenerated water for reuse, represented as follows:

$F_1, F_2, F_3, F_4, F_5, F_6, W_1, W_2, W_3, W_4, W_5, W_6, X_{12}, X_{13}, X_{14}, X_{15}, X_{16}, X_{21}, X_{23}, X_{24}, X_{25}, X_{26}, X_{31}, X_{32}, X_{34}, X_{35}, X_{36}, X_{41}, X_{42}, X_{43}, X_{45}, X_{46}, X_{51}, X_{52}, X_{53}, X_{54}, X_{56}, X_{61}, X_{62}, X_{63}, X_{64}, X_{65}, C_{11}, C_{12}, C_{13}, C_{14}, C_{21}, C_{22}, C_{23}, C_{24}, C_{31}, C_{32}, C_{33}, C_{34}, C_{41}, C_{42}, C_{43}, C_{44}, C_{51}, C_{52}, C_{53}, C_{54}, C_{61}, C_{62}, C_{63}, C_{64}, R_{11}, R_{12}, R_{13}, R_{14}, R_{15}, R_{16}, R_{17}, R_{18}, R_{19}, R_{20}, R_{21}, R_{22}$, respectively.

Where, F is for freshwater required by each industrial process, W is for wastewater produced by each industrial process, X is for wastewater reused in another industrial process, C is for the level of contaminant produced by each industrial process and R is for the regenerated water. Only the contaminant level is known all the remaining parameters are determined.

8.3.1 Representation of Multi- Contaminant, Multi-objective Water Reuse with regeneration in Matlab for Kaduna Refinery:

The five systems of equations 7.2 to 7.6 are used as the fitness function as shown in appendix F2.

As described in the work of Al-Ani (2012) and De León Almaraz *et al.*, (2016), a simple technology was found to be very effective method in the treatment of oily wastewater from an old processing plant of the North Oil Company with removal efficiencies of TDS, COD, and TSS as 99.4%, 99.2%, and 99.5% respectively. Therefore, the regeneration considered here is a typical refinery wastewater treatment plant that can remove 90% of the considered contaminants (i.e. Suspended Solid (SS), Hardness (H), Chemical oxygen demand (COD) and free hydrocarbons (FH)).

The linear constraints equations are represented in Matlab software as the matrix and vector of equalities (Aeq and beq) using the coefficient of the variables as shown in appendix F2.

The matrix and vector of inequalities are not available in the constraints, therefore (A and b) are represented as empty set as follows: $A = []$, $b = []$. The vector for lower and upper bounds (LB and UB) are represented with the set of lowest and highest value of outcome of each point as shown in appendix F2. The upper bound is assumed to be infinity. This means that there is no limit to the extent at which water can be allocated to any given industrial process. In the Nonlinear Constraints functions the regeneration terms are included and are vectorised and represented in matlab as shown in appendix F2. The code function for obtaining the solution in matlab is shown in appendix F2.

The syntax for obtaining the solution in Matlab is as follows:

```
x=gamultiobj(@FRW4REG_KAD_MULTTOBJ,nvars,A,b,Aeq,beq,lb,ub,@Constraints_FRW4REG_KADMULTI,options)
```

Where x is the local minimum values of the fitness function, `gamultiobj` is the protocol of the multi-objective genetic algorithm code, `@FRW4REG_KAD_MULTTOBJ` is

the set of fitness functions to be minimised, '@Constraints_FRW4REG_KADMULTI' is the nonlinear constraints functions of the problem, and all the other remaining parameters are as described in section 8.2.1. This syntax search for the possible solution of the problem and display the result as vector when the stopping criteria are met.

8.3.2 The result of Multi-contaminant, Multi-objective with regeneration Water Reuse for Kaduna Refinery:

The set of functions, parameters and genetic operators used by the multi-objective genetic algorithm (MOGA) for diagnostic analysis of the problem are shown in Table 7.1. The differences are Fitness function is '@FRW4REG_KAD_MULTII' with 78 number of variables, 5 Number of objectives, 30 (thirty) Equality constraints and '@Constraints_FRW4REG_KADMULTI' as the nonlinear constraint function.

Optimization come to termination when the average change in the spread of Pareto solutions is less than Function Tolerance option and constraint violation is less than Constraint Tolerance.

Switching to the hybrid optimization solver (fgoalattain) leads to Local minimum, which is the optimum result after the satisfaction of constraints.

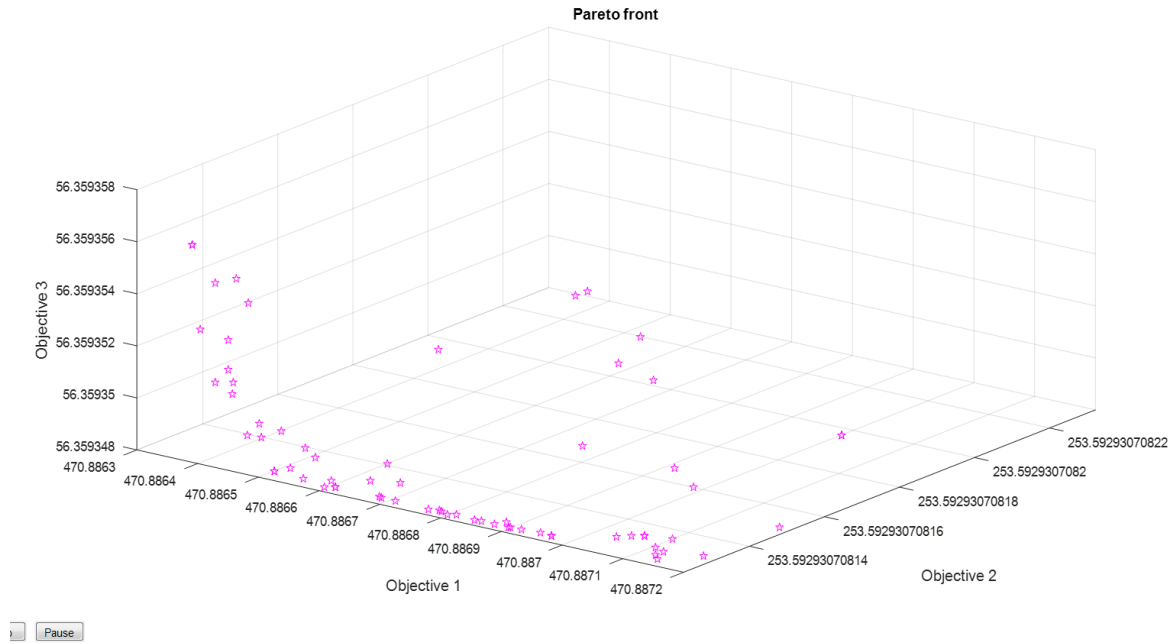


Figure 8. 7: The graphical display of the solution.

Figure 8.7 shows the graphical display of the pareto front spread as the solution search was running. This shows a wide range of search space analysed by the GA. The shape of the graph is based on all the possible solution points. Switching to the hybrid optimisation solver (fgoalattain) leads to Local minimum, which is the optimum result if Constraints are satisfied. The final end of diagnostic information for the solution is displayed as shown in Table 8.5.

Table 8. 5: End of diagnostic information for the solution of three process

Generation	f-count	Average Pareto distance	Average Pareto spread
1	311	0	0
2	611	0	0
3	911	0	0
4	1031	0	0
5	1331	0	0
6	1577	0	0
7	1823	0	0
8	2069	0	0
9	2315	0	0
10	2561	0	0
11	2807	0	0
12	3053	0	0

The final graphical display of the solution at the termination of the MOGA indicate that the MOGA get stuck at the solution of 470.0 for objective 1, 472.0 for objective 2 and 169.5 for objective 3. Objective 4 and 5 as 1 and 92 in the solution, respectively. At stuck point the hybrid function 'fgoalattain' continues and found the optimum solution as in Table 8.5

The Pareto optimal solution was obtained with the addition of hybrid function 'fgoalattain' under the median time of 47.2 seconds.

Table 8.6 present the individual values of each objective after the analysis of the hybrid function.

Table 8.6 present the individual values of each objective after the analysis.

Table 8. 6: End of diagnostic solution of three process

FRW	WWR	RWR	CWWR	RWR
430.0	430.0	90.0	1.0	90.0

The Solution of the multi-contaminant, multi-objective problem with regeneration for Kaduna refinery is shown in Table 8.7, it indicates that the sum of fresh water flow rates at the entrance of all water using processes (FRW) is 430.0 m³/h, the sum of wastewater produced by all water using processes (WWR) is 430.0 m³/h, the sum of all the values of Reuse Wastewater (RWR) is 90.0 m³/h which indicate only regeneration process takes wastewater, treat it and provide it for reused by other process. The sum of all the nodes of Wastewater reuse inter-connections (CWWR) is 1 which is the connection between process 2 and regeneration. The regenerated water flow-rate expressed as the sum of the water flow-rates going from a process to a regeneration unit and from a regeneration unit to another (RWR) is 90.0m³/h.

Table 8. 7: Solution of the problem corresponding to Figure 8.6

Process Number	Type of process	Type of water	Fresh water intake (m ³ /h)	Wastewater reuse (m ³ /h)
1	Cooling Tower	Freshwater only	150	0.0
2	Ion Exchangers	Freshwater only	280	0.0
3	Laboratory	Wastewater only	0.0	20.0
4	SWS Desalters	Wastewater only	0.0	45.0
5	FCC SWS	Wastewater only	0.0	15.0
6	Caustic treating	Wastewater only	0.0	10.0
		Total Flowrate (m ³ /h)	430	90.0

Superstructure Schematic Network:

The superstructure schematic MATLAB result network configuration for multi-contaminant and multi-objective optimum water reuse with regeneration network of the Kaduna refinery solution is shown in Figure 8.8.

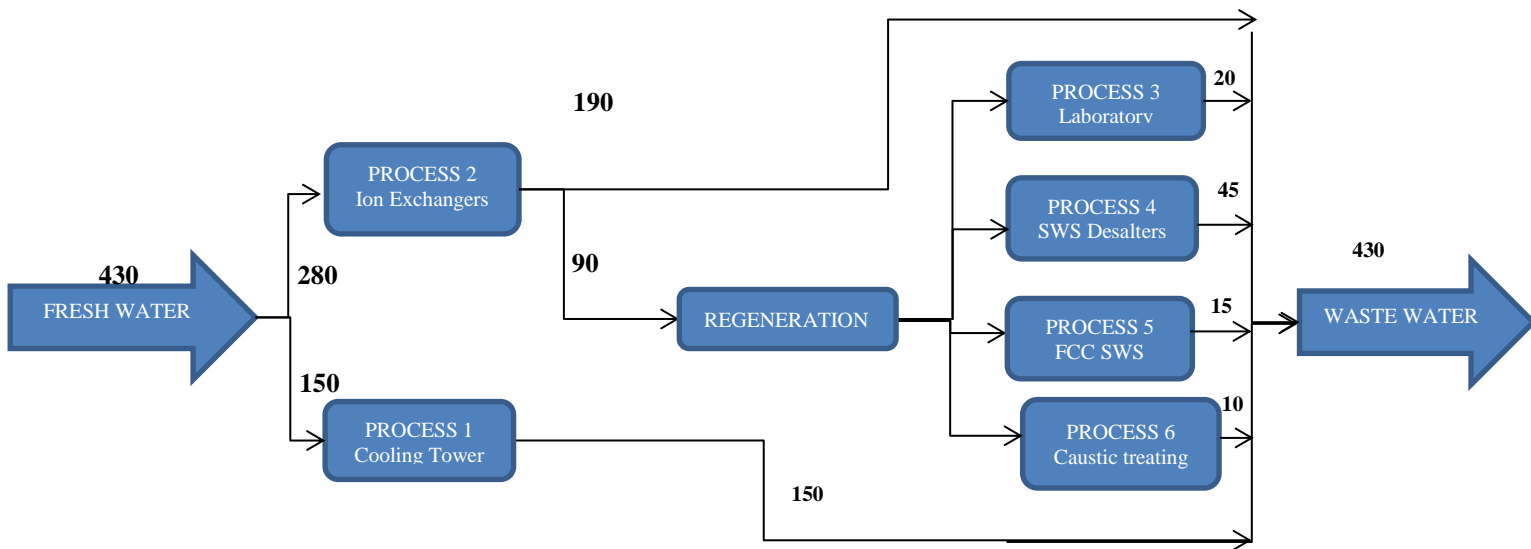


Figure 8. 8: The diagrammatical Superstructure representation of the solution of water reuse with regeneration network for Kaduna Refinery.

Figure 8.9 shows diagnostic solution of wastewater reuse with regeneration for the refinery. The connection modification required for the reuse of wastewater after regeneration from Ion exchanger process by the SWS Desalters and FCC SWS processes is shown with a bold arrow.

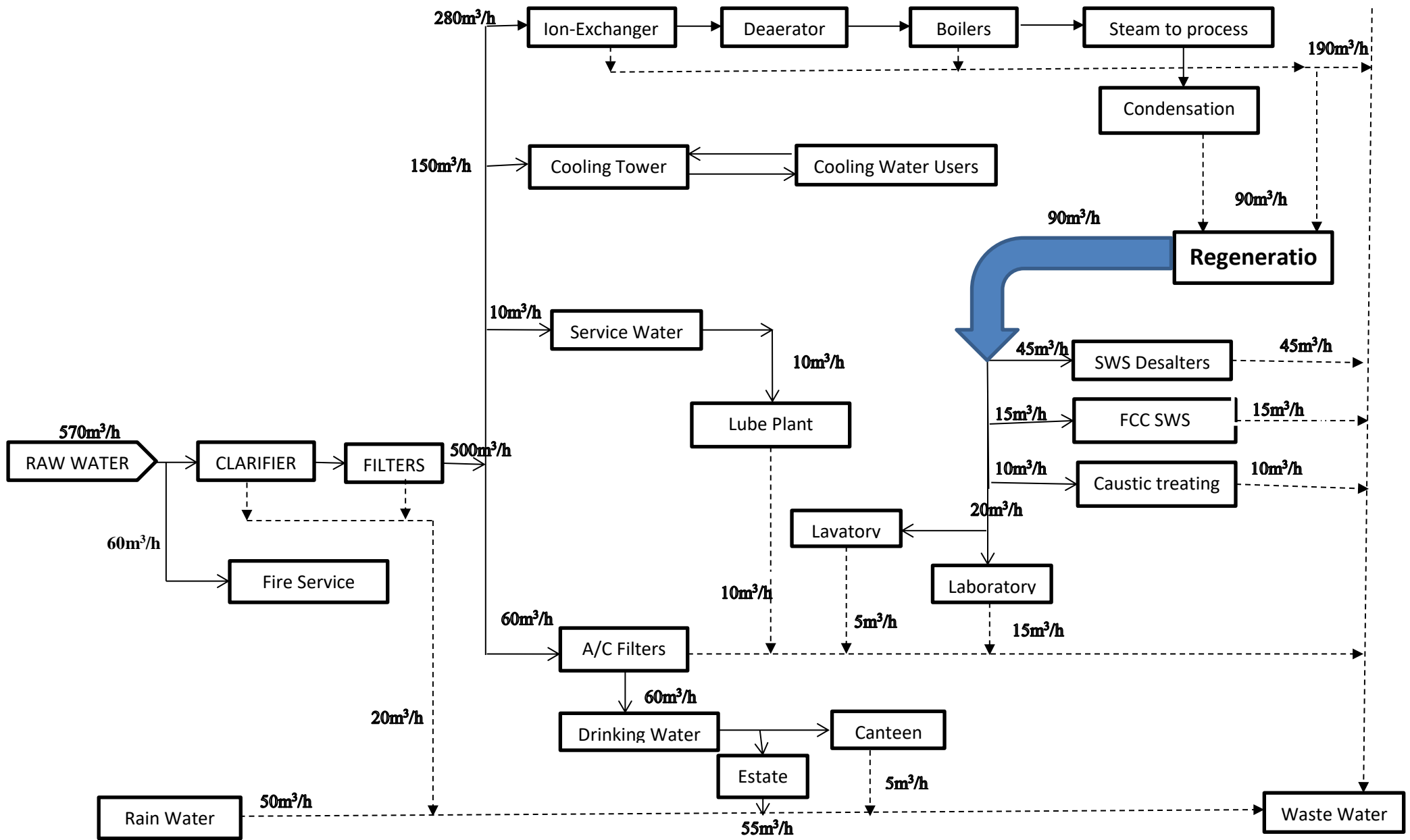


Figure 8. 9: The diagnostic solution of wastewater reuse with regeneration for the refinery.

8.4 Conclusion

This chapter has presented the data obtained from KRPC and all the necessary mathematical steps required in the application of the model for solving the WAP for a refinery. The multi-contaminants and multi-objective nature of a typical refinery was considered in the analysis of minimum freshwater requirement of this refinery. The multi objective genetic algorithm and hybrid function 'Fgoalattain' was used to analyse the WAP problem based on Pareto front for multi-contaminant water reuse with and without regeneration. The result shows that the sum of freshwater flow rates at the entrance of all water using processes (FRW) is 520.0 m³/h, but it can be reduced to 460.0 m³/h if wastewater reuse was considered and it can be further be reduced to 430.0 m³/h if regeneration reuse was considered in the refinery. This indicates that the refinery can save 60.0m³/h which is 11.5% by reusing wastewater and 90.0m³/h which is 17.3% by regeneration and reuse from the wastewater produced by process 2, which is Ion Exchangers. The readers can easily follow the steps to obtain the optimum result for other industries as demonstrated.

The next chapter will presents a summary of the research work carried out and conclusion and recommendations on the WAP results obtained.

CHAPTER NINE

9.0 CONCLUSION AND RECOMMENDATIONS

This chapter presents a summary of the significant contributions made in the solutions of many of the challenges identified in the mathematical optimization of WAP problems. The research work carried out based on the objectives that lead to achieving the main aim and discussion of the results obtained are presented. It also presents the suggestions for future work.

9.1 Introduction

Industries as one of the huge consumers of freshwater require the innovative way of minimizing its water use. This research proposed a framework for (industrial) water application planning (WAP) that minimise freshwater consumption of any given water using industry. The framework considers a network of interconnections of water streams among the water-using/water-disposing processes. It can handle single and multi-contaminant processes with and without regeneration technologies while the processes receive water of adequate quality. The framework addresses the problem of optimal water allocation in an industry by integrating the water-using and wastewater treatment processes to account for many possible water reuse and regeneration opportunities.

The research is based on systematic literature review. It starts with identification of the different classifications of the WAP problems and approaches used in solving them. The analysis of the literature leads to determination of five major research gaps on the mathematical optimisation method for solving the WAP problem. A conceptual WAP model was derived to handle all the challenges, efficiently. The Genetic Algorithm (GA) optimisation was selected to be used in the matlab software environment for solving WAP models based on its robustness in handling such challenges. The mathematical

application of WAP models used was tested in the optimisation of single contaminant water reuse network for 2 to 10 number of industrial processes. The values of the solutions obtained from the WAP model using GA with and without hybrid function were compared. The multi-contaminant and multi-objective WAP problems and their data set-up requirements were presented. Finally, the application of the model to the case study of Kaduna Refining and Petrochemical Company Limited (KRPC) and the expected minimisation of freshwater with and without regeneration of the wastewater using MOGA is presented. Therefore, the objectives of the research were achieved as follows:

9.2 First Objective: To identify optimisation methods/strategies that can be applied to single and multi- contaminant water re-use industrial processes

The general overview of the literature involved in the different Water Application Planning (WAP) methods was analysed. It assists in the identification of different methods of water reuse optimisation. The optimisation methods identified were Water Pinch Analysis (WPA) and Mathematical method. It described the basic concepts of Water pinch technology (WPT) and mathematical programming as applied to WAP problems. The stochastic mathematical algorithm optimisation method known as Genetic Algorithm (GA) has been identified as the most appropriate method to use in the solution of WAP problem. This is because it has been identified as most robust stochastic optimisation method.

9.3 Second Objective: To design a solution strategy for optimising water reuse network capable of handling single, multi-contaminants and regeneration:

The sensitivity analysis of the GA as the selected method for solving the different WAP problems in matlab software environment was carried out. This leads to identification of the best parameters setting for the solution method and achieving the best computer time for different number of industrial processes. Furthermore, the solution strategy of GA with and without hybrid function 'fmincon' was presented. This shows the advantage of using hybrid function in GA for obtaining the optimum result. Moreover, the mathematical application of WAP models used in optimisation of single contaminant and multi-contaminant water reuse network and their data set-up requirements were presented, respectively. The advantage of adding regeneration in finding the optimum minimum freshwater use in the 3 industrial processes example obtained from literature is highlighted.

9.4 Third Objective: To develop a robust solution method for the optimisation of 'Water Application Planning' (WAP) problem considering both single and multi-objective (MO)

The single and multi-objective of minimising freshwater use were considered in solving WAP problem based on Pareto front. The result shows that the method of solution is robust, since it can search a wide-ranging distribution of Pareto optimal solution and it has a noble performance and small computational time.

The Multi-objective GA (MOGA) was improved with a hybrid function 'fgoalattain' to increase its capability to search for optimum solution of WAP problem.

9.5: Fourth Objective: To assess the application of developed 'Water Application Planning' (WAP) framework for water reuse networks in a refinery:

A case study of Kaduna Refining and Petrochemical Company Limited (KRPC) was presented. This addresses the problem of optimal water application in a petroleum refinery by integrating the water-using and wastewater treatment processes to account for many possible water reuse and regeneration opportunities. The relevant data for the minimisation of freshwater use was obtained and evaluated. The analysis of the data obtained was carried out using multi-contaminant, multi-objective method of analysis. The multi objective genetic algorithm (MOGA) and hybrid function 'Fgoalattain' was used to analysed the refinery's WAP problem based on Pareto front for multi-contaminant water reuse with and without regeneration. This result indicates that the refinery can save 60.0m³/h by reusing the wastewater and 90.0m³/h by regeneration and reuse from the wastewater produced by process 2 which is Ion Exchanger.

Furthermore, the diagrammatical Superstructure representation of the solution of water reuse network was presented in all the analysed cases.

9.6: Recommendations for Future Work:

This research identifies the best method of optimisation of water reuse network for the minimisation of freshwater use in industries. The research articles published in this research area were extensively reviewed and different approaches were identified before the selection of this method. However, the performance of the method can be improved by adding more than one hybrid function to the GA to obtain the optimum solution.

It is anticipated that the combination of two robust stochastic mathematical optimisation method (e.g. Genetic Algorithm and Ant Colony Optimisation (ACO) algorithms) with two hybrid functions can improve the solution and computer time. Furthermore, the Matlab software used in the analysis is improving annually with new version, therefore, using the latest version can lead to achieving the best result and shortest computer time.

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APPENDIX A



Optimization of Water Reuse Network Using Water Pinch Technology (WPT) by Considering Single Contaminant for Kaduna Refinery and Petrochemical Company, Nigeria

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Abstract

Conventionally, freshwater has been the only source of water for processes used in the industries due to the fact that it is cheap, and the wastewater generated in these processes has been treated in a central common facility in order to remove contaminants and to meet regulatory specifications for wastewater disposal. This research identifies an optimum design of water reuse network for Kaduna refinery and petrochemical company (KRPC), while considering suspended solid (SS), hardness (H), Chemical oxygen demand (COD) and Free hydrocarbons (FH) wastewater contaminants and analysing the feasibilities of reuse and recycling for water and wastewater minimization in the water network of the company by using graphical method known as Water Pinch Technology (WPT). The analysis indicated the possibility of reducing the fresh water use by 76.8 m³/h (32.3%) if Free Hydrocarbons (FH) was considered as the reference contaminant.

Keywords: Freshwater; Optimization; Wastewater; Environment; Contaminant; Pinch

Introduction

Large quantity of water is required in many industries, which is used in many processes for washing or as part of the product. The resulting wastewater is usually treated in a central common facility in order to remove contaminants and to meet regulatory discharge requirements. In some cases, the treated wastewater may still contain certain level of pollutants. Consequently, the environmental pollution increases due to this disposal trend. As opposed to this conventional approach, reusing and re-routing the water streams in an integral water network helps in reducing the consumption of freshwater, and minimizes the amount of wastewater to be treated and disposed of to the environment. This is very important, especially in developing countries where the relatively high cost and limited manpower pose additional challenges to effective wastewater treatment. One of the methods that can be used to minimize wastewater production is by Graphical method known as Water Pinch Technology (WPT) or Water Pinch Analysis (WPA).

WPT or WPA originates from the concept of heat pinch technique. It is a systematic technique for reducing water consumption and wastewater generation through integration of water-using activities or processes. It was first introduced by Wang and Smith. They used a limiting composite curve to solve water minimization problems. Since then, it has been widely used as a tool for water conservation in industrial process plants. It was extended in 1998 by Nick Hallale at the University of Cape Town, who developed it as a special case of mass exchange networks for capital cost targeting. Manan et al. [1] applied it successfully in urban/domestic buildings. Most of the methods used in WPT/WPA are based on the mass exchange of one or several contaminants. If the mass exchange is based on mass transferring of one contaminant, the problem will be solved as a single contaminant [2-4]. Nevertheless, if it includes mass transferring of two or more key contaminants, the problem will be solved as multiple contaminants [5]. Graphical methods are so practical to solve single contaminant problems. However, they are complicated and sometimes impossible for multiple contaminant problems [6].

This paper focuses on wastewater minimisation using single-

contaminant technique using WPT/WPA based on the composite curves introduced by Wang and Smith [7] and the work of Mohammadnejad et al. [6]. Furthermore, it will address the problem of an optimum design of water minimization by using a combination of WPA, simple mathematical calculation and possible forbidden or forced water network interconnections restrictions. The proposed method tries to address shortcomings in the conventional WPA by considering the possibility of interconnections of different processes in any industry [8,9]. The method thus represents an improvement over existing state-of-the-art approaches. This paper will also test the feasibility of the method using data obtained from the Nigerian Kaduna petrochemical refinery. The feasibilities of reuse and recycling of water and wastewater minimization in the water network of the refinery will be analysed by considering suspended solid (SS), hardness (H), chemical oxygen demand (COD) and Free Hydrocarbons (FH) wastewater contaminants [10,11].

This will eventually lead to providing a means of minimizing the potential dangers facing the aquatic ecosystem as a result of the reduction in the discharge volume of industrial effluents containing harmful contaminants in concentrations above the maximum permissible levels and facilitate efficient and cost effective water usage planning and management.

Materials and Methods

This research is on the Kaduna Refining and Petrochemical Company Limited (KRPC) (Figure 1), a Subsidiary of Nigerian National Petroleum Corporation (NNPC).

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The Refinery project was completed and the Fuels Plant was commissioned in 1980. While the two other subsections of the refinery, the Lubes Plant and Petrochemical Plant were commissioned in 1983 and 1988 respectively. Kaduna Refinery occupies an area of 2.89 square kilometres. The plot plan is designed with safety and ease of maintenance in mind. The design also attempts to minimize operating costs. The refinery was designed to process both imported paraffinic and Nigerian crude oils into fuels and lubes products and was constructed by Chiyoda Chemical Engineering and Construction Company (now Chiyoda Corporation) of Japan (<http://www.nnpcgroup.ng/KRPC.aspx.htm>, 2015). The total installed capacity of the refinery is 110,000 BPSD. The water usage network existing in KRPC shows that fresh water from the river is the only source of water for process and other utilities use. The typical characteristics of this water are high suspended solids (with seasonal variation), high dissolved solids (metals), and variable turbidity. From the information obtained, the flow rate of the fresh water use is 650 m³/h. The existing water usage network by various units is shown in Figure 2.

Table 1 shows the flow rate and the maximum allowable concentration at inlet (C_{in}) and outlet (C_{out}) of major water using units. However the value for fire unit indicated as 60.0 m³/h may reach 150.0 m³/h during fire fighting.

Water pinch analysis steps

Water Pinch Analysis (WPA) was carried out using source and sink composite curves, which is a graphical tool for setting water recovery targets as well as for design of water recovery networks [12]. It considers each water-using operation as being described by the mass transfer of a certain contaminant(s) from the process itself to the water stream (Figure 3a) and represented by the Loading and Concentration Figure (Figure 3b). First of all, in order to achieve a better understanding of the composite curves, a single water using unit is analysed in this section.



Figure 1: The picture of Kaduna Refining and Petrochemical Company Limited (KRPC).

WPA involves five key steps as stated by Wan and Manan [13], they are:

1. Analysis of water network: The first step is to analyse the existing or the base case water network through plant auditing as shown in Figure 2. In general, water-using operations can be classified into two main categories, i.e., mass-transfer-based (MTB) and non-mass-transfer-based (NMTB) operations [1,14].
2. Data extraction: The second step is to identify water sources and water sinks having potential for reuse and recycling and to extract the limiting water flow rate and limiting concentration data. Non-limiting concentrations in the water system are situated at a concentration below their maximum limits and do not affect the water sink for that operation.
3. Setting the minimum utility targets: The third step is to establish the minimum possible quantity of fresh water requirement and wastewater generation, or the minimum water targets using a targeting method.
4. Water network design/retrofit: The fourth step is to design a water recovery network to realise the minimum water targets.
5. Economic evaluation: The final step is to evaluate the economics of the water network.

The processes that use large amount of water rate such as cooling tower, Ion exchangers, and Service water used in desalter, fuel carbon cracking, Lube plant, caustic treating and laboratory in the refinery were selected [15-19]. They use total rate of 565 m³/h which is equivalent to 82.5% of the total water rate used by the refinery. While the contaminants selected are Suspended solids (SS), Hardness (H), Chemical oxygen demand (COD) and free hydrocarbons (FH).

These contaminants are analysed separately using single contaminant method of WPA/WPT, by establishing the pinch point using mass load which is calculated as follows (Equation 1):

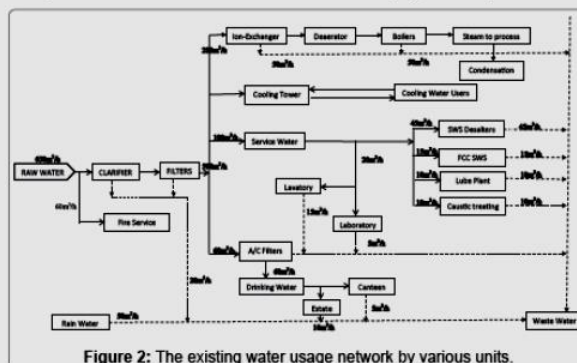


Figure 2: The existing water usage network by various units.

Unit No.	Unit name	Flow Rate of Fresh Water (m ³ /h)	Suspended Solid		Hardness		Chemical Oxygen Demand (COD)		Free Hydrocarbons	
			C_{in} (ppm)	C_{out} (ppm)	C_{in} (ppm)	C_{out} (ppm)	C_{in} (ppm)	C_{out} (ppm)	C_{in} (ppm)	C_{out} (ppm)
1	Cooling Tower	150	40	500	5	10	0	150	0	5
2	Ion Exchangers	280	10	20	20	100	0	150	0	5
3	Laboratory	20	25	250	50	200	400	1000	0	5
4	SWS Desalters	45	30	300	20	100	400	1000	0	1000
5	FCC SWS	15	15	30	20	100	600	1200	0	10
6	Caustic treating	10	15	20	20	100	600	1200	0	10
7	Drinking	60	20	150	10	200	0	0.05	0	0
8	Fire	60	-	-	-	-	-	-	-	-

Table 1: The maximum allowable value of major water using units.

$$\Delta m_{opi} = \frac{(C_{out} - C_{in})f_{opi}}{1000} \quad (1)$$

Where Δm_{opi} is the mass-load for operation i , C_{out} and C_{in} are the outlet and inlet concentration respectively, and f_{opi} is the fresh water flowrate.

The Schematic representation of water balance superstructure model of KRPC water using operations in all processes is illustrated in Figure 4. This can be used as the bases for analysis of water using single contaminant method.

Results

Water Pinch Analysis (WAP) using single contaminant method

The WAP analysis using single contaminant method is done by constructing limiting composite curve (LCC). To construct the LCC, limiting water profiles of individual processes are plotted on an impurity concentration vs load graph. The limiting water profiles are plotted according to their limiting inlet and outlet concentrations which define the concentration intervals. The impurity load is then added within each concentration interval to form the limiting composite curve [20-25].

The limiting water use data for suspended solids (SS), Hardness (H), Chemical oxygen demand (COD) and free hydrocarbons (FH)

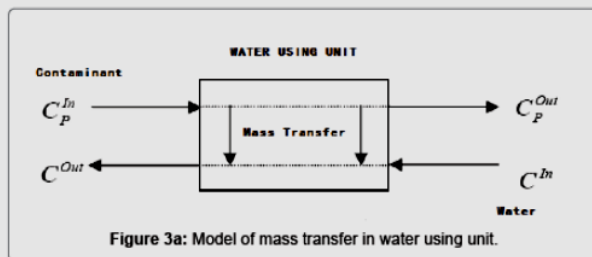


Figure 3a: Model of mass transfer in water using unit.

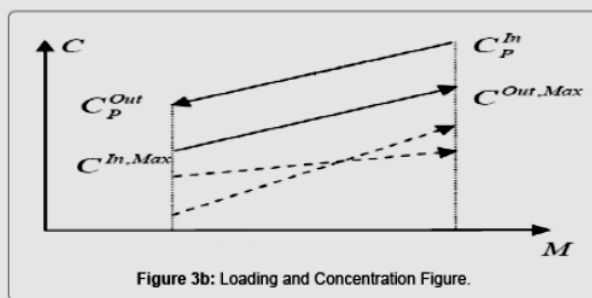


Figure 3b: Loading and Concentration Figure.

contaminants and their calculated cumulative mass load (ppm) are shown in Tables 2-5 respectively. The data were established by referring to the water consuming units as sink and water generating units as source and it was used to construct the limiting composite curves which indicate the pinch point for the particular contaminant considered as a single contaminant to all the processes [26-28]. The sink and source were arranged in ascending order from lower contaminant value process to the higher one. The curves are shown in Figures 5-8.

Figure 5 is the graphical representation of limiting water use data for suspended solids (SS) in Table 2. The graph indicates a pinch point at 20 ppm concentration of SS, and 3.07 ppm cumulative mass load. This means that there is possibility of reduction of fresh water source of 365 m³/h if SS was considered as the only contaminant in the refinery water supply, which is 56% of the total fresh water use.

Figure 6 is the graphical representation of limiting water use data for hardness (H). The graph indicates a pinch point at 100 ppm concentration of H, and 23.15 ppm cumulative mass load. This means that there is possibility of reduction of fresh water source of 430 m³/h if H was considered as the only contaminant in the refinery water supply, which is 66% of the total fresh water use.

Figure 7 is the graphical representation of limiting water use data for Chemical oxygen Demand (COD). The graph indicates a pinch point at 150 ppm concentration of COD, and 64.5 ppm cumulative mass load. This means that there is possibility of reduction of fresh water source of 490 m³/h if COD was considered as the only contaminant in the refinery water supply, which is 75.4% of the total fresh water use.

Figure 8 is the graphical representation of limiting water use data for Free Hydrocarbon (FH). The graph indicates a pinch point at 10 ppm concentration of FH, and 2.49 ppm cumulative mass load. This means that there is possibility of reduction of fresh water source of 534 m³/h if FH was considered as the only contaminant in the refinery water supply, which is 82% of the total fresh water use, because of the range of acceptance of pollution level of FH by different processes.

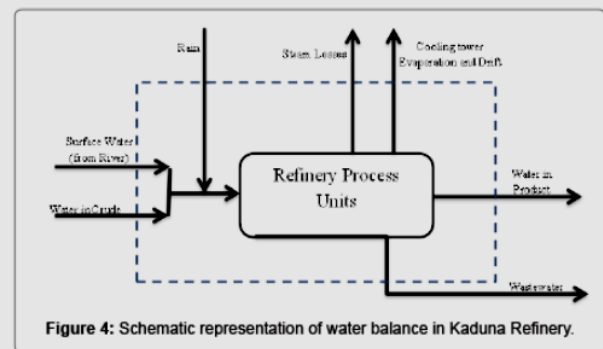


Figure 4: Schematic representation of water balance in Kaduna Refinery.

Process number	Sink	Sink Flow Rate	C_{in} (ppm)	Source	Source Flow Rate m ³ /h	C_{out} (ppm)	Mass Load	Cummulative Mass Load (ppm)	Cumulative Flow m ³ /h
		m ³ /h					(ppm)		
8	SK8	60	-	SR8	60	-	-	-	60
2	SK2	280	10	SR2	280	20	2.8	2.8	340
5	SK5	15	15	SR5	15	30	0.225	3.025	355
6	SK6	10	15	SR6	10	20	0.05	3.075	365
7	SK7	60	20	SR7	60	150	7.8	10.875	425
3	SK3	20	25	SR3	20	250	4.5	15.375	445
4	SK4	50	30	SR4	45	300	12.15	27.525	490
1	SK1	150	40	SR1	150	500	69	96.525	640

Table 2: Limiting water data for suspended solid (SS) contaminant.

Process number	Sink	Sink Feed Flow Rate m ³ /h	C _m (ppm)	source	Source Flow Rate m ³ /h	C _{out} (ppm)	Mass load	Cumulative massload (ppm)	cumulative flow m ³ /h
							(ppm)		
1	SK1	150	5	SR1	150	10	0.75	0.75	150
2	SK2	280	20	SR2	280	100	22.4	23.15	430
4	SK4	45	20	SR4	45	100	3.6	26.75	475
5	SK5	15	20	SR5	15	100	1.2	27.95	490
6	SK6	10	20	SR6	10	100	0.8	28.75	500
7	SK7	60	10	SR7	60	200	11.4	40.15	560
3	SK3	20	50	SR3	20	200	3	43.15	580
8	SK8	60	-	SR8	60	-	-	-	640

Table 3: Limiting water data for hardness (H).

Process number	Sink	Sink Feed Flow Rate m ³ /h	C _m (ppm)	Source	Source Flow Rate m ³ /h	C _{out} (ppm)	Mass load	Cumulative massload (ppm)	Cumulative flow m ³ /h
							(ppm)		
7	SK7	60	0	SR7	60	0.05	0.003	0.003	60
1	SK1	150	0	SR1	150	150	22.5	22.503	210
2	SK2	280	0	SR2	280	150	42	64.503	490
3	SK3	20	400	SR3	20	1000	12	76.503	510
4	SK4	45	400	SR4	45	1000	27	103.503	555
5	SK5	15	600	SR5	15	1200	9	112.503	570
5	SK6	10	600	SR6	10	1200	6	118.503	580
8	SK8	60	-	SR8	60	-	-	-	640

Table 4: Limiting water data for chemical oxygen demand (COD).

Process number	Sink	Sink Feed Flow Rate m ³ /h	C _m (ppm)	Source	Source Flow Rate m ³ /h	C _{out} (ppm)	Mass load	Cumulative massload (ppm)	Cumulative flow m ³ /h
							(ppm)		
7	SK7	60	0	TSR7	60	0	0	0	60
1	SK1	150	0	SR1	150	5	0.75	0.75	210
2	SK2	280	0	SR2	280	5	1.4	2.15	490
3	SK3	20	0	SR3	20	5	0.1	2.25	510
5	SK5	15	0	SR5	15	10	0.15	2.4	525
6	SK6	10	0	SR6	10	10	0.1	2.5	535
4	SK4	45	0	SR4	45	1000	45	47.5	580
8	SK8	60	-	SR8	60	-	-	-	640

Table 5: Limiting water data for free hydrocarbons (FH).

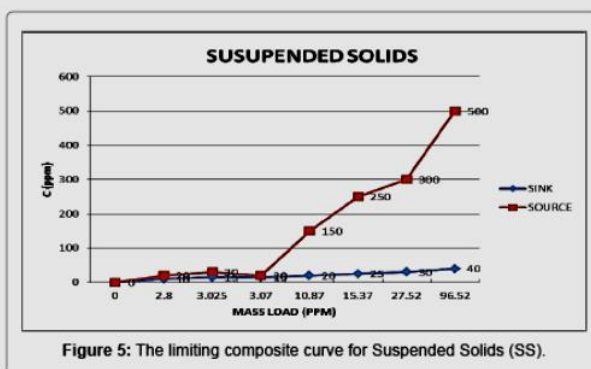


Figure 5: The limiting composite curve for Suspended Solids (SS).

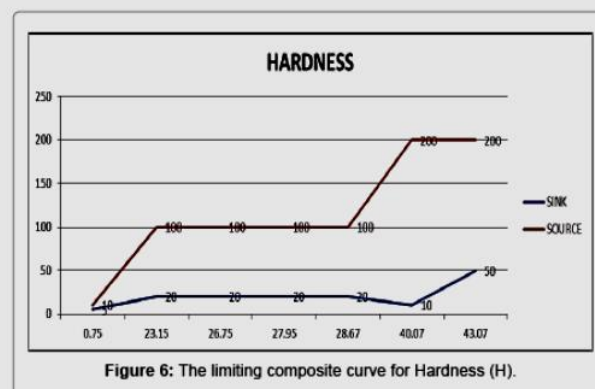


Figure 6: The limiting composite curve for Hardness (H).

The result obtained by this graphical analysis of pinch point can be justified by analysing the concentration grid of each contaminant and considering that a water generating process with output concentration lower than the minimum input concentration of another process can be re-used if the process allow re-use of water from another process [26].

The concentration grid for suspended solids (SS) contaminant is shown in Figure 9. The result indicate that water from three processes namely; Ion Exchangers, FCC SWS, Caustic treating and Drinking can be re-used in the refinery which gives a total saving of fresh water

source of 365 m³/h if SS is considered as the only contaminant as shown by the pinch graphical analysis. This agrees with the result obtained from WPT analysis [29-31].

The concentration grid for Hardness (H) contaminant is shown in Figure 10. The result indicate that only water from Cooling Tower and Drinking can be re-used in the refinery which gives a total saving of fresh water source of 210 m³/h if H is considered as the only contaminant, which is 32.3% of the total fresh water use. This contradicts the value

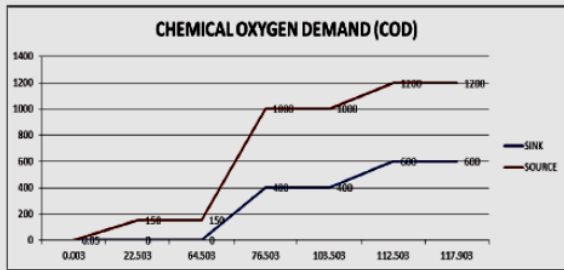


Figure 7: The limiting composite curve for Chemical Oxygen Demand (COD).

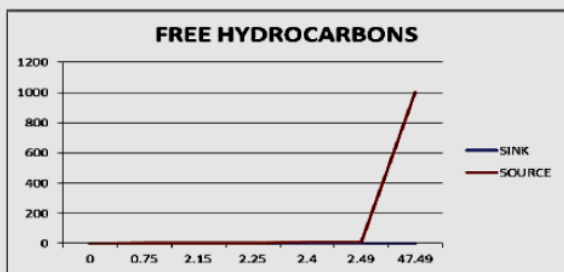


Figure 8: The limiting composite curve for Free Hydrocarbons (FH).

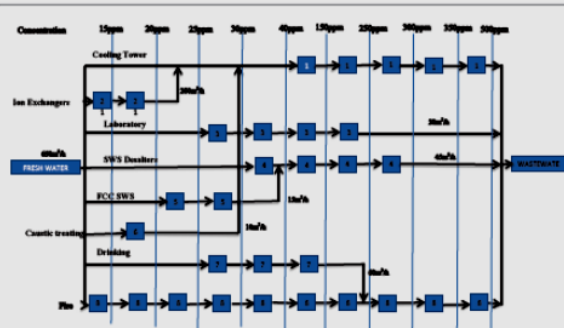


Figure 9: The concentration grid for Suspended Solids (SS).

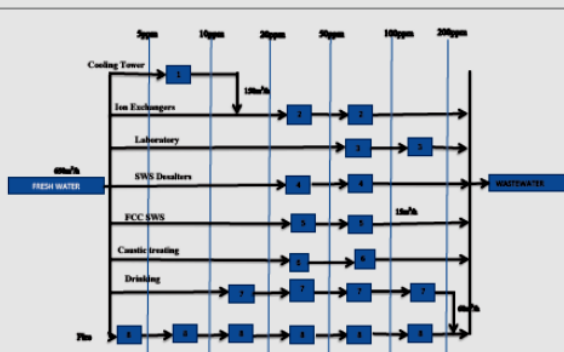


Figure 10: The concentration grid for Hardness (H).

shown by the pinch graphical analysis. Possibly due to the presence of four processes (Ion Exchangers, SWS Desalter, FCC SWS, and caustic treating) that has equal concentration ranges of 20 ppm to 100 ppm.

Furthermore, the concentration grid for Chemical Oxygen Demand (COD) contaminant is shown in Figure 11. The result indicate that water from three processes namely; Cooling Tower, Ion Exchangers, and Drinking can be re-used in the refinery which gives a total saving of fresh water source of 490 m³/h if COD is considered as the only contaminant as shown by the pinch graphical analysis.

The concentration grid for Free Hydrocarbons (FH) contaminant is shown in Figure 12. The result indicate that only water from Drinking can be re-used in the refinery which gives a total saving of fresh water source of 60 m³/h if FH is considered as the only contaminant, which is 9.2% of the total fresh water use. This contradicts the value shown by the pinch graphical analysis. Possibly due to the fact that all the processes have equal input concentration ranges of 0 ppm.

Therefore, the pinch analysis for a single contaminant should be used only in the situation where all the processes have different concentration ranges. Otherwise equal concentration ranges should be eliminated before carrying out the analysis.

Based on the above analysis of single contaminant, the amount

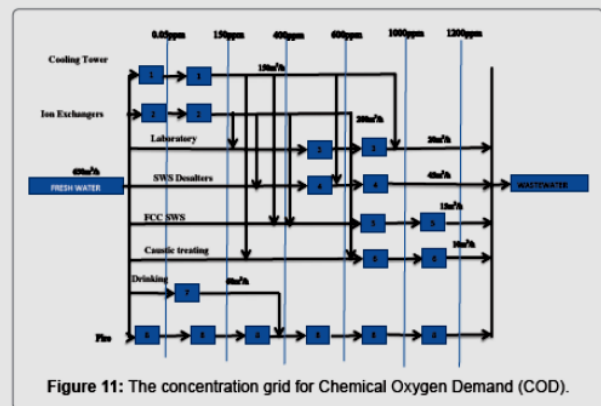


Figure 11: The concentration grid for Chemical Oxygen Demand (COD).

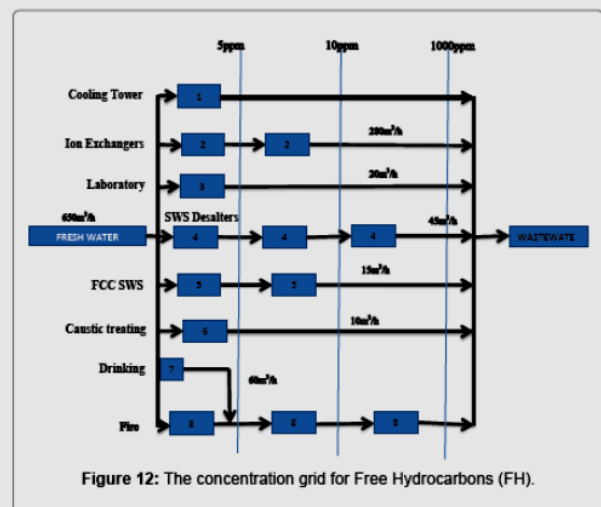


Figure 12: The concentration grid for Free Hydrocarbons (FH).

of fresh water can be reduced by re-using 365 m³/h (56%) if SS was considered as the only contaminant, in the refinery water supply, by 210 m³/h (32.3%) if H was considered as the only contaminant, by 490 m³/h (75.4%) if COD was considered as the only contaminant, and by 60 m³/h (9.2%) if FH was considered as the only contaminant.

Conclusion

In this paper, an optimum design of water reuse network for Kaduna refinery by considering suspended solid (SS), hardness (H), chemical oxygen demand (COD) and Free Hydrocarbons (FH) wastewater contaminants was achieved. The analysis of the feasibilities of reuse and recycling for water and wastewater minimization in the water network of the refinery was also carried out. The result indicate that there are possibilities of reduction of fresh water use of 365 m³/h, 430 m³/h, 490 m³/h, and 534 m³/h if SS, H, COD, and FH are considered as the single-contaminant in the refinery water supply, respectively. This will leads to 56%, 66%, 75.4%, and 82% reduction of the total fresh water use if SS, H, COD, and FH are considered as the single-contaminant in the refinery water supply, respectively. However, these results were further analysed by using the concentration grid of each contaminant. The values obtained for SS and COD agree with the result obtained from WPT analysis, but give the values of 210 m³/h and 60 m³/h, which correspond to the reduction of 32.3% and 9.2% for H and FH respectively.

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APPENDIX B

B1. Equations for Single Contaminant Water Reuse without Regeneration for 3 Industrial Processes

The fitness function is the Sum of fresh water flow rates at the entrance of each water using process as shown in equation 5.5:

$$F = \text{Min} \sum_{i=1}^3 F_i \dots \dots \dots 5.5a$$

$$F = F_1 + F_2 + F_3 \dots \dots \dots 5.5b$$

The Linear Constraints functions of the water and contaminant mass balance are represented in equation 5.6 and 5.7 as follows:

1. The constraint of the water mass balance of all process

$$F_i + \sum_{j \neq i} X_{i,j} - W_i - \sum_{j \neq i} X_{j,i} = 0 \dots \dots \dots 5.6a$$

$$F_1 + X_{1,2} + X_{1,3} - W_1 - X_{2,1} - X_{3,1} = 0 \dots \dots \dots 5.6b$$

$$F_2 + X_{2,1} + X_{2,3} - W_2 - X_{1,2} - X_{3,2} = 0 \dots \dots \dots 5.6c$$

$$F_3 + X_{3,1} + X_{3,2} - W_3 - X_{1,3} - X_{2,3} = 0 \dots \dots \dots 5.6d$$

2. The constraint of the contaminant mass balance of all processes:

$$\sum_{j \neq i} C_{j,out} X_{i,j} + \Delta M_i - C_{i,out} \left(W_i + \sum_{j \neq i} X_{j,i} \right) = 0 \dots \dots \dots 5.7a$$

$$C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + \Delta M_1 - C_{1,out} (W_1 + X_{2,1} + X_{3,1}) = 0 \dots \dots \dots 5.7b$$

$$C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + \Delta M_2 - C_{2,out} (W_2 + X_{1,2} + X_{3,2}) = 0 \dots \dots \dots 5.7c$$

$$C_{1,out} X_{3,1} + C_{2,out} X_{3,2} + \Delta M_3 - C_{3,out} (W_3 + X_{1,3} + X_{2,3}) = 0 \dots \dots \dots 5.7d$$

3. The nonlinear constraint function of the maximum contaminant inlet concentration are represented in equation 5.8 as follows:

$$C_{j,in} = \frac{\sum_{j \neq i} C_{j,out} X_{i,j}}{\sum_{j \neq i} X_{i,j} + F_i} \leq C_{i,in}^{max} \dots \dots \dots 5.8a$$

$$C_{2,out} = \frac{C_{2,out} X_{1,2} + C_{3,out} X_{1,3}}{F_1 + X_{1,2} + X_{1,3}} \leq C_{1,in}^{max} \dots\dots\dots 5.8b$$

$$C_{1,out} = \frac{C_{1,out} X_{2,1} + C_{3,out} X_{2,3}}{F_2 + X_{2,1} + X_{2,3}} \leq C_{2,in}^{max} \dots\dots\dots 5.8c$$

$$C_{1,out} = \frac{C_{1,out} X_{3,1} + C_{2,out} X_{3,2}}{F_3 + X_{3,1} + X_{3,2}} \leq C_{3,in}^{max} \dots\dots\dots 5.8d$$

B2. Equations for Single Contaminant Water Reuse without Regeneration for 4 Industrial Processes

The fitness function is the Sum of fresh water flow rates at the entrance of each water using process as shown in equation 5.9:

$$F = \sum_{i=1}^4 F_i \dots\dots\dots 5.9a$$

$$F = F_1 + F_2 + F_3 + F_4 \dots\dots\dots 5.9a$$

The Linear Constraints functions of the water and contaminant mass balance are represented in equation 5.10 and 5.11 as follows:

Linear Constraints functions

1. The constraint of the water mass balance of all process

$$F_i + \sum_{j \neq i} X_{i,j} - W_i - \sum_{j \neq i} X_{j,i} = 0 \dots\dots\dots 5.10a$$

$$F_1 + X_{1,2} + X_{1,3} + X_{1,4} - W_1 - X_{2,1} - X_{3,1} - X_{4,1} = 0 \dots\dots\dots 5.10b$$

$$F_2 + X_{2,1} + X_{2,3} + X_{2,4} - W_2 - X_{1,2} - X_{3,2} - X_{4,2} = 0 \dots\dots\dots 5.10c$$

$$F_3 + X_{3,1} + X_{3,2} + X_{3,4} - W_3 - X_{1,3} - X_{2,3} - X_{4,3} = 0 \dots\dots\dots 5.10d$$

$$F_4 + X_{4,1} + X_{4,2} + X_{4,3} - W_4 - X_{1,4} - X_{2,4} - X_{3,4} = 0 \dots\dots\dots 5.10e$$

2. The constraint of the contaminant mass balance of all processes

$$\sum_{j \neq i} C_{j,out} X_{i,j} + \Delta M_i - C_{i,out} \left(W_i + \sum_{j \neq i} X_{j,i} \right) = 0 \dots\dots\dots 5.11a$$

$$C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4} + \Delta M_1 - C_{1,out} (W_1 + X_{2,1} + X_{3,1} + X_{4,1}) = 0 \dots\dots\dots 5.11b$$

$$C_{1,out}X_{2,1} + C_{3,out}X_{2,3} + C_{4,out}X_{2,4} + \Delta M_2 - C_{2,out}(W_2 + X_{1,2} + X_{3,2} + X_{4,2}) = 0 \dots \dots \dots 5.11c$$

$$C_{1,out}X_{3,1} + C_{2,out}X_{3,2} + C_{4,out}X_{3,4} + \Delta M_3 - C_{3,out}(W_3 + X_{1,3} + X_{2,3} + X_{4,3}) = 0 \dots \dots \dots 5.11d$$

$$C_{1,out}X_{4,1} + C_{2,out}X_{4,2} + C_{4,out}X_{4,3} + \Delta M_4 - C_{4,out}(W_4 + X_{1,4} + X_{2,4} + X_{3,4}) = 0 \dots \dots \dots 5.11e$$

3. The nonlinear constraint function of the maximum contaminant inlet concentration are represented in equation 5.12 (b-e) as follows:

$$C_{j,in} = \frac{\sum_{j \neq i} X_{i,j} C_{j,out}}{\sum_{j \neq i} X_{i,j} + F_i} \leq C_{i,in}^{max} \dots \dots \dots 5.12a$$

$$C_{2,out} = \frac{C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4}}{F_1 + X_{1,2} + X_{1,3} + X_{1,4}} \leq C_{1,in}^{max} \dots \dots \dots 5.12b$$

$$C_{1,out} = \frac{C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + C_{4,out} X_{2,4}}{F_2 + X_{2,1} + X_{2,3} + X_{2,4}} \leq C_{2,in}^{max} \dots \dots \dots 5.12c$$

$$C_{1,out} = \frac{C_{1,out} X_{3,1} + C_{2,out} X_{3,2} + C_{4,out} X_{3,4}}{F_3 + X_{3,1} + X_{3,2} + X_{3,4}} \leq C_{3,in}^{max} \dots \dots \dots 5.12d$$

$$C_{1,out} = \frac{C_{1,out} X_{4,1} + C_{2,out} X_{4,2} + C_{3,out} X_{4,3}}{F_4 + X_{4,1} + X_{4,2} + X_{4,3}} \leq C_{4,in}^{max} \dots \dots \dots 5.12e$$

B3. Equations for Single Contaminant Water Reuse without Regeneration for 5 Industrial Processes

The fitness function is the Sum of fresh water flow rates at the entrance of each water using process as shown in equation 5.13 (a-b):

$$F = \sum_{i=1}^4 F_i \dots \dots \dots 5.13a$$

$$F = F_1 + F_2 + F_3 + F_4 + F_5 \dots \dots \dots 5.13b$$

The Linear Constraints functions of the water and contaminant mass balance are represented in equation 5.14 (a-f) and 5.15 (a-f) as follows:

1. The constraint of the water mass balance of all process:

$$F_i + \sum_{j \neq i} X_{i,j} - W_i - \sum_{j \neq i} X_{j,i} = 0 \dots \dots \dots 5.14a$$

$$F_1 + X_{1,2} + X_{1,3} + X_{1,4} + X_{1,5} - W_1 - X_{2,1} - X_{3,1} - X_{4,1} - X_{5,1} = 0 \dots \dots \dots 5.14b$$

$$F_2 + X_{2,1} + X_{2,3} + X_{2,4} + X_{2,5} - W_2 - X_{1,2} - X_{3,2} - X_{4,2} - X_{5,2} = 0 \dots \dots \dots 5.14c$$

$$F_3 + X_{3,1} + X_{3,2} + X_{3,4} + X_{3,5} - W_3 - X_{1,3} - X_{2,3} - X_{4,3} - X_{5,3} = 0 \dots \dots \dots 5.14d$$

$$F_4 + X_{4,1} + X_{4,2} + X_{4,3} + X_{4,5} - W_4 - X_{1,4} - X_{2,4} - X_{3,4} - X_{5,4} = 0 \dots \dots \dots 5.14e$$

$$F_5 + X_{5,1} + X_{5,2} + X_{5,3} + X_{5,4} - W_5 - X_{1,5} - X_{2,5} - X_{3,5} - X_{4,5} = 0 \dots \dots \dots 5.14f$$

2. The constraint of the contaminant mass balance of all processes:

$$\sum_{j \neq i} C_{j,out} X_{i,j} + \Delta M_i - C_{i,out} \left(W_i + \sum_{j \neq i} X_{j,i} \right) = 0 \dots \dots \dots 5.15a$$

$$C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4} + C_{5,out} X_{1,5} + \Delta M_1 - C_{1,out} (W_1 + X_{2,1} + X_{3,1} + X_{4,1} + X_{5,1}) = 0 \dots \dots \dots 5.15b$$

$$C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + C_{4,out} X_{2,4} + C_{5,out} X_{2,5} + \Delta M_2 - C_{2,out} (W_2 + X_{1,2} + X_{3,2} + X_{4,2} + X_{5,2}) = 0 \dots \dots \dots 5.15c$$

$$C_{1,out} X_{3,1} + C_{2,out} X_{3,2} + C_{4,out} X_{3,4} + C_{5,out} X_{3,5} + \Delta M_3 - C_{3,out} (W_3 + X_{1,3} + X_{2,3} + X_{4,3} + X_{5,3}) = 0 \dots \dots \dots 5.15d$$

$$C_{1,out} X_{4,1} + C_{2,out} X_{4,2} + C_{3,out} X_{4,3} + C_{5,out} X_{4,5} + \Delta M_4 - C_{4,out} (W_4 + X_{1,4} + X_{2,4} + X_{3,4} + X_{5,4}) = 0 \dots \dots \dots 5.15e$$

$$C_{1,out} X_{5,1} + C_{2,out} X_{5,2} + C_{3,out} X_{5,3} + C_{4,out} X_{5,4} + \Delta M_5 - C_{5,out} (W_5 + X_{1,5} + X_{2,5} + X_{3,5} + X_{4,5}) = 0 \dots \dots \dots 5.15f$$

3. The nonlinear constraint function of the maximum contaminant inlet concentration

are represented in equation 5.16 as follows:

$$C_{j,in} = \frac{\sum_{j \neq i} X_{i,j} C_{j,out}}{\sum_{j \neq i} X_{i,j} + F_i} \leq C_{i,in}^{max} \dots \dots \dots 5.16a$$

$$C_{2,out} = \frac{C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4} + C_{5,out} X_{1,5}}{F_1 + X_{1,2} + X_{1,3} + X_{1,4} + X_{1,5}} \leq C_{1,in}^{max} \dots \dots \dots 5.16b$$

$$C_{1,out} = \frac{C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + C_{4,out} X_{2,4} + C_{5,out} X_{2,5}}{F_2 + X_{2,1} + X_{2,3} + X_{2,4} + X_{2,5}} \leq C_{2,in}^{max} \dots \dots \dots 5.16c$$

$$C_{1,out} = \frac{C_{1,out} X_{3,1} + C_{2,out} X_{3,2} + C_{4,out} X_{3,4} + C_{5,out} X_{3,5}}{F_3 + X_{3,1} + X_{3,2} + X_{3,4} + X_{3,5}} \leq C_{3,in}^{max} \dots \dots \dots 5.16d$$

$$C_{1,out} = \frac{C_{1,out} X_{4,1} + C_{2,out} X_{4,2} + C_{3,out} X_{4,3} + C_{5,out} X_{4,5}}{F_4 + X_{4,1} + X_{4,2} + X_{4,3} + X_{4,5}} \leq C_{4,in}^{max} \dots \dots \dots 5.16e$$

$$C_{1,out} = \frac{C_{1,out} X_{5,1} + C_{2,out} X_{5,2} + C_{3,out} X_{5,3} + C_{4,out} X_{5,4}}{F_5 + X_{5,1} + X_{5,2} + X_{5,3} + X_{5,4}} \leq C_{5,in}^{max} \dots \dots \dots 5.16f$$

B4. Equations for Single Contaminant Water Reuse without Regeneration for 6 Industrial Processes

The fitness function is the Sum of fresh water flow rates at the entrance of each water using process as shown in equation 5.17 (a-b):

$$F = \sum_{i=1}^6 F_i \dots \dots \dots \dots \dots \dots 5.17a$$

$$F = F_1 + F_2 + F_3 + F_4 + F_5 + F_6 \dots \dots \dots \dots \dots \dots 5.17b$$

The Linear Constraints functions of the water and contaminant mass balance are represented in equation 5.18 and 5.19 as follows:

CONSTRAINTS

Linear Constraints functions

1. The constraint of the water mass balance of all process

$$F_i + \sum_{j \neq i} X_{i,j} - W_i - \sum_{j \neq i} X_{j,i} = 0 \dots \dots \dots \dots \dots \dots 5.18a$$

$$F_1 + X_{1,2} + X_{1,3} + X_{1,4} + X_{1,5} + X_{1,6} - W_1 - X_{2,1} - X_{3,1} - X_{4,1} - X_{5,1} - X_{6,1} = 0 \dots 5.18b$$

$$F_2 + X_{2,1} + X_{2,3} + X_{2,4} + X_{2,5} + X_{2,6} - W_2 - X_{1,2} - X_{3,2} - X_{4,2} - X_{5,2} - X_{6,2} = 0 \dots 5.18c$$

$$F_3 + X_{3,1} + X_{3,2} + X_{3,4} + X_{3,5} + X_{3,6} - W_3 - X_{1,3} - X_{2,3} - X_{4,3} - X_{5,3} - X_{6,3} = 0 \dots 5.18d$$

$$F_4 + X_{4,1} + X_{4,2} + X_{4,3} + X_{4,5} + X_{4,6} - W_4 - X_{1,4} - X_{2,4} - X_{3,4} - X_{5,4} - X_{6,4} = 0 \dots 5.18e$$

$$F_5 + X_{5,1} + X_{5,2} + X_{5,3} + X_{5,4} + X_{5,6} - W_5 - X_{1,5} - X_{2,5} - X_{3,5} - X_{4,5} - X_{6,5} = 0 \dots 5.18f$$

$$F_6 + X_{6,1} + X_{6,2} + X_{6,3} + X_{6,4} + X_{6,5} - W_6 - X_{1,6} - X_{2,6} - X_{3,6} - X_{4,6} - X_{5,6} = 0 \dots 5.18g$$

2. The constraint of the contaminant mass balance of all processes

$$\sum_{j \neq i} C_{j,out} X_{i,j} + \Delta M_i - C_{i,out} \left(W_i + \sum_{j \neq i} X_{j,i} \right) = 0 \dots \dots \dots \dots \dots \dots 4.19a$$

$$C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4} + C_{5,out} X_{1,5} + C_{6,out} X_{1,6} + \Delta M_1 - C_{1,out} (W_1 + X_{2,1} + X_{3,1} + X_{4,1} + X_{5,1} + X_{6,1}) = 0 \dots 4.19b$$

$$C_{1,out}X_{2,1} + C_{3,out}X_{2,3} + C_{4,out}X_{2,4} + C_{5,out}X_{2,5} + C_{6,out}X_{2,6} + \Delta M_2 - C_{2,out}(W_2 + X_{1,2} + X_{3,2} + X_{4,2} + X_{5,2} + X_{6,2}) = 0 \dots 4.19c$$

$$C_{1,out}X_{3,1} + C_{2,out}X_{3,2} + C_{4,out}X_{3,4} + C_{5,out}X_{3,5} + C_{6,out}X_{3,6} + \Delta M_3 - C_{3,out}(W_3 + X_{1,3} + X_{2,3} + X_{4,3} + X_{5,3} + X_{6,3}) = 0 \dots 4.19d$$

$$C_{1,out}X_{4,1} + C_{2,out}X_{4,2} + C_{3,out}X_{4,3} + C_{5,out}X_{4,5} + C_{6,out}X_{4,6} + \Delta M_4 - C_{4,out}(W_4 + X_{1,4} + X_{2,4} + X_{3,4} + X_{5,4} + X_{6,4}) = 0 \dots 4.19e$$

$$C_{1,out}X_{5,1} + C_{2,out}X_{5,2} + C_{3,out}X_{5,3} + C_{4,out}X_{5,4} + C_{6,out}X_{5,6} + \Delta M_5 - C_{5,out}(W_5 + X_{1,5} + X_{2,5} + X_{3,5} + X_{4,5} + X_{6,5}) = 0 \dots 4.19f$$

$$C_{1,out}X_{6,1} + C_{2,out}X_{6,2} + C_{3,out}X_{6,3} + C_{4,out}X_{6,4} + C_{5,out}X_{6,5} + \Delta M_6 - C_{6,out}(W_6 + X_{1,6} + X_{2,6} + X_{3,6} + X_{4,6} + X_{5,6}) = 0 \dots 4.19g$$

3. The nonlinear constraint function of the maximum contaminant inlet concentration are represented in equation 5.20 as follows:

$$C_{j,in} = \frac{\sum_{j \neq i} X_{i,j} C_{j,out}}{\sum_{j \neq i} X_{i,j} + F_i} \leq C_{i,in}^{max} \dots \dots \dots 5.20a$$

$$C_{2,out} = \frac{C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4} + C_{5,out} X_{1,5} + C_{6,out} X_{1,6}}{F_1 + X_{1,2} + X_{1,3} + X_{1,4} + X_{1,5} + X_{1,6}} \leq C_{1,in}^{max} \dots 5.20b$$

$$C_{1,out} = \frac{C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + C_{4,out} X_{2,4} + C_{5,out} X_{2,5} + C_{6,out} X_{2,6}}{F_2 + X_{2,1} + X_{2,3} + X_{2,4} + X_{2,5} + X_{2,6}} \leq C_{2,in}^{max} \dots 5.20c$$

$$C_{1,out} = \frac{C_{1,out} X_{3,1} + C_{2,out} X_{3,2} + C_{4,out} X_{3,4} + C_{5,out} X_{3,5} + C_{6,out} X_{3,6}}{F_3 + X_{3,1} + X_{3,2} + X_{3,4} + X_{3,5} + X_{3,6}} \leq C_{3,in}^{max} \dots 5.20d$$

$$C_{1,out} = \frac{C_{1,out} X_{4,1} + C_{2,out} X_{4,2} + C_{3,out} X_{4,3} + C_{5,out} X_{4,5} + C_{6,out} X_{4,6}}{F_4 + X_{4,1} + X_{4,2} + X_{4,3} + X_{4,5} + X_{4,6}} \leq C_{4,in}^{max} \dots 5.20e$$

$$C_{1,out} = \frac{C_{1,out} X_{5,1} + C_{2,out} X_{5,2} + C_{3,out} X_{5,3} + C_{4,out} X_{5,4} + C_{6,out} X_{5,6}}{F_5 + X_{5,1} + X_{5,2} + X_{5,3} + X_{5,4} + X_{5,6}} \leq C_{5,in}^{max} \dots 5.20f$$

$$C_{1,out} = \frac{C_{1,out} X_{6,1} + C_{2,out} X_{6,2} + C_{3,out} X_{6,3} + C_{4,out} X_{6,4} + C_{5,out} X_{6,5}}{F_6 + X_{6,1} + X_{6,2} + X_{6,3} + X_{6,4} + X_{6,5}} \leq C_{6,in}^{max} \dots 5.20g$$

B5. Equations for Single Contaminant Water Reuse without Regeneration for 7 Industrial Processes

The fitness function is the Sum of fresh water flow rates at the entrance of each water using process as shown in equation 5.5:

$$F = \sum_{i=1}^7 F_i \dots\dots\dots 5.21a$$

$$F = F_1 + F_2 + F_3 + F_4 + F_5 + F_6 + F_7 \dots\dots\dots 5.21b$$

The Linear Constraints functions of the water and contaminant mass balance are represented in equation 5.22 and 5.23 as follows:

CONSTRAINTS

Linear Constraints functions

1. The constraint of the water mass balance of all process

$$F_i + \sum_{j \neq i} X_{i,j} - W_i - \sum_{j \neq i} X_{j,i} = 0 \dots\dots\dots 5.22a$$

$$F_1 + X_{1,2} + X_{1,3} + X_{1,4} + X_{1,5} + X_{1,6} + X_{1,7} - W_1 - X_{2,1} - X_{3,1} - X_{4,1} - X_{5,1} - X_{6,1} - X_{7,1} = 0 \dots\dots\dots 5.22b$$

$$F_2 + X_{2,1} + X_{2,3} + X_{2,4} + X_{2,5} + X_{2,6} + X_{2,7} - W_2 - X_{1,2} - X_{3,2} - X_{4,2} - X_{5,2} - X_{6,2} - X_{7,2} = 0 \dots\dots\dots 5.22c$$

$$F_3 + X_{3,1} + X_{3,2} + X_{3,4} + X_{3,5} + X_{3,6} + X_{3,7} - W_3 - X_{1,3} - X_{2,3} - X_{4,3} - X_{5,3} - X_{6,3} - X_{7,3} = 0 \dots\dots\dots 5.22d$$

$$F_4 + X_{4,1} + X_{4,2} + X_{4,3} + X_{4,5} + X_{4,6} + X_{4,7} - W_4 - X_{1,4} - X_{2,4} - X_{3,4} - X_{5,4} - X_{6,4} - X_{7,4} = 0 \dots\dots\dots 5.22e$$

$$F_5 + X_{5,1} + X_{5,2} + X_{5,3} + X_{5,4} + X_{5,6} + X_{5,7} - W_5 - X_{1,5} - X_{2,5} - X_{3,5} - X_{4,5} - X_{6,5} - X_{7,5} = 0 \dots\dots\dots 5.22f$$

$$F_6 + X_{6,1} + X_{6,2} + X_{6,3} + X_{6,4} + X_{6,5} + X_{6,7} - W_6 - X_{1,6} - X_{2,6} - X_{3,6} - X_{4,6} - X_{5,6} - X_{7,6} = 0 \dots\dots\dots 5.22g$$

$$F_7 + X_{7,1} + X_{7,2} + X_{7,3} + X_{7,4} + X_{7,5} + X_{7,6} - W_7 - X_{1,7} - X_{2,7} - X_{3,7} - X_{4,7} - X_{5,7} - X_{6,7} = 0 \dots\dots\dots 5.22h$$

2. The constraint of the contaminant mass balance of all processes

$$\sum_{j \neq i} C_{j,out} X_{i,j} + \Delta M_i - C_{i,out} \left(W_i + \sum_{j \neq i} X_{j,i} \right) = 0 \dots\dots\dots 5.23a$$

$$C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4} + C_{5,out} X_{1,5} + C_{6,out} X_{1,6} + C_{7,out} X_{1,7} + \Delta M_1 - C_{1,out} (W_1 + X_{2,1} + X_{3,1} + X_{4,1} + X_{5,1} + X_{6,1} + X_{7,1}) = 0 \dots\dots\dots 5.23b$$

$$C_{1,out}X_{2,1} + C_{3,out}X_{2,3} + C_{4,out}X_{2,4} + C_{5,out}X_{2,5} + C_{6,out}X_{2,6} + C_{7,out}X_{2,7} + \Delta M_2 - C_{2,out}(W_2 + X_{1,2} + X_{3,2} + X_{4,2} + X_{5,2} + X_{6,2} + X_{7,2}) = 0 \dots \dots \dots 5.23c$$

$$C_{1,out}X_{3,1} + C_{2,out}X_{3,2} + C_{4,out}X_{3,4} + C_{5,out}X_{3,5} + C_{6,out}X_{3,6} + C_{7,out}X_{3,7} + \Delta M_3 - C_{3,out}(W_3 + X_{1,3} + X_{2,3} + X_{4,3} + X_{5,3} + X_{6,3} + X_{7,3}) = 0 \dots \dots \dots 5.23d$$

$$C_{1,out}X_{4,1} + C_{2,out}X_{4,2} + C_{3,out}X_{4,3} + C_{5,out}X_{4,5} + C_{6,out}X_{4,6} + C_{7,out}X_{4,7} + \Delta M_4 - C_{4,out}(W_4 + X_{1,4} + X_{2,4} + X_{3,4} + X_{5,4} + X_{6,4} + X_{7,4}) = 0 \dots \dots \dots 5.23e$$

$$C_{1,out}X_{5,1} + C_{2,out}X_{5,2} + C_{3,out}X_{5,3} + C_{4,out}X_{5,4} + C_{6,out}X_{5,6} + C_{7,out}X_{5,7} + \Delta M_5 - C_{5,out}(W_5 + X_{1,5} + X_{2,5} + X_{3,5} + X_{4,5} + X_{6,5} + X_{7,5}) = 0 \dots \dots \dots 5.23f$$

$$C_{1,out}X_{6,1} + C_{2,out}X_{6,2} + C_{3,out}X_{6,3} + C_{4,out}X_{6,4} + C_{5,out}X_{6,5} + C_{7,out}X_{6,7} + \Delta M_6 - C_{6,out}(W_6 + X_{1,6} + X_{2,6} + X_{3,6} + X_{4,6} + X_{5,6} + X_{7,6}) = 0 \dots \dots \dots 5.23g$$

$$C_{1,out}X_{7,1} + C_{2,out}X_{7,2} + C_{3,out}X_{7,3} + C_{4,out}X_{7,4} + C_{5,out}X_{7,5} + C_{6,out}X_{7,6} + \Delta M_7 - C_{7,out}(W_7 + X_{1,7} + X_{2,7} + X_{3,7} + X_{4,7} + X_{5,7} + X_{6,7}) = 0 \dots \dots \dots 5.23h$$

3. The nonlinear constraint function of the maximum contaminant inlet concentration are represented in equation 5.24 as follows:

$$C_{j,in} = \frac{\sum_{j \neq i} X_{i,j} C_{j,out}}{\sum_{j \neq i} X_{i,j} + F_i} \leq C_{i,in}^{max} \dots \dots \dots 5.24a$$

$$C_{2,out} = \frac{C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4} + C_{5,out} X_{1,5} + C_{6,out} X_{1,6} + C_{7,out} X_{1,7}}{F_1 + X_{1,2} + X_{1,3} + X_{1,4} + X_{1,5} + X_{1,6} + X_{1,7}} \leq C_{1,in}^{max} \dots \dots 5.24b$$

$$C_{1,out} = \frac{C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + C_{4,out} X_{2,4} + C_{5,out} X_{2,5} + C_{6,out} X_{2,6} + C_{7,out} X_{2,7}}{F_2 + X_{2,1} + X_{2,3} + X_{2,4} + X_{2,5} + X_{2,6} + X_{2,7}} \leq C_{2,in}^{max} \dots \dots 5.24c$$

$$C_{1,out} = \frac{C_{1,out} X_{3,1} + C_{2,out} X_{3,2} + C_{4,out} X_{3,4} + C_{5,out} X_{3,5} + C_{6,out} X_{3,6} + C_{7,out} X_{3,7}}{F_3 + X_{3,1} + X_{3,2} + X_{3,4} + X_{3,5} + X_{3,6} + X_{3,7}} \leq C_{3,in}^{max} \dots \dots 5.24d$$

$$C_{1,out} = \frac{C_{1,out} X_{4,1} + C_{2,out} X_{4,2} + C_{3,out} X_{4,3} + C_{5,out} X_{4,5} + C_{6,out} X_{4,6} + C_{7,out} X_{4,7}}{F_4 + X_{4,1} + X_{4,2} + X_{4,3} + X_{4,5} + X_{4,6} + X_{4,7}} \leq C_{4,in}^{max} \dots \dots 5.24e$$

$$C_{1,out} = \frac{C_{1,out} X_{5,1} + C_{2,out} X_{5,2} + C_{3,out} X_{5,3} + C_{4,out} X_{5,4} + C_{6,out} X_{5,6} + C_{7,out} X_{5,7}}{F_5 + X_{5,1} + X_{5,2} + X_{5,3} + X_{5,4} + X_{5,6} + X_{5,7}} \leq C_{5,in}^{max} \dots \dots 5.24f$$

$$C_{1,out} = \frac{C_{1,out} X_{6,1} + C_{2,out} X_{6,2} + C_{3,out} X_{6,3} + C_{4,out} X_{6,4} + C_{5,out} X_{6,5} + C_{7,out} X_{6,7}}{F_6 + X_{6,1} + X_{6,2} + X_{6,3} + X_{6,4} + X_{6,5} + X_{6,7}} \leq C_{6,in}^{max} \dots \dots 5.24g$$

$$C_{1,out} = \frac{C_{1,out} X_{7,1} + C_{2,out} X_{7,2} + C_{3,out} X_{7,3} + C_{4,out} X_{7,4} + C_{5,out} X_{7,5} + C_{6,out} X_{7,6}}{F_7 + X_{7,1} + X_{7,2} + X_{7,3} + X_{7,4} + X_{7,5} + X_{7,6}} \leq C_{7,in}^{max} \dots \dots 5.24h$$

$$\sum_{j \neq i} C_{j,out} X_{i,j} + \Delta M_i - C_{i,out} \left(W_i + \sum_{j \neq i} X_{j,i} \right) = 0 \dots \dots \dots 5.27a$$

$$C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4} + C_{5,out} X_{1,5} + C_{6,out} X_{1,6} + C_{7,out} X_{1,7} + C_{8,out} X_{1,8} + \Delta M_1 - C_{1,out} (W_1 + X_{2,1} + X_{3,1} + X_{4,1} + X_{5,1} + X_{6,1} + X_{7,1} + X_{8,1}) = 0 \dots \dots \dots 5.27b$$

$$C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + C_{4,out} X_{2,4} + C_{5,out} X_{2,5} + C_{6,out} X_{2,6} + C_{7,out} X_{2,7} + C_{8,out} X_{2,8} + \Delta M_2 - C_{2,out} (W_2 + X_{1,2} + X_{3,2} + X_{4,2} + X_{5,2} + X_{6,2} + X_{7,2} + X_{8,2}) = 0 \dots \dots \dots 5.27c$$

$$C_{1,out} X_{3,1} + C_{2,out} X_{3,2} + C_{4,out} X_{3,4} + C_{5,out} X_{3,5} + C_{6,out} X_{3,6} + C_{7,out} X_{3,7} + C_{8,out} X_{3,8} + \Delta M_3 - C_{3,out} (W_3 + X_{1,3} + X_{2,3} + X_{4,3} + X_{5,3} + X_{6,3} + X_{7,3} + X_{8,3}) = 0 \dots \dots \dots 5.27d$$

$$C_{1,out} X_{4,1} + C_{2,out} X_{4,2} + C_{3,out} X_{4,3} + C_{5,out} X_{4,5} + C_{6,out} X_{4,6} + C_{7,out} X_{4,7} + C_{8,out} X_{4,8} + \Delta M_4 - C_{4,out} (W_4 + X_{1,4} + X_{2,4} + X_{3,4} + X_{5,4} + X_{6,4} + X_{7,4} + X_{8,4}) = 0 \dots \dots \dots 5.27e$$

$$C_{1,out} X_{5,1} + C_{2,out} X_{5,2} + C_{3,out} X_{5,3} + C_{4,out} X_{5,4} + C_{6,out} X_{5,6} + C_{7,out} X_{5,7} + C_{8,out} X_{5,8} + \Delta M_5 - C_{5,out} (W_5 + X_{1,5} + X_{2,5} + X_{3,5} + X_{4,5} + X_{6,5} + X_{7,5} + X_{8,5}) = 0 \dots \dots \dots 5.27f$$

$$C_{1,out} X_{6,1} + C_{2,out} X_{6,2} + C_{3,out} X_{6,3} + C_{4,out} X_{6,4} + C_{5,out} X_{6,5} + C_{7,out} X_{6,7} + C_{8,out} X_{6,8} + \Delta M_6 - C_{6,out} (W_6 + X_{1,6} + X_{2,6} + X_{3,6} + X_{4,6} + X_{5,6} + X_{7,6} + X_{8,6}) = 0 \dots \dots \dots 5.27g$$

$$C_{1,out} X_{7,1} + C_{2,out} X_{7,2} + C_{3,out} X_{7,3} + C_{4,out} X_{7,4} + C_{5,out} X_{7,5} + C_{6,out} X_{7,6} + C_{8,out} X_{7,8} + \Delta M_7 - C_{7,out} (W_7 + X_{1,7} + X_{2,7} + X_{3,7} + X_{4,7} + X_{5,7} + X_{6,7} + X_{8,7}) = 0 \dots \dots \dots 5.27h$$

$$C_{1,out} X_{8,1} + C_{2,out} X_{8,2} + C_{3,out} X_{8,3} + C_{4,out} X_{8,4} + C_{5,out} X_{8,5} + C_{6,out} X_{8,6} + C_{7,out} X_{8,7} + \Delta M_8 - C_{8,out} (W_8 + X_{1,8} + X_{2,8} + X_{3,8} + X_{4,8} + X_{5,8} + X_{6,8} + X_{7,8}) = 0 \dots \dots \dots 5.27i$$

3. The nonlinear constraint function of the maximum contaminant inlet concentration are represented in equation 5.28 as follows:

$$C_{j,in} = \frac{\sum_{j \neq i} X_{i,j} C_{j,out}}{\sum_{j \neq i} X_{i,j} + F_i} \leq C_{i,in}^{max} \dots \dots \dots 5.28a$$

$$C_{2,out} = \frac{C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4} + C_{5,out} X_{1,5} + C_{6,out} X_{1,6} + C_{7,out} X_{1,7} + C_{8,out} X_{1,8}}{F_1 + X_{1,2} + X_{1,3} + X_{1,4} + X_{1,5} + X_{1,6} + X_{1,7} + X_{1,8}} \leq C_{1,in}^{max} \dots \dots 5.28b$$

$$C_{1,out} = \frac{C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + C_{4,out} X_{2,4} + C_{5,out} X_{2,5} + C_{6,out} X_{2,6} + C_{7,out} X_{2,7} + C_{8,out} X_{2,8}}{F_2 + X_{2,1} + X_{2,3} + X_{2,4} + X_{2,5} + X_{2,6} + X_{2,7} + X_{2,8}} \leq C_{2,in}^{max} \dots 5.28c$$

$$C_{1,out} = \frac{C_{1,out} X_{3,1} + C_{2,out} X_{3,2} + C_{4,out} X_{3,4} + C_{5,out} X_{3,5} + C_{6,out} X_{3,6} + C_{7,out} X_{3,7} + C_{8,out} X_{3,8}}{F_3 + X_{3,1} + X_{3,2} + X_{3,4} + X_{3,5} + X_{3,6} + X_{3,7} + X_{3,8}} \leq C_{3,in}^{max} \dots 5.28d$$

$$C_{1,out} = \frac{C_{1,out} X_{4,1} + C_{2,out} X_{4,2} + C_{3,out} X_{4,3} + C_{5,out} X_{4,5} + C_{6,out} X_{4,6} + C_{7,out} X_{4,7} + C_{8,out} X_{4,8}}{F_4 + X_{4,1} + X_{4,2} + X_{4,3} + X_{4,5} + X_{4,6} + X_{4,7} + X_{4,8}} \leq C_{4,in}^{max} \dots 5.28e$$

$$C_{1,out} = \frac{C_{1,out} X_{5,1} + C_{2,out} X_{5,2} + C_{3,out} X_{5,3} + C_{4,out} X_{5,4} + C_{6,out} X_{5,6} + C_{7,out} X_{5,7} + C_{8,out} X_{5,8}}{F_5 + X_{5,1} + X_{5,2} + X_{5,3} + X_{5,4} + X_{5,6} + X_{5,7} + X_{5,8}} \leq C_{5,in}^{max} \dots 5.28f$$

$$C_{1,out} = \frac{C_{1,out} X_{6,1} + C_{2,out} X_{6,2} + C_{3,out} X_{6,3} + C_{4,out} X_{6,4} + C_{5,out} X_{6,5} + C_{7,out} X_{6,7} + C_{8,out} X_{6,8}}{F_6 + X_{6,1} + X_{6,2} + X_{6,3} + X_{6,4} + X_{6,5} + X_{6,7} + X_{6,8}} \leq C_{6,in}^{max} \dots 5.28g$$

$$C_{1,out} = \frac{C_{1,out} X_{7,1} + C_{2,out} X_{7,2} + C_{3,out} X_{7,3} + C_{4,out} X_{7,4} + C_{5,out} X_{7,5} + C_{6,out} X_{7,6} + C_{8,out} X_{7,8}}{F_7 + X_{7,1} + X_{7,2} + X_{7,3} + X_{7,4} + X_{7,5} + X_{7,6} + X_{7,8}} \leq C_{7,in}^{max} \dots 5.28h$$

$$C_{1,out} = \frac{C_{1,out} X_{8,1} + C_{2,out} X_{8,2} + C_{3,out} X_{8,3} + C_{4,out} X_{8,4} + C_{5,out} X_{8,5} + C_{6,out} X_{8,6} + C_{7,out} X_{8,7}}{F_8 + X_{8,1} + X_{8,2} + X_{8,3} + X_{8,4} + X_{8,5} + X_{8,6} + X_{8,7}} \leq C_{8,in}^{max} \dots 5.28i$$

B7. Equations for Single Contaminant Water Reuse without Regeneration for 9 Industrial Processes

The fitness function is the Sum of fresh water flow rates at the entrance of each water using process as shown in equation 5.5:

$$F = \sum_{i=1}^9 F_i \dots 5.29a$$

$$F = F_1 + F_2 + F_3 + F_4 + F_5 + F_6 + F_7 + F_8 + F_9 \dots \dots \dots 5.29b$$

The Linear Constraints functions of the water and contaminant mass balance are represented in equation 5.6 and 5.7 as follows:

CONSTRAINTS

Linear Constraints functions

1. The constraint of the water mass balance of all process

$$F_i + \sum_{j \neq i} X_{i,j} - W_i - \sum_{j \neq i} X_{j,i} = 0 \dots \dots \dots 5.30a$$

$$F_1 + X_{1,2} + X_{1,3} + X_{1,4} + X_{1,5} + X_{1,6} + X_{1,7} + X_{1,8} + X_{1,9} - W_1 - X_{2,1} - X_{3,1} - X_{4,1} - X_{5,1} - X_{6,1} - X_{7,1} - X_{8,1} - X_{9,1} = 0 \dots \dots \dots 5.30b$$

$$F_2 + X_{2,1} + X_{2,3} + X_{2,4} + X_{2,5} + X_{2,6} + X_{2,7} + X_{2,8} + X_{2,9} - W_2 - X_{1,2} - X_{3,2} - X_{4,2} - X_{5,2} - X_{6,2} - X_{7,2} - X_{8,2} - X_{9,2} = 0 \dots \dots \dots 5.30c$$

$$F_3 + X_{3,1} + X_{3,2} + X_{3,4} + X_{3,5} + X_{3,6} + X_{3,7} + X_{3,8} + X_{3,9} - W_3 - X_{1,3} - X_{2,3} - X_{4,3} - X_{5,3} - X_{6,3} - X_{7,3} - X_{8,3} - X_{9,3} = 0 \dots \dots \dots 5.30d$$

$$F_4 + X_{4,1} + X_{4,2} + X_{4,3} + X_{4,5} + X_{4,6} + X_{4,7} + X_{4,8} + X_{4,9} - W_4 - X_{1,4} - X_{2,4} - X_{3,4} - X_{5,4} - X_{6,4} - X_{7,4} - X_{8,4} - X_{9,4} = 0 \dots \dots \dots 5.30e$$

$$F_5 + X_{5,1} + X_{5,2} + X_{5,3} + X_{5,4} + X_{5,6} + X_{5,7} + X_{5,8} + X_{5,9} - W_5 - X_{1,5} - X_{2,5} - X_{3,5} - X_{4,5} - X_{6,5} - X_{7,5} - X_{8,5} - X_{9,5} = 0 \dots \dots \dots 5.30f$$

$$F_6 + X_{6,1} + X_{6,2} + X_{6,3} + X_{6,4} + X_{6,5} + X_{6,7} + X_{6,8} + X_{6,9} - W_6 - X_{1,6} - X_{2,6} - X_{3,6} - X_{4,6} - X_{5,6} - X_{7,6} - X_{8,6} - X_{9,6} = 0 \dots \dots \dots 5.30g$$

$$F_7 + X_{7,1} + X_{7,2} + X_{7,3} + X_{7,4} + X_{7,5} + X_{7,6} + X_{7,8} + X_{7,9} - W_7 - X_{1,7} - X_{2,7} - X_{3,7} - X_{4,7} - X_{5,7} - X_{6,7} - X_{8,7} - X_{9,7} = 0 \dots \dots \dots 5.30h$$

$$F_8 + X_{8,1} + X_{8,2} + X_{8,3} + X_{8,4} + X_{8,5} + X_{8,6} + X_{8,7} + X_{8,9} - W_8 - X_{1,8} - X_{2,8} - X_{3,8} - X_{4,8} - X_{5,8} - X_{6,8} - X_{7,8} - X_{9,8} = 0 \dots \dots \dots 5.30i$$

$$F_9 + X_{9,1} + X_{9,2} + X_{9,3} + X_{9,4} + X_{9,5} + X_{9,6} + X_{9,7} + X_{9,8} - W_9 - X_{1,9} - X_{2,9} - X_{3,9} - X_{4,9} - X_{5,9} - X_{6,9} - X_{7,9} - X_{8,9} = 0 \dots \dots \dots 5.30j$$

2. The constraint of the contaminant mass balance of all processes

$$\sum_{j \neq i} C_{j,out} X_{ij} + \Delta M_i - C_{i,out} \left(W_i + \sum_{j \neq i} X_{ji} \right) = 0 \dots \dots \dots 5.31a$$

$$C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4} + C_{5,out} X_{1,5} + C_{6,out} X_{1,6} + C_{7,out} X_{1,7} + C_{8,out} X_{1,8} + C_{9,out} X_{1,9} + \Delta M_1 - C_{1,out} (W_1 + X_{2,1} + X_{3,1} + X_{4,1} + X_{5,1} + X_{6,1} + X_{7,1} + X_{8,1} + X_{9,1}) = 0 \dots \dots \dots 5.31b$$

$$C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + C_{4,out} X_{2,4} + C_{5,out} X_{2,5} + C_{6,out} X_{2,6} + C_{7,out} X_{2,7} + C_{8,out} X_{2,8} + C_{9,out} X_{2,9} + \Delta M_2 - C_{2,out} (W_2 + X_{1,2} + X_{3,2} + X_{4,2} + X_{5,2} + X_{6,2} + X_{7,2} + X_{8,2} + X_{9,2}) = 0 \dots \dots \dots 5.31c$$

$$C_{1,out} X_{3,1} + C_{2,out} X_{3,2} + C_{4,out} X_{3,4} + C_{5,out} X_{3,5} + C_{6,out} X_{3,6} + C_{7,out} X_{3,7} + C_{8,out} X_{3,8} + C_{9,out} X_{3,9} + \Delta M_3 - C_{3,out} (W_3 + X_{1,3} + X_{2,3} + X_{4,3} + X_{5,3} + X_{6,3} + X_{7,3} + X_{8,3} + X_{9,3}) = 0 \dots \dots \dots 5.31d$$

$$C_{1,out} X_{4,1} + C_{2,out} X_{4,2} + C_{3,out} X_{4,3} + C_{5,out} X_{4,5} + C_{6,out} X_{4,6} + C_{7,out} X_{4,7} + C_{8,out} X_{4,8} + C_{9,out} X_{4,9} + \Delta M_4 - C_{4,out} (W_4 + X_{1,4} + X_{2,4} + X_{3,4} + X_{5,4} + X_{6,4} + X_{7,4} + X_{8,4} + X_{9,4}) = 0 \dots \dots \dots 5.31e$$

$$C_{1,out}X_{5,1} + C_{2,out}X_{5,2} + C_{3,out}X_{5,3} + C_{4,out}X_{5,4} + C_{6,out}X_{5,6} + C_{7,out}X_{5,7} + C_{8,out}X_{5,8} + C_{9,out}X_{5,9} + \Delta M_5 - C_{5,out}(W_5 + X_{1,5} + X_{2,5} + X_{3,5} + X_{4,5} + X_{6,5} + X_{7,5} + X_{8,5} + X_{9,5}) = 0 \dots \dots \dots 5.31f$$

$$C_{1,out}X_{6,1} + C_{2,out}X_{6,2} + C_{3,out}X_{6,3} + C_{4,out}X_{6,4} + C_{5,out}X_{6,5} + C_{7,out}X_{6,7} + C_{8,out}X_{6,8} + C_{9,out}X_{6,9} + \Delta M_6 - C_{6,out}(W_6 + X_{1,6} + X_{2,6} + X_{3,6} + X_{4,6} + X_{5,6} + X_{7,6} + X_{8,6} + X_{9,6}) = 0 \dots \dots \dots 5.31a$$

$$C_{1,out}X_{7,1} + C_{2,out}X_{7,2} + C_{3,out}X_{7,3} + C_{4,out}X_{7,4} + C_{5,out}X_{7,5} + C_{6,out}X_{7,6} + C_{8,out}X_{7,8} + C_{9,out}X_{7,9} + \Delta M_7 - C_{7,out}(W_7 + X_{1,7} + X_{2,7} + X_{3,7} + X_{4,7} + X_{5,7} + X_{6,7} + X_{8,7} + X_{9,7}) = 0 \dots \dots \dots 5.31g$$

$$C_{1,out}X_{8,1} + C_{2,out}X_{8,2} + C_{3,out}X_{8,3} + C_{4,out}X_{8,4} + C_{5,out}X_{8,5} + C_{6,out}X_{8,6} + C_{7,out}X_{8,7} + C_{9,out}X_{8,9} + \Delta M_8 - C_{8,out}(W_8 + X_{1,8} + X_{2,8} + X_{3,8} + X_{4,8} + X_{5,8} + X_{6,8} + X_{7,8} + X_{9,8}) = 0 \dots \dots \dots 5.31h$$

$$C_{1,out}X_{9,1} + C_{2,out}X_{9,2} + C_{3,out}X_{9,3} + C_{4,out}X_{9,4} + C_{5,out}X_{9,5} + C_{6,out}X_{9,6} + C_{7,out}X_{9,7} + C_{8,out}X_{9,8} + \Delta M_9 - C_{9,out}(W_9 + X_{1,9} + X_{2,9} + X_{3,9} + X_{4,9} + X_{5,9} + X_{6,9} + X_{7,9} + X_{8,9}) = 0 \dots \dots \dots 5.31i$$

3. The nonlinear constraint function of the maximum contaminant inlet concentration are represented in equation 5.4 as follows:

$$C_{j,in} = \frac{\sum_{j \neq i} X_{i,j} C_{j,out}}{\sum_{j \neq i} X_{i,j} + F_i} \leq C_{i,in}^{max} \dots \dots \dots 5.32a$$

$$\begin{aligned} & C_{2,out} \\ &= \frac{C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4} + C_{5,out} X_{1,5} + C_{6,out} X_{1,6} + C_{7,out} X_{1,7} + C_{8,out} X_{1,8} + C_{9,out} X_{1,9}}{F_1 + X_{1,2} + X_{1,3} + X_{1,4} + X_{1,5} + X_{1,6} + X_{1,7} + X_{1,8} + X_{1,9}} \\ &\leq C_{1,in}^{max} \dots \dots \dots 5.32b \end{aligned}$$

$$\begin{aligned} & C_{1,out} \\ &= \frac{C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + C_{4,out} X_{2,4} + C_{5,out} X_{2,5} + C_{6,out} X_{2,6} + C_{7,out} X_{2,7} + C_{8,out} X_{2,8} + C_{9,out} X_{2,9}}{F_2 + X_{2,1} + X_{2,3} + X_{2,4} + X_{2,5} + X_{2,6} + X_{2,7} + X_{2,8} + X_{2,9}} \\ &\leq C_{2,in}^{max} \dots \dots \dots 5.32c \end{aligned}$$

$$C_{1,out} = \frac{C_{1,out} X_{3,1} + C_{3,out} X_{3,2} + C_{4,out} X_{3,4} + C_{5,out} X_{3,5} + C_{6,out} X_{3,6} + C_{7,out} X_{3,7} + C_{8,out} X_{3,8} + C_{9,out} X_{3,9}}{F_3 + X_{3,1} + X_{3,2} + X_{3,4} + X_{3,5} + X_{3,6} + X_{3,7} + X_{3,8} + X_{3,9}} \leq C_{3,in}^{max} \dots \dots \dots 5.32d$$

$$C_{1,out} = \frac{C_{1,out} X_{4,1} + C_{2,out} X_{4,2} + C_{3,out} X_{4,3} + C_{5,out} X_{4,5} + C_{6,out} X_{4,6} + C_{7,out} X_{4,7} + C_{8,out} X_{4,8} + C_{9,out} X_{4,9}}{F_4 + X_{4,1} + X_{4,2} + X_{4,3} + X_{4,5} + X_{4,6} + X_{4,7} + X_{4,8} + X_{4,9}} \leq C_{4,in}^{max} \dots \dots \dots 5.32e$$

$$C_{1,out} = \frac{C_{1,out} X_{5,1} + C_{2,out} X_{5,2} + C_{3,out} X_{5,3} + C_{4,out} X_{5,4} + C_{6,out} X_{5,6} + C_{7,out} X_{5,7} + C_{8,out} X_{5,8} + C_{9,out} X_{5,9}}{F_5 + X_{5,1} + X_{5,2} + X_{5,3} + X_{5,4} + X_{5,6} + X_{5,7} + X_{5,8} + X_{5,9}} \leq C_{5,in}^{max} \dots \dots \dots 5.32f$$

$$C_{1,out} = \frac{C_{1,out} X_{6,1} + C_{2,out} X_{6,2} + C_{3,out} X_{6,3} + C_{4,out} X_{6,4} + C_{5,out} X_{6,5} + C_{7,out} X_{6,7} + C_{8,out} X_{6,8} + C_{9,out} X_{6,9}}{F_6 + X_{6,1} + X_{6,2} + X_{6,3} + X_{6,4} + X_{6,5} + X_{6,7} + X_{6,8} + X_{6,9}} \leq C_{6,in}^{max} \dots \dots \dots 5.32g$$

$$C_{1,out} = \frac{C_{1,out} X_{7,1} + C_{2,out} X_{7,2} + C_{3,out} X_{7,3} + C_{4,out} X_{7,4} + C_{5,out} X_{7,5} + C_{6,out} X_{7,6} + C_{8,out} X_{7,8} + C_{9,out} X_{7,9}}{F_7 + X_{7,1} + X_{7,2} + X_{7,3} + X_{7,4} + X_{7,5} + X_{7,6} + X_{7,8} + X_{7,9}} \leq C_{7,in}^{max} \dots \dots \dots 5.32h$$

$$C_{1,out} = \frac{C_{1,out} X_{8,1} + C_{2,out} X_{8,2} + C_{3,out} X_{8,3} + C_{4,out} X_{8,4} + C_{5,out} X_{8,5} + C_{6,out} X_{8,6} + C_{7,out} X_{8,7} + C_{9,out} X_{8,9}}{F_8 + X_{8,1} + X_{8,2} + X_{8,3} + X_{8,4} + X_{8,5} + X_{8,6} + X_{8,7} + X_{8,9}} \leq C_{8,in}^{max} \dots \dots \dots 5.32i$$

$$C_{1,out} = \frac{C_{1,out} X_{9,1} + C_{2,out} X_{9,2} + C_{3,out} X_{9,3} + C_{4,out} X_{9,4} + C_{5,out} X_{9,5} + C_{6,out} X_{9,6} + C_{7,out} X_{9,7} + C_{8,out} X_{9,8}}{F_9 + X_{9,1} + X_{9,2} + X_{9,3} + X_{9,4} + X_{9,5} + X_{9,6} + X_{9,7} + X_{9,8}} \leq C_{9,in}^{max} \dots \dots \dots 5.32j$$

B8. Equations for Single Contaminant Water Reuse without Regeneration for 10 Industrial Processes

The fitness function is the Sum of fresh water flow rates at the entrance of each water using process as shown in equation 5.33:

$$F = \sum_{i=1}^4 F_i \dots \dots \dots 5.33a$$

$$F = F_1 + F_2 + F_3 + F_4 + F_5 + F_6 + F_7 + F_8 + F_9 + F_{10} \dots \dots \dots 5.33b$$

The Linear Constraints functions of the water and contaminant mass balance are represented in equation 5.6 and 5.7 as follows:

CONSTRAINTS:

Linear Constraints functions:

1. The constraint of the water mass balance of all process:

$$F_i + \sum_{j \neq i} X_{i,j} - W_i - \sum_{j \neq i} X_{j,i} = 0 \dots \dots \dots 5.34a$$

$$F_1 + X_{1,2} + X_{1,3} + X_{1,4} + X_{1,5} + X_{1,6} + X_{1,7} + X_{1,8} + X_{1,9} + X_{1,10} - W_1 - X_{2,1} - X_{3,1} - X_{4,1} - X_{5,1} - X_{6,1} - X_{7,1} - X_{8,1} - X_{9,1} - X_{10,1} = 0 \dots 5.34b$$

$$F_2 + X_{2,1} + X_{2,3} + X_{2,4} + X_{2,5} + X_{2,6} + X_{2,7} + X_{2,8} + X_{2,9} + X_{2,10} - W_2 - X_{1,2} - X_{3,2} - X_{4,2} - X_{5,2} - X_{6,2} - X_{7,2} - X_{8,2} - X_{9,2} - X_{10,2} = 0 \dots 5.34c$$

$$F_3 + X_{3,1} + X_{3,2} + X_{3,4} + X_{3,5} + X_{3,6} + X_{3,7} + X_{3,8} + X_{3,9} + X_{3,10} - W_3 - X_{1,3} - X_{2,3} - X_{4,3} - X_{5,3} - X_{6,3} - X_{7,3} - X_{8,3} - X_{9,3} - X_{10,3} = 0 \dots 5.34d$$

$$F_4 + X_{4,1} + X_{4,2} + X_{4,3} + X_{4,5} + X_{4,6} + X_{4,7} + X_{4,8} + X_{4,9} + X_{4,10} - W_4 - X_{1,4} - X_{2,4} - X_{3,4} - X_{5,4} - X_{6,4} - X_{7,4} - X_{8,4} - X_{9,4} - X_{10,4} = 0 \dots 5.34e$$

$$F_5 + X_{5,1} + X_{5,2} + X_{5,3} + X_{5,4} + X_{5,6} + X_{5,7} + X_{5,8} + X_{5,9} + X_{5,10} - W_5 - X_{1,5} - X_{2,5} - X_{3,5} - X_{4,5} - X_{6,5} - X_{7,5} - X_{8,5} - X_{9,5} - X_{10,5} = 0 \dots 5.34f$$

$$F_6 + X_{6,1} + X_{6,2} + X_{6,3} + X_{6,4} + X_{6,5} + X_{6,7} + X_{6,8} + X_{6,9} + X_{6,10} - W_6 - X_{1,6} - X_{2,6} - X_{3,6} - X_{4,6} - X_{5,6} - X_{7,6} - X_{8,6} - X_{9,6} - X_{10,6} = 0 \dots 5.34g$$

$$F_7 + X_{7,1} + X_{7,2} + X_{7,3} + X_{7,4} + X_{7,5} + X_{7,6} + X_{7,8} + X_{7,9} + X_{7,10} - W_7 - X_{1,7} - X_{2,7} - X_{3,7} - X_{4,7} - X_{5,7} - X_{6,7} - X_{8,7} - X_{9,7} - X_{10,7} = 0 \dots 5.34h$$

$$F_8 + X_{8,1} + X_{8,2} + X_{8,3} + X_{8,4} + X_{8,5} + X_{8,6} + X_{8,7} + X_{8,9} + X_{8,10} - W_8 - X_{1,8} - X_{2,8} - X_{3,8} - X_{4,8} - X_{5,8} - X_{6,8} - X_{7,8} - X_{9,8} - X_{10,8} = 0 \dots 5.34i$$

$$F_9 + X_{9,1} + X_{9,2} + X_{9,3} + X_{9,4} + X_{9,5} + X_{9,6} + X_{9,7} + X_{9,8} + X_{9,10} - W_9 - X_{1,9} - X_{2,9} - X_{3,9} - X_{4,9} - X_{5,9} - X_{6,9} - X_{7,9} - X_{8,9} - X_{10,9} = 0 \dots 5.34j$$

$$F_{10} + X_{10,1} + X_{10,2} + X_{10,3} + X_{10,4} + X_{10,5} + X_{10,6} + X_{10,7} + X_{10,8} + X_{10,9} - W_{10} - X_{1,10} - X_{2,10} - X_{3,10} - X_{4,10} - X_{5,10} - X_{6,10} - X_{7,10} - X_{8,10} - X_{9,10} = 0 \dots 5.34k$$

2. The constraint of the contaminant mass balance of all processes:

$$\sum_{j \neq i} C_{j,out} X_{i,j} + \Delta M_i - C_{i,out} \left(W_i + \sum_{j \neq i} X_{j,i} \right) = 0 \dots \dots \dots 5.35a$$

$$C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4} + C_{5,out} X_{1,5} + C_{6,out} X_{1,6} + C_{7,out} X_{1,7} + C_{8,out} X_{1,8} + C_{9,out} X_{1,9} + C_{10,out} X_{1,10} + \Delta M_1 - C_{1,out} (W_1 + X_{2,1} + X_{3,1} + X_{4,1} + X_{5,1} + X_{6,1} + X_{7,1} + X_{8,1} + X_{9,1} + X_{10,1}) = 0 \dots 5.35b$$

$$C_{1,out}X_{2,1} + C_{3,out}X_{2,3} + C_{4,out}X_{2,4} + C_{5,out}X_{2,5} + C_{6,out}X_{2,6} \\ + C_{7,out}X_{2,7} + C_{8,out}X_{2,8} + C_{9,out}X_{2,9} + C_{10,out}X_{2,10} + \Delta M_2 - C_{2,out}(W_2 + X_{1,2} \\ + X_{3,2} + X_{4,2} + X_{5,2} + X_{6,2} + X_{7,2} + X_{8,2} + X_{9,2} + X_{10,2}) = 0 \dots 5.35c$$

$$C_{1,out}X_{3,1} + C_{2,out}X_{3,2} + C_{4,out}X_{3,4} + C_{5,out}X_{3,5} + C_{6,out}X_{3,6} \\ + C_{7,out}X_{3,7} + C_{8,out}X_{3,8} + C_{9,out}X_{3,9} + C_{10,out}X_{3,10} + \Delta M_3 - C_{3,out}(W_3 + X_{1,3} \\ + X_{2,3} + X_{4,3} + X_{5,5} + X_{6,3} + X_{7,3} + X_{8,3} + X_{9,3} + X_{10,3}) = 0 \dots 5.35d$$

$$C_{1,out}X_{4,1} + C_{2,out}X_{4,2} + C_{3,out}X_{4,3} + C_{5,out}X_{4,5} + C_{6,out}X_{4,6} \\ + C_{7,out}X_{4,7} + C_{8,out}X_{4,8} + C_{9,out}X_{4,9} + C_{10,out}X_{4,10} + \Delta M_4 - C_{4,out}(W_4 + X_{1,4} \\ + X_{2,4} + X_{3,4} + X_{5,4} + X_{6,4} + X_{7,4} + X_{8,4} + X_{9,4} + X_{10,4}) = 0 \dots 5.35e$$

$$C_{1,out}X_{5,1} + C_{2,out}X_{5,2} + C_{3,out}X_{5,3} + C_{4,out}X_{5,4} + C_{6,out}X_{5,6} \\ + C_{7,out}X_{5,7} + C_{8,out}X_{5,8} + C_{9,out}X_{5,9} + C_{10,out}X_{5,10} + \Delta M_5 - C_{5,out}(W_5 + X_{1,5} \\ + X_{2,5} + X_{3,5} + X_{4,5} + X_{6,5} + X_{7,5} + X_{8,5} + X_{9,5} + X_{10,5}) = 0 \dots 5.35f$$

$$C_{1,out}X_{6,1} + C_{2,out}X_{6,2} + C_{3,out}X_{6,3} + C_{4,out}X_{6,4} + C_{5,out}X_{6,5} \\ + C_{7,out}X_{6,7} + C_{8,out}X_{6,8} + C_{9,out}X_{6,9} + C_{10,out}X_{6,10} + \Delta M_6 - C_{6,out}(W_6 + X_{1,6} \\ + X_{2,6} + X_{3,6} + X_{4,6} + X_{5,6} + X_{7,6} + X_{8,6} + X_{9,6} + X_{10,6}) = 0 \dots 5.35g$$

$$C_{1,out}X_{7,1} + C_{2,out}X_{7,2} + C_{3,out}X_{7,3} + C_{4,out}X_{7,4} + C_{5,out}X_{7,5} \\ + C_{6,out}X_{7,6} + C_{8,out}X_{7,8} + C_{9,out}X_{7,9} + C_{10,out}X_{7,10} + \Delta M_7 - C_{7,out}(W_7 + X_{1,7} \\ + X_{2,7} + X_{3,7} + X_{4,7} + X_{5,7} + X_{6,7} + X_{8,7} + X_{9,7} + X_{10,7}) = 0 \dots 5.35h$$

$$C_{1,out}X_{8,1} + C_{2,out}X_{8,2} + C_{3,out}X_{8,3} + C_{4,out}X_{8,4} + C_{5,out}X_{8,5} + C_{6,out}X_{8,6} \\ + C_{7,out}X_{8,7} + C_{9,out}X_{8,9} + C_{10,out}X_{8,10} + \Delta M_8 - C_{8,out}(W_8 + X_{1,8} + X_{2,8} + X_{3,8} \\ + X_{4,8} + X_{5,8} + X_{6,8} + X_{7,8} + X_{9,8} + X_{10,8}) = 0 \dots 5.35i$$

$$C_{1,out}X_{9,1} + C_{2,out}X_{9,2} + C_{3,out}X_{9,3} + C_{4,out}X_{9,4} + C_{5,out}X_{9,5} + C_{6,out}X_{9,6} \\ + C_{7,out}X_{9,7} + C_{8,out}X_{9,8} + C_{10,out}X_{9,10} + \Delta M_9 - C_{9,out}(W_9 + X_{1,9} + X_{2,9} + X_{3,9} \\ + X_{4,9} + X_{5,9} + X_{6,9} + X_{7,9} + X_{8,9} + X_{10,9}) = 0 \dots 5.35j$$

$$C_{1,out}X_{10,1} + C_{2,out}X_{10,2} + C_{3,out}X_{10,3} + C_{4,out}X_{10,4} + C_{5,out}X_{10,5} + C_{6,out}X_{10,6} \\ + C_{7,out}X_{10,7} + C_{8,out}X_{10,8} + C_{9,out}X_{10,9} + \Delta M_{10} - C_{10,out}(W_{10} + X_{1,10} + X_{2,10} \\ + X_{3,10} + X_{4,10} + X_{5,10} + X_{6,10} + X_{7,10} + X_{8,10} + X_{9,10}) = 0 \dots 5.35k$$

3. Maximum Contaminant inlet concentration:

$$C_{j,in} = \frac{\sum_{j \neq i} X_{i,j} C_{j,out}}{\sum_{j \neq i} X_{i,j} + F_i} \leq C_{i,in}^{max} \dots \dots \dots 5.36a$$

$$C_{2,out} = \frac{C_{2,out} X_{1,2} + C_{3,out} X_{1,3} + C_{4,out} X_{1,4} + C_{5,out} X_{1,5} + C_{6,out} X_{1,6} + C_{7,out} X_{1,7} + C_{8,out} X_{1,8} + C_{9,out} X_{1,9} + C_{10,out} X_{1,10}}{F_1 + X_{1,2} + X_{1,3} + X_{1,4} + X_{1,5} + X_{1,6} + X_{1,7} + X_{1,8} + X_{1,9} + X_{1,10}} \\ \leq C_{1,in}^{max} \dots 5.36b$$

$$C_{1,out} = \frac{C_{1,out} X_{2,1} + C_{3,out} X_{2,3} + C_{4,out} X_{2,4} + C_{5,out} X_{2,5} + C_{6,out} X_{2,6} + C_{7,out} X_{2,7} + C_{8,out} X_{2,8} + C_{9,out} X_{2,9} + C_{10,out} X_{2,10}}{F_2 + X_{2,1} + X_{2,3} + X_{2,4} + X_{2,5} + X_{2,6} + X_{2,7} + X_{2,8} + X_{2,9} + X_{2,10}} \leq C_{2,in}^{max}$$

$$C_{1,out} = \frac{C_{1,out} X_{3,1} + C_{2,out} X_{3,2} + C_{4,out} X_{3,4} + C_{5,out} X_{3,5} + C_{6,out} X_{3,6} + C_{7,out} X_{3,7} + C_{8,out} X_{3,8} + C_{9,out} X_{3,9} + C_{10,out} X_{3,10}}{F_3 + X_{3,1} + X_{3,2} + X_{3,4} + X_{3,5} + X_{3,6} + X_{3,7} + X_{3,8} + X_{3,9} + X_{3,10}} \\ \leq C_{3,in}^{max} \dots 5.36d$$

$$C_{1,out} = \frac{C_{1,out} X_{4,1} + C_{2,out} X_{4,2} + C_{3,out} X_{4,3} + C_{5,out} X_{4,5} + C_{6,out} X_{4,6} + C_{7,out} X_{4,7} + C_{8,out} X_{4,8} + C_{9,out} X_{4,9} + C_{10,out} X_{4,10}}{F_4 + X_{4,1} + X_{4,2} + X_{4,3} + X_{4,5} + X_{4,6} + X_{4,7} + X_{4,8} + X_{4,9} + X_{4,10}} \\ \leq C_{4,in}^{max} \dots 5.36e$$

$$C_{1,out} = \frac{C_{1,out} X_{5,1} + C_{2,out} X_{5,2} + C_{3,out} X_{5,3} + C_{4,out} X_{5,4} + C_{6,out} X_{5,6} + C_{7,out} X_{5,7} + C_{8,out} X_{5,8} + C_{9,out} X_{5,9} + C_{10,out} X_{5,10}}{F_5 + X_{5,1} + X_{5,2} + X_{5,3} + X_{5,4} + X_{5,6} + X_{5,7} + X_{5,8} + X_{5,9} + X_{5,10}} \\ \leq C_{5,in}^{max} \dots 5.36f$$

$$C_{1,out} = \frac{C_{1,out} X_{6,1} + C_{2,out} X_{6,2} + C_{3,out} X_{6,3} + C_{4,out} X_{6,4} + C_{5,out} X_{6,5} + C_{7,out} X_{6,7} + C_{8,out} X_{6,8} + C_{9,out} X_{6,9} + C_{10,out} X_{6,10}}{F_6 + X_{6,1} + X_{6,2} + X_{6,3} + X_{6,4} + X_{6,5} + X_{6,7} + X_{6,8} + X_{6,9} + X_{6,10}} \\ \leq C_{6,in}^{max} \dots 5.36g$$

$$C_{1,out} = \frac{C_{1,out} X_{7,1} + C_{2,out} X_{7,2} + C_{3,out} X_{7,3} + C_{4,out} X_{7,4} + C_{5,out} X_{7,5} + C_{6,out} X_{7,6} + C_{8,out} X_{7,8} + C_{9,out} X_{7,9} + C_{10,out} X_{7,10}}{F_7 + X_{7,1} + X_{7,2} + X_{7,3} + X_{7,4} + X_{7,5} + X_{7,6} + X_{7,8} + X_{7,9} + X_{7,10}} \\ \leq C_{7,in}^{max} \dots 5.36h$$

$$C_{1,out} = \frac{C_{1,out} X_{8,1} + C_{2,out} X_{8,2} + C_{3,out} X_{8,3} + C_{4,out} X_{8,4} + C_{5,out} X_{8,5} + C_{6,out} X_{8,6} + C_{7,out} X_{8,7} + C_{9,out} X_{8,9} + C_{10,out} X_{8,10}}{F_8 + X_{8,1} + X_{8,2} + X_{8,3} + X_{8,4} + X_{8,5} + X_{8,6} + X_{8,7} + X_{8,9} + X_{8,10}} \leq C_{8,in}^{max}$$

$$C_{1,out} = \frac{C_{1,out} X_{9,1} + C_{2,out} X_{9,2} + C_{3,out} X_{9,3} + C_{4,out} X_{9,4} + C_{5,out} X_{9,5} + C_{6,out} X_{9,6} + C_{7,out} X_{9,7} + C_{8,out} X_{9,8} + C_{10,out} X_{9,10}}{F_9 + X_{9,1} + X_{9,2} + X_{9,3} + X_{9,4} + X_{9,5} + X_{9,6} + X_{9,7} + X_{9,8} + X_{9,10}} \leq C_{9,in}^{max}$$

$$C_{1,out} = \frac{C_{1,out} X_{10,1} + C_{2,out} X_{10,2} + C_{3,out} X_{10,3} + C_{4,out} X_{10,4} + C_{5,out} X_{10,5} + C_{6,out} X_{10,6} + C_{7,out} X_{10,7} + C_{8,out} X_{10,8} + C_{9,out} X_{10,9}}{F_{10} + X_{10,1} + X_{10,2} + X_{10,3} + X_{10,4} + X_{10,5} + X_{10,6} + X_{10,7} + X_{10,8} + X_{10,9}} \leq$$

APPENDIX C

C1. Matlab Code for Single Contaminant Water Reuse without Regeneration for 3(three) Industrial Processes

Fitness function

```
Function f=FRW(x)
% return the sum of all the values of fresh water x
f =x(:,1)+x(:,2)+x(:,3);
End
```

Constraint function

```
Function [c,ceq] = Constraints_FRW(x)
% return the values of the nonlinear constraints
C1out = 75; C2out = 100; C3out = 125; C1in = 0; C2in = 50; C3in = 75;
c = [(( C2out*x(:,7)+ C3out*x(:,8))/(x(:,1)+x(:,7)+x(:,8)))-C1in;
((C1out*x(:,9)+ C3out*x(:,10))/(x(:,2)+x(:,9)+x(:,10)))-C2in;
((C1out*x(:,11)+ C2out*x(:,12))/(x(:,3)+x(:,11)+x(:,12)))-C3in];
ceq=[];
End
```

The Code function

```
function [x,fval,exitflag,output,population,score] =
FRW_code(nvars,Aeq,beq,lb,ub,PopulationSize_Data,CrossoverFraction_Data)
%% This is MATLAB file for the solution of Water Application Planning (WAP)
Model using Genetic Algorithm (GA) Optimisation with hybrid function
fmincon for three industrial process.
% The Required Data shown below:
nvars=12; A=[]; b=[];
Aeq = [1,0,0,-1,0,0,1,1,-1,0,-1,0;0,1,0,0,-1,0,-1,0,1,1,0,-1;0,0,1,0,0,-1,0
,-1,0,-1,1,1;0,0,0,-75,0,0,100,125,-75,0,-75,0;0,0,0,0,-100,0,-100,0,75,125
,0,-100;0,0,0,0,0,-125,0,-125,0,-125,75,100];
beq = [0;0;0;-3750;-1000;-1000];
% Lower bounds:
lb = [0,0,0,0,0,0,0,0,0,0,0,0];
% Upper bounds:
ub = [inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf];
% Non-linear Constraint:
nonlcon=@Constraints_FRW;
%% Start with the default options
options = gaoptimset;
%% Modify options setting
options = gaoptimset(options,'PopulationSize', 10);
options = gaoptimset(options,'CrossoverFraction', 0.8);
options = gaoptimset(options,'SelectionFcn', @selectionuniform);
options = gaoptimset(options,'CrossoverFcn', {@crossoverheuristic, 1.2});
options = gaoptimset(options,'MutationFcn', {@mutationadaptfeasible [] []});
options = gaoptimset(options,'HybridFcn', { @fmincon [] });
options = gaoptimset(options,'Display', 'diagnose');
options = gaoptimset(options,'PlotFcns', {@gaplotbestf @gaplotbestindiv
@gaplotexpectation @gaplotrange @gaplotscorediversity @gaplotscores });
[x,fval,exitflag,output,population,score]=ga(@FRW,nvars,A,b,Aeq,beq,lb,ub,n
onlcon,options);
end
```

C2. Matlab Code for Single Contaminant Water Reuse without Regeneration for 4(Four) Industrial Processes

Fitness function

```
function f=FRW2(x)
% return the sum of all the values of fresh water x for 4(Four) processes
f =x(:,1)+x(:,2)+x(:,3)+x(:,4);
End
```

Constraint function

```
function [c,ceq] = Constraints_FRW2(x)
% return the values of the nonlinear constraints
C1out=100;C2out=100;C3out=800;C4out=800;C1in=0; C2in=50; C3in=50; C4in=400;
c=[((C2out*x(:,9)+C3out*x(:,10)+C4out*x(:,11))/(x(:,1)+x(:,9)+x(:,10)+x(:,11)))-C1in;((C1out*x(:,15)+C3out*x(:,12)+C4out*x(:,13))/(x(:,2)+x(:,15)+x(:,12)+x(:,13)))-C2in;((C1out*x(:,16)+C2out*x(:,17)+C4out*x(:,14))/(x(:,3)+x(:,16)+x(:,17)+x(:,14)))-C3in;((C1out*x(:,18)+C2out*x(:,19)+C3out*x(:,20))/(x(:,4)+x(:,18)+x(:,19)+x(:,20)))-C4in];
ceq=[];
end
```

The Code function

```
function [x,fval,exitflag,output,population,score] =
FRW2_code(nvars,Aeq,beq,lb,ub,PopulationSize_Data,CrossoverFraction_Data)
%% This is MATLAB file for the solution of Water Application Planning (WAP)
Model using Genetic Algorithm(GA)Optimisation with hybrid function fmincon
for four industrial process.
% The Required Data is shown below:
InitialPopulation_Data=rand(1,110);
nvars = 20; A=[]; b=[];
Aeq = [1,0,0,0,-1,0,0,0,1,1,1,0,0,0,-1,-1,0,-1,0,0;0,1,0,0,0,-1,0,0,-1,0,1,0,1,0,1,1,0,0,-1;
0,0,0,1,0,0,0,-1,0,0,-1,0,-1,-1,0,0,0,1,1,1;0,0,0,0,-100,0,0,0,100,800,
800,0,0,0,-100,-100,0,-100,0,0;0,0,0,0,0,-100,0,0,-100,0,0,800,800,0,100,
0,-100,0,-100,0;0,0,0,0,0,0,-800,0,0,-800,0,-800,0,800,0,100,100,0,0,-800;
0,0,0,0,0,0,0,-800,0,0,-800,0,-800,-800,0,0,0,100,100,-800];
beq = [0;0;0;0;-2000;-5000;-30000;-4000];
% Lower bounds:
lb = [0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0];
% Upper bounds:
ub = [inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf];
% Non-linear Constraint:
nonlcon=@Constraints_FRW2;
%% Start with the default options
options = gaoptimset;
%% Modify options setting
options = gaoptimset(options,'PopulationSize', 10);
options = gaoptimset(options,'CrossoverFraction', 0.8);
options = gaoptimset(options,'SelectionFcn', @selectionuniform);
options = gaoptimset(options,'CrossoverFcn', {@crossoverheuristic, 1.2});
options = gaoptimset(options,'MutationFcn', {@mutationadaptfeasible[][] });
options = gaoptimset(options,'Display', 'diagnose');
options = gaoptimset(options,'PlotFcns', { @gaplotbestf @gaplotbestindiv
@gaplotexpectation @gaplotrange @gaplotscorediversity @gaplotscores });
[x,fval,exitflag,output,population,score]=ga(@FRW2,nvars,A,b,Aeq,beq,lb,ub,
nonlcon,options);
End
```

C3. Matlab Code for Single Contaminant Water Reuse without Regeneration for 5(Five) Industrial Processes

Fitness function

```
function f=FRW3(x)
% return the sum of all the values of fresh water x for 5(Five) processes
f =x(:,1)+x(:,2)+x(:,3)+x(:,4)+x(:,5);
End
```

Constraint function

```
function [c,ceq] = Constraints_FRW3(x)
% return the values of the nonlinear constraints
C1out=100; C2out=50; C3out=100; C4out=200; C5out=300; Clin=0; C2in=0;
C3in=50; C4in=75; C5in=100;
c=[((C2out*x(:,11)+C3out*x(:,12)+C4out*x(:,13)+C5out*x(:,14))/(x(:,1)+x(:,11)+x(:,12)+x(:,13)+x(:,14)))-Clin;
((C1out*x(:,20)+C3out*x(:,15)+C4out*x(:,16)+C5out*x(:,17))/(x(:,2)+x(:,20)+x(:,15)+x(:,16)+x(:,17)))-C2in;
((C1out*x(:,21)+C2out*x(:,22)+C4out*x(:,18)+C5out*x(:,19))/(x(:,3)+x(:,21)+x(:,22)+x(:,18)+x(:,19)))-C3in;
((C1out*x(:,23)+C2out*x(:,24)+C3out*x(:,25)+C5out*x(:,26))/(x(:,4)+x(:,23)+x(:,24)+x(:,25)+x(:,26)))-C4in;
((C1out*x(:,27)+C2out*x(:,28)+C3out*x(:,29)+C5out*x(:,30))/(x(:,5)+x(:,27)+x(:,28)+x(:,29)+x(:,30)))-C5in];
ceq=[];
end
```

The Code function

```
function [x,fval,exitflag,output,population,score] =
FRW3_code(nvars,Aeq,beq,lb,ub,PopulationSize_Data,CrossoverFraction_Data)
%% This is MATLAB file for the solution of Water Application Planning (WAP)
Model using Genetic Algorithm (GA) Optimisation with hybrid function
fmincon for five industrial process.
% The Required Data shown below:
nvars=30; A=[]; b=[];
Aeq = [1,0,0,0,0,-1,0,0,0,0,1,1,1,1,0,0,0,0,0,-1,-1,0,-1,0,0,0,-1,0,0,0;
0,1,0,0,0,0,-1,0,0,0,-1,0,0,0,1,1,1,0,0,1,0,-1,0,-1,0,0,0,-1,0,0;
0,0,1,0,0,0,0,-1,0,0,0,-1,0,0,-1,0,0,1,1,0,1,1,0,0,-1,0,0,0,-1,0;
0,0,0,1,0,0,0,0,-1,0,0,0,-1,0,0,-1,0,-1,0,0,0,0,1,1,1,1,0,0,0,-1;
0,0,0,0,1,0,0,0,0,-1,0,0,0,-1,0,0,-1,0,-1,0,0,0,0,0,0,-1,1,1,1,1;
0,0,0,0,0,-100,0,0,0,0,50,100,200,300,0,0,0,0,0,-100,-100,0,-100,0,0,0,
-100,0,0,0;0,0,0,0,0,0,-50,0,0,0,-50,0,0,0,100,200,300,0,0,100, 0,-50,0,-
50,0,0,0,-50,0,0;0,0,0,0,0,0,0,-100,0,0,0,-100,0,0,-100,0,0,200,300,0,100,
50,0,0,-100,0,0,0,-100,0;0,0,0,0,0,0,0,0,-200,0,0,0,-200,0,0,-200,0,-200,0,
0,0,0,100,50,100,300,0,0,0,-200;0,0,0,0,0,0,0,0,0,-300,0,0,0,-300,0,0,-300,
0,-300,0,0,0,0,0,0,-300,100,50,100,200];
beq = [0;0;0;0;0;-1000;-1000;-500;-625;-4000];
% Lower bounds:
lb = [0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0];
% Upper bounds:
ub =
[inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf];
% Non-linear Constraint:
nonlcon=@Constraints_FRW3;
%% Start with the default options
options = gaoptimset;
%% Modify options setting
```

```

options = gaoptimset(options, 'PopulationSize', 10);
options = gaoptimset(options, 'CrossoverFraction', 0.8);
options = gaoptimset(options, 'SelectionFcn', @selectionuniform);
options = gaoptimset(options, 'CrossoverFcn', {@crossoverheuristic, 1.2});
options = gaoptimset(options, 'MutationFcn', {@mutationadaptfeasible[] []});
options = gaoptimset(options, 'HybridFcn', { @fmincon [] });
options = gaoptimset(options, 'Display', 'diagnose');
options = gaoptimset(options, 'PlotFcns', { @gaplotbestf @gaplotbestindiv
@gaplotexpectation @gaplotrange @gaplotscorediversity @gaplotscores });
[x,fval,exitflag,output,population,score] =
ga(@FRW3,nvars,A,b,Aeq,beq,lb,ub,nonlcon,options);
end

```

C4. Matlab Code for Single Contaminant Water Reuse without Regeneration for 6(Six) Industrial Processes

Fitness function

```

function f=FRW4(x)
% return the sum of all the values of fresh water x for 6(Six) processes
f =x(:,1)+x(:,2)+x(:,3)+x(:,4)+x(:,5)+x(:,6);
end

```

Constraint function

```

function [c,ceq] = Constraints_FRW4(x)
% return the values of the nonlinear constraints
C1out=80; C2out=100; C3out=200; C4out=100; C5out=800; C6out=800; C1in=25;
C2in=25; C3in=25; C4in=50; C5in=50; C6in=400;
c=[((C2out*x(:,13)+C3out*x(:,14)+C4out*x(:,15)+C5out*x(:,16)+C6out*x(:,17))
/(x(:,1)+x(:,13)+x(:,14)+x(:,15)+x(:,16)+ x(:,17)))-C1in;
((C1out*x(:,18)+C3out*x(:,19)+C4out*x(:,20)+C5out*x(:,21)+C6out*x(:,22))/(x
(:,2)+x(:,18)+x(:,19)+x(:,20)+x(:,21)+ x(:,22)))-C2in;
((C1out*x(:,23)+C2out*x(:,24)+C4out*x(:,25)+C5out*x(:,26)+C6out*x(:,27))/(x
(:,3)+x(:,23)+x(:,24)+x(:,24)+x(:,26)+ x(:,27)))-C3in;
((C1out*x(:,28)+C2out*x(:,29)+C3out*x(:,30)+C5out*x(:,31)+C6out*x(:,32))/(x
(:,4)+x(:,28)+x(:,29)+x(:,30)+x(:,31)+ x(:,32)))-C4in;
((C1out*x(:,33)+C2out*x(:,34)+C3out*x(:,35)+C4out*x(:,36)+C6out*x(:,37))/(x
(:,5)+x(:,33)+x(:,34)+x(:,35)+x(:,36)+ x(:,37)))-C5in;
((C1out*x(:,38)+C2out*x(:,39)+C3out*x(:,40)+C4out*x(:,41)+C5out*x(:,42))/(x
(:,6)+x(:,38)+x(:,39)+x(:,40)+x(:,41)+ x(:,42)))-C6in];
ceq=[];
end

```

The Code function

```

function [x,fval,exitflag,output,population,score] =
FRW4_code(nvars,Aeq,beq,lb,ub,PopulationSize_Data,CrossoverFraction_Data)
%% This is MATLAB file for the solution of Water Application Planning (WAP)
Model using Genetic Algorithm(GA)Optimisation with hybrid function fmincon
for six industrial process.
% The Required Data shown below:
nvars=42; A=[]; b=[];
Aeq = [1,0,0,0,0,0,-1,0,0,0,0,0,1,1,1,1,1,-1,0,0,0,0,-1,0,0,0,0,-1,0,0,0,0,
-1,0,0,0,0,-1,0,0,0,0;0,1,0,0,0,0,0,-1,0,0,0,0,-1,0,0,0,0,1,1,1,1,1,0,-1,0,
0,0,0,-1,0,0,0,0,-1,0,0,0,0,-1,0,0,0;0,0,1,0,0,0,0,0,-1,0,0,0,0,-1,0,0,0,0,
-1,0,0,0,0,1,1,1,1,1,0,0,-1,0,0,0,0,-1,0,0;0,0,0,1,0,0,0,0,0,-1,0,
0,0,0,-1,0,0,0,0,-1,0,0,0,0,0,-1,0,0,0,0,0,-1,0,0,0,0,0,-1,0,0,0,0,0,
1,0,0,0,0,0,-1,0,0,0,0,-1,0,0,0,0,-1,0,0,0,0,-1,0,1,1,1,1,1,0,0,
0,0,-1;0,0,0,0,0,1,0,0,0,0,0,-1,0,0,0,0,-1,0,0,0,0,-1,0,0,0,0,-1,0,0,0,0,-1
,0,0,0,0,0,-1,1,1,1,1,1,1;0,0,0,0,0,0,0,0,-80,0,0,

```



```

C1out=80; C2out=90; C3out=200; C4out=100; C5out=800; C6out=800; C7out=600;
C8out=100; C9out=100; C1in=25; C2in=25; C3in=25; C4in=50; C5in=50;
C6in=400; C7in=400; C8in=0; C9in=0;
c=[((C2out*x(:,19)+C3out*x(:,20)+C4out*x(:,21)+C5out*x(:,22)+C6out*x(:,23)+
C7out*x(:,24)+C8out*x(:,25)+C9out*x(:,26))/(x(:,1)+x(:,19)+x(:,20)+x(:,21)+
x(:,22)+ x(:,23)+ x(:,24)+ x(:,25)+ x(:,26)))-C1in;
((C1out*x(:,27)+C3out*x(:,28)+C4out*x(:,29)+C5out*x(:,30)+C6out*x(:,31)+C7o
ut*x(:,32)+C8out*x(:,33)+C9out*x(:,34))/(x(:,2)+x(:,27)+x(:,28)+x(:,29)+x(
:,30)+ x(:,31)+ x(:,32)+ x(:,33)+ x(:,34)))-C2in;
((C1out*x(:,35)+C2out*x(:,36)+C4out*x(:,37)+C5out*x(:,38)+C6out*x(:,39)+C7o
ut*x(:,40)+C8out*x(:,41)+C9out*x(:,42))/(x(:,3)+x(:,35)+x(:,36)+x(:,37)+x(
:,38)+ x(:,39)+ x(:,40)+ x(:,41)+ x(:,42)))-C3in;
((C1out*x(:,43)+C2out*x(:,44)+C3out*x(:,45)+C5out*x(:,46)+C6out*x(:,47)+C7o
ut*x(:,48)+C8out*x(:,49)+C9out*x(:,50))/(x(:,4)+x(:,43)+x(:,44)+x(:,45)+x(
:,46)+ x(:,47)+ x(:,48)+ x(:,49)+ x(:,50)))-C4in;
((C1out*x(:,51)+C2out*x(:,52)+C3out*x(:,53)+C4out*x(:,54)+C6out*x(:,55)+C7o
ut*x(:,56)+C8out*x(:,57)+C9out*x(:,58))/(x(:,5)+x(:,51)+x(:,52)+x(:,53)+x(
:,54)+ x(:,55)+ x(:,56)+ x(:,57)+ x(:,58)))-C5in;
((C1out*x(:,59)+C2out*x(:,60)+C3out*x(:,61)+C4out*x(:,62)+C5out*x(:,63)+C7o
ut*x(:,64)+C8out*x(:,65)+C9out*x(:,66))/(x(:,6)+x(:,59)+x(:,60)+x(:,61)+x(
:,62)+ x(:,63)+ x(:,64)+ x(:,65)+ x(:,66)))-C6in;
((C1out*x(:,67)+C2out*x(:,68)+C3out*x(:,69)+C4out*x(:,70)+C5out*x(:,71)+C6o
ut*x(:,72)+C8out*x(:,73)+C9out*x(:,74))/(x(:,7)+x(:,67)+x(:,68)+x(:,69)+x(
:,70)+ x(:,71)+ x(:,72)+ x(:,73)+ x(:,74)))-C7in;
((C1out*x(:,75)+C3out*x(:,76)+C4out*x(:,77)+C5out*x(:,78)+C6out*x(:,79)+C7o
ut*x(:,80)+C7out*x(:,81)+C9out*x(:,82))/(x(:,8)+x(:,75)+x(:,76)+x(:,77)+x(
:,78)+ x(:,79)+ x(:,80)+ x(:,81)+ x(:,82))) - C8in;
((C1out*x(:,83)+C3out*x(:,84)+C4out*x(:,85)+C5out*x(:,86)+C6out*x(:,87)+C7o
ut*x(:,88)+C8out*x(:,89)+C8out*x(:,90))/(x(:,9)+x(:,83)+x(:,84)+x(:,85)+x(
:,86)+ x(:,87)+ x(:,88)+ x(:,89)+ x(:,90)))- C9in];
ceq=[];
end

```

The Code function

```

function [x,fval,exitflag,output,population,score] =
FRW7_code(nvars,Aeq,beq,lb,ub,PopulationSize_Data,CrossoverFraction_Data)
% This is MATLAB file for the solution of Water Application Planning (WAP)
Model using Genetic Algorithm(GA)Optimisation with hybrid function fmincon
for nine industrial process.
% The Required Data shown below:
nvars=90; A=[]; b=[];
Aeq=[1,0,0,0,0,0,0,0,0,0,-1,0,0, 0 , 0 , 0 , 0 , 0 , 0 , 1 , 1 , 1 , 1 , 1 ,
1 , 1 , 1 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 ,
-1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 ,
0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 ,
0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ;0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , -1 , 0 ,0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 1 ,
1 , 1 , 1 , 1 , 1 , 1 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 ,
0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 ,
0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 ,
0 , 0 , 0 , 0 , 0 ;0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 ,
0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 ,
0 , 1 , 1 , 1 , 1 , 1 , 1 , 1 , 1 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 ,
-1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 ,
0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 ,
;0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 ,
, 0 , 0 , 0 , 0 , 1 , 1 , 1 , 1 , 1 , 1 , 1 , 1 , 0 , 0 , 0 , -1 ,0 , 0 , 0 ,
, 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 ;0 , 0 , 0 , 0 , 1
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0 , 0 , 0 , 0 , 0 , -1 ,0 , 0

```



```

0 , 0 , -200 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -200 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , -200 , 0 , 0 , 0 , 0 , 0 , 0 ; 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , 0
, 80 , 90 , 200 , 800 , 800 , 600 , 100 , 300 , 300 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 ; 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , 0 , 0 , -800 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -800 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , -800 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -800 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , -800 , 0 , 0 , 0 , 0 , 0 , 80 , 90 , 200 , 100 , 800 , 600 , 100
, 300 , 300 , 0 , 0 , 0 , 0 , -800 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -800 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , -800 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -800 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , -800 , 0 , 0 , 0 , 0 ; 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -800 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -800
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -800 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -800
, 0 , 0 , 0 , 0 , 80 , 90 , 200 , 100 , 800 , 600 , 100 , 300 , 300 , 0 , 0 , 0 ,
0 , 0 , -800 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -800 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , -800 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -800 , 0 , 0 , 0 ; 0 , 0 , 0 , 0 ,
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -600 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , -600 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -600 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , -600 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -600 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , -600 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -600 , 0 , 0 , 0 , 80 , 90
, 200 , 100 , 800 , 800 , 100 , 300 , 300 , 0 , 0 , 0 , 0 , 0 , 0 , -600 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , -600 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -600 , 0 , 0 ; 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 80 , 90 , 200 , 100 , 800 , 800 , 600
, 300 , 300 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -
100 , 0 ; 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , -300 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -300 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , -300 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -300 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, -300 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -300 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -
300 , 0 , 80 , 90 , 200 , 100 , 800 , 800 , 600 , 100 , 300 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , -300 ; 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , -300 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -300 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , -300 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -300 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , -300 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -300 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , -300 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -300 , 80 , 90 , 200 , 100
, 800 , 800 , 600 , 100 , 300];
beq =[0;0;0;0;0;0;0;0;0;0;0;-2000;-2880;-4000;-3000;-30000;-5000;-2000;-1000;
-20000;-6500];
%% Modify options setting
options = gaoptimset(options, 'PopulationSize', PopulationSize_Data);
options = gaoptimset(options, 'CrossoverFraction', 0.8);
options = gaoptimset(options, 'SelectionFcn', @selectionuniform);
options = gaoptimset(options, 'CrossoverFcn', {@crossoverheuristic, 1.5});
options = gaoptimset(options, 'MutationFcn', @mutationadaptfeasible);
options = gaoptimset(options, 'HybridFcn', { @fmincon
[optimoptions('fmincon','Display','iter','Algorithm','sqp')] });
options = gaoptimset(options, 'Display', 'diagnose');
options = gaoptimset(options, 'PlotFcns', { @gaplotbestf @gaplotbestindiv
@gaplotexpectation @gaplotrange @gaplotscorediversity @gaplotscores});
[x,fval,exitflag,output,population,score] =
ga(@FRW8,nvars,A,b,Aeq,beq,lb,ub,@Constraints_FRW8,options);
End

```


APPENDIX D

D1. Matlab Code for Multi-Contaminant Water Reuse without Regeneration for 3 Industrial.

Fitness function

```
function f=FRW(x)
% return the sum of all the values of fresh water x
f =x(:,1)+x(:,2)+x(:,3);
end
```

Constraint function

```
function [c,ceq] = ConstraintsMULT_FRW(x)
% return the values of the nonlinear constraints
C11out=100; C12out=80; C13out=60; C21out=150; C22out=115; C23out=105;
C31out=125; C32out=80; C33out=130; C11in=0; C12in=0; C13in=0; C21in=50;
C22in=50; C23in=50; C31in=75; C32in=75; C33in=75;
c=[(( C21out*x(:,7)+ C31out*x(:,8))/(x(:,1)+x(:,7)+x(:,8))-C11in);
(( C22out*x(:,7)+ C32out*x(:,8))/(x(:,1)+x(:,7)+x(:,8))-C12in);
(( C23out*x(:,7)+ C33out*x(:,8))/(x(:,1)+x(:,7)+x(:,8))-C13in);
((C11out*x(:,9)+ C31out*x(:,10))/(x(:,2)+x(:,9)+x(:,10))-C21in);
((C12out*x(:,9)+ C32out*x(:,10))/(x(:,2)+x(:,9)+x(:,10))-C22in);
((C13out*x(:,9)+ C33out*x(:,10))/(x(:,2)+x(:,9)+x(:,10))-C23in);
((C11out*x(:,11)+ C21out*x(:,12))/(x(:,3)+x(:,11)+x(:,12))-C31in);
((C12out*x(:,11)+ C22out*x(:,12))/(x(:,3)+x(:,11)+x(:,12))-C32in);
((C13out*x(:,11)+ C23out*x(:,12))/(x(:,3)+x(:,11)+x(:,12))-C33in)];
ceq=[];
end
```

The Code function

```
function [x,fval,exitflag,output,population,score] =
FRW_MULT_CONTT_code(nvars,Aeq,beq,lb,ub,PopulationSize_Data,CrossoverFracti
on_Data)
%% This is MATLAB file for the solution of Water Application Planning (WAP)
Model using Genetic Algorithm (GA) Optimisation with hybrid function
fmincon for three industrial process.
% The Required Data shown below:
nvars=21; A=[]; b=[];
Aeq = [1,0,0,-1,0,0,1,1,-1,0,-1,0,0,0,0,0,0,0,0,0,0;0,1,0,0,-1,0,-1,0,1,1,0
,-1,0,0,0,0,0,0,0,0,0;0,0,1,0,0,-1,0,-1,1,0,1,1,0,0,0,0,0,0,0,0,0;0,0,0,-
100,0,0,150,125,-100,0,-100,0,1,0,0,0,0,0,0,0,0;0,0,0,-80,0,0,115,80,-80,0,
-80,0,0,1,0,0,0,0,0,0,0;0,0,0,-60,0,0,105,130,-60,0,-60,0,0,0,0,1,
0,0,0,0,0;0,0,0,0,0,0,-150,0,-150,0,100,125
,0,-150,0,0,0,1,0,0,0,0;0,0,0,0,-115,0
,-115,0,80,80,0,-115,0,0,0,0,1,0,0,0,0;0,0,0
,0,0,-105,0,-105,0,60,130,0,-105,0,0,0,0,0,0,
1,0,0,0;0,0,0,0,0,-125,0,-125,0,-125,100,
150,0,0,0,0,0,0,1,0,0;0,0,0,0,0,-80,0,-80
,0,-80,80,115,0,0,0,0,0,0,1,0;0,0,0,0,0,
-130,0,-130,0,-130,60,105,0,0,0,0,0,0,0,1];
beq = [0;0;0;-3000;-2400;-1800;-4000;-3000;-3600;-1500;-600;-2000];
% Lower bounds:
lb = [0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0];
% Upper bounds:
ub = [100,100,100,100,100,100,100,100,100,100,100,100,100,100,100,100,100,100,100,100,100];
% Non-linear Constraint:
```

```

nonlcon=@ConstraintsMULT_FRW;
%% Start with the default options
options = gaoptimset;
%% Modify options setting
options = gaoptimset(options, 'PopulationSize', 10);
options = gaoptimset(options, 'CrossoverFraction', 0.8);
options = gaoptimset(options, 'SelectionFcn', @selectionuniform);
options = gaoptimset(options, 'CrossoverFcn', {@crossoverheuristic, 1.2});
options = gaoptimset(options, 'MutationFcn', {@mutationadaptfeasible [] []});
options = gaoptimset(options, 'HybridFcn', { @fmincon [] });
options = gaoptimset(options, 'Display', 'diagnose');
options = gaoptimset(options, 'PlotFcns', { @gaplotbestf @gaplotbestindiv
@gaplotexpectation @gaplotrange @gaplotscorediversity @gaplotscores });
[x, fval, exitflag, output, population, score] =
ga(@FRW, nvars, A, b, Aeq, beq, lb, ub, nonlcon, options);
end

```

D2. Matlab Code for Multi-Contaminant Water Reuse with Regeneration for 3(three) Industrial Processes

Fitness function

```

function f=FRW(x)
% return the sum of all the values of fresh water x
f =x(:,1)+x(:,2)+x(:,3);
end

```

Constraint function

```

function [c,ceq] = ConstraintsMULT_REG_FRW(x)
% return the values of the nonlinear constraints
C11out=100; C12out=80; C13out=60; C21out=150; C22out=115; C23out=105;
C31out=125; C32out=80; C33out=130; C11in=0; C12in=0; C13in=0; C21in=50;
C22in=50; C23in=50; C31in=75; C32in=75; C33in=75; Co1=25; Co2=25; Co3=25;
c=[(( C21out*x(:,7)+ C31out*x(:,8)+Co1*x(:,13)))/(x(:,1)+x(:,7)+x(:,8)+
(:,13))-C11in);(( C22out*x(:,7)+ C32out*x(:,8)+ Co2*x(:,13)))/(x(:,1)+x(:,7)
+x(:,8)+x(:,13))-C12in);(( C23out*x(:,7)+ C33out*x(:,8)+ Co3*x(:,13)))/
(x(:,1)+x(:,7)+x(:,8)+x(:,13))-C13in);((C11out*x(:,9)+ C31out*x(:,10)+
Co1*x(:,14)))/(x(:,2)+x(:,10)+x(:,9)+x(:,14))-C21in);((C12out*x(:,9)+
C32out*x(:,10)+Co2*x(:,14)))/(x(:,2)+x(:,10)+x(:,9)+x(:,14))-C22in);
((C13out*x(:,9)+C33out*x(:,10)+Co3*x(:,14)))/(x(:,2)+x(:,10)+x(:,9)+x(:,14))
-C23in);((C11out*x(:,11)+ C21out*x(:,12)+Co1*x(:,15)))/(x(:,3)+x(:,11)+
x(:,12)+x(:,15))-C31in);((C12out*x(:,11)+ C22out*x(:,12)+Co2*x(:,15)))/
(x(:,3)+x(:,11)+x(:,12)+x(:,15))-C32in);((C13out*x(:,11)+ C23out*x(:,12)+
Co3*x(:,15)))/(x(:,3)+x(:,11)+x(:,12)+x(:,15))-C33in)];
ceq=[];
end

```

The Code function

```

function [x, fval, exitflag, output, population, score] =
FRWREG_code(nvars, Aeq, beq, lb, ub, PopulationSize_Data, CrossoverFraction_Data)
%% This is MATLAB file for the solution of Water Application Planning (WAP)
Model using Genetic Algorithm (GA) Optimisation with hybrid function
fmincon for three industrial process with regeneration.
% The Required Data shown below:
nvars=27; A=[]; b=[];
Aeq = [1,0,0,-1,0,0,1,1,-1,0,-1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,-1,0,0;0,1,0,0,-1,0,0,-1,0,1,1,0,-1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,-1,0,-1,0,-1,1,1,

```

```

0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,-1;0,0,0,-100,0,0,150,125,-100,0,-100,0,1,0,0,0
,0,0,0,0,0,25,0,0,-100,0,0;0,0,0,-80,0,0,115,80,-80,0,-80,0,0,1,0,0,0,0,0,0
,0,25,0,0,-80,0,0;0,0,0,-60,0,0,105,130,-60,0,-60,0,0,0,1,0,0,0,0,0,25,0,
0,-60,0,0;0,0,0,0,-150,0,-150,0,100,125,0,-150,0,0,0,1,0,0,0,0,0,25,0,0,-
150,0;0,0,0,0,-115,0,-115,0,80,80,0,-115,0,0,0,0,1,0,0,0,0,0,25,0,0,-115,0;
0,0,0,0,-105,0,-105,0,60,130,0,-105,0,0,0,0,0,1,0,0,0,0,25,0,0,-105,0;
0,-105,0;0,0,0,0,0,0,-125,0,-125,0,-125,100,150,0,
0,0,0,0,0,0,1,0,0,0,0,25,0,0,-125;0,0,0,0,
0,-80,0,-80,0,-80,80,115,0,0,0,0,0,0,0,0,1,0,0
,0,25,0,0,-80;0,0,0,0,0,-130,0,-130,0,-130,
60,105,0,0,0,0,0,0,1,0,0,25,0,0,-130];
beq=[0;0;0;-3000;-2400;-1800;-4000;-3000;-3600;-1500;-600;-2000];
% Lower bounds:
lb = [0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0];
% Upper bounds:
ub = [inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,inf,
inf,inf,inf,inf,inf,inf, inf,inf, inf,inf, inf];
nonlcon=@ConstraintsREG_FRW;
%% Start with the default options
options = optimoptions('gamultiobj');
%% Modify options setting
options = optimoptions(options, 'PopulationSize', 10);
options = optimoptions(options, 'CreationFcn', @gacreationnonlinearfeasible);
options = optimoptions(options, 'CrossoverFraction', 0.8);
options = optimoptions(options, 'ParetoFraction', 0.35);
options = optimoptions(options, 'MigrationInterval', 6);
options = optimoptions(options, 'MigrationFraction', 0.5);
options = optimoptions(options, 'SelectionFcn', {@selectiontournament 3 });
options = optimoptions(options, 'CrossoverFcn', {@crossoverheuristic 1.3 });
options = optimoptions(options, 'MutationFcn', @mutationadaptfeasible);
options = optimoptions(options, 'Display', 'diagnose');
options = optimoptions(options, 'HybridFcn', @fgoalattain);
options = optimoptions(options, 'PlotFcn', {@gaplotdistance @gaplotgenealogy
@gaplotscorediversity @gaplotselection @gaplotpareto @gaplotrankhist
@gaplotspread });
[x,fval,exitflag,output,population,score] =
ga(@FRWR,nvars,A,b,Aeq,beq,lb,ub,nonlcon,options);
end

```

APPENDIX E

E1. Matlab Code for Multi-objective Water Reuse in Matlab for 3(three) Industrial.

Fitness function

```
function f=FRW_MULTOBJ(x)
% f(1)return the sum of all the values of fresh water x
f(1) =x(:,1)+x(:,2)+x(:,3);
% f(2)return the sum of all the values of Wastewater x
f(2) =x(:,4)+x(:,5)+x(:,6);
% f(3)return the sum of all the values of Reuse Wastewater x
f(3) =x(:,7)+x(:,8)+x(:,9)+x(:,10)+x(:,11)+x(:,12);
% f(4)return the sum of all the nodes of Wastewater reuse interconnections
for i = 7:12;
    if x(:,i) >= 1;
        y(i) = 1;
    else
        y(i) = 0;
    end
end
f(4) = sum(y(i));
end.
```

E2. Matlab Code for Multi-objective Water Reuse in Matlab for 3(three) Industrial.

Fitness function

```
function f=FRWREG_MULTOBJ(x)
% f(1)return the sum of all the values of fresh water x
f(1) =x(:,1)+x(:,2)+x(:,3);
% f(2)return the sum of all the values of Wastewater x
f(2) =x(:,4)+x(:,5)+x(:,6);
% f(3)return the sum of all the values of Reuse Wastewater x
f(3) =x(:,7)+x(:,8)+x(:,9)+x(:,10)+x(:,11)+x(:,12);
% f(4)return the sum of all the nodes of Wastewater reuse interconnections
for i = 7:12;
    if x(:,i) >= 1;
        y(i) = 1;
    else
        y(i) = 0;
    end
end
f(4) = sum(y(i));
% f(5)return the sum of all the values of Reuse Wastewater x
f(5) =x(:,13)+x(:,14)+x(:,15)+x(:,16)+x(:,17)+x(:,18);
end
```

APPENDIX F

F1. Matlab Code for Multi- Contaminant, Multi-objective Water Reuse in Matlab for Kaduna Refinery.

Fitness function

```
function f=FRW4KAD_MULTOBJ(x)
% f(1) return the sum of all the values of fresh water x
f(1)=x(:,1)+x(:,2)+x(:,3)+x(:,4)+x(:,5)+x(:,6);
% f(2) return the sum of all the values of Wastewater x
f(2)=x(:,7)+x(:,8)+x(:,9)+x(:,10)+x(:,11)+x(:,12);
% f(3) return the sum of all the values of Reuse Wastewater x
f(3)=x(:,13)+x(:,14)+x(:,15)+x(:,16)+x(:,17)+x(:,18)+x(:,19)+x(:,20)+x(:,21)
+x(:,22)+x(:,23)+x(:,24)+x(:,25)+x(:,26)+x(:,27)+x(:,28)+x(:,29)+x(:,30)+x
(:,31)+x(:,32)+x(:,33)+x(:,34)+x(:,35)+x(:,36)+x(:,37)+x(:,38)+x(:,39)+x(:,
40)+x(:,41)+x(:,42);
% f(4) return the sum of all the nodes of Wastewater reuse interconnections
for i = 13:42;
    if x(:,i) >= 1;
        y(i) = 1;
    else
        y(i) = 0;
    end
end
f(4) = sum(y(i));
end.
```

Constraint function

```
function [c,ceq] = Constraints_FRW4KADMULTI(x)
```

% Suspended Solid = C1

```
%Cin (ppm) Cout (ppm)
%40      500
%10      20
%25      250
%30      300
%15      30
%15      20
```

%Hardness = C2

```
%Cin (ppm) Cout (ppm)
%5        10
%20       100
%50       200
%20       100
%20       100
%20       100
```

%Chemical oxygen demand (COD)= C3

```
%Cin (ppm) Cout (ppm)
%0         150
%0         150
%400       1000
%400       1000
%600       1200
%600       1200
```

%Free hydrocarbons = C4

```
%Cin (ppm) Cout (ppm)
%0         5
%0         5
```



```

%0      5
%0     1000
%0     10
%0     10
%return the values of the nonlinear constraints
C11out=500; C21out=20; C31out=250; C41out=300; C51out=30; C61out=20;
C12out=10; C22out=100; C32out=200; C42out=100; C52out=100; C62out=100;
C13out=150; C23out=150; C33out=1000; C43out=1000; C53out=1200; C63out=1200;
C14out=5; C24out=5; C34out=5; C44out=1000; C54out=10; C64out=10;
C11in=40; C21in=10; C31in=25; C41in=30; C51in=15; C61in=15;
C12in=5; C22in=20; C32in=50; C42in=20; C52in=20; C62in=20;
C13in=0; C23in=0; C33in=400; C43in=400; C53in=600; C63in=600;
C14in=0; C24in=0; C34in=0; C44in=0; C54in=0; C64in=0;
c=[((C21out*x(:,13)+C31out*x(:,14)+C41out*x(:,15)+C51out*x(:,16)+C61out*x(:,17)))/(x(:,1)+x(:,13)+x(:,14)+x(:,15)+x(:,16)+ x(:,17)))-C11in;
((C22out*x(:,13)+C32out*x(:,14)+C42out*x(:,15)+C52out*x(:,16)+C62out*x(:,17)))/(x(:,1)+x(:,13)+x(:,14)+x(:,15)+x(:,16)+ x(:,17)))-C12in;
((C23out*x(:,13)+C33out*x(:,14)+C43out*x(:,15)+C53out*x(:,16)+C63out*x(:,17)))/(x(:,1)+x(:,13)+x(:,14)+x(:,15)+x(:,16)+ x(:,17)))-C13in;
((C24out*x(:,13)+C34out*x(:,14)+C44out*x(:,15)+C54out*x(:,16)+C64out*x(:,17)))/(x(:,1)+x(:,13)+x(:,14)+x(:,15)+x(:,16)+ x(:,17)))-C14in;
((C11out*x(:,18)+C31out*x(:,19)+C41out*x(:,20)+C51out*x(:,21)+C61out*x(:,22)))/(x(:,2)+x(:,18)+x(:,19)+x(:,20)+x(:,21)+ x(:,22)))-C21in;
((C12out*x(:,18)+C32out*x(:,19)+C42out*x(:,20)+C52out*x(:,21)+C62out*x(:,22)))/(x(:,2)+x(:,18)+x(:,19)+x(:,20)+x(:,21)+ x(:,22)))-C22in;
((C13out*x(:,18)+C33out*x(:,19)+C43out*x(:,20)+C53out*x(:,21)+C63out*x(:,22)))/(x(:,2)+x(:,18)+x(:,19)+x(:,20)+x(:,21)+ x(:,22)))-C23in;
((C14out*x(:,18)+C34out*x(:,19)+C44out*x(:,20)+C54out*x(:,21)+C64out*x(:,22)))/(x(:,2)+x(:,18)+x(:,19)+x(:,20)+x(:,21)+ x(:,22)))-C24in;
((C11out*x(:,23)+C21out*x(:,24)+C41out*x(:,25)+C51out*x(:,26)+C61out*x(:,27)))/(x(:,3)+x(:,23)+x(:,24)+x(:,24)+x(:,26)+ x(:,27)))-C31in;
((C12out*x(:,23)+C22out*x(:,24)+C42out*x(:,25)+C52out*x(:,26)+C62out*x(:,27)))/(x(:,3)+x(:,23)+x(:,24)+x(:,24)+x(:,26)+ x(:,27)))-C32in;
((C13out*x(:,23)+C23out*x(:,24)+C43out*x(:,25)+C53out*x(:,26)+C63out*x(:,27)))/(x(:,3)+x(:,23)+x(:,24)+x(:,24)+x(:,26)+ x(:,27)))-C33in;
((C14out*x(:,23)+C24out*x(:,24)+C44out*x(:,25)+C54out*x(:,26)+C64out*x(:,27)))/(x(:,3)+x(:,23)+x(:,24)+x(:,24)+x(:,26)+ x(:,27)))-C34in;
((C11out*x(:,28)+C21out*x(:,29)+C31out*x(:,30)+C51out*x(:,31)+C61out*x(:,32)))/(x(:,4)+x(:,28)+x(:,29)+x(:,30)+x(:,31)+ x(:,32)))-C41in;
((C12out*x(:,28)+C22out*x(:,29)+C32out*x(:,30)+C52out*x(:,31)+C62out*x(:,32)))/(x(:,4)+x(:,28)+x(:,29)+x(:,30)+x(:,31)+ x(:,32)))-C42in;
((C13out*x(:,28)+C23out*x(:,29)+C33out*x(:,30)+C53out*x(:,31)+C63out*x(:,32)))/(x(:,4)+x(:,28)+x(:,29)+x(:,30)+x(:,31)+ x(:,32)))-C43in;
((C14out*x(:,28)+C24out*x(:,29)+C34out*x(:,30)+C54out*x(:,31)+C64out*x(:,32)))/(x(:,4)+x(:,28)+x(:,29)+x(:,30)+x(:,31)+ x(:,32)))-C44in;
((C11out*x(:,33)+C21out*x(:,34)+C31out*x(:,35)+C41out*x(:,36)+C61out*x(:,37)))/(x(:,5)+x(:,33)+x(:,34)+x(:,35)+x(:,36)+ x(:,37)))-C51in;
((C12out*x(:,33)+C22out*x(:,34)+C32out*x(:,35)+C42out*x(:,36)+C62out*x(:,37)))/(x(:,5)+x(:,33)+x(:,34)+x(:,35)+x(:,36)+ x(:,37)))-C52in;
((C13out*x(:,33)+C23out*x(:,34)+C33out*x(:,35)+C43out*x(:,36)+C63out*x(:,37)))/(x(:,5)+x(:,33)+x(:,34)+x(:,35)+x(:,36)+ x(:,37)))-C53in;
((C14out*x(:,33)+C24out*x(:,34)+C34out*x(:,35)+C44out*x(:,36)+C64out*x(:,37)))/(x(:,5)+x(:,33)+x(:,34)+x(:,35)+x(:,36)+ x(:,37)))-C54in;
((C11out*x(:,38)+C21out*x(:,39)+C31out*x(:,40)+C41out*x(:,41)+C51out*x(:,42)))/(x(:,6)+x(:,38)+x(:,39)+x(:,40)+x(:,41)+ x(:,42)))-C61in;
((C12out*x(:,38)+C22out*x(:,39)+C32out*x(:,40)+C42out*x(:,41)+C62out*x(:,42)))/(x(:,6)+x(:,38)+x(:,39)+x(:,40)+x(:,41)+ x(:,42)))-C62in;
((C13out*x(:,38)+C23out*x(:,39)+C33out*x(:,40)+C43out*x(:,41)+C63out*x(:,42)))/(x(:,6)+x(:,38)+x(:,39)+x(:,40)+x(:,41)+ x(:,42)))-C63in;
((C14out*x(:,38)+C24out*x(:,39)+C34out*x(:,40)+C44out*x(:,41)+C64out*x(:,42)))/(x(:,6)+x(:,38)+x(:,39)+x(:,40)+x(:,41)+ x(:,42)))-C64in];

```



```

-250 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ;0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -200 ,
0 , 0 , 0 , 0 , -200 , 0 , 0 , 0 , 0 , -200 , 0 , 0 , 0 , 10 , 100 , 100 ,
100 , 100 , 0 , 0 , -200 , 0 , 0 , 0 , 0 , -200 , 0 , 0 , 0 , 0 , 0 , -200 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 ;0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0
, 0 , -1000 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 150,150,1000,1200 , 1200 ,
0 , 0 , -1000 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 ,
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , 0 ;0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -5 , 0 , 0 , 0 , 0 , -5 , 0
, 0 , 0 , 0 , -5 ,0 , 0 , 0 , 5 , 5 ,1000,10, 10 , 0 , 0 , -5 , 0 , 0 , 0 ,
0 , -5 , 0 , 0 , 0 , 0 , -5 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ;0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , -300 ,0 , 0 , 0 , 0 , -300 , 0 , 0 , 0 , 0 , -300 , 0 , 0
, 0 , 0 , -300 , 0 , 0 , 500,20,250,30 , 20 , 0 , 0 , 0 , -300 , 0 , 0 , 0
, 0 , -300 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ;0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -
100 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , -100 ,
0 , 0 , 10 ,100,200,100,100,0,0,0,-100 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 ;0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 0 , -
1000 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 150 ,150 ,
1000 , 1200 , 1200 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 ;0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 0 , -
1000 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 5 , 5 , 5 ,
10 , 10 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
;0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -30 , 0 , 0 , 0 , 0 , -30 , 0 , 0
, 0 , -30 , 0 , 0 , 0 , 0 , -30 , 0 , 0 , 0 , 0 , -30 , 0 , 500 , 20 ,250 ,
300 , 20 , 0 , 0 , 0 , 0 , -30 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ;0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , -100 , 0 , 0
, 0 , 0 , -100 , 0 , 0 , 0 , 0 , -100 , 0 , 10 , 100 , 200 , 100 , 100 , 0 ,
0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 ;0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, -1200 , 0 , 0 , 0 , 0 , -1200 , 0 , 0 , 0 , 0 , -1200 , 0 , 0 , 0 , 0 ,
-1200 , 0 , 0 , 0 , 0 , -1200,0,150,150,1000,1000,1200,0 , 0 , 0 , 0 , -1200
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1
, 0 , 0 , 0 , 0 , 0 ;0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -10 , 0 , 0 ,
0 , 0 , -10 , 0 , 0 , 0 , 0 , -10 , 0 , 0 , 0 , 0 , -10 , 0 , 0 , 0 , 0 , 0 , -
10 , 0 , 5 , 5 , 5 , 1000 ,10,0 , 0 , 0 , 0 , 0 , -10 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 ;0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -20 , 0 , 0 , 0 , -20 , 0 , 0 ,
0 , 0 , -20 , 0 , 0 , 0 , 0 , -20 , 0 , 0 , 0 , -20 , 0 , 0 , 0 , 0 , 0
, -20 , 500,20,250,300,30,0,0,0,0,0,0,0,0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 ;0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, -100 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , -100
, 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , -100 , 10 , 100 , 200 ,100,100 ,
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 1 , 0 , 0 ;0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -1200 , 0 ,
0 , 0 , 0 , -1200 , 0 , 0 , 0 , 0 , -1200 , 0 , 0 , 0 , 0 , -1200 , 0 , 0 ,
0 , 0 , -1200 , 0 , 0 , 0 , 0 , -1200 , 150 , 150 , 1000 , 1000 , 1200 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 1 , 0 ;0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -10 , 0 , 0 , 0
, 0 , -10 , 0 , 0 , 0 , 0 , -10 , 0 , 0 , 0 , 0 , -10 , 0 , 0 , 0 , 0 , 0 , -
10 , 0 , 0 , 0 , 0 , -10 , 5 , 5 , 5 , 1000 , 10 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 ] ;
beq=[0;0;0;0;0;0;-69000;-750;-22500;-750;-2800;-22400;-42000;-1400;-4500;-
3000;-12000;-100;-12150;-3600;-27000;-45000;-225;-1200;-9000;-150;-50;-
800;-6000;-100];

```



```
f(5)=x(:,67)+x(:,68)+x(:,69)+x(:,70)+x(:,71)+x(:,72)+x(:,73)+x(:,74)+x(:,75)
)+x(:,76)+x(:,77)+x(:,78);
end.
```

Constraint function

```
function [c,ceq] = Constraints_FRW4REG_KADMULTI(x)
```

% Suspended Solid = C1

```
%Cin (ppm)  Cout (ppm)
%40         500
%10         20
%25         250
%30         300
%15         30
%15         20
```

%Hardness = C2

```
%Cin (ppm)  Cout (ppm)
%5          10
%20         100
%50         200
%20         100
%20         100
%20         100
```

%Chemical oxygen demand (COD)= C3

```
%Cin (ppm)  Cout (ppm)
%0          150
%0          150
%400        1000
%400        1000
%600        1200
%600        1200
```

%Free hydrocarbons = C4

```
%Cin (ppm)  Cout (ppm)
%0          5
%0          5
%0          5
%0          1000
%0          10
%0          10
```

```
%return the values of the nonlinear constraints
```

```
C11out=500; C21out=20; C31out=250; C41out=300; C51out=30; C61out=20;
C12out=10; C22out=100; C32out=200; C42out=100; C52out=100; C62out=100;
C13out=150; C23out=150; C33out=1000; C43out=1000; C53out=1200; C63out=1200;
C14out=5; C24out=5; C34out=5; C44out=1000; C54out=10; C64out=10; C11in=40;
C21in=10; C31in=25; C41in=30; C51in=15; C61in=15; C12in=5; C22in=20;
C32in=50; C42in=20; C52in=20; C62in=20; C13in=0; C23in=0; C33in=400;
C43in=400; C53in=600; C63in=600; C14in=0; C24in=0; C34in=0; C44in=0;
C54in=0; C64in=0; Co1=2;Co2=1;Co3=15;Co4=0.5;
c=[((C21out*x(:,13)+C31out*x(:,14)+C41out*x(:,15)+C51out*x(:,16)+C61out*x(:,17)
)+ Co1*x(:,67)))/(x(:,1)+x(:,13)+x(:,14)+x(:,15)+x(:,16)+x(:,17)))-C11in;
((C22out*x(:,13)+C32out*x(:,14)+C42out*x(:,15)+C52out*x(:,16)+C62out*x(:,17)
)+ Co2*x(:,67)))/(x(:,1)+x(:,13)+x(:,14)+x(:,15)+x(:,16)+ x(:,17)))-C12in;
((C23out*x(:,13)+C33out*x(:,14)+C43out*x(:,15)+C53out*x(:,16)+C63out*x(:,17)
)+ Co3*x(:,67)))/(x(:,1)+x(:,13)+x(:,14)+x(:,15)+x(:,16)+ x(:,17)))-C13in;
((C24out*x(:,13)+C34out*x(:,14)+C44out*x(:,15)+C54out*x(:,16)+C64out*x(:,17)
)+ Co4*x(:,67)))/(x(:,1)+x(:,13)+x(:,14)+x(:,15)+x(:,16)+ x(:,17)))-C14in;
((C11out*x(:,18)+C31out*x(:,19)+C41out*x(:,20)+C51out*x(:,21)+C61out*x(:,22)
)+ Co1*x(:,68)))/(x(:,2)+x(:,18)+x(:,19)+x(:,20)+x(:,21)+ x(:,22)))-C21in;
((C12out*x(:,18)+C32out*x(:,19)+C42out*x(:,20)+C52out*x(:,21)+C62out*x(:,22)
)+ Co2*x(:,68)))/(x(:,2)+x(:,18)+x(:,19)+x(:,20)+x(:,21)+ x(:,22)))-C22in;
```


1 , 0 , 0 , 0 , 0 , -1 , 1 , 1 , 1 , 1 , 1 , 0 , 0 ,
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 ,
, 0 , 0 , 0 , 0 , 0 , -1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , -500 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 20 , 250 ,
300 , 30 , 20 , -500 , 0 , 0 , 0 , 0 , 0 , 0 , -500 , 0 ,
, 0 , 0 , 0 , 0 , 0 , -500 , 0 , 0 , 0 , 0 , 0 , -500 ,
, 0 , 0 , 0 , 0 , 0 , 0 , -500 , 0 , 0 , 0 , 0 , 0 , 0 , 1 ,
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , 0 , 0 , 0 , 0 , 25 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , -500 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , -10 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 100 ,
, 200 , 100 , 100 , 100 , -10 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
-10 , 0 , 0 , 0 , 0 , 0 , 0 , -10 , 0 , 0 , 0 , 0 , 0 , 0 ,
, -10 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -10 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , -10 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , 0 , 0 , 0 , -150 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 150 , 1000 , 1000 , 1200 , 1200 , -150 , 0 , 0 , 0 ,
, 0 , -150 , 0 , 0 , 0 , 0 , 0 , -150 , 0 , 0 , 0 ,
0 , 0 , -150 , 0 , 0 , 0 , 0 , 0 , -150 , 0 , 0 , 0 ,
, 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 25 , 0 , 0 ,
;0 , 0 , 0 , 0 , 0 , 0 , 0 , -150 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , 5 , 5 , 1000 , 10 , 10 , -5 , 0 , 0 ,
0 , 0 , 0 , 0 , -5 , 0 , 0 , 0 , 0 , 0 , 0 , -5 , 0 ,
, 0 , 0 , 0 , 0 , -5 , 0 , 0 , 0 , 0 , 0 , 0 , -5 ,
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 ,
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 25 ,
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , -5 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -20 ,
0 , 0 , 0 , 0 , 0 , -20 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 500 ,
, 250 , 300 , 30 , 20 , 0 , 0 , -20 , 0 , 0 , 0 , 0 , 0 ,
0 , -20 , 0 , 0 , 0 , 0 , 0 , 0 , -20 , 0 , 0 , 0 , 0 ,
1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 25 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -20 , 0 ,
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
, -100 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 10 , 200 , 100 , 100 , 100 , 0 , -100 , 0 , 0 , 0 ,
, 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 ,
, 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , 0 , 0 , 25 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
-100 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , -150 , 0 , 0 , 0 , 0 , 0 , -150 , 0 , 0 , 0 ,
, 0 , 0 , 0 , 150 , 1000 , 1000 , 1200 , 1200 , 0 , -150 ,
, 0 , 0 , 0 , 0 , 0 , -150 , 0 , 0 , 0 , 0 , 0 , 0 , - ,
150 , 0 , 0 , 0 , 0 , 0 , 0 , -150 , 0 , 0 , 0 , 0 , 0 , 0 ,
0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 ,
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 25 , 0 , 0 , 0 , 0 , 0 ,

1200 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 0 , -1000
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
25 , 0 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 0 , 0
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -1000 , 0 , 0
, 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 0 , 0 , -1000 , 0 , 0
0 , 10 , 0 , 0 , -1000 , 0 , 0 , 0 , 5 , 5 , 5 , 10
, 0 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 0 , 0 , -1000 , 0
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 25
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , -1000 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -30 , 0
, 0 , 0 , 0 , 0 , 0 , -30 , 0 , 0 , 0 , 0 , 0 , 0 , -30 , -30
, 0 , 500 , 20 , 250 , 300 , 20 , 0 , 0 , 0 , 0 , 0 , 0
0 , -30 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 25 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -30 , 0 , 0 , 0
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -
100 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , 0
-100 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , -100
, 0 , 10 , 100 , 200 , 100 , 100 , 0 , 0 , 0 , 0 , 0 , 0 , 0
-100 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 25 , 0 , 0 , 0 , 0
0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
0 , 0 , 0 , -1200 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -1200 , 0
, 0 , 0 , 0 , 0 , -1200 , 0 , 0 , 0 , 0 , 0 , -1200 ,
0 , 0 , 0 , 0 , 0 , -1200 , 0 , 0 , 150 , 150 , 1000 ,
1000 , 1200 , 0 , 0 , 0 , 0 , 0 , -1200 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0
, 0 , 0 , -1200 , 0 , 0 , 0 , 0 , 0 , 0 , 25 , 0 , 0 , 0 , 0
0 , 0 , 0 , 0 , 0 , 0 , -10 , 0 , 0 , 0 , 0 , 0 , 0 , -10
-10 , 0 , 0 , 0 , 0 , 0 , 0 , -10 , 0 , 0 , 0 , 5 , 5 , 5
, 1000 , 10 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -10 , 0 , 0 , 0 , 0
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 25 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , -10 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
0 , 0 , 0 , -20 , 0 , 0 , 0 , 0 , 0 , 0 , -20 , 0 , 0 , 0
, 0 , 0 , 0 , -20 , 0 , 0 , 0 , 0 , 0 , 0 , -20 , 0 , 0 , 0
0 , 0 , 0 , 0 , -20 , 500 , 20 , 250 , 300 , 30 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
25 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -20 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0
, 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0 , 0 , 0 , -100 , 0
0 , 0 , 0 , 0 , 0 , -100 , 10 , 100 , 200 , 100 ,
100 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
0 , 0 , 0 , 0 , 0 , 1 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0
, 0 , 25 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , -100 , 0 , 0 , 0

APPENDIX G

G1. Fitness function values for Single-Contaminant Water Reuse:

Population Size	Fitness function values With Hybrid Function (For the Number of Industrial processes) (m ³ /h)									Percentage of best Optimum result (%)
	Two	Three	Four	Five	Six	Seven	Eight	Nine	Ten	
3	25.4	57.95311	91.1924	30.0011	156	115.9929	138.2445	158.0817	165.9313	60
4	25.0	56.66734	91.0679	30.0001	156	115.9929	138.2899	158.0982	165.9313	60
5	25.0	56.66724	90.0002	30	156	115.9929	138.2698	158.0886	165.9313	70
6	25.4	56.66753	90.2133	30.0001	156	115.9929	138.2427	158.0975	165.9313	60
7	26.0	56.66749	90	30.0002	156	115.9929	138.2472	158.1342	165.9313	80
8	25.0	56.66692	90.9204	30.0011	156	115.9929	138.2375	158.1309	165.9313	80
9	25.5	56.66701	90	30	156	115.994	138.2718	158.1701	165.9313	60
10	25.0	56.66688	90	30.0011	156	115.9929	138.2271	158.0902	165.9313	90
20	25.0	56.66709	90.9924	30	156	115.9929	138.2961	158.1084	165.9313	70
30	25.0	56.66729	91.2742	30.0002	156	115.9929	138.2068	158.1169	165.9313	70
40	25.0	56.66709	91.3834	30.0002	156	115.9929	138.2177	158.1534	165.9313	60
50	25.0	56.66725	91.3058	30.0003	156.0001	115.9929	138.2682	158.1085	165.9313	60
60	25.0	56.6671	90	30.0011	156	115.9929	138.2295	158.1026	165.9313	70
70	25.0	56.66677	90.001	30.0002	156	115.9929	138.274	158.1437	165.9313	70
80	25.0	56.66725	91.4661	30.0001	156	115.9929	138.2769	158.1709	165.9313	60
90	25.0	56.66732	91.153	30.0056	156	115.9929	138.2904	158.1858	165.9313	70
100	25.0	56.6673	91.2474	30.0023	156	115.9929	138.2993	158.175	165.9313	70
200	25.0	56.66722	90	30.0002	156	115.9929	138.2583	158.1217	165.9313	70
300	25.0	56.66727	91.0174	30.0001	156	115.9929	138.2358	158.1204	165.9313	70
400	25.0	56.66738	90	30.0011	156	115.9929	138.2595	158.1086	165.9313	80
500	25.0	56.66705	90.0001	30.0002	156	115.9929	138.2934	158.1233	165.9313	70
600	25	56.7	90.9522	30.0011	156	115.9929	138.2698	158.1076	165.9313	80
700	25	56.7	90.9802	30.0002	156	115.9929	138.2041	158.1254	165.9313	70
800	25	56.7	90.9793	30	156	115.9929	138.2576	158.1169	165.9313	80
900	25	56.7	90.0004	30.0001	156	115.9929	138.2757	158.1953	165.9313	70
1000	24.9996	56.7	91.0334	30	156	115.9929	138.2664	158.1616	165.9313	80

