SINGLE CONTAMINANT
BASED
WATER PINCH ANALYSIS

A PROJECT REPORT

SUBMITTED BY

MANEET GOYAL

IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE AWARD OF THE DEGREE OF

BACHELOR OF ENGINEERING

IN

PETROCHEMICAL ENGINEERING

TO

SAVITRIBAI PHULE PUNE UNIVERSITY

MAY 2016

DEPARTMENT OF PETROCHEMICAL ENGINEERING

MAEER'S MAHARASHTRA INSTITUTE OF TECHNOLOGY

MAEER'S
MAHARASHTRA INSTITUTE OF TECHNOLOGY

affiliated to

SAVITRIBAI PHULE PUNE UNIVERSITY

BONA FIDE CERTIFICATE

This is to certify that this project report, entitled, **Single Contaminant Based Water Pinch Analysis,** is submitted by **Mr Maneet Goyal,** PRN No. 71300362G**,** in partial fulfilment of the requirements of the Savitribai Phule Pune University for the award of Degree of Bachelor of Engineering in Petrochemical Engineering. It is the record of his own work carried out by him under my guidance.

Prof Datta B. Dandge
Project Supervisor, and Head of the Department
Department of Petrochemical Engineering
MAEER's Maharashtra Institute of Technology

Place: Pune, Maharashtra
Date: 6th June 2016

CONTENTS

Chapter	Title	Page No.
	Acknowledgements	6
	Abstract	7
	List of Figures	8
	List of Tables	9
	Chapters	
1.	Need for Water Minimization	10
1.1.	Groundwater Depletion	12
1.2.	Wastewater Contamination	15
2.	Water Cascade Analysis and the Nearest Neighbour Algorithm for Water Minimization	20
2.1.	Water Pinch Analysis	21
2.1.1.	Water Cascade Analysis	27
2.1.2.	Nearest Neighbour Algorithm	30
2.1.2.1	A Note on LR Elimination	33
3.	Targeting using Water Cascade Analysis	35
3.1.	Generating Base Case: No Water Reuse/Recycle	35
3.1.1.	crude.m Algorithm	35
3.1.2.	Major Assumption in crude.m	36

3.1.3.	Program Objectives	36
3.1.4.	crude.m	37
3.2.	Targeting using WCA	43
3.2.1.	intprt_v2.m Algorithm	45
3.2.2.	Major Assumptions in intprt_v2.m	47
3.2.3.	Program Objectives	48
3.2.4.	Alternate Approach for Multiple Source Targeting	48
3.2.5.	intprt_v2.m	50
4.	Network Design using NNA	58
4.1.	nnaup.m Algorithm	58
4.1.1.	Major Limitations	60
4.1.2.	Program Objectives	60
4.1.3	nnaup.m	60
	Concluding Remarks	74
	Appendices	
A	Some Helpful Explanations	76
A.1.	Fresh Water requirement in Fixed Contaminant Load Systems	76
A.2.	Mathematical Reasoning behind the applicability of LR Elimination	78
B	Sub-routines Developed for Targeting	81
B.1.	mysort.m	81

B.2.	imnor.m	81
B.3.	trgt.m	83
B.4.	wca.m	84
B.5.	fzbl.m	85
B.6.	nantonill.m	86
B.7.	FWAug_v2.m	86
B.8.	thresh2.m	87
B.9.	thresh2aliter.m	88
B.10.	row.m	90
B.11.	PurityFresh.m	90
C	Sub-routines Developed for Network Design	91
C.1.	Shenoy.m	91
C.2.	ShenFun.m	91
C.3.	concUpdate.m	91
C.4.	searcon.m	92
	References	93

ACKNOWLEDGEMENTS

First and foremost, I would like to thank my supervisor, **Prof Datta B Dandge,** for guiding me in this work with a liberal approach, and sharing his invaluable ideas that inspired me to stay passionate about this Project. More than anything else, I would like to thank him for teaching me how to learn. Under his guidance, learning, to me, became enjoyable and empowering.

Thanks are due to **Dr Neeta Kankane**, Department of Mathematics, MAEER's Maharashtra Institute of Technology. Her guidance helped me confidently explore new areas of science, and her appreciation motivated me to push my boundaries.

I also wish to thank my Project Coordinators, **Dr Somnath Nandi**, Department of Technology, Savitribai Phule Pune University and **Dr Dinesh Bhutada**, Department of Petrochemical Engineering, MAEER's Maharashtra Institute of Technology for always showing faith in me.

Last but not the least, I would like to extend my sincere gratitude towards **my family** for inspiring me to persevere, for their unconditional love and support, and for always being there for me.

Maneet Goyal

ABSTRACT

The current increase in water stress at both global and national levels can only be checked through the execution of effective water management plans. Regulation of water usage in process industry will form an integral part of many such plans. Water Pinch Analysis (WPA) is a systematic technique used to carry out water minimization in industries, civil complexes, etc. by exploiting water reuse opportunities to the maximum possible extent. In this work, we discuss the use of Water Cascade Analysis and the Nearest Neighbour Algorithm in establishing the minimum water requirements of a process and subsequently, designing networks which will help us realize those targets. Both targeting and network synthesis are facilitated by a set of MATLAB programs that we are currently expanding to deal with a wide variety of water recovery problems. The analysis is based on single contaminant, and is applicable for continuous-type operations.

Key Words: Water Pinch Analysis, Targeting, Network Design, Fixed Load, Fixed Flowrate, Single Contaminant, Water Minimization, MATLAB, Water Cascade, Nearest Neighbour, Continuous-type Operations

LIST OF FIGURES

Figure 1	Global scenario of the per capita availability of renewable water resource
Figure 2	Baseline Water Stress Levels in India in 2010
Figure 3	Outcome of Process Synthesis: Step Change in Cost Savings
Figure 4	The Water Management Hierarchy
Figure 5	Steps involved in WPA
Figure 6	Output generated by nnaup.m for Data Set IX
Figure 7	Conventional Representation of Source-Sink Matching Matrix for Data Set VII
Figure 8	Output generated source exchanges and LR eliminations
Figure 9	Conventional Representation of Source-Sink Matching Matrix given in Figure 8
Figure 10	Network Matrix for the Brewery Case

LIST OF TABLES

Table 1	Application of Water Minimization in Industries
Table 2	Complete Water Cascade Table
Table 3	Source Data Set I
Table 4	Demand Data Set I
Table 5	Source Data Set II
Table 6	Demand Data Set II
Table 7	Source Data Set III
Table 8	Demand Data Set III
Table 9	Source Data Set IV
Table 10	Demand Data Set IV
Table 11	MATLAB Programs used in the targeting process
Table 12	Alternate WCA for Multiple Source Targeting
Table 13	Source Data Set V
Table 14	Demand Data Set V
Table 15	Source Data Set VI
Table 16	Demand Data Set VI
Table 17	Source Data Set VII
Table 18	Demand Data Set VII
Table 19	MATLAB Programs used in the network design process
Table 20	Source Data Set VIII
Table 21	Demand Data Set VIII
Table 22	Source Data Set IX
Table 23	Demand Data Set IX
Table 24	Representative Data of the Beer Brewery's Water Network

CHAPTER 1

Need for Water Minimization

It's not just about the money!

Water minimization, in a broad sense, refers to the reduction in water usage by means of adopting reuse, recycle, and/or regeneration (Wang & Smith 1994) strategies and/or employing alternatives with lower inherent water demands. A more refined explanation which is specific to the scope of this work can be derived from Westerberg's definition (Westerberg 1987) of process synthesis: "the discrete decision making activities of conjecturing (a) which of the many available component parts one should use, and (b) how they should be interconnected to structure the optimum solution to a given design problem." In water minimization, the available component parts assume the form of available water resources and the design problem concerns itself with finding an optimum water network. In this chapter, we highlight the need for carrying out water minimization in the light of one of the pressing global problems - water stress.

Water stress in its extreme form leads to water scarcity. According to one classification (UN-Water 2014), when the availability of renewable fresh water per capita per annum in a country falls below 1700 m^3, it may begin to experience regular or periodic 'water stress'. The condition worsens when the same falls below 1000 m^3 as the nation's health and economy starts getting affected due to 'water scarcity' (Fry 2005). At the extreme, when this availabiltiy falls even below 500 m^3, 'absolute scarcity' is declared.

Factors such as groundwater depletion, wastewater contamination and other accessibility concerns (Schulte 2014) give rise to the condition of water stress. These factors can be broadly attributed to 'unsustainable development pathways', ‘governance failures’, or both. Socio-economic phenomenona like globalization, industrialization, overpopulation, urbanization, etc. have not only put tremendous pressure on the existing groundwater resources but have also resulted in climate change and variability. The situation is exacerbated by wastewater contamination which further limits the availability of ‘immediately accessible’ water resources (Millennium-ecosystem-assessment 2005). Moreover, some of the current food & energy security policies, civil & military conflicts, and transboundary issues (UN-WWAP 2015) further intensify water stress and give another strong blow to the possibility of the existence of a safe and sustainable future. Figure 1, showing a significant portion of the population worldwide under the grip of water stress, stands as a testimony to the above mentioned facts. Narrowing down to a national level perspective, we also present figure 2 which gives the Baseline Water Stress levels (India-Water-Tool n.d.) in India for the year 2010. Clearly, majority of the regions in India (more than 54% of the area (Shiao et al. 2015)) are experiencing high to extremely high water stress, and consequently, counter-measures are the need of the hour.

Note: In the light of water minimization, our focus is not on tackling accessibility issues which are rooted in societal failures to meet the public water demand even when there are ample resources available. A simlar situation is posed by Syria (UNICEF 2013) where water supply services are declining due to regional conflicts. Clearly, in such cases, water minimization measures alone may not produce satisfactory results in reducing water stress.

We now discuss two important factors contributing to water stress.

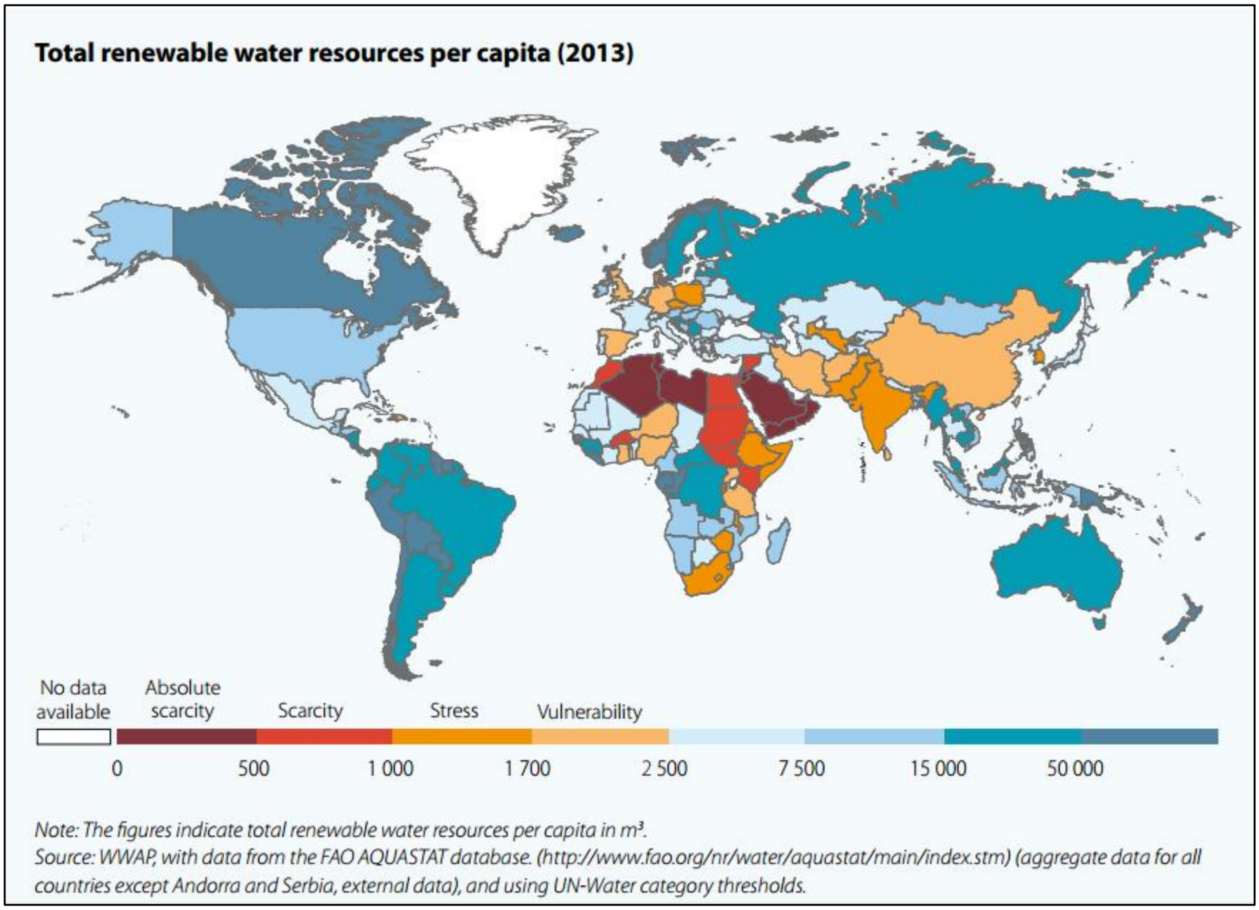

Figure 1: Global scenario of the per capita availability of renewable water resource

1.1. Groundwater Depletion

Excessive water usage for agricultural, industrial, and domestic purposes has significantly contributed towards the overexploitation of ground water resources which in turn has led to many detrimental consequences. For instance, let us first consider the case of the North China Plain (NCP) where persistent high rate of groundwater removal has led to a significant reduction in the water table levels. According to one estimate, the density of pumped wells in this region has exceeded 19 wells per km^2. The Hebei Plain that lie in the northern part of the NCP makes a serious and convincing case: due to rapid urbanization, industrialization and agricultural expansion, the water demand here has doubled in comparison with the trend witnessed during the 1950s and 60s. Furthermore, some claim that by 1980s, the water level decline rates went up to 2-3 m/year in some of the intensively exploited artesian aquifers of the Hebei Province. (Changming et al. 2001)

One of the serious consequences of overexploitation in the NCP is the deterioration of the ground water quality. By 1993, Laizhou City had witnessed 20-40% decrease in the agricultural production due to salinization resulting from sea water intrusion (Jing-jie et al. 1999). Salinization, however, may also occur due to the introduction of saline ground water into fresh water aquifers. Moreover, the interaction between ground water and various wastewater discharges induced by the increased hydraulic gradients may also easily affect human health. (Changming et al. 2001)

The ramifications of the overexploitation of groundwater are being witnessed in other regions also. In Mexico, we see another example wherein excessive exploitation of water resources has led to some serious problems such as high decline in water level in the Valley of Toluca aquifer, land subsidence, decreased river flow in Lerma river, drying up of wetlands, etc. The wetlands of Almoloya del Rio have been deteriorated because the springs that used to charge the lagoons are now catering to the basic needs of the residents of Mexico City. This arrangement has affected both the local flora and fauna and the agricultural produce of this region (Esteller & Diaz-Delgado 2002). One work indicates that many Middle East and North African countries have also suffered a similar fate (Salameh 2008).

Through water minimization, the rate of depletion of ground water resources can be reduced and consequently, the ecosystem can be benefitted and risks to human lives lowered. However, ground water depletion is not the only cause of

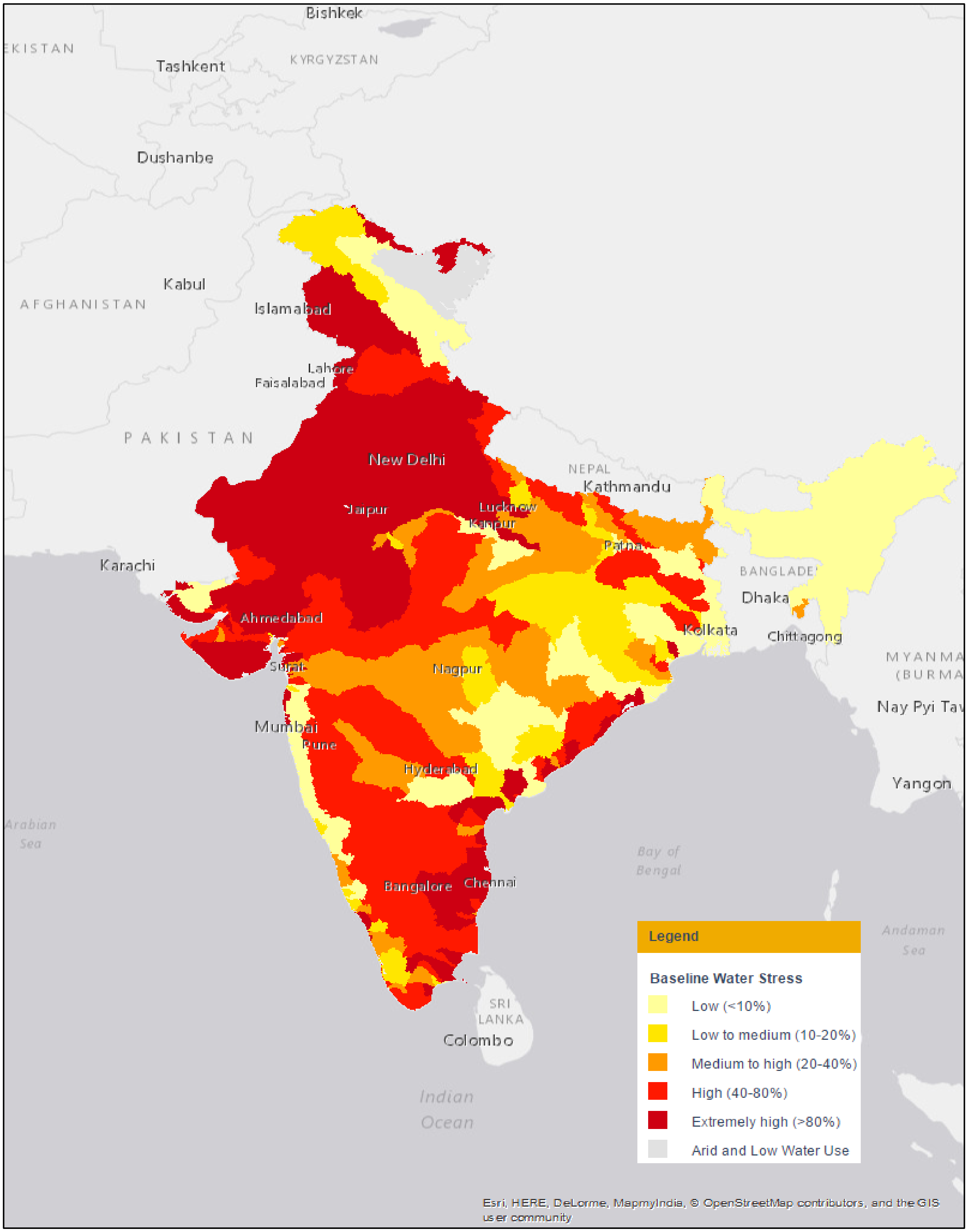

Figure 2: Baseline Water Stress Levels in India in 2010

worry and other factors like wastewater contamination and climate change and variability have to be also dealt with.

Note: Another severe effect of the overexploitation of groundwater depletion is land subsidence. Some report that till 1995, 17 land-subsidence areas were identified in the entire NCP, and in the Xushui County, Hebei Province alone, the land collapses caused damage to more than 200 buildings. (Changming et al. 2001)

1.2. Wastewater Contamination

Wastewater originating in anthropogenic activities pose a major threat to the society because of its toxic and/or hazardous constituents. For instance, the wastewater from sheep dipping industries has high arsenic content, from explosive and chemical works industries large amount of nitro compounds, from paper and textile industries large concentrations of Chromium, Mercury and free Chlorine, and from fertilizer indutries and petroleum refineries fatal amounts of Cadmium, Lead, Nickel ions, etc. (Bond et al. 1972). These pollutants harm both ecosystem (Camargo & Alonso 2006) and human health (Schwarzenbach et al. 2010). For example, heavy metals in high concentrations can be lethal for human beings: cadmium poisoning can cause damage to kidneys and tearing down of testicular tissues and red blood cells, lead poisonong can cause dysfunctions in the brain and nervous systems, and mercury poisoning can result in paralysis, blindness, and even birth defects (Alturkmani n.d.). As regards Chromium, Cr(VI) is carcinogenic in nature and causes irritation. Cr(III) is also lethal in high concentration (Singanan & Peters 2013). Copper poisoning may cause diarrhea, liver and kidney failure, respiratory difficulties, and even death (Tapiero et al. 2003). Fortunately, World Health Organization (WHO) has prescribed standards specifying the permissible limits of various chemical contaminants in drinking water (World-Health-Organization 2008). As indicated earlier, the threat is not limited to humans: one widely referred work (Camargo & Alonso 2006) shows that high concentration of inorganic nitrogen in fresh water can lead to its acidification, eutrophication, and even the loss of aquatic life.

Water minimization, and hence, wastewater minimization leading to lower contamination of water bodies can drive more water resources under the fit-for-consumption category, and benefit both ecosystem and human health. Moreover, in process industries, it can also lead to advantages which they may be most interested in, i.e., reduced cost of production. Water minimization leads to lower water usage and hence, lower utility costs. Moreover, the subsequent reduction in wastewater generation may also result in reduced treatment costs and in some cases, reduced capital costs associated with both process vessels and effluent treatment facilities. These cost reducing factors clearly cannot be overlooked and may serve as the USPs for promoting a culture of water minimization. Some of the promising results of employing water minimization in industries are reported in Table 1. Clearly, water minimization alone may not be able to fully prevent the life-threatening situations arising due to increasing water pollution but is definitely an important step towards combatting it.

In effect, adopting sustainable development pathways and better governance strategies, and reaching a global consensus over sustainable management of water resources are required to take a detour to a better future. Water minimization, certainly, constitutes an inherent part of this action plan.

Table 1: Application of Water Minimization in Industries

S. No.	Industry	Technique	Comments	Reference
1.	Agrochemical Plants	Insight based pinch analysis	Targeting studies over an agrochemical facility consisting of three process (batch type) resulted in more than 57% fresh water savings for a certain type of mode of operation.	(Majozi et al. 2006)
2.	Chemical Manufacturing	Insight based pinch analysis	Various retrofit projects pertaining to reuse/recycle of process water in a chlor-alkali complex point towards an annual saving of the order of 11,69,000 RMB.	(Liao et al. 2011)
3.	Electroplating Industries	Mathematical Optimization	Reduction in fresh water requirement (FWR) and wastewater discharge (WWD) in an electroplating industry indicates a 39.3% reduction in the annualized costs.	(Zhou et al. 2001)

4.	Food and Beverage Plants	Insight based pinch analysis	Application of water pinch analysis (WPA) in a citrus juice processing plant shows that around 22% reduction in both FWR and WWD can be obtained by careful exploitation of the water reuse opportunities. Moreover, the payback period associated with the physical modifications required for employing an optimal water network is just 0.14 years.	(Thevendiraraj et al. 2003)
5.	Oil Refineries	Insight based pinch analysis	Dual contaminant (COD and Hardness) based WPA in Tehran Oil Refinery predicted a 42% reduction in the FWR of the refinery.	(Nabi Bidhendi et al. 2010)

6.	Palm Oil Mills	Mathematical Optimization	Mathematical optimization studies in Thaksin Palm Oil Mill indicates that wastewater recycle/reuse could reduce the FWR and WWD by 65% and 67% respectively.	(Chungsiriporn et al. 2006)
7.	Pulp and Paper Mills	Insight based pinch analysis	Targeting studies using Water Cascade Analysis (Manan et al. 2004) in an Indian Paper Mill predicts around 56% reduction in WWD. Moreover, the resultant reduction in the pollution costs is reported to be around 35%.	(Shukla et al. 2013)
8.	Textile/fabric Mills	Insight based pinch analysis	Water and wastewater minimization in the first textile mill of Malaysia was performed using WPA. Incorporation of regeneration-reuse strategy points to around 50% reduction in the FWR.	(Wenzel et al. 2001)

CHAPTER 2

Water Cascade Analysis and the Nearest Neighbour Algorithm for Water Minimization

With a pinch of Pinch!

Process Synthesis

The U.S. National Park Service gives a lucid meaning of the term, conservation – "*the proper use of nature*" (National Park Service n.d.). Similarly, by extension, the notion of resource conservation can be developed. In the context of process industries, it relates to the efficient use of resources such that their consumption is minimized and benefits are reaped, majorly in the forms of lower production costs and/or compliance with the environmental laws. Hence, in response to various resource conservation problems, the designer/engineer should generate optimal solutions to maximize the related benefits. Here, the bigger picture includes the greater good of environmental and global welfare. Process synthesis, defined in Chapter 1, serves as a very powerful tool in completing this task. It not only helps us in generating the minimum targets corresponding to a given resource recovery problem, but also helps us in figuring out how to actually realize those targets. Moreover, the targets and/or network solutions are not based on the previous designs but rather draw input from fundamental and more representative factors such as operating conditions (Wan Alwi & Manan 2013) of the process units, qualitative (thermodynamic driving force) and the associated quantitative (flux) data, etc. Such an analysis leads to finding out the 'true' minimum targets, and ultimately, aids engineers/designers in "*beating the learning curve*" (see figure 3) (Kemp 2007).

Pinch analysis, an insightful and systematic technique used for carrying out process synthesis, is the focus of this work.

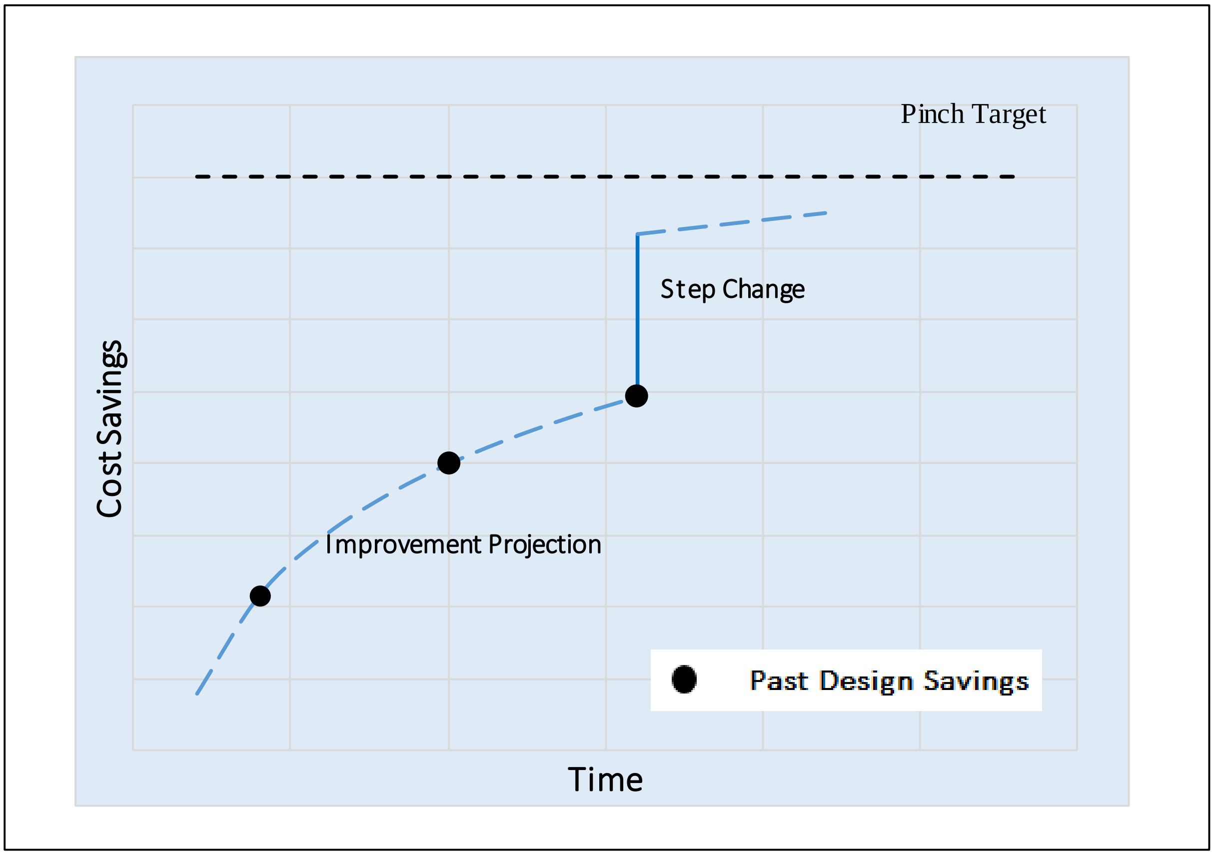

Figure 3: Outcome of Process Synthesis: Step Change in Cost Savings

2.1. Water Pinch Analysis

With regard to water conservation, Wan Alwi and Manan (2006) discussed the use of Water Management Hierarchy (WMH) which allows industries to greatly lower their water demands in a systematic manner, and make their water usage "*economically legitimate*". In WMH (presented in figure 4), elimination of water usage takes precedence over all other options, the least preferable one being 'fresh water' usage (Wan Alwi & Manan 2006). If water use cannot be eliminated completely, then WMH directs the industry towards reducing its water usage by bringing necessary changes to the demand units (processes and/or equipment). When both elimination and reduction measures are exhausted, industries should consider implementing Levels 3 and 4 of WMH.

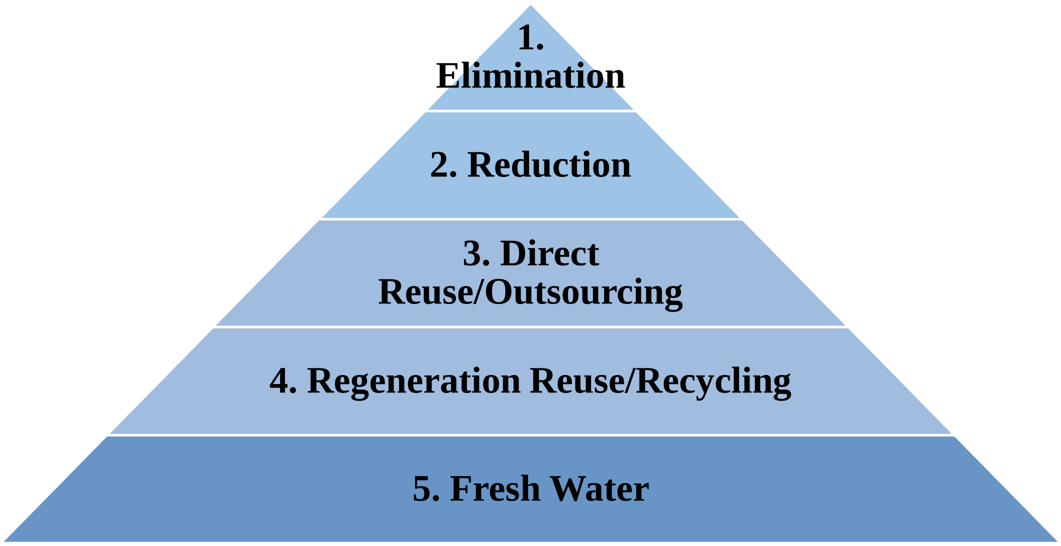

Figure 4: The Water Management Hierarchy

Level 3 involves directly reusing the wastewater discharge and/or employing external sources such as lakes, rivers, etc. (i.e., outsourcing) in demand units that can tolerate lower quality water feed without adversely affecting the specifications of the final product. Level 4 involves a qualified version of reuse which is implemented when demand units cannot tolerate the quality of the available wastewater streams. Therefore, partial treatment (i.e., regeneration) of select wastewater streams is carried out to reduce their contaminant concentrations to acceptable levels. If the regenerated stream is used in the same unit it was derived from, it is referred to as regeneration-recycling, otherwise, it is referred to a regeneration-reuse. Finally, the least preferable option of fresh water usage has to be employed, mainly when:

1. there exist units which cannot tolerate water feeds of lower quality (as compared to that of fresh water), and the available regeneration measures also do not reduce the contaminant level of the input streams to that of fresh water, and
2. dilution of wastewater streams with fresh water (Wan Alwi & Manan 2013) is necessary to aid the reuse/recycle process.

Water Pinch Analysis (WPA), is a powerful technique used to carry out water minimization in industries, civil complexes (Manan et al. 2006), etc. In relation to WMH, it is employed after Levels 1 and 2 have been fully implemented. It involves 5 steps (Wan Alwi & Manan 2013) as given in figure 5.

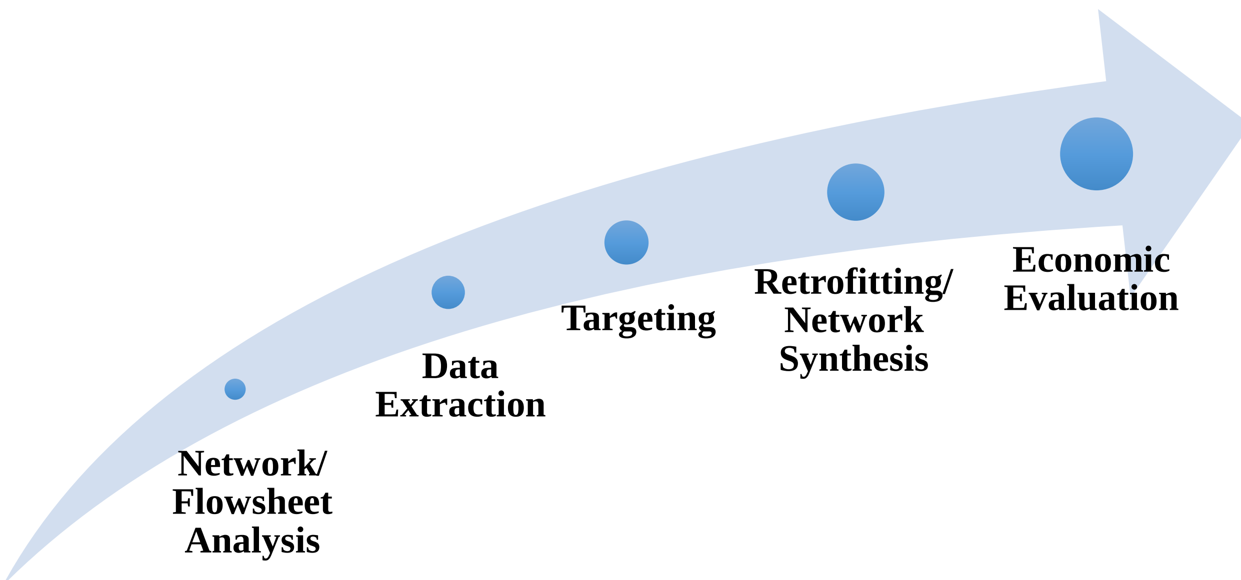

Figure 5: Steps involved in WPA

The first step of **network analysis** requires obtaining water network of the concerned plant/process by studying its PFDs and P&IDs. Once the network has been obtained, a water mass balance, with at least 90% accountability (Smith 2005), is to be performed which gives us information related to the existing fresh water requirements, wastewater discharge, water losses and gains, different flowrates, etc. Mass balance data can be obtained from *"existing material balances, computer* *monitoring, routine measurements, previous plant studies, laboratory data"*, etc. (Liu et al. 2004; Wan Alwi & Manan 2013). Another important task in the first step is to classify the various water using operations.

In WPA, we deal with 2 types of operations: mass transfer based (fixed contaminant load) and non-mass transfer based (fixed flowrate). In fixed contaminant load based operations, water acts as a mass separating agent (Manan et al. 2004). The examples of such operations include washing of equipment, gas absorption, solvent extraction, etc. These operations are quality controlled (Prakash & Shenoy 2005b) and are limited by the maximum values of inlet and outlet concentrations of the concerned contaminant(s). The flowrate of water in these operation can take any *practically feasible* value as long as the specified contaminant load is transfer from the rich stream to the lean stream (water), and the concentration constraints are not violated. In contrast, fixed flowrate based operations are quantity controlled (Prakash & Shenoy 2005b) operations wherein water is used as anything but a mass separating agent. The examples of such operations include heating or cooling applications, water acting as a reactant or product, etc. In these operations, the inlet and outlet flowrates are of primary importance and are fixed (Manan et al. 2004).

The utility of the flowrate data and the classification obtained from the first step is in determining the source and sink streams having potential for water reuse/recycle. For instance, a process identified as that of fixed contaminant load type can be assessed for the operating outlet contaminant concentrations and if the same are found to less than the limiting values, then there exists potential for water savings. Further, by identifying losses though flowrate data, steps can be taken to prevent all the avoidable losses and hence, lower the water demands. In the **data extraction** step, the key contaminants restricting water reuse are identified and a decision is made regarding the kind of approach to be followed – single contaminant or multiple contaminants based. If the concentration constraints have to be adhered to with respect to more than one contaminant type, multiple contaminants based approach involving complex mathematical modeling and optimization has to be adopted instead of the simple insight-based pinch analysis techniques. In some cases, multiple contaminants of similar nature (for example, suspended solids, dissolved solids, organic content/COD, etc.) can be aggregated (The-Institute-of-Chemical-Engineers 2000) to obtain a pseudo-single contaminant based system that can be treated using pinch analysis techniques.

Once the key contaminants have been identified, limiting flowrate and concentration data corresponding to both source and sink streams need to be 'extracted'. Such data correspond to the system constraints and help generate minimum targets. The constraints may be physical (design related), economic, environmental, etc. For instance, a certain minimum amount of flowrate may be strictly specified to ensure that the solids deliberately introduced in the feed water, remain suspended, or a fixed heat load is transferred from the process stream to the water (coolant) stream in a heat exchanger, for a maximum allowable temperature difference (between the inlet and outlet temperature of the coolant). Similarly, the upper limit of the flowrate may be specified keeping in mind pumping power requirements, excessive friction losses in pipes, etc.

As regards concentration, the maximum values are mainly governed by the ability of a processing unit to handle that particular quality of water (fouling and corrosion limitations), maximum solubility, minimum mass transfer driving force, minimum flowrate requirements, environmental regulations, etc. (Smith 2005). The minimum values may be influenced by the limited availability of 'pure' fresh water source due to which impure fresh water sources also have to be allocated.

As mentioned earlier, the availability of limiting data helps in carrying out **targeting**, i.e., finding out the minimum fresh water requirement and the minimum wastewater discharge of a plant/process. Once the targets have been determined, efforts are directed toward **designing water networks** which will help us in actually realizing the targets generated earlier. In this work, water cascade analysis (WCA) (Manan et al. 2004) is used for carrying out targeting because it is one of the most versatile (Foo 2009) targeting techniques; it caters to problems involving impure sources (Foo 2007), multiple sources (Foo 2007), threshold cases (Foo 2008), etc. Moreover, if the targets are not satisfactory, and some regeneration strategy is adopted, this technique can also be used to generate the 'ultimate flowrate targets' (Ng, Foo, Tan, et al. 2007; Ng et al. 2008). Total network targeting which includes both fresh water targeting and wastewater treatment targeting can also be performed using WCA targeting (Ng, Foo & Tan 2007a; Ng, Foo & Tan 2007b).

As regards Network Design, the Nearest Neighbour Algorithm (Prakash & Shenoy 2005b; Shenoy 2012) is selected as the preferred tool because of the same reasons applicable to the selection of WCA: versatility and amenability to computer programs. If the generated networks are found to be too complex, their complexity can be reduced by eliminating some interconnections by employing 2 source shifts (Prakash & Shenoy 2005a). However, in the process, fresh water penalty may be incurred or the quality of wastewater may worsen. In some cases, even with the same number of interconnections (or complexity) and fresh water requirements, one network may be preferred over others due to economic factors, operability issues, etc. Source shift algorithm facilitates the generation of these alternate networks also.

Ultimately, the various process changes, regeneration strategies, water networks, etc. proposed by the engineer/designer must be subjected to some sort of **economic evaluation,** for example, a cost benefit analysis or a payback period calculation, to figure out the feasibilities of the projects.

Now, we will give a brief description of the WCA and the NNA techniques.

2.1.1. Water Cascade Analysis

WCA is a systematic algebraic technique used to find out the minimum fresh water requirement, minimum wastewater discharge, minimum regeneration flowrate, pinch point(s), etc. of the process under consideration (Manan et al. 2004; Foo 2007; Ng, Foo, Tan, et al. 2007). The step-by-step procedure for single source targeting (without regeneration) is mentioned as under.

1. All the source and sink concentrations, denoted by C_k, are arranged in the ascending order in column 2 of the Water Cascade Table (WCT) (see Table 2) with their index/level, k, placed in column 1. The repeated entries are excluded. The last entry in the concentration column is the maximum possible contaminant concentration, i.e., 10^6 ppm. It facilitates in impure load cascading in the later steps, but can and should be excluded in certain cases (Parand et al. 2013).
2. Next step is to evaluate the water content in the streams at various concentration level. This parameter is typically referred to as water purity (denoted by P_k) and given by equation 1 (Hallale 2002). These values are placed in column 3 of the WCT.

$$P = \frac{1000000 - C}{1000000}$$

3. Then, the difference between the consecutive purity levels, ΔP_k (defined in equation 2), are calculated in column 4.

$$\Delta P_k = P_k - P_{k+1}$$

4. In columns 5 and 6, the total sources, $\sum S_k$, and demands, $\sum D_k$, existing at the concentration level, k, are placed. Column 7 contains the net interval water flowrate which is given by $\sum S_k - \sum D_k$. A positive value at level k in column 7

Table 2: Complete Water Cascade Table

Index	Concentration	Purity	Purity Difference	Source	Demand	Net Interval Water Flowrate	Cumulative Net Demand/Source	Pure Water Surplus/Deficit	Cumulative Pure Water Surplus/Deficit	Interval Fresh Water Demand
k -	C_k [ppm]	P_k -	ΔP_k	$\sum S_k$ [kg/h]	$\sum D_k$ [kg/h]	$\sum S_k - \sum D_k$ [kg/h]	$F_{C,k}$ [kg/h]	Δm_k [kg/h]	Cum. Δm_k [kg/h]	$F_{FW,k}$ [kg/h]
							F_{FW}			
1	C_1	P_1		S_1	D_1	$S_1 - D_1$			0	
			P_1-P_2				$F_{C,1}$	Δm_1		
2	C_2	P_2		S_2	D_2	$S_2 - D_2$			Cum. Δm_2	$F_{FW,2}$
			P_2-P_3				$F_{C,2}$	Δm_2		
3	C_3	P_3		S_3	D_3	$S_3 - D_3$			Cum. Δm_3	$F_{FW,3}$
			:				$F_{C,3}$	Δm_3		
:	:	:		:	:	:			:	:
			:				:	:		
:	:	:		:	:	:			:	:
			:				:	:		
n-3	C_{n-3}	P_{n-3}		S_{n-3}	D_{n-3}	$S_{n-3} - D_{n-3}$			Cum. Δm_{n-3}	$F_{FW,n-3}$
			P_{n-3}-P_{n-2}				$F_{C,n-3}$	Δm_{n-3}		
n-2	C_{n-2}	P_{n-2}		S_{n-2}	D_{n-2}	$S_{n-2} - D_{n-2}$			Cum. Δm_{n-2}	$F_{FW,n-2}$
			P_{n-2}-P_{n-1}				$F_{C,n-2}$	Δm_{n-2}		
n-1	C_{n-1}	P_{n-1}		S_{n-1}	D_{n-1}	$S_{n-1} - D_{n-1}$			Cum. Δm_{n-1}	$F_{FW,n-1}$
			P_{n-1}-P_n				$F_{C,n-1}$	Δm_{n-1}		
n	C_n	P_n		S_n	D_n	$S_n - D_n$			Cum. Δm_n	$F_{FW,n}$
			P_n-P_{n+1}				$F_{C,n}$	Δm_n		
n+1	10,000,00	P_{n+1}		S_{n+1}	D_{n+1}	$S_{n+1} - D_{n+1}$			Cum. Δm_{n+1}	$F_{FW,n+1}$

indicates an excess of water source, whereas, a negative value indicates that the water demand at that level is not fully met.

5. In column 8, the interval flowrates are cascaded down to obtain the cumulative input and output flowrate of the entire process. The first value in the column depicts the fresh water (concentration level 1) requirement, however, initially it is assumed to be zero to figure out the preliminary water balance and pure water surplus/deficit. At a later stage, these two sets of derived values help us in checking whether there is any violation of flowrate and concentration constraints, respectively.
6. Pure water surplus is recorded in column 9 and is defined as the product of the purity difference and the cumulative water flowrate across two purity levels. A positive value (surplus) indicates that the quality of water in the concerned region is better than what is required. On the other hand, a negative value (deficit) calls for a better quality feed.
7. In column 10, the pure water surplus/deficit is cascaded down to obtain the cumulative values at different levels. As mentioned earlier, the negative values point towards an infeasibility pertaining to the quality of the feed, which considering the definition of water surplus/deficit, is the fresh water availability at that level. However, the infeasibilities, if present, corresponds to our initial assumption of zero fresh water flowrate. So by providing a sufficient amount of fresh water feed, the infeasibilities or the shortages of fresh water availability can be overcome.
8. To do this, in column 11, the interval fresh water demand/availability, $F_{FW,\,k}$, is calculated at each level using equation 3. A positive value denotes fresh water availability where as a negative value denotes a demand for the same. To ensure that fresh water demand at each level is met and the consumption of fresh water

is at its minimum, fresh water equal to maximum interval fresh water demand is introduced in the process.

$$F_{FW,k} = \frac{cumulative\ pure\ water\ surplus/deficit}{P_{FW} - P_k}$$

The level at which the cumulative fresh water surplus becomes zero denotes the pinch point of the process network. Moreover, the final value of cumulative net flowrate denotes the minimum wastewater discharge from the process. A detailed description of this technique is presented elsewhere (Manan et al. 2004).

2.1.2. Nearest Neighbour Algorithm

The Nearest Neighbour Algorithm was proposed by Prakash and Shenoy (2005) for designing minimum fresh water networks once the water targets have been identified. The optimality of NNA is proven elsewhere (Prakash & Shenoy 2005b). Although it is applicable to both fixed load (modeled as FF units with equal inlet and outlet flowrates) and fixed flowrate problems, the networks generated for the former case are found to be *"unnecessarily complex"* and had a relatively high *"water flow-through rate"* (Prakash & Shenoy 2005b; Shenoy 2012). In order to deal with these problem, a few design rules were proposed by the authors, however, later Shenoy (2012) proposed an enhanced version of the NNA which accommodates those design rules. Hence, the enhanced NNA serves as a tool which can be used for both FF and FC problems but without the problems associated with the use of the former version. The steps involved in applying the enhanced version of NNA are as under.

1. Arrange the demand and source concentrations in ascending order in the source sink matching matrix horizontally and vertically, respectively. Then, put the corresponding flowrates in the same manner as shown in figure 3.

2. Since the pinch point has already been determined in the targeting stage, use it to identify and subsequently gray-out the cross pinch regions. This is in accordance with the one of the pinch heuristics associated with network design: there may not be any cross-pinch interconnections (Hallale 2002).
3. While satisfying demands, for fixed flowrate problems, sources at the same level are given the maximum preference followed by the nearest neighbours (in terms of concentration). Satisfying a demand implies satisfying its flowrate and mass load. In contrast, for fixed load problems, local recycle (LR) match and the cleanest possible source are preferred the most (Prakash & Shenoy 2005b; Shenoy 2012). However, if LR matches are neither available (the corresponding source is exhausted) nor accessible (the corresponding source is present on the other side of the pinch), the same concentration source and the nearest neighbours are considered for meeting the demand.
4. Once all the demands have been met, the remaining sources are discharged as wastewater (WW).

		C_{D1} **($C_{D1} \leq C_{S3}$)**	C_{D2} **($C_{D2} \leq C_{S3}$)**	C_{D3} **($C_{D3} \leq C_{S3}$)**	C_{D4} **($C_{D4} > C_{S3}$)**	WW_C **($C_{WW} > C_{S3}$)**
		F_{D1}	F_{D2}	F_{D3}	F_{D4}	WW_F
C_{S1} **($C_{S1} \leq C_{S3}$)**	F_{S1}					
C_{S2} **($C_{S2} \leq C_{S3}$)**	F_{S2}					
C_{S3} **(Pinch)**	F_{S3}					
C_{S4} **($C_{S4} > C_{S3}$)**	F_{S4}					

Figure 3: Grayed Out Source-Sink Matching Matrix

The difference in the network design approach exists because, for FF units, it is desirable that the inlet concentrations are at their maximum possible value so that the maximum amount of contaminants is taken up by the process units. This results in wastewater of the best quality and hence, end-of-pipe treatment becomes easier. Whereas, for FC units, the minimum inlet concentrations are preferred to simplify the water networks. The minimum inlet concentration is achieved by giving priority to LR match and the cleanest available source(s). Later, the LR match can be eliminated without any change to the contaminant load transferred provided that any flowrate constraint(s), if present, is not violated. This leads to reduction in the number of interconnections and hence, reduced complexity. Further, post LR elimination, the input(s) to the unit is that of the highest possible quality, therefore, the flow-through rate is also lowered. Reduced flow-through rate leads to lower capital (due to smaller unit sizes) (Prakash & Shenoy 2005b) and operating costs (due to handling of smaller volumes, e.g., lower mixing power requirements) associated with the unit. *An inherent assumption, here, is that residence times of water in the units are kept constant.* However, the inlet concentration for an FC unit should be minimized only when the corresponding demand and source lie on the same side of the pinch, otherwise, pinch violation may occur (Prakash & Shenoy 2005b). The contaminant load for an FC unit is given by equation 4, where, F is the input flowrate and C_{in} and C_{out} are the inlet and outlet concentrations, respectively.

$$\Delta m = F * (C_{out} - C_{in})$$

As regards the outlet concentrations of the FF and FC units, they should be kept at their maximum allowable value (Prakash & Shenoy 2005b). For FC units, it helps in minimizing the water demand because for a fixed contaminant load and inlet concentration, the amount of water required to take up that load decreases. See

Appendix A for related insights. However, it is a little hard to deduce a relation for FF units because, by their very definition, the flowrates have to be fixed.

2.1.2.1. A Note on LR Elimination

In the previous section, we mentioned that eliminating an LR match does not violate the contaminant load constraint. A mathematical explanation to that is given in Appendix A.

Eliminating an LR does not lead to the load violation because:

1. The flowrates of the recycle stream and the other source stream(s) are so adjusted that the initial flowrate requirement of and the initial inlet concentration to the demand unit are at their limiting (maximum) values.
2. The allocations in the first step ensure that sufficient driving force is available for the transfer of the specified contaminant load to the lean stream.
3. We are assuming that the mass load specified is based on the consideration of the minimum mass transfer driving force. So, after taking up the contaminant load, the increase in the lean stream's concentration leads to a driving force that is not capable of transferring any more contaminants. Hence, the outlet stream has reached the maximum possible concentration.
4. However, since the recycle stream (a part of the outlet) is at its maximum possible concentration, it is the portion contributed by the other stream(s) in the mixed feed that takes up all the contaminants.
5. Hence, the recycle match can be treated as redundant and eliminated if it does not violate the flowrate constraints that may be associated with the concerned operation.

It is not problematic to find out the flowrate of the cleanest source to be allocated without considering the local recycle match, but the present arrangement complies well with NNA framework wherein instead of the nearest neighbours, the LR match and cleanest source will be prioritized.

CHAPTER 3

Targeting using Water Cascade Analysis

Standing on the shoulders of MATLAB®

As a part of this project, we make an attempt to treat various types of targeting and network design problems that may be encountered while carrying out water minimization studies over a system using the pinch methodology.

3.1. Generating Base Case: No Water Reuse/Recycle

First, we present a MATLAB program, **crude.m**, which gives fresh water requirement of a system with no water reuse or recycle. This data can help us in generating a base case, having maximum fresh water consumption, with which networks with maximum water reuse/recycle can be compared.

The inputs to this program include the location of the source and demand data and the concentration(s) of the fresh water source(s) available for use. The outputs are the fresh water requirements for each quality of fresh water, and the total wastewater generation.

3.1.1. crude.m Algorithm

1. Import the source and demand data.
2. Arrange the data in ascending order of concentration. For this step, we developed **mysort.m**.
3. For all the demands, find out the fresh water requirement:

i. If the demand is of fixed flowrate type, allocate the dirtiest fresh water source such that the fresh water concentration is less than or equal to the limiting inlet concentration, and flowrate is equal to the specified one.

ii. If the demand is of fixed contaminant load type, allocate the dirtiest fresh water source such that the fresh water concentration is less than or equal to the limiting inlet concentration, and the contaminant load remains intact. Note: While determining the flowrate that satisfies the contaminant load constraint, the outlet concentration is kept at its limiting value. This minimizes the flowrate requirement. See Appendix A.

4. Sum up the allocations corresponding to each fresh water quality.
5. Calculate the total loss and gains in the process.

i. Calculate the losses by finding the difference between inlet and outlet flowrates for each process. Negative losses will be treated as gains.
ii. If independent source exists, treat it as gain.
iii. If independent demand exists, treat is as loss.
iv. Sum up all the losses (and gains).

6. Calculate the wastewater discharge by subtracting the total losses from the fresh water requirement.

Examples are provided later to aid the understanding of the algorithm.

3.1.2. Major Assumptions in crude.m

1. Losses occur in the outlet flow for any process. This assumption has been made elsewhere also (Shenoy 2012).
2. Losses in fixed contaminant load processes are independent of the outlet flowrate. If this assumption cannot be accommodated, then the wastewater flowrate may be ignored.

3.1.3. Program Objectives (In the order of precedence)

1. Maximize the use of dirtier sources.
2. Minimize the amount of the source used.

3.1.4. crude.m

```
function [FData,WW] = crude(FileName,Sheet,SPoints,DPoints,FWConc)

% FWConc = [0 25 50 75 100 125];
% [NumS,TxtS,SData] = xlsread('Sample Matrices.xlsm',16,'L11:Q13'); % Source Data
% [NumD,TxtD,DData] = xlsread('Sample Matrices.xlsm',16,'F11:K13'); % Demand Data
% FWConc = [0 50];
% [NumS,TxtS,SData] = xlsread('Sample Matrices.xlsm',23,'L9:Q16'); % Source Data
% [NumD,TxtD,DData] = xlsread('Sample Matrices.xlsm',23,'F9:K15'); % Demand Data
[NumS,TxtS,SData] = xlsread(FileName,Sheet,SPoints); % Source Data
[NumD,TxtD,DData] = xlsread(FileName,Sheet,DPoints); % Demand Data
```

Sorting Data in ascending order of Concentration

```
FWConc = sort([FWConc 1000000]);
SData = mysort(NumS,TxtS,SData);
DData = mysort(NumD,TxtD,DData);
FW = zeros(length(FWConc),1);
for jj = 1:row(DData)
    for ii = 1:length(FWConc)
        if FWConc(ii) > DData{jj,4} && strcmp(DData{jj,5},'FF') == 1
            FW(ii-1) = FW(ii-1) + DData{jj,3};
            break;
        elseif FWConc(ii) > DData{jj,4} && strcmp(DData{jj,5},'FC') == 1
            for mm = 1:row(SData)
                if strcmp(SData{mm,2},DData{jj,2}) == 1
                    Cout = SData{mm,4};
                    break;
                end
            end
            FW(ii-1) = FW(ii-1) + (DData{jj,6}/(Cout-FWConc(ii-1)));
            break;
        end
    end
end
FW = FW(1:end-1);
FWConc = FWConc(1:end-1);
FData = [FWConc' FW];
Loss = 0;
for ii = 1:row(DData)
    for jj = 1:row(SData)
        if SData{jj,2} == DData{ii,2}
           Loss = Loss + DData{ii,3} - SData{jj,3};
        end
    end
end
for jj = 1:row(SData)
    if sum(NumS(jj,1) == NumD(:,1)) == 0
        Loss = Loss - NumS(jj,3);
    end
end
```

```
for ii = 1:row(DData)
    if sum(NumD(ii,1) == NumS(:,1)) == 0
        Loss = Loss + NumD(ii,3);
    end
end
WW = sum(FW) - Loss;

end
```

Example 3.1.1. Data is adopted from a elsewhere (Deng & Feng 2009). Refer to Tables 3 and 4.

Table 3: Source Data Set I

Stream No.	**Process Name**	**Flow Rate**	**Concentration**	**Type**	**Mass Load**
Out	-	t/h	ppm	-	1e-6 t/h
1	A	30	60	FF	
2	B	25	100	FC	1200
3	C	150	80	FF	
4	D	80	200	FC	16000
5	E	40	60	FF	
6	F	120	80	FF	
7	G	0	200	FF	
8	H	83.33	20	FF	

Given that the fresh water is available in 2 concentrations: 0 and 50 ppm, the program gives following results: for 0 ppm fresh water, the requirement is 450 t/h, and for 50 ppm fresh water, 200.67 t/h. The total wastewater generated is 469 t/h.

In the demand data set, we can see that there are 3 demands (at 60, 100, and 80 ppm) which have concentration equal to or than that of the dirtier source (50 ppm), two of which are FC type. As per step 3(ii) of the algorithm, their FW requirements are found to be 24, 106.67, and 80 t/h, respectively. The first 2 flowrates are different from the flowrates given in the demand data table because the operations are of FC type. Hence, for 60 ppm demand (Process A), the dirtiest acceptable source being 50 ppm, mass load 1200 g/h, and outlet concentration 100 ppm, fresh water requirement can be calculated as 1200/(100-50) = 24 t/h. Similarly, the other demands can be calculated. As regards the remaining demands, all are of FF type and have inlet concentration less than 50 ppm. Therefore, the only remaining FW source of concentration 0 ppm will be used, and the fresh water requirement will simply be the summation of the concerned demand flowrates which comes out to be 450 t//h.

Table 4: Demand Data Set I

Stream No.	**Process Name**	**Flow Rate**	**Concentration**	**Type**	**Mass Load**
In	-	t/h	ppm	-	1e-6 t/h
1	A	40	20	FF	
2	B	30	60	FC	1200
3	C	200	20	FF	
4	D	160	100	FC	16000
5	E	60	20	FF	
6	F	150	20	FF	
7	G	70	80	FF	

Example 3.1.2. Data is adopted from a seminal work on WPA, entitled, “Wastewater Minimization” (Wang & Smith 1994). Refer to Tables 5 and 6.

Table 5: Source Data Set II

Stream No.	**Process Name**	**Flow Rate**	**Concentration**	**Type**	**Load**
Out	-	t/h	ppm	-	1e-6 t/h
1	A	20	100	FC	2000
2	B	100	100	FC	5000
3	C	40	800	FC	30000

Table 6: Demand Data Set II

Stream No.	**Process Name**	**Flow Rate**	**Concentration**	**Type**	**Load**
In	-	t/h	ppm	-	1e-6 t/h
1	A	20	0	FC	2000
2	B	100	50	FC	5000
3	C	40	50	FC	30000

Given that the fresh water is available in 2 concentrations: 0 and 50 ppm, the program gives following results: for 0 ppm fresh water, the requirement is 20 t/h, and for 50 ppm fresh water, 140 t/h. The total wastewater generated is 160 t/h.

Similar to the previous case, the demands can be calculated from mass load, concentration of the dirtiest acceptable source, and the outlet concentration of the concerned unit. Processes B and C can be fed with 50 ppm source, hence, their fresh water requirement can be calculated as 5000/(100-50) = 100 t/h and 30000/(800-50)

= 40 t/h, respectively. Similarly, for Process A, the fresh water requirements, with 0 ppm FW, can be calculated as 2000/(100-0) = 20 t/h. Here, the total demand flowrates and source flowrates are equal (no losses and no gains), therefore, the wastewater discharge will simple be equal to the total fresh water requirements, i.e., (20+100+40) = 140 t/h.

Example 3.1.3. Data is adopted from a book by R. Smith (Smith 2005). Refer to Tables 7 and 8.

Table 7: Source Data Set III

Stream No.	**Process Name**	**Flow Rate**	**Concentration**	**Type**	**Load**
Out	-	t/h	ppm	-	1e-6 t/h
1	A	10	100	FC	1000
2	B	20	100	FC	1000
3	C	20	400	FC	6000
4	D	20	10	FC	200
5	E	30	200	FC	4000

Table 8: Demand Data Set III

Stream No.	**Process Name**	**Flow Rate**	**Concentration**	**Type**	**Load**
In	$	t/h	ppm	-	1e-6 t/h
1	A	10	0	FC	1000
2	B	20	50	FC	1000
3	C	20	100	FC	6000
4	D	20	0	FC	200
5	E	40	100	FC	4000

Given that the fresh water is available in 3 concentrations: 0, 50, and 100 ppm, the program gives following results: for 0 ppm fresh water, the requirement is 30 t/h, for 50 ppm fresh water, 20 t/h, and for 100 ppm fresh water, 60 t/h. The total wastewater generated is 100 t/h since there is a loss of 10 t/h in process E. Moreover, it can be seen that priority is first given towards using the maximum dirtiest source possible – all the sources which can tolerate 100 ppm fresh water are fed by it. In this case there are 2 such processes: Processes C and E. Since, they are of FC type, their demand is minimized by maximizing their outlet concentration.

Example 3.1.4. Data is adopted from two works (Polley & Polley 2000; Wang & Smith 1994). Refer to Tables 9 and 10.

Table 9: Source Data Set IV

Stream No.	**Process Name**	**Flow Rate**	**Concentration**	**Type**	**Load**
Out	$	t/h	ppm	-	1e-6 t/h
1	A	20	100	FC	2000
2	B	50	50	FF	
3	C	100	100	FC	5000
4	D	40	800	FC	30000
5	E	100	100	FF	
6	F	70	150	FF	
7	G	60	250	FF	
8	H	10	800	FC	4000

Given that the fresh water is available in 3 concentrations: 0, 50, and 100 ppm, the program gives following results: for 0 ppm fresh water, the requirement is 70 t/h, for 50 ppm fresh water, 240 t/h, and for 100 ppm fresh water, 155.71 t/h. The total wastewater generated is 445.71 t/h.

Table 10: Demand Data Set IV

Stream No.	**Process Name**	**Flow Rate**	**Concentration**	**Type**	**Load**
In	$	t/h	ppm	-	1e-6 t/h
1	A	20	0	FC	2000
2	B	50	20	FF	
3	C	100	50	FC	5000
4	D	40	50	FC	30000
5	E	100	50	FF	
6	F	80	100	FF	
7	G	70	200	FF	
8	H	10	400	FC	4000

3.2. Targeting using WCA

Second, we present a set of programs that carry out fresh water targeting of fixed contaminant load, fixed flowrate and even hybrid systems. They give the pinch point(s), fresh water requirement and wastewater generation of a system after exploiting water reuse opportunities to the maximum possible extent. The programs are based on the Water Cascade Table (WCT) technique developed by Manan et al. (2004) and deal with problems involving:

1. Multiple fresh water sources (pure and impure) (Foo 2007)
2. Availability Constraints, i.e., limited availability of fresh water of a certain quality (Foo 2007)
3. Threshold Problems (Foo 2008)

Moreover, we also introduce an **alternate approach** for targeting of multiple fresh water sources. The conventional 3-step approach (Foo 2007) has been replaced by a dual step approach and can easily accommodate any number of fresh water sources. A description of the alternate procedure is presented later.

The WCA technique was chosen because of the following reasons.

1. Considering the wide variety of problems it can handle, it is one of the most well developed (Foo 2009) techniques available for carrying out targeting in single contaminant based systems.
2. Its algebraic nature (Manan et al. 2004) makes it amenable to computer programming, leading to highly accurate solutions in just fractions of a second.
3. Large and complex problems can be solved with lesser effort and higher accuracy (Foo 2012) as compared to its graphical counter parts.

However, the algebraic procedures such as WCT may not be as insightful (Foo 2012) for the designers as the graphical ones. Two highly developed graphical techniques involve the use of limiting composite curves (Wang & Smith 1994) and material recovery pinch diagrams (El-Halwagi et al. 2003; Prakash & Shenoy 2005b), respectively.

The programs which aid in the targeting process are:

Table 11: MATLAB Programs used in the targeting process

intprt_v2.m	trgt.m	nantonill.m	wca.m	thresh2.m
imnor.m	fzbl.m	FWAug_v2.m	row.m	thresh2aliter.m

intprt_v2.m is the parent function in the targeting process and caters to problems involving multiple pinch points, impure sources, multiple sources, availability constraints, etc. The inputs to this program are the locations of the source and demand data. Other optional inputs are concentration(s) of the fresh water sources and the corresponding availabilities (in terms of mass flowrate). However, if the availabilities are not mentioned, the program will assume it to be infinite. Similarly, under the absence of fresh concentration, the program will assume a single source of 0 ppm concentration at infinite availability.

3.2.1. intprt_v2.m Algorithm

1. Import the source and demand data.
2. Organize the data as is done in the WCT. Refer to section 2.1.1. This task is performed by **imnor.m.** Only six columns of the WCT containing levels/indices, concentrations, purity, demands, sources and net interval flowrates are generated.
3. Carry out targeting by generating the remaining columns of the WCT. This task is performed by **wca.m**. Once the complete cascade has been made, targeting is done by **trgt.m**. The final output is the target values corresponding to different fresh water sources available for use.
4. Once the targets have been evaluated, check whether the fresh water sources are available at the required mass flowrates. If there exist any fresh water source with targeted flowrate higher than the available flowrate, then use that source completely by considering it as an additional inherent source in the WCT. Do this by increasing the net interval flowrate at the level of that 'limited' source by the same amount as is available for that particular fresh water source. This task is done by **fzbl.m**. One of the outputs is the updated WCT (containing the six columns specified earlier).
5. After introducing the limited fresh water source as an inherent source of the network, it is no longer considered as fresh water source. Therefore, update the vectors containing the fresh water concentrations and corresponding

levels/indices. This task is also performed by fzbl.m and the updated vectors are the other remaining outputs.

6. The limited availability sources have been considered as inherent sources of the network, for the ease of calculation. In reality, they fresh water sources only, so store their concentration and flowrate (availability) and later augment it to the matrix containing the other targeted flowrates. In intprt_v2.m, this is done by **FWAug_v2.m**.
7. If the availability of all the fresh water sources is less than the corresponding targeted values, produce an error and terminate the program. One may restart after increasing the availabilities. Directly go to step 8 if this is not the case.
8. For the fresh water sources with availabilities lower than the required amounts, changes have been made to the WCT. Now update the availability vector also by discarding entries corresponding to ‘limited’ availabilities.
9. After changes have been made in the WCT, re-target the cascade using trgt.m and again check whether the availability of the remaining sources (not removed earlier/made an inherent part of the WCT) is more than the targeted flowrates. If again some availabilities are less than what is required, go to step 4.
10. After all the availabilities have been satisfied, there may be a region for which targeting haven’t been performed. Check the existence of such region by analysis the interval fresh water demand/availability (IFWD) of the final cascade. The IFWD was pre-allocated a vector of ‘NaN’. And the first value in that vector, after all the demands have been satisfied stays ‘NaN’. Therefore, if more than one occurrences of ‘NaN’ are there, terminate the run. One may restart after introducing a higher quality source.
11. If all the demands are satisfied (indicated by 1 ‘NaN’ entry and remaining non-negative values in IFWD), look for the zero IFWD value(s). The concentration corresponding to this value(s) is the pinch point(s).

12. At this stage, the contaminant load constraints have been satisfied, but there may be a violation of the flowrate constraint – negative wastewater flowrate. So whatever deficit is there, add the same amount in either of the fresh water source. A choice of 2 sub-routines, viz., thresh2.m and thresh2aliter.m, has been provided to do this.
13. If sources aren't available to tackle the flowrate constraint, terminate the run and start again with higher availability. The source whose availability is increased can be such that the water costs is minimized.
14. If both flowrate and contaminant load constraints are satisfied, look for fresh water source whose flowrates are zero. These sources are flagged off as redundant sources and may show excess pinch point(s) in the process network.

All the sub-routines mentioned in the algorithm are presented in Appendix B.

3.2.2. Major Assumptions in intprt_v2.m

The primary assumption in Foo (2007) is that the pure fresh water has to be purchased from external vendors and hence, incurs cost, whereas, all the impure fresh water sources, like lakes, rivers, rain harvest, etc., are virtually free. Moreover, the author proposes the use of only the highest quality impure source when multiple impure sources are available. A cogent reasoning is provided which correctly points that the use of lower quality sources leads to higher fresh water flowrates and hence, greater wastewater discharge. Clearly, this will call for higher treatment costs.

Moreover, higher flowrates may also lead to higher operational costs (pumping power) and higher capital costs (larger unit sizes) (Prakash & Shenoy 2005b). This understanding encourages the user to employ maximum 2 sources: the highest quality impure source and the pure fresh water source (if needed).

The use of WCA for multiple sources has been reported in the literature (Foo 2007). It follows a three step approach (considering two sources only) where firstly, lower quality source flowrate is determined followed by the higher quality one. Thereafter, an adjustment is made to the lower quality source, to remove the excess flowrate cascaded down from the purer source. This approach may be easy to follow for 2 sources, but it may start becoming tedious due to flowrate adjustments as the number of sources increases.

In this work, we assume that cost is associated with each type of water source. The purer the source, the more costly it is (Parand et al. 2013). So, a trade-off will exist between the resource (water) costs and the operational & capital costs. In order to find out the optimum flowrate which minimizes cost, we may need to carry targeting involving more than 2 sources multiple times and hence, an easier targeting approach will be preferred. We discuss one such approach in Section 3.2.1.

3.2.3. Program Objectives

The primary objective in this algorithm is to minimize the use of higher quality sources.

3.2.4. Alternate Approach for Multiple Source Targeting

The alternate approach for multiple source targeting is also based on WCA wherein all the columns except the one containing the interval fresh water demand (IFWD) are calculated in the conventional (Manan et al. 2004; Foo 2007) way. In the IFWD, the values are calculated differently in that the fresh water sources are sequentially targeted in multiple iterations. The approach proposed by Foo (2007) also works with sequential targeting with multiple iterations but each iteration also involves a flowrate adjustment. Considering the above factors, we can conclude that the alternate approach leads to slightly more effective utilization of computational resources.

Consider 10 different purities (P_1 to P_{10}) arranged in the descending order such that the fresh water sources are available at, say, P_1, P_3, and P_7. Assuming that the cumulative mass load corresponding to each level is given as cum. Δm_i, where, i is the purity level ranking from 2 to 10, the minimum flowrates for each source can be calculated as given in Table 12.

Table 12: Alternate WCA for Multiple Source Targeting

Level	Purity	Net Interval Flowrate	Cumulative Mass Load	Interval Fresh Water Demand
1	P_1	$F_{N,1} + (F_{FW,1} = 0)$	0	
2	P_2	$F_{N,2}$	cum. Δm_2	cum. $\Delta m_2/(P_1-P_2)$
3	P_3	$F_{N,3} + (F_{FW,1} = 0)$	cum. Δm_3	cum. $\Delta m_3/(P_1-P_3)$
4	P_4	$F_{N,4}$	cum. Δm_4	cum. $\Delta m_4/(P_3-P_4)$
5	P_5	$F_{N,5}$	cum. Δm_5	cum. $\Delta m_5/(P_3-P_5)$
6	P_6	$F_{N,6}$	cum. Δm_6	cum. $\Delta m_6/(P_3-P_6)$
7	P_7	$F_{N,7} + (F_{FW,1} = 0)$	cum. Δm_7	cum. $\Delta m_7/(P_3-P_7)$
8	P_8	$F_{N,8}$	cum. Δm_8	cum. $\Delta m_8/(P_7-P_8)$
9	P_9	$F_{N,9}$	cum. Δm_9	cum. $\Delta m_9/(P_7-P_9)$
10	P_{10}	$F_{N,10}$	cum. Δm_{10}	cum. $\Delta m_{10}/(P_7-P_{10})$

The region which will be fed with P_1 purity ranges from P_1 to P_3 (Region 1). Similarly, the regions for P_3 and P_7 fresh waters range from P_4 to P_7 (Region 2) and P_8 to P_{10} (Region 3), respectively. Initially, the fresh water flowrates are assumed to be zero, to check whether the cascade is feasible or not. If the cascade is not feasible, then the maximum interval fresh water demand or absolute of the maximum negative fresh water surplus in the region 1 is added to the net interval flowrate at the level of purity, P_1. The targeted flowrates are added to the appropriate net interval flowrates because they are considered as additional sources. Later, when the net flowrates are again cascaded, the cumulative mass load and hence, the interval fresh water demands are updated. Since, the fresh water demand for region 1 has already been met, we look for the maximum interval fresh water demand in region 2 and then add the same to the net interval flowrate at the level of purity P_3. If the no interval fresh water demand is observed, we simply move to region 3. From the description, one more distinction between the earlier and the alternate approach can be figured, i.e., the targeting in latter starts from high quality source moving towards lower quality sources. However, as mentioned earlier, in the former approach, targeting is performed in the opposite direction starting from the lowest quality source.

3.2.5. intprt_v2.m

Program to interpret WCT for Pinch Point(s), Fresh Water and Wastewater Targets.

```
function [PinchP,F_Matrix, WW] = intprt_v2(FileName,Sheet,SPoints,DPoints,FWConc,Availability)
```

Different Forms the function can take.

```
if nargin == 5 % If the availabilities of different sources are not mentioned, then they are
assumed to be infinite.
    Availability = inf*ones(1,length(FWConc));
end
if nargin == 4 % If the FWConc(s) are not given, then only one pure fresh water source is
assumed. Pure FW source implies that its contaminant concentration is zero.
    FWConc = 0;
    Availability = inf*ones(1,length(FWConc));
end
Availability = Availability'; % In this program, the availablities are required in the column
form.
Availability_Dupli = Availability; % This Dupli variable is to be used while making the augmented
```

```
matrix. Dupli variable is required because this variable gets updated in size if the availability
of any FW source is less than the targeted value at the same concentration.
```

Initial importing, organizing and targeting.

```
[FWConc,J] = sort(FWConc,'ascend');
FWConc_Dupli = FWConc; % Duplicating this variable for use in the "The Limitated Availability"
Case.
Availability = Availability(J);
[N, Ind] = imnor(FileName,Sheet,SPoints,DPoints,FWConc); % First Six Columns of WCT generated
along with Concentraion Levels of the fed FW Concentrations.
FW_f = trgt(N,Ind,FWConc); % Multi/Single Pure/Impure Source Targeting
FW_f_Dupli = FW_f; % Duplicating this variable for use in the "The Limitated Availability" Case.
```

Availability Check

```
F_Matrix_Augment = [];
xx = 1; % First index of F_Matrix_Augment
while sum(FW_f > Availability) >= 1
    [New_FWConc,New_N,New_Ind] = fzbl(FW_f,Availability,FWConc,N,Ind); % Performing the
availability/feasibility check.
    FWConc = New_FWConc; % Updated variable after the feasibility check.
    N = New_N; % Updated variable after the feasibility check.
    Ind = New_Ind; % Updated variable after the feasibility check.
    if isempty(FWConc) && isempty(Ind)
        error('The availability of the input FW concentration(s) is to be increased to make the
WCT feasible.');
    end
    for j = 1:length(Availability) % For discarding the sources which are completely
exhausted/emptied.
        if FW_f(j) > Availability(j)
            Availability(j) = nan; % If the availability is less than the targeted value, that
source is completely dried/exhausted. Thereafter, the corresponding availability is reduced to
'NaN'. This 'NaN' is also discarded from the Availability Vector.
        end
    end
    Availability = nantonill(Availability); % Discarding the 'NaN' entries from the Availability
vector.
    FW_f = trgt(N,Ind,FWConc); % Retargeting with update N (the limited sources have been added
in the cascade).
    [F_Matrix_Augment(xx,:), FWConc_Dupli, Availability_Dupli] =
FWAug_v2(FWConc_Dupli,Availability_Dupli,FWConc);
    xx = xx + 1;
end
```

Updating Water Cascade

```
[~, F_C, ~, ~, IFWD] = wca(N,Ind,FW_f,FWConc); % Updating the water cascade using Targeted
Values.
```

Contaminant Load Check

All IFWD values should be non-negative.

```
if sum(isnan(IFWD)) >= 2
    error('The given FW concentration(s) are not satisfying Contaminant Load Constraints. Add a
higher quality source.');
end
if sum(IFWD < 0) >= 1
    error('The availability of the input FW concentration(s) is to be increased to make the WCT
feasible.');
end
```

Recording Pinch Points

```
PinchP = []; % Initiating the vector which will contain Pinch Points.
for i = 2:row(N)
    if IFWD(i) == 0 % If Interval Fresh Water Demand is zero, then the corresponding Source
cocnetration is a Pinch Point.
      PinchP = [PinchP; N(i,2)];
    end
end
PinchP_Duplicate = PinchP; % We want to copy the value of PinchP because if the threshold case
holds for the concerned problem, the new points given by PinchP1 will be set to PinchP and
further use of orginal value of PinchP will not be possible.
```

Zero Network Discharge: Threshold Case

```
Availability = Availability - FW_f;
if F_C(end) == 0 || F_C(end) < 0
    [UpdatedInput1,UpdatedInput2,UpdatedInput3,~] =
thresh2(F_C,N,Ind,FW_f,FWConc,PinchP,PinchP_Duplicate,Availability);
    FW_f = UpdatedInput1;
    F_C = UpdatedInput2;
    PinchP = UpdatedInput3;
end
```

Recording WW Flowrate and Fresh Water Flowrates

```
WW = F_C(end); % Recording WW Flowrate.
if WW < 0
    error('Flowrate Constraint is not satisfied. Go for debugging');
end
F_Matrix = [(sort(FWConc,'ascend'))' FW_f]; % This will make a matrix which will contain the FW
concentrations (that were already fed as input) along with the corresponding targeted FW values.
```

Limited Availability Case

In the limited availability case, if the targeted value is more than the available value, then targeting is carried out by adding the limited available value to the source of the same concentration. In this arrangement, the limited value source does not appear in the final answer. So in this portion of the code, we present a sub-routine that will restore the limited availability source in the final answer (i.e. in F_Matrix.)

```
F_Matrix = [F_Matrix; F_Matrix_Augment];
```

Flagging the Redundant Fresh Water Sources

```
for i = 1:row(F_Matrix)
    if F_Matrix(i,2) == 0
        fprintf('Fresh Water Source No. %d is a Redundant Source.\n',i);
    end
end

end
```

Example 3.2.1: Data is adopted from an acrylonitrile case study (El-Halwagi 1997). Refer to tables 13 and 14.

Table 13: Source Data Set V

Stream No.	**Process Name**	**Flow Rate**	**Concentration**	**Type**	**Load**
Out	$	t/h	ppm		1e-6 t/h
1	A	120	100	FC	12000
2	B	80	140	FC	7200
4	D	140	180	FC	5600
5	E	80	230	FC	4800
6	F	195	250	FC	1950

Given: a fresh water source of 0 ppm contaminant concentration is available at infinite availability. Running intprt_v2.m with the above data generated the correct fresh water and wastewater targets of 200 t/h and 120 t/h respectively. The pinch points are at 100 and 120 ppm. The lower concentration pinch point is called the limiting pinch point and greatly influences the utility targets (Hallale 2002). crude.m gives the fresh water demand to be 311.2 t/h. Hence, by maximizing reuse, we are witnessing a saving of 35.7 %. As regards wastewater discharge, crude.m generate 231.2 t/h, therefore, a wastewater reduction 48.1 % is achieved.

Table 14: Demand Data Set V

Stream No.	**Process Name**	**Flow Rate**	**Concentration**	**Type**	**Load**
In	$	t/h	ppm		1e-6 t/h
1	A	120	0	FC	12000
2	B	80	50	FC	7200
3	C	80	50	FF	
4	D	140	140	FC	5600
5	E	80	170	FC	4800
6	F	195	240	FC	1950

Example 3.2.2: Demand and Source Data Sets II are used.

Given: fresh water sources of 0 and 50 ppm contaminant concentration are available with infinite availability. intprt_v2.m generates fresh water target of 20 t/h (0 ppm) and 140 t/h (50 ppm) and wastewater discharge of 160 t/h. The pinch points are at 50 and 100 ppm, with the limiting pinch point being at the lower concentration.

In this case, fresh water requirements and wastewater discharge generated by crude.m and intprt_v2.m are same. These results imply that for this particular case, there are no reuse opportunities that can be exploited. This has happened because we have an impure fresh water source also, and the program, intprt_v2.m tries to maximize its use (because it is of lower quality). As a result, both operations B and C are fed with 50 ppm fresh water source and the outlet generated at 100 and 800 ppm, respectively, cannot be reused since it will lead to contaminant constraint violation. Similarly, for operation A, the outlet contaminant concentration will be 100 ppm making it unfit for reuse in operations B and C.

Example 3.2.3.: Threshold case with zero fresh water requirements (Jacob et al. 2002). Refer to table 15 and 16.

Table 15: Source Data Set VI

Stream No.	Process Name	Flow Rate	Concentration	Type	Load
Out	-	t/h	ppm	-	1e-6 t/h
-	-	500	100	-	-
-	-	2000	110	-	-
-	-	400	110	-	-
-	-	300	60	-	-

Table 16: Demand Data Set VI

Stream No.	Process Name	Flow Rate	Concentration	Type	Load
In	$	t/h	ppm	-	1e-6 t/h
-	-	1200	120	-	-
-	-	800	105	-	-
-	-	500	80	-	-

Given: a fresh water source of 0 ppm contaminant concentration is available at infinite availability. intprt_v2.m generates the following results: zero fresh water requirement, wastewater discharge at 700 t/h, and pinch point at 60 ppm contaminant concentration. Although this particular process can operate without any fresh water requirements, a feed inlet should be provided for emergency situations arising from operation upsets (Foo 2008).

Cases like these are categorized as under threshold problems (Foo 2008). They include process networks with zero fresh water requirement, zero wastewater discharge, or both.

Example 3.2.4: Threshold case with zero wastewater discharge (Foo 2008).

Table 17: Source Data Set VII

Stream No.	Process Name	Flow Rate	Concentration	Type	Load
Out	-	t/h	ppm	-	1e-6 t/h
-	-	50	100	-	-
-	-	20	20	-	-
-	-	40	250	-	-

Table 18: Demand Data Set VII

Stream No.	Process Name	Flow Rate	Concentration	Type	Load
In	$	t/h	ppm	-	1e-6 t/h
-	-	50	20	-	-
-	-	20	50	-	-
-	-	100	400	-	-

Given: a fresh water source of 0 ppm contaminant concentration is available at infinite availability. intprt_v2.m generates the following results: 60 t/h fresh water requirement, zero wastewater discharge, and no pinch point. Here, 59.97 t/h of fresh water satisfied all the contaminant load constraints but the flowrate constraint was violated (negative wastewater discharge of 0.03 t/h). This violation was removed by simply adding the requisite amount of fresh water in the cascade.

Threshold problems are *“rare but realistic cases”* (Foo 2008) observed in the process synthesis domain. In heat pinch analysis, they corresponding to process networks without any cold or hot utility requirements (Linnhoff et al. 1982).

CHAPTER 4

Network Design using NNA

Simply connecting the dots!

In this chapter, we execute the task of network design using the Nearest Neighbour Algorithm (Prakash & Shenoy 2005b). A MATLAB program, **nnaup.m**, is developed for carrying out network design. Table 19 presents some major sub-routines of the program, nnaup.m. However, since, it is not the enhanced version (Shenoy 2012), the networks generated have limitations such as high flow-through rate and large number of interconnections.

Table 19: MATLAB Programs used in the network design process

nnaup.m	intprt_v2.m	mysort.m
searcon.m	concUpdate.m	Shenoy.m

4.1. nnaup.m Algorithm

1. Import the source and demand data.
2. Carry out targeting using intprt_v2.m to find out the minimum fresh water requirements, wastewater flowrate, and pinch point(s).
3. If multiple pinch points exist, terminate the run. *The current version is not tailored to carry out design of such networks.*
4. For single pinch networks, initialize the Source-Sink matching matrix by placing the source concentration and flowrate data horizontally and the corresponding demand data vertically. See figure 3 for a detailed visual.
5. Gray out the cross pinch regions. This is done by allocating the value of ‘NaN’ to the gray region elements.

6. Start the matching process for below-the-pinch region.

(i) Start with the demand with the most stringent requirement/cleanest source requirement.

(ii) Give priority to the source having the same concentration as that of the demand.

(iii) While allocating source, check the amount available and keep updating their availabilities after each allocation.

(iv) If the source of same concentration does not exist or isn't available in sufficient amount, go for the nearest neighbours. Nearest Neighbours selection is done by **Shenoy.m**. A detailed description of rules governing the allocation process is presented (Prakash & Shenoy 2005b; Foo 2012).

(v) The flowrate and contaminant load constraints/equations are updated as required, and are represented by **ShenFun.m**. Further, they simultaneously solved by using the **fsolve** command. After the demand of the concerned source has been met, move to the next source.

7. Once all the demands in below-the-pinch region have been met, move to above-the-pinch region with a new pool of source concentrations (that do not lead to cross pinch allocation). The same process presented in Prakash and Shenoy (2005b) is to be followed.
8. After the demands in above-the-pinch region have also been met, check whether the wastewater flowrate reported by intprt_v2.m is equal to the remaining sources. If they are not equal, terminate the run and go for debugging.
9. If the above condition is satisfied, discharge the remaining sources as wastewater streams by allocating them in the last column of the source-sink matching matrix.

4.1.1. Major Limitations

The current version of the program is limited to the design of networks with:

1. Only single pinch point.
2. Only single fresh water feed. Note: With some manual adjustments in the source data post targeting, multiple fresh water feeds may be accommodated.

4.1.2. Program Objectives

The primary program objective is to satisfy all the sources such that flowrate and contaminant load constraints associated with them are satisfied and minimum amount of fresh water is required.

4.1.3. nnaup.m

Program to generate a Water Network for Single Contaminant Based Hybrid Systems.

```
function N = nnaup(FileName,Sheet,SPoints,DPoints,FWConc,Availability)
```

Fetching the Data from MS-Excel Worksheet

```
[NumS,TxtS,SData] = xlsread(FileName,Sheet,SPoints); % Source Data
[NumD,TxtD,DData] = xlsread(FileName,Sheet,DPoints); % Demand Data
```

Sorting Data in ascending order of Concentration

```
SData = mysort(NumS,TxtS,SData);
DData = mysort(NumD,TxtD,DData);
```

Getting the FW and WW Targets and Pinch Point(s)

```
[PinchP,F_Matrix, WW] = intprt_v2(FileName,Sheet,SPoints,DPoints,FWConc,Availability);
FW = F_Matrix(2);
if numel(PinchP) > 1
    error('Multiple Pinch Points exist for this process network.\n');
end
```

Initializing the First Two Rows and Columns of the Network Matrix

```
Source_Size = row(SData) + 1;
flag = 'y'; % If flag is equal to y, then FW conc sources are not present in the initial data.
for ii = 1:row(SData)
    if FWConc == SData{ii,4};
        Source_Size = row(SData);
        flag = 'n'; % If flag is equal to n, then there exists a source which has a conc. equal
to that of fresh water.
        break;
    end
end
Demand_Size = row(DData) + 1; % +1 for WW Stream
SCon = zeros(Source_Size,1); % Initializing the First Column of Network Matrix. Contains Source
Concentrations.
SFlow = zeros(Source_Size,1); % Initializing the Second Column of Network Matrix. Contains Source
Flowrates.
DCon = zeros(Demand_Size,1); % Initializing First Row of Network Matrix. Contains Demand
Concentrations.
DFlow = zeros(Demand_Size,1); % Initializing Second Row of Network Matrix. Contains Demand
Flowrates.
```

Setting the Source Parents in the Network Matrix

```
if flag == 'y' % If flag is equal to y, then FW conc sources are not present in the initial data.
    SCon(1) = FWConc;
    SFlow(1) = FW;
    for ii = 2:Source_Size
        SCon(ii) = SData{ii-1,4};
        SFlow(ii) = SData{ii-1,3};
    end
elseif flag == 'n' % If flag is equal to n, then there exists a source which has a conc. equal to
that of fresh water.
    SCon(1) = FWConc;
    SFlow(1) = SData{1,4} + FW;
    for ii = 2:Source_Size
        SCon(ii) = SData{ii,4};
        SFlow(ii) = SData{ii,3};
    end
end
```

Setting the Demand Parents in the Network Matrix

```
for ii = 1:Demand_Size-1
DCon(ii) = DData{ii,4};
DFlow(ii) = DData{ii,3};
end
DFlow(end) = WW;
```

Initializing the Network Matrix

```
N = zeros(length(SCon)+2,length(DCon)+2);
N(1:2,1:2) = nan;
N(3:end,1:2) = [SCon SFlow];
N(1:2,3:end) = [DCon'; DFlow'];
```

Graying Out the Cross Pinch Regions

```
PinchConcCount = sum(SCon == PinchP);
for ii = 1:length(SCon) % For Finding the Row Index
    if SCon(ii) == PinchP
        DIR = (ii+2); % Desired Index (Row)
    end
end
DIC = []; % Initializing Desired Index (Column). Sometimes, there may be no demand concentration
which is higher than the source pinch concnetration and as a result DIC will remain an empty
matrix.
for ii = 1:length(DCon) % For Finding the Column Index
    if DCon(ii) > PinchP
        DIC = (ii+2); % Desired Index (Column)
        break; % Because we want the nearest higher concentration.
    end
end
if ~isempty(DIC) % Setting Gray Area.
    N(DIR+1:end,3:DIC-1) = nan;
    N(3:DIR-1-(PinchConcCount-1),DIC:end-1) = nan;
elseif DIR == length(SCon)+2
    fprintf('No Gray Area.\n');
else
    N(DIR+1:end,3:end-1) = nan;
end
N(2,end) = WW; % Introduced WW Flow rate in the Network Matrix
N(3:DIR-1-(PinchConcCount-1),end) = nan; % Sources whose concentrations are 'less' than pinch
concentration will not be discarded as wastewater.
Grayed = N;
```

Making the Network using NNA (Shenoy,2012): Below Pinch

```
[rN,cN] = size(N);
SourcePool1 = N(3:DIR,1);
if isempty(DIC)
    DIC = cN-1;
end
% Source-Sink Mapping in Below the Pinch Region.
for ii = 3:DIC-1 % Demands
    FCEqualBefore = 0;
    for jj = 3:DIR % Sources
        if N(1,ii) == N(jj,1) % If conc. of demand = conc. of source
            if N(2,ii) >= N(jj,2) && N(2,ii) > 0 % Demand >= Source
                N(jj,ii) = N(jj,2); % Allocating
                N(2,ii) = N(2,ii) - N(jj,2); % Updating demand
```

```
                FCEqualBefore = FCEqualBefore + N(1,ii)*N(jj,2); % This is added for the
conditions wherein equal concentration source doesn't satisfy the demand. So whatever amount of
equal-concentration-source is available, it is fed to the demand amd the equivalent contaminant
load is also recorded to be later fed in to the fsolve function.
                N(jj,2) = 0; % Updating Source
                SourcePool1 = concUpdate(SourcePool1,N(1,ii));
                N(jj,1) = NaN;
            elseif N(2,ii) < N(jj,2) && N(2,ii) > 0 % Demand < Source
                N(jj,ii) = N(2,ii); % Allocating
                N(jj,2) = N(jj,2) - N(2,ii); % Updating Source
                FCEqualBefore = FCEqualBefore + N(1,ii)*N(2,ii); % This is added for the
conditions wherein equal concentration source is more than the demand. So whatever amount of
equal-concentration-source is required, it is fed to the demand amd the equivalent contaminant
load is also recorded to be later fed in to the fsolve function.
                N(2,ii) = 0; % Updating Demand
            end
        end
    end
        FlCl_Before = 0; FhCh_Before = 0; % Initial Values of some inputs to ShenFun
        while N(2,ii) > 0 % While the demand is not met.
            [Cl, Ch] = Shenoy(SourcePool1,N(1,ii));
            for mm = 3:DIR % mm is just a loop index
                if N(mm,1) == Cl
                    Fl = round(N(mm,2),1); % Available Flowrate of Lower Concentration
                    ss = mm; % Storing this index for its use in correcting the Lower Conc.
Source Availability after allocation.
                elseif N(mm,1) == Ch
                    Fh = round(N(mm,2),1); % Available Flowrate of Higher Concentration
                    qq = mm; % Storing this index for its use in correcting the Higher Conc.
Source Availability after allocation.
                    break; % Added because the required info on Conc and Flowrate has already
been taken.
                end
            end
            y = round((fsolve(@(x)
ShenFun(x,Cl,Ch,N(2,ii),Grayed(2,ii),N(1,ii),FlCl_Before,FhCh_Before,FCEqualBefore),[Fl;Fh])),1);
% Finding the demands of Cl and Ch
            if y(1) < Fl && y(2) < Fh % Both the demands are lower than availabilities. So the
demand will be completely met.
                N(2,ii) = 0; % Demand has been reduced to zero since it is completely met.
                N(ss,2) = N(ss,2) - y(1); % Availability of Cl is now reduced since some of it is
allocated to the demand.
                N(qq,2) = N(qq,2) - y(2); % Availability of Cl is now reduced since some of it is
allocated to the demand.
                N(ss,ii) = y(1); % Allocation of Cl in the Network Matrix.
                N(qq,ii) = y(2); % Allocation of Ch in the Network Matrix.
            elseif y(1) > Fl && y(2) <= Fh % Only Ch availability is more than the demand. So
whatever Cl is available will be used completely.
                N(2,ii) = N(2,ii) - Fl; % The demand is updated.
                N(ss,2) = 0; % Availability of Cl is now reduced to 0 since all of it is
allocated to the demand.
                N(ss,ii) = Fl; % Allocation of Cl in the Network Matrix.
                FlCl_Before = FlCl_Before + Fl*Cl; % Updating the contaminant load.
                SourcePool1 = concUpdate(SourcePool1,Cl); % Updating the number of available
```

```
sources.
                N(:,1) = searcon(Cl,N(:,1)); % Replacing Cl with nan in the Source Concentration
Column.
            elseif y(1) <= Fl && y(2) > Fh % Only Cl availability is more than the demand. So
whatever Ch is available will be used completely.
                N(2,ii) = N(2,ii) - Fh; % The demand is updated.
                N(qq,2) = 0; % Availability of Ch is now reduced to 0 since all of it is
allocated to the demand.
                N(qq,ii) = Fh; % Allocation of Ch in the Network Matrix.
                FhCh_Before = FhCh_Before + Fh*Ch; % Updating the contaminant load.
                SourcePool1 = concUpdate(SourcePool1,Ch); % Updating the number of available
sources.
                N(:,1) = searcon(Ch,N(:,1)); % Replacing Ch with nan in the Source Concentration
Column.
            elseif y(1) >= Fl && y(2) >= Fh % Both Cl and Ch availability is less than that
required so both of them will be used completely.
                N(2,ii) = N(2,ii) - y(1) - y(2);
                N(ss,2) = 0; % Availability of Cl is now reduced to 0 since all of it is
allocated to the demand.
                N(qq,2) = 0; % Availability of Ch is now reduced to 0 since all of it is
allocated to the demand.
                N(ss,ii) = Fl; % Allocation of Cl in the Network Matrix.
                N(qq,ii) = Fh; % Allocation of Ch in the Network Matrix.
                FlCl_Before = FlCl_Before + Fl*Cl; % Updating the contaminant load.
                FhCh_Before = FhCh_Before + Fh*Ch; % Updating the contaminant load.
                SourcePool1 = concUpdate(SourcePool1,Cl); % Updating the number of available
sources.
                N(:,1) = searcon(Cl,N(:,1)); % Replacing Cl with nan in the Source Concentration
Column.
                SourcePool1 = concUpdate(SourcePool1,Ch); % Updating the number of available
sources.
                N(:,1) = searcon(Ch,N(:,1)); % Replacing Ch with nan in the Source Concentration
Column.
            elseif y(1) == Fl && y(2) < Fh
                N(2,ii) = 0; % Demand has been reduced to zero since it is completely met.
                N(ss,2) = 0; % Availability of Cl is now reduced since some of it is allocated to
the demand.
                N(qq,2) = N(qq,2) - y(2); % Availability of Cl is now reduced since some of it is
allocated to the demand.
                N(ss,ii) = y(1); % Allocation of Cl in the Network Matrix.
                N(qq,ii) = y(2); % Allocation of Ch in the Network Matrix.
                SourcePool1 = concUpdate(SourcePool1,Cl);
                N(:,1) = searcon(Cl,N(:,1));
            elseif y(1) < Fl && y(2) == Fh
                N(2,ii) = 0; % Demand has been reduced to zero since it is completely met.
                N(ss,2) = N(ss,2) - y(1); % Availability of Cl is now reduced since some of it is
allocated to the demand.
                N(qq,2) = 0; % Availability of Cl is now reduced since some of it is allocated to
the demand.
                N(ss,ii) = y(1); % Allocation of Cl in the Network Matrix.
                N(qq,ii) = y(2); % Allocation of Ch in the Network Matrix.
                SourcePool1 = concUpdate(SourcePool1,Ch);
                N(:,1) = searcon(Ch,N(:,1));
            end
```

```
        end
end
```

Making the Network using NNA (Shenoy,2012): Above Pinch

```
SourcePool2 = N(DIR:rN,1);
for ii = DIC:cN-1 % Source-Sink Mapping in Below the Pinch Region.
     FCEqualBefore = 0;
    for jj = DIR-(PinchConcCount-1):rN
        if N(1,ii) == N(jj,1) % If conc. of demand = conc. of source
            if N(2,ii) >= N(jj,2) && N(2,ii) > 0 % Demand >= Source
                N(jj,ii) = N(jj,2); % Allocating
                N(2,ii) = N(2,ii) - N(jj,2); % Updating demand
                FCEqualBefore = FCEqualBefore + N(1,ii)*N(jj,2); % This is added for the
conditions wherein equal concentration source doesn't satisfy the demand. So whatever amount of
equal-concentration-source is available, it is fed to the demand amd the equivalent contaminant
load is also recorded to be later fed in to the fsolve function.
                N(jj,2) = 0; % Updating Source
                SourcePool2 = concUpdate(SourcePool2,N(1,ii));
                N(jj,1) = NaN;
            elseif N(2,ii) < N(jj,2) && N(2,ii) > 0 % Demand < Source
                N(jj,ii) = N(2,ii); % Allocating
                N(jj,2) = N(jj,2) - N(2,ii); % Updating Source
                FCEqualBefore = FCEqualBefore + N(1,ii)*N(2,ii); % This is added for the
conditions wherein equal concentration source is more than the demand. So whatever amount of
equal-concentration-source is required, it is fed to the demand amd the equivalent contaminant
load is also recorded to be later fed in to the fsolve function.
                N(2,ii) = 0; % Updating Demand
            end
        end
    end
        FlCl_Before = 0; FhCh_Before = 0; % Initial Values of some inputs to ShenFun
        while N(2,ii) > 0 % While the demand is not met.
            [Cl, Ch] = Shenoy(SourcePool2,N(1,ii));
            for mm = DIR:rN % mm is just a loop index
                if N(mm,1) == Cl
                    Fl = round(N(mm,2),1); % Available Flowrate of Lower Concentration
                    ss = mm; % Storing this index for its use in correcting the Lower Conc.
Source Availability after allocation.
                elseif N(mm,1) == Ch
                    Fh = round(N(mm,2),1); % Available Flowrate of Higher Concentration
                    qq = mm; % Storing this index for its use in correcting the Higher Conc.
Source Availability after allocation.
                    break; % Added because the required info on Conc and Flowrate has already
been taken.
                end
            end
            y = round((fsolve(@(x)
ShenFun(x,Cl,Ch,N(2,ii),Grayed(2,ii),N(1,ii),FlCl_Before,FhCh_Before,FCEqualBefore),[Fl;Fh])),1);
% Finding the demands of Cl and Ch
            if y(1) < Fl && y(2) < Fh % Both the demands are lower than availabilities. So the
demand will be completely met.
                N(2,ii) = 0; % Demand has been reduced to zero since it is completely met.
```

```
                N(ss,2) = N(ss,2) - y(1); % Availability of Cl is now reduced since some of it is
allocated to the demand.
                N(qq,2) = N(qq,2) - y(2); % Availability of Cl is now reduced since some of it is
allocated to the demand.
                N(ss,ii) = y(1); % Allocation of Cl in the Network Matrix.
                N(qq,ii) = y(2); % Allocation of Ch in the Network Matrix.
             elseif y(1) > Fl && y(2) <= Fh % Only Ch availability is more than the demand. So
whatever Cl is available will be used completely.
                N(2,ii) = N(2,ii) - Fl; % The demand is updated.
                N(ss,2) = 0; % Availability of Cl is now reduced to 0 since all of it is
allocated to the demand.
                N(ss,ii) = Fl; % Allocation of Cl in the Network Matrix.
                FlCl_Before = FlCl_Before + Fl*Cl; % Updating the contaminant load.
                SourcePool2 = concUpdate(SourcePool2,Cl); % Updating the number of available
sources.
                N(:,1) = searcon(Cl,N(:,1)); % Replacing Cl with nan in the Source Concentration
Column.
            elseif y(1) <= Fl && y(2) > Fh % Only Cl availability is more than the demand. So
whatever Ch is available will be used completely.
                N(2,ii) = N(2,ii) - Fh; % The demand is updated.
                N(qq,2) = 0; % Availability of Ch is now reduced to 0 since all of it is
allocated to the demand.
                N(qq,ii) = Fh; % Allocation of Ch in the Network Matrix.
                FhCh_Before = FhCh_Before + Fh*Ch; % Updating the contaminant load.
                SourcePool2 = concUpdate(SourcePool2,Ch); % Updating the number of available
sources.
                N(:,1) = searcon(Ch,N(:,1)); % Replacing Ch with nan in the Source Concentration
Column.
            elseif y(1) >= Fl && y(2) >= Fh % Both Cl and Ch availability is less than that
required so both of them will be used completely.
                N(2,ii) = N(2,ii) - y(1) - y(2);
                N(ss,2) = 0; % Availability of Cl is now reduced to 0 since all of it is
allocated to the demand.
                N(qq,2) = 0; % Availability of Ch is now reduced to 0 since all of it is
allocated to the demand.
                N(ss,ii) = Fl; % Allocation of Cl in the Network Matrix.
                N(qq,ii) = Fh; % Allocation of Ch in the Network Matrix.
                FlCl_Before = FlCl_Before + Fl*Cl; % Updating the contaminant load.
                FhCh_Before = FhCh_Before + Fh*Ch; % Updating the contaminant load.
                SourcePool2 = concUpdate(SourcePool2,Cl); % Updating the number of available
sources.
                N(:,1) = searcon(Cl,N(:,1)); % Replacing Cl with nan in the Source Concentration
Column.
                SourcePool2 = concUpdate(SourcePool2,Ch); % Updating the number of available
sources.
                N(:,1) = searcon(Ch,N(:,1)); % Replacing Ch with nan in the Source Concentration
Column.
            elseif y(1) == Fl && y(2) < Fh
                N(2,ii) = 0; % Demand has been reduced to zero since it is completely met.
                N(ss,2) = 0; % Availability of Cl is now reduced since some of it is allocated to
the demand.
                N(qq,2) = N(qq,2) - y(2); % Availability of Cl is now reduced since some of it is
allocated to the demand.
                N(ss,ii) = y(1); % Allocation of Cl in the Network Matrix.
```

```
                N(qq,ii) = y(2); % Allocation of Ch in the Network Matrix.
                SourcePool2 = concUpdate(SourcePool2,Cl);
                N(:,1) = searcon(Cl,N(:,1));
            elseif y(1) < Fl && y(2) == Fh
                N(2,ii) = 0; % Demand has been reduced to zero since it is completely met.
                N(ss,2) = N(ss,2) - y(1); % Availability of Cl is now reduced since some of it is
allocated to the demand.
                N(qq,2) = 0; % Availability of Cl is now reduced since some of it is allocated to
the demand.
                N(ss,ii) = y(1); % Allocation of Cl in the Network Matrix.
                N(qq,ii) = y(2); % Allocation of Ch in the Network Matrix.
                SourcePool2 = concUpdate(SourcePool2,Ch);
                N(:,1) = searcon(Ch,N(:,1));
            end
        end
 end
```

Sketching the Wastewater Stream

```
 N(DIR-(PinchConcCount-1):end,end) = N(DIR-(PinchConcCount-1):end,2);
 N(DIR-(PinchConcCount-1):end,2) = 0; % Updating the Sources which supply to Wastewater Stream.
 if N(2,end) - sum(N(DIR-(PinchConcCount-1):end,end)) > 1e-1 % The sum of the remaining amounts
of sources including and above the Pinch Point must be equal to the targetted value.
     error('Wastewater Flowrate is not matching with targetted value.');
 end
 N(1,end) = sum(Grayed(DIR-(PinchConcCount-1):end,1).*N(DIR-(PinchConcCount-
1):end,end))/N(2,end); % Wastewater Concentration
 WWCon = N(1,end);
 N(2,end) = 0; % Updating the wastewater target since there is no error above.
```

Network Dressing

```
 if sum(N(3:end,2) == 0) == length(N(3:end,2)) && sum(N(2,3:end) == 0) == length(N(2,3:end))
     N(:,1:2) = Grayed(:,1:2);
     N(1:2,3:end) = Grayed(1:2,3:end);
     N(1,end) = WWCon; % The wastewater concentration was removed due to dressing, therefore, it
is again fed to the network.
 else
     error('Either the Leftover Sources or the Satisfied Demands (including Wastewater Target)
are not summing upto zero.');
 end
format short;

end
```

Example 4.1: Data is adopted from an early work on WPA (Polley & Polley 2000).

It has been assumed that S_i and D_i are input and output of the same unit i, in order to present the conventional network design.

Table 20: Source Data Set VIII

Stream No.	Process Name	Flow Rate	Concentration	Type	Load
Out	$	t/h	Ppm	-	1e-6 t/h
S_A	A	50	50	FF	-
S_B	B	100	100	FF	-
S_C	C	70	150	FF	-
S_D	D	60	200	FF	-

Table 21: Demand Data Set VIII

Stream No.	Process Name	Flow Rate	Concentration	Type	Load
In	$	t/h	Ppm	-	1e-6 t/h
D_A	A	50	20	FF	-
D_B	B	100	50	FF	-
D_C	C	80	100	FF	-
D_D	D	70	200	FF	-

Given: a pure (0 ppm) fresh water feed at infinite availability. The network generated by nnaup.m (in the form of a matrix) was exported to an Excel Sheet using the 'xlswrite' command. The same is presented in figure 4. Since all the operations are of fixed flowrate type, flow-through rates for these operations cannot be changed. It is to be noted that the network generated in figure 4 is just one possible solution. Other networks can also be generated by varying the order in which the demands are satisfied (Shenoy 2012). Figure 4 gives a rather crude representation of the water network which may be hard to understand. Here, empty spaces denote cross-pinch region. Figure 5 presents the same network in a conventional form.

		Unit	A	B	C	D	WW
		Demand Concnetration	20	50	100	200	200
Unit	Source Concentration	Demand Flowrate / Source Flowrate	50	100	80	70	50
FF	0	70	30	35	5		
A	50	50	20	30	0		
B	100	100	0	35	65		
C	150	70	0	0	10	35	25
D	250	60				35	25

Figure 4: Output generated by nnaup.m for Data Set VII

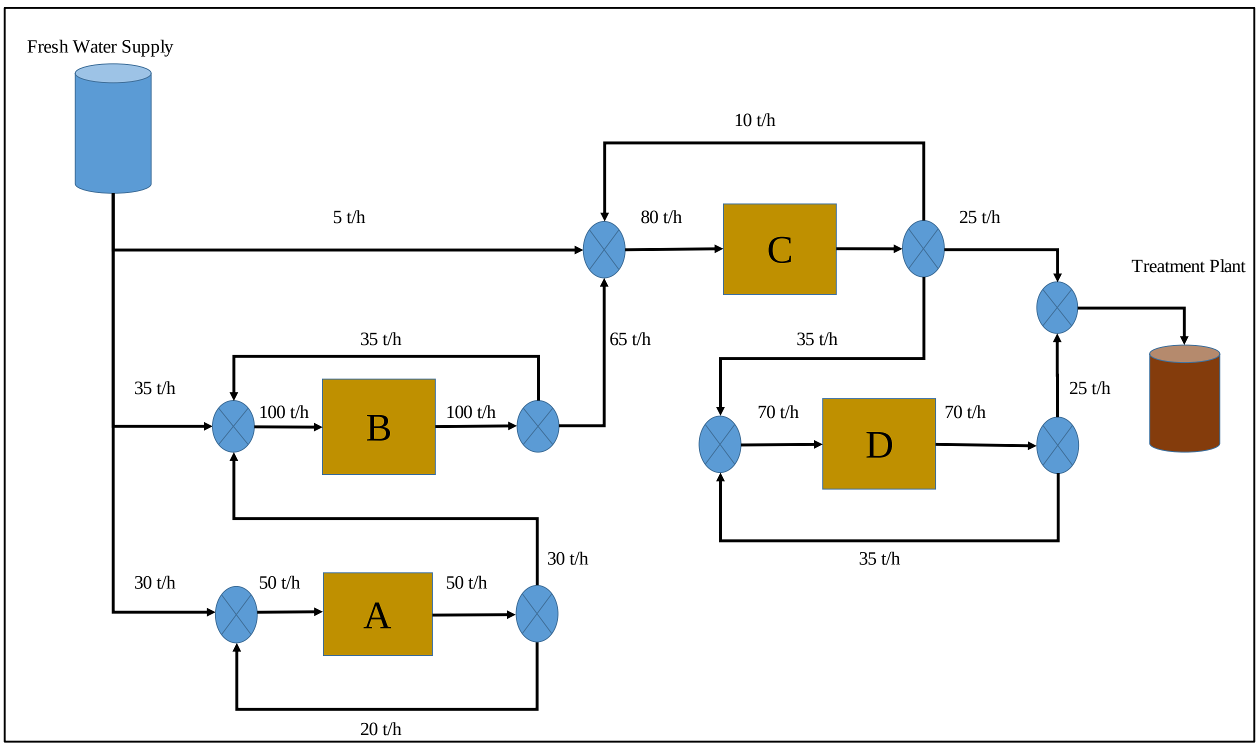

Figure 5: Conventional Representation of Source-Sink Matching Matrix for Data Set VII

Example 4.2: Data is adopted from Wang and Smith (1994).

Table 22: Source Data Set IX

Stream No.	Process Name	Flow Rate	Concentration	Type	Load
Out	$	t/h	Ppm	-	1e-6 t/h
1	A	20	100	FC	2000
2	B	100	100	FC	5000
3	C	40	800	FC	30000
4	D	10	800	FC	4000

Table 23: Demand Data Set IX

Stream No.	Process Name	Flow Rate	Concentration	Type	Load
In	$	t/h	Ppm	-	1e-6 t/h
1	A	20	0	FC	2000
2	B	100	50	FC	5000
3	C	40	50	FC	30000
4	D	10	400	FC	4000

Given: a pure (0 ppm) fresh water feed at infinite availability. The output generated by nnaup.m is presented in figure 6, and the conventional representation is given in figure 7. Unlike the previous case, this case has only FC units. Therefore, we may eliminate any LR matches, if present. The allocation matrix presented in figure 6, depicts an LR match. It can also be seen in the conventional network (figure 7) around unit B. After eliminating, the number of matches will reduce from 11 to 10, and the total water flowrate through units will decrease to 140 t/h from 170 t/h. Accordingly, the inlet feed concentration to source B will also decrease to approximately 28.57 ppm (concentration of the mixture of 50 t/h of pure freshwater and 20 t/h of impure/reused water (100 ppm).

		Unit	A	B	C	D	WW
		Demand Concnetration	0	50	50	400	455.44
Unit	Source Concentration	Demand Flowrate / Source Flowrate	20	100	40	10	90
FF	0	90	20	50	20		
A	100	20	0	20	0	0	0
B	100	100	0	30	20	5.7	44.3
C	800	40				4.3	35.7
D	800	10				0	10

Figure 6: Output generated by nnaup.m for Data Set IX

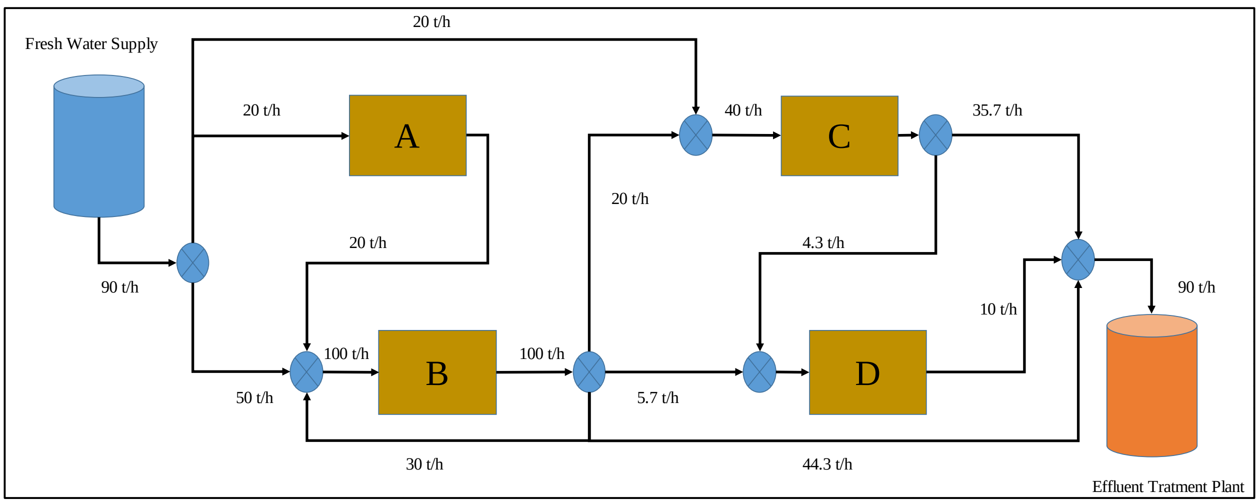

Figure 7: Conventional Representation of Source-Sink Matching Matrix for Data Set VII

We can also simply interchange source allocations of same quality sources and generate alternate designs with LR matches. In this case, the match between unit C (source) and unit D (demand) can be exchanged for an LR match around unit D. Similarly, the match between unit B (source) and unit C (demand) can be exchanged for an LR match around unit B. After they are eliminated, the flowrates of unit B and D will become 50 t/h and 5.7 t/h, respectively. Their inlet concentrations will also change to 0 ppm and 100 ppm, respectively. The resultant network has only 8 interconnections and the flow-through rate is also reduced by approximately 32% (as compared to the original network generated by nnaup.m). The final network is shown in figures 8 and 9.

		Unit	A	B	C	D	WW
		Demand Concnetration	0	0	50	100	455.44
Unit	Source Concentration	Demand Flowrate / Source Flowrate	20	50	40	5.7	90
FF	0	90	20	50	20		
A	100	20	0	0	20	0	0
B	100	50	0	0	0	5.7	44.3
C	800	40				0	40
D	800	5.7				0	5.7

Figure 8: Output generated source exchanges and LR eliminations

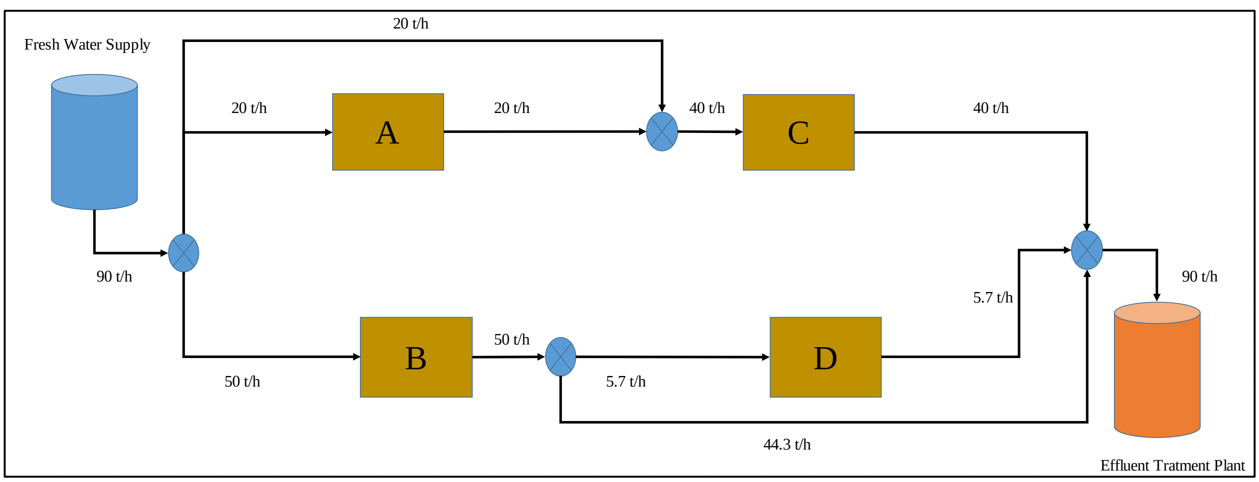

Figure 9: Conventional Representation of Source-Sink Matching Matrix given in Figure 8

Example 4.3. Data is adopted from a work on water minimization in breweries (Olankule & Ityokumbul 2014). Refer to Table 24.

Table 24: Representative Data of the Beer Brewery's Water Network

Operation	Limiting Flowrate (t/h)	Limiting Inlet Concentration (ppm)	Limiting Outlet Concentration (ppm)	Mass Load (kg/h)
Mashing (B)	70.00	0.00	1570.00	109.90
Mash Filtering (D)	56.58	1596.00	8474.00	389.16
Wort Boiling (C)	75.92	442.00	1695.00	95.13
1^0 Fermentation (E)	71.54	1950.00	9010.00	505.07
2^0 Fermentation (A)	42.64	857.00	1464.00	25.88
Beer Filtration (F)	13.46	990.00	9684.00	117.02

Given: Pure fresh water feed with infinite availability. After decomposing the limiting data given in table 23 into the conventional forms of source and demand data, network design was carried out using nnaup.m. The results are presented in figure 9. Here, all the operations are of FC type so there lies a potential for lowering the number of interconnections/matches and the flow-through rate.

		Unit	B	C	A	F	D	E	WW
		Demand Concnetration	0	442	857	990	1596	1950	8507.7
Unit	Source Concentration	Demand Flowrate / Source Flowrate	70	75.92	42.64	13.46	56.58	71.54	146
FF	0	146.004484	70	52.999	18.033	4.9725			
A	1464	42.64	0	22.921	19.719	0			
B	1570	70	0	0	4.888	8.4875	44.811	4.6125	7.2006
C	1695	75.92					11.769	64.151	0
D	8474	56.58					0	2.7761	53.804
E	9010	71.54					0	0	71.54
F	9684	13.46					0	0	13.46

Figure 10: Network Matrix for the Brewery Case

CONCLUDING REMARKS

Increasing water stress arising due to the abuse of water resources has posed a serious threat to the ecosystem which also includes human population. However, these availability and accessibility concerns can be dealt with through effective execution of sustainable water management plans. Water minimization shall form an inherent part of many such plans, and is critical to combatting water stress. In this work, we discussed the use of an insight based technique, namely, water pinch analysis which can guide industries in judiciously using their water resources and consequently, minimizing their water consumption.

A MATLAB based toolbox which facilitates single contaminant based water pinch analysis has been developed. Moreover, examples from numerous classical works are presented to help the users in understanding the working of the toolbox. However, the types of problems it can solve are currently limited. For instance, the algorithms in their current forms cannot cater to problems involving regeneration recycle/reuse (Ng, Foo, Tan, et al. 2007; Ng et al. 2008), wastewater treatment targeting and network design (Ng, Foo & Tan 2007a; Ng, Foo & Tan 2007b), batch operations, and multiple key contaminants. The toolbox is very much capable of dealing with multiple pinch points, multiple sources (Foo 2007) and threshold cases (Foo 2008) as far as targeting is concerned. But as regards network design, the toolbox cannot generate a source-sink allocation matrix for a process network having multiple pinch points and sources. In order to overcome the above mentioned limitations, efforts are in order to enhance this toolbox to a level where it can deal with most single contaminant, continuous operations based problems.

In the process of toolbox development, an improvement was noted in the use of WCA for carrying out multiple source targeting. The alternate approach eliminates the need for flowrate adjustment which was inherent in the previous technique. Moreover, the toolbox allows its users to prioritize the use of fresh water sources with respect to their qualities (contaminant concentration levels) in that they can adopt the assumptions presented by Foo (2007) and employ the use of only the highest quality impure source in addition to the pure water source (if required) or else they can adopt our assumptions wherein we maximize the use of the dirtier source(s). As mentioned earlier, the choice between the two sets of assumptions should be made by carefully evaluating fresh water costs, associated capital costs, and other operating costs. The latter set may be preferred when considerable resource costs are associated with the use of some or all fresh water types, and the same increase with increasing purity.

The applications of this toolbox lies in both academia and industries wherein it can aid its users in developing a basic understanding of targeting and network design procedures, and generating practical water network solutions for real life processes. Furthermore, being a computer based tool, it offers an overwhelming speed and accuracy. One of the main ideas behind this work was to develop a freely accessible and robust toolbox for regulating water use in process industries and with the proposed modifications, this tool can prove to be a valuable asset for these industries.

APPENDIX A

Some Helpful Explanations

A.1. Fresh Water Requirement in Fixed Contaminant Load Systems: A Conceptual Perspective

The underlying explanation paves a way to understand how water requirement is being reduced when a pure fresh water source instead of an impure one is fed into a fixed contaminant load system. A fixed contaminant load process is one in which the mass load (typically, in kg/h) transferred from the process stream to the mass separating agent is fixed (Prakash & Shenoy 2005b) and is of prime concern to the designer/engineer.

Consider a contaminant-rich process stream which is fed into a separator unit (extractor unit, gas absorber, etc.). Due to the process requirements, it may be desirable to get the process stream to a certain purity level. So, if a process stream is input to the separator at flowrate, $\mathbf{F_P}$ m^3/h, and contaminant concentration, $\mathbf{C_{P,\,in}}$ $kmol/m^3$, and the desired outlet concentration is $\mathbf{C_{P,\,out}}$ $kmol/m^3$, then the number of moles, **M** (or, mass load) to be transferred out of the process stream is $\mathbf{F_P\ (C_{P,\,in} - C_{P,\,out})}$, assuming no volumetric loss or gain in the process stream**.** This constant volumetric flow rate assumption accommodates the following: there are no leakages due to which any part of the process stream is lost, and water neither gets reacted nor it is generated to an extent that practically affects the volumetric flow rate. Moreover, we assume that the process stream forms a **dilute solution** such that the transfer of contaminants does not practically effect its volume. Clearly, we have considered:

$$M = F_P\left(C_{P,in} - C_{P,out}\right)$$

In the above mas transfer model, we are assuming a linear relation between the mass transfer rate and the concentration difference, which usually holds true only for dilute solutions (Wang & Smith 1994). However, any non-linearity between these two entities can also be treated using the above model by splitting the non-linear behaviour into various linear segments (Wang & Smith 1994).

If water at flowrate, $\mathbf{F_W}$ and contaminant concentration $\mathbf{C_{W,\,in}}$ is used as the mass separating agent, then the contaminant load taken up by the water stream will lead to an increase in its outlet concentration to, say, $\mathbf{C_{W,\,out}}$. Now, if we are able to supply a higher quality (lower contaminant concentration) water feed to the process, the water requirements can be reduced. Let $\mathbf{C^{II}_{W,\,in}}$ be the new inlet concentration such that $\mathbf{C^{II}_{W,\,in}} < \mathbf{C_{W,\,in}}$.

Now, in one hour, if the concentration of $\mathbf{F_W}$ m^3 of water increased from $\mathbf{C_{W,\,in}}$ to $\mathbf{C_{W,\,out}}$ kmol/m^3 after taking up **M** moles of contaminant, we can say that the concentration of same volume of water can go from $\mathbf{C^{II}_{W,\,in}}$ **to** $\mathbf{C^{II}_{W,\,out}}$ such that $\mathbf{C^{II}_{W,\,out}} < \mathbf{C_{W,\,out}}$. However, it is to be noted that the outlet water concentration should be restricted to its maximum value which is governed by various factors as pointed out by R. Smith (Smith 2005). Some of these factors are *"maximum solubility, corrosion limitations, fouling limitations, minimum of mass transfer driving force, minimum flowrate requirements, maximum inlet concentration for downstream processing"*, etc. So, at this position, for the same mass load of **M** moles, we want the concentration of water to go up from $\mathbf{C^{II}_{W,\,in}}$ to $\mathbf{C_{W,\,out}}$. This can be achieved if we reduce the volume of water fed to the process unit since a fixed amount of mass in a lesser volume implies higher concentration. Hence, we can reduce the flow rate of water to the process unit. A reduction in flowrate can also be achieved if the outlet concentration of water stream is less than the maximum allowable value. However, for a fixed inlet concentration, maximum outlet concentration is required in order to

minimize the water requirement. Figure A1 depicts the concentration profile of various water streams having different limiting inlet and outlet concentrations with respect to a process stream.

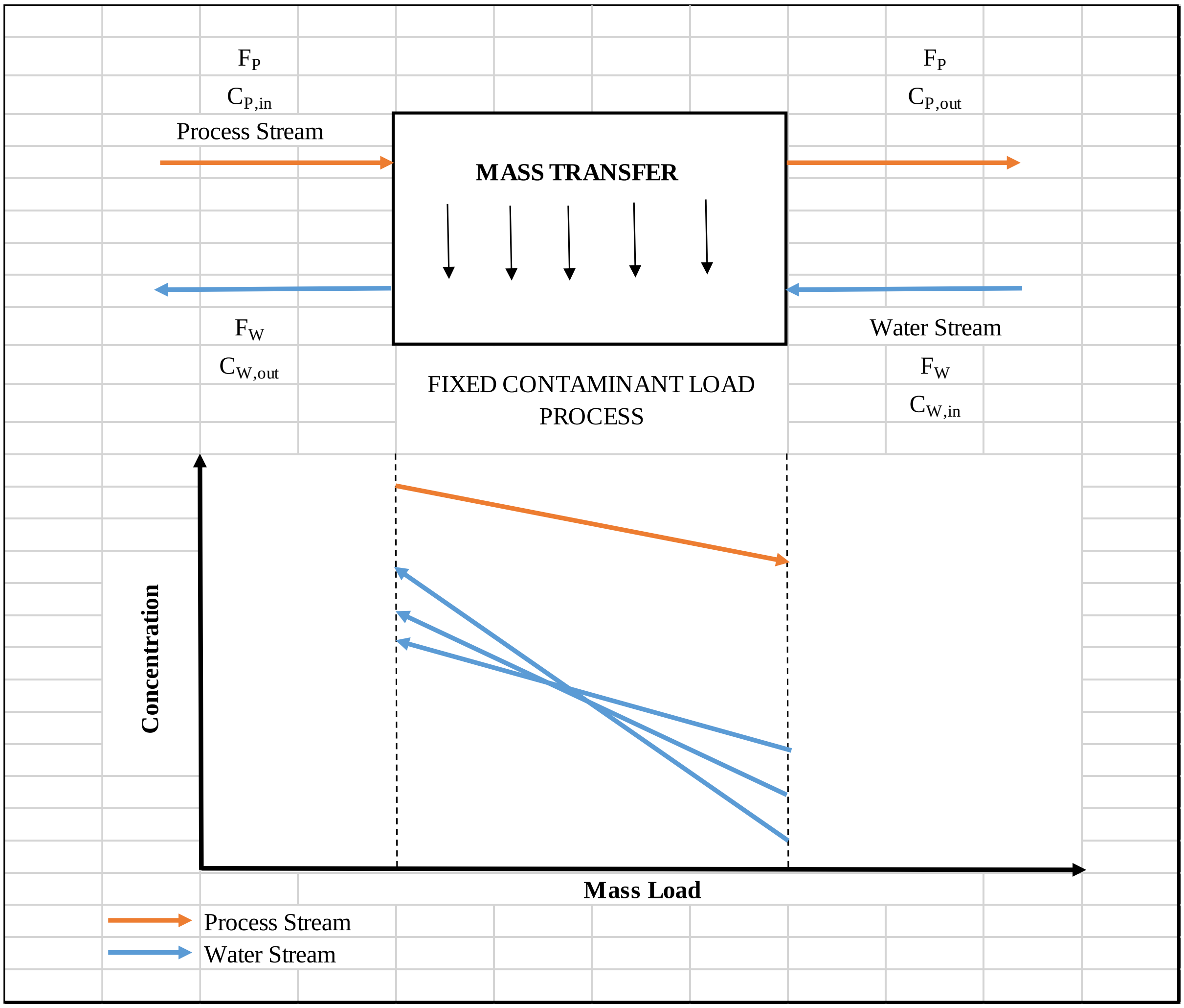

Figure A1: Concentration Profile of Water and Process Streams for a Fixed Contaminant Load Process

A.2. Mathematical Reasoning behind the applicability of LR Elimination

Here, we will prove why eliminating the LR match does not lead to contaminant load constraint violation. The LR match can be depicted as in figure A2.

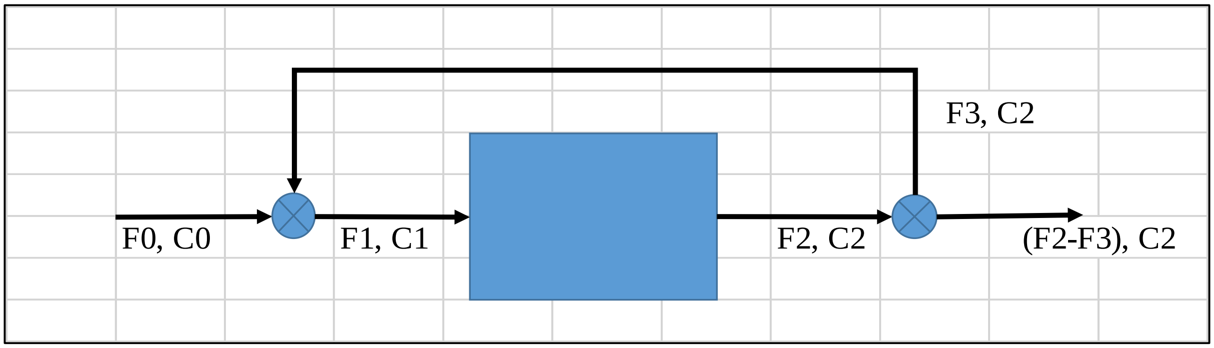

Figure A2: An LR Match

Since the FC operation must ensure a specified contaminant load transfer (as dictated by the process requirements), equation A2 will hold:

$$\Delta m_{specified} = F_2 C_2 - F_1 C_1$$

Further, an FC operation, is assumed to work with no losses and gains. Therefore, the inlet flowrate will be equal to the outlet flowrate. Hence, equation A2 becomes:

$$\Delta m_{specified} = F_1 (C_2 - C_1)$$

Moreover, considering the overall arrangement (figure A2), two more relations can be derived. Equations A3 and A4 for summing junction and overall load transfer, respectively.

$$F_1 C_1 = F_0 C_0 + F_3 C_2$$

$$\Delta m_{overall} = (F_2 - F_3) C_2 - F_0 C_0$$

Substituting equation A3 in equation A4 gives:

$$\Delta m_{overall} = F_2 C_2 - F_1 C_1 = \Delta m_{specified}$$

Clearly, the contaminant concentration load remains satisfied without the involvement of the LR, and hence, it can be eliminated as in figure A3.

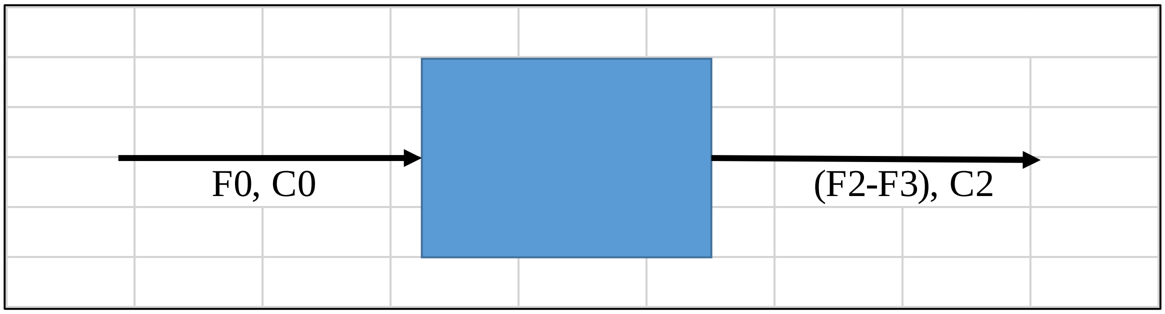

Figure A3: FC Operation after LR Elimination

Appendix B

Sub-routines Developed for Targeting

B.1. mysort.m

Function for sorting the input matrices in such a way that the concentrations are in ascending order in the output matrix containing the source/demand data.

```
function outS = mysort(NumS,TxtS,SData)
[NumS(:,4),I1] = sort(NumS(:,4));
NumS(:,1:3) = NumS(I1,1:3);
NumS(:,6) = NumS(I1,6);
TxtS = TxtS(I1,:);
SData(:,2) = TxtS(:,1);
SData(:,5) = TxtS(:,4);
for ii = 1:row(SData)
  SData{ii,1} = NumS(ii,1);
  SData{ii,3} = NumS(ii,3);
  SData{ii,4} = NumS(ii,4);
  SData{ii,6} = NumS(ii,6);
end
outS = SData;
end
```

B.2. imnor.m

Program for Importing and Organizing the source and demand data in the form of WCT. Inputs are the location of the source and demand data and the concentration of different fresh water (FW) sources available. Outputs are: a partial WCT containing levels/indices, concentrations, purity, demands, sources, and net interval flowrates and a vector containing the indices of the fresh water sources.

```
function [N, Ind] = imnor(FileName,Sheet,SPoints,DPoints,FWConc)
```

Fetching the Data from MS-Excel Worksheet

```
[~,~,SData] = xlsread(FileName,Sheet,SPoints); % Source Data
[~,~,DData] = xlsread(FileName,Sheet,DPoints); % Demand Data
FWConc = sort(FWConc,'ascend');
```

Setting Levels, Concentration and Purity Columns

```
r1 = row(DData);
r2 = row(SData);
Conc_Vector_Initial = [FWConc DData{:,4} SData{:,4} 10^6]; % All the Concentrations that are
there in the Data Sets
Conc = unique(Conc_Vector_Initial); % The duplicate entries are removed and the modified data is
arranged in ascending order.
k = (1:length(Conc))'; % Purity Levels
format long; % This is required because purity calculations lead to same purities for close
concentrations upon rounding off.
Pury = PurityFresh(Conc);
```

Allocation of Flowrates

```
Demand = zeros(length(Conc),1);
for ii = 1:length(Conc) % Allocation of Demands
    for jj = 1:r1
        if Conc(ii) == DData{jj,4}
            Demand(ii) = Demand(ii) + DData{jj,3};
        end
    end
end
Source = zeros(length(Conc),1);
for ii = 1:length(Conc) % Allocation of Sources
    for jj = 1:r2
        if Conc(ii) == SData{jj,4}
            Source(ii) = Source(ii) + SData{jj,3};
        end
    end
end
NetDemand = Source - Demand;
N = [k Conc' Pury' Demand Source NetDemand];
```

Getting Level/Index of Fresh Water Concentrations

```
Ind = zeros(length(FWConc),1);
for i = 1:length(FWConc)
    for j = 1:length(k)
        if FWConc(i) == Conc(j)
            Ind(i) = j;
            break;
        end
    end
end

end
```

B.3. trgt.m

Program for carrying out targeting of different Fresh Water sources. The input to the program is the output of imnor.m and the concentrations of the fresh water sources available for use. The output includes targeted values of all the fresh water sources available. If multiple sources are fed as input, then the algorithm works towards maximizing the use of sources of poorer quality or alternately, minimizing the use of sources of higher quality. This is discussed in a little depth in Chapter 3.

```
function FW_f = trgt(N,Ind,FWC)
FWC = sort(FWC,'ascend');
FW_f = zeros(length(Ind),1); % Preallocating Fresh water Source Values. The number of sources
will be equal to the number of Fresh water Conc. available.
[~, ~, ~, ~, IFWD] = wca(N,Ind,FW_f,FWC); % Need only Interval fresh water demand because the
nature of these values (positive or negative) will detemine the fresh water deficit in the
concerned interval.
Ind = sort(Ind,'ascend'); % Ind will already be in ascending order but we are still doing sorting
as a preventive measure for errors not thought of till now. This vector is generated by 'imnor'
where concentrations are already arranged in the ascending order by the program.
if min(IFWD) >= 0
    fprintf('Threshold Case: No Fresh Water Required.\n');
    return;
    % The threshold concentration will be...
end
if length(Ind) > 1 % If there are more than one FW concentrations, then FW targets will be be
calculated for each of them.
    for i = 1:length(Ind)-1
        a = Ind(i)+1;
        b = Ind(i+1);
        if min(IFWD(a:b)) < 0 % If the min value is >= 0, then that particular FW source will
remain zero only.
            FW_f(i) = -1*min(IFWD(a:b));
        end
        [~, ~, ~, ~, IFWD] = wca(N,Ind,FW_f,FWC);
    end
    a = b + 1;
    b = N(end,1);
    if min(IFWD(a:b)) < 0
        FW_f(end) = -1*min(IFWD(a:b));
    end
else % Simple single targeting for only one FW source, whether impure or pure.
    a = Ind(1) + 1;
    b = N(end,1);
    if min(IFWD(a:b)) < 0
        FW_f = -1*min(IFWD(a:b));
    end
```

```
end
end
```

B.4. wca.m

Program to carry out the complete WCA. Using the partial WCT, it completes the WCT and therefore, makes it ready to be analyzed by trgt.m for target value(s) and pinch point(s).

```
function [delP, F_C, PWSurp, cumPWSurp, IFWD] = wca(N,Ind,FW,FWC)
```

Putting the FW Concentration and Indices in descending order.

```
Ind = sort(Ind,'descend');
[~, I] = sort(FWC,'descend');
FW = FW(I); % Accordingly, the flowrates have to be set in the right order, corresponding to the
right concentration.
```

Updating the Sources Values of the FW Concentration Sources

```
N(Ind,6) = N(Ind,6) + FW;
```

Calculating the remaining columns of the WCT

```
delP = -1*diff(N(:,3));
F_C = cumsum(N(1:end-1,6));
PWSurp = delP.*F_C;
cumPWSurp = cumsum(PWSurp);
cumPWSurp = [NaN;cumPWSurp];
```

Calculating the Interval Fresh Water Demand

```
IFWD = nan(row(N),1); % Pre-allocating the Interval Fresh water Demand Column
a = Ind(1);
b = row(N);
if length(Ind) > 1
    for i = 1:length(Ind)-1 % The value of the lower index is changed. For i = length(Ind), a
will try to access out-of-bounds/non-existent value of Ind. Hence, it is restricted to
length(Ind)-1.
        for j = a+1:b
            IFWD(j) = cumPWSurp(j)/(N(a,3)-N(j,3));
        end
    b = a; % The value of the lower index is changed.
    a = Ind(i+1);
    end
    for j = a+1:b % For the last index set. For interval fresh water demand calculation.
        IFWD(j) = cumPWSurp(j)/(N(a,3)-N(j,3));
```

```
    end
else % If only one FW Source is there!
    for j = a+1:b
        IFWD(j) = cumPWSurp(j)/(N(a,3)-N(j,3));
    end
end
% IFWD(1) = nan. This is non-existent because the denominator terms contain the difference b/w
the same values, i.e., 0. The conceptual reason is...
IFWD = round(IFWD,6); % Rounding off to 6 significant digits because more accuracy may not be
required. Moreover, excessively small value can be treated as pinch point itself because...

end
```

B.5. fzbl.m

Program to Update the vectors containing fresh water concentrations and corresponding indices/levels and the WCT (partial) depending upon fresh water source availability. Inputs: targeted flowrates of fresh water sources, their availabilities, concentrations and indices/levels, and the partial WCT (denoted by N).

```
function [New_FWConc,New_N,New_Ind] = fzbl(FW_f,Availability,FWConc,N,Ind)
for i = 1:length(Ind)
    if FW_f(i) > Availability(i) % If the targeted flowrate at the concentration under
consideration is more than what is available, then whatever is available is added to the source
of that particular concentration.
        N(Ind(i),6) = N(Ind(i),6) + Availability(i);
        FWConc(i) = []; % The concentration corresponding to the new greater source is removed or
put to 'nill' for re-targeting.
        Ind(i) = []; % The concentration index (index: level at which that particular
concentration lies in the second column of the WCT) corresponding to the new greater source is
removed or put to 'nill' for re-targeting.
    end
end
New_FWConc = FWConc; % Updated set of FW Cocentration(s) is the output.
New_N = N; % N is the matrix containing the first six columns of the WCT. Here, it is updated if
some of the sources have been updated.
New_Ind = Ind; % The index column is updated and is one of the outputs. It contains new reduced
number of levels.
end
```

B.6. nantonill.m

Program to discard 'NaN' from the input vector. In MATLAB, NaN denotes ‘not a number’. The output is new vector in the same order but without the ‘NaN’ entries.

```
function out = nantonill(in)
j = 1;
count = 0;
for i = 1:length(in) % Loop for counting the number of 'NaN' occurences. This no. of occurences
will then be equal to the length of the output 'out'.
    if ~isnan(in(i))
        count = count + 1;
    end
end
out = zeros(count,1);
for i = 1:length(in) % Loop for filling up the output 'out'. It will have all the non 'NaN'
members of the input '
    if ~isnan(in(i))
        out(j) = in(i);
        j = j+1;
    end
end
end
```

B.7. FWAug_v2.m

Program to produce rows which will be augmented to the final FW matrix when the availability of a certain input source is less than the targeted value of the same concentration. This type of arrangement is required because when a particular source is lower than its target/required value, retargeting is carried out after increasing the source value (in WCT) at the level of the limited FW Source in the cascade table. In the process, the concerned FW source is lost. This program will allow us to retain that particular FW Source and later augment the same to the final fresh water matrix (FW_Matrix). Inputs: vectors containing FW concentrations before and after availability check done by fzbl.m, and availability before the availability check. Outputs: Row containing concentration and flowrate of the limited fresh water which was earlier considered as an inherent part of the network, updated vectors of FW concentrations and availabilities. The concentration and availability of the FW source(s) extracted as row(s) is discarded from the input vectors.

```
function [F_Row_Augment, FWConc_Dupli, Availability_Dupli] =
FWAug_v2(FWConc_Dupli,Availability_Dupli,FWConc)
[~, i] = setdiff(FWConc_Dupli,FWConc);
F_Row_Augment = [FWConc_Dupli(i) Availability_Dupli(i)];
FWConc_Dupli(i) = [];
Availability_Dupli(i) = [];
end
```

B.8. thresh2.m

Program to update Pinch Point, fresh water flowrates (FW_f), and wastewater flowrate (F_C) for Zero Wastewater Discharge Case. Preference to lower quality sources is given in order to remove the flowrate constraint violation. After evaluating the Zero Network Discharge Threshold Case, if the flowrate constraint is not satisfied, this program will first update FW_f and then, F_C and pinch point (PinchP) after retargeting with the updated FW_f. The availability of the sources is also considered. If the lowest quality source, doesn't have the required availability, whatever amount is available is used, and then the remaining flowrate deficit is tried to recovered with the second lowest quality source and so on.

```
function [UpdatedInput1,UpdatedInput2,UpdatedInput3,UpdatedInput4] =
thresh2(F_C,N,Ind,FW_f,FWConc,PinchP,PinchP_Duplicate,Availability)
if F_C(end) == 0
    fprintf('Threshold Case: Zero Network Discharge.\n');
    fprintf('Here, the WW water discharge was already zero, post trageting.\n');
    % The threshold concetration will/will not exist because...
end
F_C_dummy = -F_C(end); % This dummy variable is being created for aiding the availability check.
if F_C(end) < 0
    for m = length(Availability):-1:1
        if Availability(m) <= F_C_dummy && F_C_dummy > 0 && Availability(m) > 0
            F_C_dummy = F_C_dummy - Availability(m);
            FW_f(m) = FW_f(m) + Availability(m);
            Availability(m) = 0;
        elseif Availability(m) > F_C_dummy && F_C_dummy > 0
            Availability(m) = Availability(m) - F_C_dummy;
```

```
            FW_f(m) = FW_f(m) + F_C_dummy;
            F_C_dummy = 0;
            break;
        end
    end
    if round(F_C_dummy,6) ~= 0
        error('The availability of sources is lower than what is required for satisfying the
flowrate constraints.');
    end
    fprintf('Threshold Case: Zero Network Discharge.\n');
    [~, F_C, ~, ~, IFWD] = wca(N,Ind,FW_f,FWConc); % Updating the water cascade using Targeted
Values.
    PinchP1 = []; % Initiating the vector which will contain Pinch Points.
    for i = 2:row(N)
        if IFWD(i) == 0 % If Interval Fresh Water Demand is zero, then the corresponding Source
concentration is a Pinch Point.
            PinchP1 = [PinchP1; N(i,2)]; % Making new pinch concentration column after the
flowrates have been adjusted.
        end
    end
    PinchP = PinchP1; % Updating the New Pinch Points
%     %% Defining the Threshold Concentration(s)
%     fprintf('The Threshold Concentration(s) are:\n');
%     ThreshCon = setdiff(PinchP_Duplicate,PinchP1);
%     fprintf('%d \n',ThreshCon);
end
UpdatedInput1 = FW_f;
UpdatedInput2 = F_C;
UpdatedInput3 = PinchP;
UpdatedInput4 = Availability;
end
```

B.9. thresh2aliter.m

Alternate Program to update Pinch Point, FW_f, and F_C for Zero Wastewater Discharge Case. Preference is given to higher quality sources. The same updates as in thresh2.m are made. The flowrate deficit is tried to recovered by using the highest quality impure source and then moving towards the second best impure source and so on. If the impure sources are not able to able to recover the deficit, then the pure FW source is considered.

```
function [UpdatedInput1,UpdatedInput2,UpdatedInput3,UpdatedInput4] =
thresh2aliter(F_C,N,Ind,FW_f,FWConc,PinchP,PinchP_Duplicate,Availability)
if F_C(end) == 0
    fprintf('Threshold Case: Zero Network Discharge.\n');
    fprintf('Here, the WW water discharge was already zero, post trageting.\n');
```

```
end
F_C_dummy = -F_C(end); % This dummy variable is being created for aiding the availability check.
if F_C(end) < 0
    [FW_Impure, Availability_Impure, FW_Pure, Availability_Pure] =
alitersort(FWConc,FW_f,Availability);
    for m = 1:length(FW_Impure)
        if Availability_Impure(m) <= F_C_dummy && F_C_dummy > 0 && Availability_Impure(m) > 0
            F_C_dummy = F_C_dummy - Availability_Impure(m);
            FW_Impure(m) = FW_Impure(m) + Availability_Impure(m);
            Availability_Impure(m) = 0;
        elseif Availability_Impure(m) > F_C_dummy && F_C_dummy > 0
            Availability_Impure(m) = Availability_Impure(m) - F_C_dummy;
            FW_Impure(m) = FW_Impure(m) + F_C_dummy;
            F_C_dummy = 0;
            break;
        end
    end
    if round(F_C_dummy,6) ~= 0
        if ~isempty(Availability_Pure) && Availability_Pure < F_C_dummy
           error('The availability of pure and impure sources is lower than what is required to
satisfy the flowrate constraints.');
        elseif ~isempty(Availability_Pure) && Availability_Pure >= F_C_dummy
            Availability_Pure = Availability_Pure - F_C_dummy;
            FW_Pure = FW_Pure + F_C_dummy;
            F_C_dummy = 0;
        elseif isempty(Availability_Pure)
            error('The availability of impure sources is lower than what is required to satisfy
the flowrate constrints. Moreover, no pure source is available to overcome the flowrate
deficit.');
        end
    end
    fprintf('Threshold Case: Zero Network Discharge.\n');
    Availability = [Availability_Pure; Availability_Impure];
    FW_f = [FW_Pure; FW_Impure];
    [~, F_C, ~, ~, IFWD] = wca(N,Ind,FW_f,FWConc); % Updating the water cascade using Targeted
Values.
    PinchP1 = []; % Initiating the vector which will contain Pinch Points.
    for i = 2:row(N)
        if IFWD(i) == 0 % If Interval Fresh Water Demand is zero, then the corresponding Source
concentration is a Pinch Point.
            PinchP1 = [PinchP1; N(i,2)]; % Making new pinch concentration column after the
flowrates have been adjusted.
        end
    end
    PinchP = PinchP1; % Updating the New Pinch Points
%     %% Defining the Threshold Concentration(s)
%     fprintf('The Threshold Concentration(s) are:\n');
%     ThreshCon = setdiff(PinchP_Duplicate,PinchP1);
%     fprintf('%d \n',ThreshCon);
end
UpdatedInput1 = FW_f;
UpdatedInput2 = F_C;
UpdatedInput3 = PinchP;
```

```
UpdatedInput4 = Availability;
end
```

B.10. row.m

Function that gives the number of rows (r) of the Matrix (in).

```
function r = row(in)
[r,~] = size(in);
end
```

B.11. PurityFresh.m

Function that gives the purity, P, (Hallale 2002) of a feed of concentration, C. The function is vectorized and hence, can run with a vector of concentrations also.

```
function P = PurityFresh(C)
P = (10^6 - C)./(10^6);
end
```

APPENDIX C

Sub-routines Developed for Network Design

C.1. Shenoy.m

Program that gives nearest neighbours to a particular concentration (d) from a pool of the concentrations (SourceC).

```
function [Cl,Ch] = Shenoy(SourceC,d)
S = unique([SourceC',d]);
if d == S(1) || d == S(end)
    disp(d);
    error('The concerned sink cannot be satisfied by the available sources.');
end
for ii = 1:length(S)
    if S(ii) == d
        Cl = S(ii-1); % Lower Conc. than given.
        Ch = S(ii+1); % Higher Conc. than given.
        break;
    end
end
end
```

C.2. ShenFun.m

Program that represents the flowrate and contaminant load constraints.

```
function y = ShenFun(x,Cl,Ch,F_Req,Gray_F,Gray_C,FlCl_Before,FhCh_Before,FCEqualBefore)
y(1) = x(1)*Cl + x(2)*Ch + FlCl_Before + FhCh_Before + FCEqualBefore - Gray_F*Gray_C;
y(2) = x(1) + x(2) - F_Req;
end
```

C.3. concUpdate.m

This Program updates the Source/Demand Pool (in) after water allocation lead to complete exhaustion of a source of concentration, ‘flag’.

```
function out = concUpdate(in,flag)
for i = 1:length(in)
    if in(i) == flag
        in(i) = [];
        break;
    end
end
out = in;
end
```

C.4. searcon.m

Program to search the index (out) of a concentration (C) in a vector N.

```
function out = searcon(C,N)
for i = 1:length(N)
    if N(i) == C
        N(i) = nan;
        out = N;
        break;
    end
end
```

References

Alturkmani, A., *INDUSTRIAL WASTEWATER*, Homs - Syria. Available at: http://www.4enveng.com/userimages/INDUSTRIAL WASTEWATER.pdf.

Bond, R.G. et al., 1972. *CRC Handbook of Environmental Control*, CRC Press. Available at: https://books.google.co.in/books?id=HQOOjgEACAAJ.

Camargo, J.A. & Alonso, Á., 2006. Ecological and toxicological effects of inorganic nitrogen pollution in aquatic ecosystems: A global assessment. *Environment International*, 32(6), pp.831–849.

Changming, L., Jingjie, Y. & Kendy, E., 2001. Groundwater exploitation and its impact on the environment in the North China Plain. *Water International*, 26(2), pp.265–272. Available at: https://apps.webofknowledge.com/full_record.do?product=UA&search_mode=GeneralSearch&qid=8&SID=X2FPEOB44D1gbBBey3B&page=1&doc=2&cacheurlFromRightClick=no.

Chungsiriporn, J., Prasertsan, S. & Bunyakan, C., 2006. Minimization of water consumption and process optimization of palm oil mills. *Clean Technologies and Environmental Policy*, 8, pp.151–158.

Deng, C. & Feng, X., 2009. Optimal water network with zero wastewater discharge in an alumina plant. *WSEAS Trans. Environ. Dev.*, 2(5), pp.146–156.

El-Halwagi, M.M., 1997. *Pollution Prevention through Process Integration: Systematic Design Tools*, San Diego: Academic Press.

El-Halwagi, M.M., Gabriel, F. & Harell, D., 2003. Rigorous Graphical Targeting for Resource Conservation via Material Recycle/Reuse Networks. *Industrial & Engineering Chemistry Research*, 42(19), pp.4319–4328. Available at: http://pubs.acs.org/doi/abs/10.1021/ie030318a.

Esteller, M.V. & Diaz-Delgado, C., 2002. Environmental effects of aquifer overexploitation: A case study in the highlands of Mexico. *Environmental Management*, 29(2), pp.266–278.

Foo, D.C.Y., 2008. Flowrate targeting for threshold problems and plant-wide integration for water network synthesis. *Journal of Environmental Management*, 88, pp.253–274.

Foo, D.C.Y., 2012. *Process Integration for Resource Conservation*,

Foo, D.C.Y., 2009. State-of-the-Art Review of Pinch Analysis Techniques for Water Network Synthesis. *Industrial & Engineering Chemistry Research*, 48(11), pp.5125–5159. Available at: http://dx.doi.org/10.1021/ie801264c\nhttp://pubs.acs.org/doi/pdfplus/10.1021/ie801264c\nhttp://pubs.acs.org/doi/abs/10.1021/ie801264c.

Foo, D.C.Y., 2007. Water Cascade Analysis for Single and Multiple Impure Fresh Water Feed. *Chemical Engineering Research and Design*, 85(8), pp.1169–1177. Available at: http://www.sciencedirect.com/science/article/pii/S0263876207731556\nhttp://linkinghub.elsevier.com/retrieve/pii/S0263876207731556.

Fry, A., 2005. *Facts and Trends, Water*, Conches-Geneva.

Hallale, N., 2002. A new graphical targeting method for water minimisation. *Advances in Environmental Research*, 6(3), pp.377–390.

India-Water-Tool, India Water Tool: Water Stress Indicators - Baseline Water Stress.

Jacob, J. et al., 2002. Water network analysis in pulp and paper processes by pinch and linear programming techniques. *Chemical Engineering Communications*, 189(2), pp.184–206. Available at: http://www.tandfonline.com/doi/abs/10.1080/00986440211836.

Jing-jie, Y., Guo-bin, F. & Hong-zun, R., 1999. Environmental problems in coastal zone of China-sea-level rise and groundwater table decline. *JOURNAL OF CHINESE GEOGRAPHY*, 9(3), pp.307–312.

Kemp, I.C., 2007. *Pinch Analysis and Process Integration: A User Guide on Process Integration for the Efficient Use of Energy*, Butterworth-Heinemann.

Liao, Z., Wang, J. & Yang, Y., 2011. Wastewater Minimization in a Chlor-Alkali Complex. In F. S. G. Einschlag, ed. *Waste Water - Treatment and Reutilization*. InTech, pp. 407–426. Available at: http://www.intechopen.com/books/waste-water-treatment-andreutilization/wastewater-minimization-in-a-chlor-alkali-complex.

Linnhoff, B. et al., 1982. *A User Guide on Process Integration for the Efficience Use of Energy*, Rugby: IChemE.

Liu, Y.A., Lucas, B. & Mann, J., 2004. Up-to-date tools for water-system optimization. *Chemical Engineering Magazine*, pp.30–41.

Majozi, T., Brouckaert, C.J. & Buckley, C.A., 2006. A graphical technique for wastewater minimisation in batch processes. *Journal of Environmental Management*, 78(4), pp.317–329.

Manan, Z. a., Wan Alwi, S.R. & Ujang, Z., 2006. Water pinch analysis for an urban system: a case study on the Sultan Ismail Mosque at the Universiti Teknologi Malaysia (UTM). *Desalination*, 194(1-3), pp.52–68.

Manan, Z.A., Tan, Y.L. & Foo, D.C.Y., 2004. Targeting the minimum water flow rate using water cascade analysis technique. *AIChE Journal*, 50(12), pp.3169–3183.

Millennium-ecosystem-assessment, 2005. *MEA (Millennium ecosystem assessment) Ecosystems and Human Well-Being: Current State and Trends.*, Washington, DC.

Nabi Bidhendi, G.R., Mehrdadi, N. & Mohammadnejad, S., 2010. Water and Wastewater Minimization in Tehran Oil Refinery using Water Pinch Analysis. *International Journal of Environmental Research*, 4(4), pp.583–594. Available at: http://ijer.ut.ac.ir/article_244_1.html.

National Park Service, Conservation vs Preservation and the National Park Service. Available at: https://www.nps.gov/klgo/learn/education/classrooms/conservation-vs-preservation.htm [Accessed March 6, 2016].

Ng, D.K.S. et al., 2008. Extension of targeting procedure for " Ultimate Flowrate Targeting with Regeneration Placement " by Ng et al ., Chem . Eng . Res . Des ., 85 (A9): 1253 – 1267. *Chemical Engineering Research and Design*, 6, pp.1182–1186.

Ng, D.K.S., Foo, D.C.Y., Tan, R.R., et al., 2007. ULTIMATE FLOWRATE TARGETING WITH REGENERATION PLACEMENT. *Chemical Engineering Research and Design*, A9(September), pp.1253–1267.

Ng, D.K.S., Foo, D.C.Y. & Tan, R.R., 2007a. Targeting for total water network. 1. Waste stream identification. In *Industrial and Engineering Chemistry Research*. pp. 9107–9113.

Ng, D.K.S., Foo, D.C.Y. & Tan, R.R., 2007b. Targeting for total water network. 2. Waste treatment targeting and interactions with water system elements. *Industrial and Engineering Chemistry Research*, 46(26), pp.9114–9125.

Olankule, M.S. & Ityokumbul, M.T., 2014. Industrial Wastewater Management: The Water Pinch Analysis Approach. *IMPACT; International Journal of*

Research in Engineering & Technology, 2(7), pp.33–40.

Parand, R. et al., 2013. Targeting water utilities for the threshold problem without waste discharge. *Chemical Engineering Research and Design*, 91(12), pp.2569–2578. Available at: http://dx.doi.org/10.1016/j.cherd.2013.05.004.

Polley, G.T. & Polley, H.L., 2000. Design better water networks. *Chemical Engineering Progress*, 96(2), pp.47–52.

Prakash, R. & Shenoy, U. V., 2005a. Design and evolution of water networks by source shifts. *Chemical Engineering Science*, 60(7), pp.2089–2093. Available at: http://www.sciencedirect.com/science/article/pii/S0009250904008966 [Accessed January 16, 2016].

Prakash, R. & Shenoy, U. V., 2005b. Targeting and design of water networks for fixed flowrate and fixed contaminant load operations. *Chemical Engineering Science*, 60(1), pp.255–268. Available at: http://www.sciencedirect.com/science/article/pii/S0009250904005998 [Accessed January 16, 2016].

Salameh, E., 2008. Over-exploitation of groundwater resources and their environmental and socio-economic implications: The case of Jordan. *Water International*, 33(1), pp.55–68.

Schulte, P., 2014. Defining Water Scarcity, Water Stress, and Water Risk: It's Not Just Semantics. Available at: http://pacinst.org/water-definitions/ [Accessed February 10, 2016].

Schwarzenbach, R.P. et al., 2010. Global Water Pollution and Human Health. *Annual Review of Environment and Resources*, 35(1), pp.109–136.

Shenoy, U. V., 2012. Enhanced nearest neighbors algorithm for design of water networks. *Chemical Engineering Science*, 84, pp.197–206. Available at: http://www.sciencedirect.com/science/article/pii/S000925091200509X [Accessed January 16, 2016].

Shiao, T. et al., 2015. 3 Maps Explain India's Growing Water Risks. *World Resources Institute*.

Shukla, S.K. et al., 2013. Designing plant scale process integration for water management in an Indian paper mill. *Journal of environmental management*, 128, pp.602–14. Available at: http://www.sciencedirect.com/science/article/pii/S0301479713004155 [Accessed May 29, 2016].

Singanan, M. & Peters, E., 2013. Removal of toxic heavy metals from synthetic wastewater using a novel biocarbon technology. *Journal of Environmental Chemical Engineering*, 1(4), pp.884–890.

Smith, R., 2005. Water System Design. In *Chemical Process Design and Integration*. John Wiley and Sons Ltd., pp. 581–624.

Tapiero, H., Townsend, D.M. & Tew, K.D., 2003. Trace elements in human physiology and pathology. Copper. *Biomedicine and Pharmacotherapy*, 57(9), pp.386–398.

The-Institute-of-Chemical-Engineers, 2000. *Guide to Industrial Water Conservation. Part 1. Water re-use in Single Contamiant Systems*, Rugby.

Thevendiraraj, S. et al., 2003. Water and wastewater minimisation study of a citrus plant. *Resources, Conservation and Recycling*, 37(3), pp.227–250.

UNICEF, 2013. UNICEF (United Nations Children's Fund) WASH Sector, Syria.

UN-Water, 2014. Water scarcity. Available at: http://www.un.org/waterforlifedecade/scarcity.shtml [Accessed February 7, 2016].

UN-WWAP, 2015. *WWAP (United Nations World Water Assessment Programme). The United Nations World Water Development Report 2015: Water for a Sustainable World.*, Paris.

Wan Alwi, S.R. & Manan, Z.A., 2006. SHARPS - A new cost-screening technique to attain cost-effective minimum water utilisation netwrok. *AIChE Journal*, 11(52), pp.3981–3988.

Wan Alwi, S.R. & Manan, Z.A., 2013. Water Pinch Analysis for Water Management and Minimisation: An Introduction. In *Handbook of Process Integration (PI)*. pp. 353 – 380.

Wang, Y. & Smith, R., 1994. Wastewater Minimization. *Computers & Chemical Engineering*, 49(7), pp.981–1006. Available at: http://www.sciencedirect.com/science/article/pii/0009250994800065.

Wenzel, H. et al., 2001. Process integration design methods for water conservation and wastewater reduction in industry. Part 3: Experience of industrial application. *Clean Technologies and Environmental Policy*, 4, pp.16–25. Available at: http://dx.doi.org/10.1007/s10098-001-0122-y\nhttp://dx.doi.org/10.1007/s100980100121.

Westerberg, A.W., 1987. Process Synthesis: A Morphology Review. In Y. A. Liu,

H. A. McGee, & W. R. Epperly, eds. *Recent Developments in Chemical Process and Plant Design*. New York: John Wiley and Sons.

World-Health-Organization, 2008. *Guidelines for drinking-water quality: recommendations* Third., Geneva: World Health Organization.

Zhou, Q.., Lou, H.H.. & Huang, Y.L.., 2001. Design of a switchable water allocation network based on process dynamics. *Industrial and Engineering Chemistry Research*, 40(22), pp.4866–4873. Available at: http://www.scopus.com/inward/record.url?eid=2-s2.0-0035980422&partnerID=40&md5=5a55387a6b7643b454bd441db7083e0b.

Cite this work as:

Goyal, M. (2016). *Single Contaminant Based Water Pinch Analysis*. B. Engg. Project. Department of Petrochemical Engineering, Maharashtra Institute of Technology, Savitribai Phule Pune University, Pune, India.