

# **WASTEWATER MINIMIZATION USING ASPEN WATER**

*A Project Report submitted by*

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*In partial fulfillment of the requirements  
of the degree of*

**Bachelor of Technology in Chemical Engineering**

**Under the guidance of**

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## **CERTIFICATE**

This is to certify that the thesis entitled, “**Wastewater Minimization using Aspen Water**” submitted by **S R Shubham**, Roll No. 107CH029, in partial fulfillment of the requirements for the award of Bachelor of Technology Degree in Chemical Engineering at the National Institute of Technology, Rourkela is an authentic work carried out by him under my supervision and guidance.

To the best of my knowledge, the matter embodied in the thesis has not been submitted to any other university / institute for the award of any Degree or Diploma.

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## **ABSTRACT**

This thesis lays out the basic principles for analyzing a water using operation and then compares the freshwater and wastewater flowrates for a system with and without reuse. The methods of reuse, recycle and regeneration are discussed to solve the problems of multiple contaminants with multiple constraints. The preliminary mass exchange network is designed and further optimization is carried out by using ASPEN WATER software. Along with network optimizations for minimum water use, minimum network costs which include water costs or discharge costs, can also be determined with help of the software. Minimizing water use as well as the wastewater discharged from a water network are main priorities of the present work.

Two industrial case studies are discussed to illustrate the significance of wastewater minimization and the results obtained are compared with that predicted using published method. The first one is a multiple contaminants problem for a starch industry in which water saving was found to be 41% for Demineralised water and 80% for freshwater with water cost savings of about 45% and the second is a analysis of streams in petroleum refining complex in which freshwater savings was around 82%.

**Key Words:** Wastewater minimization, multiple contaminants, ASPEN WATER

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## NOMENCLATURE AND ABBREVIATIONS

C: Concentration of Contaminants, ppm

m: Mass of Contaminants, kg/hr

C<sub>proc, in</sub>: Concentration of Contaminants in inlet process stream, ppm

C<sub>proc, out</sub>: Concentration of Contaminants in outlet process stream, ppm

C<sub>w, in</sub>: Concentration of contaminants in inlet water stream, ppm

C<sub>w, out</sub>: Concentration of contaminants in outlet water stream, ppm

ppm: Parts per Million

t/h: Tons per Hour

TDS: Total Dissolved Solids

TSS: Total Suspended Solids

TOC: Total Organic Content

DM Water: Demineralised Water

H<sub>2</sub>S: Hydrogen Sulfide

### INTRODUCTION

With increasing population and decreasing water resources, a lot of focus has now shifted towards conservation of water both in domestic as well as industrial processes. The process industries, which includes chemicals, petrochemicals, petroleum refining, pharmaceuticals, pulp and papers and certain food and consumer products, represents a major portion of the world economy, use a huge quantity of water in their various processes and as a result generate a lot of wastewater. The generation of vast quantities of wastewater demands that methods are to be developed to minimize the freshwater requirements of these processes for the optimization of the process industries. (Mann and Liu, 1999)

Moreover, the increasing cost of freshwater and the treatment of wastewater compels the process plants to focus on the minimization of freshwater consumption. A direct consequence of this step is a reduction in generation of effluent and reduced treatment costs. Hence, the systematic approach to design of water recovery network has become a topic of interest in the field of research in the past few years. (Gomes et al., 2005)

Many of the industrial users of fresh water are under increasing pressure to reuse water within their facilities. Their main goal is to minimize the amount of water that is discharged, either to a receiving stream or a publicly-owned treatment works. There are a variety of reasons for this pressure, such as: (McIntyre, 1993)

- The cost of fresh water
- The cost of additional treatment to reach discharge limits fixed by governments

- Water availability in the area
- Environmental awareness
- Community relations

Wastewater minimization practices are carried in many heavy industries, process industries etc. such as:

- Complex organic chemical industry: Many industries manufacture or use complex organic chemicals. E.g. pesticides, pharmaceuticals, petrochemicals, pulp and paper etc.
- Water treatment: Industries are always in need water of high quality for processes free from one contaminant or multiple contaminants.
- Food industry: Wastewater produced here is biodegradable, non-toxic but has high concentration of biological oxygen demand (BOD) and suspended solids.
- Petroleum Refining: Wastewater is produced in number of unit like distillation unit, a hydrodesulphurization (HDS) reactor, and desalter unit.

The synthesis of a water recovery network can be stated as “*Given a set of water-using processes, it is desired to determine a network of interconnections of water streams among the water-using processes so that the overall fresh water consumption is minimized while the processes receive water of adequate quality*”. (Savelski and Bagejewicz, 2000)

In the present work the water network is proposed for water minimization in starch industry with large number of water using units like reactor, separator, washing unit, cooling towers etc using demineralized water and fresh water and a petroleum refinery complex consisting of a steam stripper, a hydrodesulphurization unit (HDS) and a desalter using fresh

water. The starch industry has contaminants like Total Organic Content (TOC), Total Dissolved solids (TDS) and Total suspended solids (TSS) while the refinery complex has contaminants like hydrocarbons, H<sub>2</sub>S and salt.

To carry out water management for above processes following objectives are to be aimed:

1. *Analysis of the problem* - This involves studying the requirements of the problem, setting targets, identifying the minimum freshwater consumption and wastewater generation in the water using operations.
2. *Design of the network* - This involves designing a water using network that achieves the identified flowrate targets given present water utilizing network using ASPEN WATER.
3. *Optimization of the network* - This involves optimizing the designed network to reduce the effluent discharge and to make the process economically viable i.e. reducing the cost of water using ASPEN WATER.
4. *Comparison of result with published work* - The results obtained from the above analysis are compared with the published work to determine their validity and significance.

### LITERATURE REVIEW

The concept of reusing water started to be investigated systematically in the 1980s. This problem has received the name of Water/Wastewater Allocation Planning (WAP) problem. The search for optimal wastewater reuse solutions was addressed by industry itself more than 20 years ago. Two major systematic strategies were developed: the use of superstructures coupled with mathematical programming and a graphic targeting procedure coupled with loop breaking. (Savelski and Bagejewicz, 2000)

If we exclude the possibility of making fundamental changes to processes to reduce their inherent demand for water, there are three possibilities for reducing wastewater:

(i) *Re-use*: Wastewater can be re-used directly in other operations providing the level of previous contamination does not interfere with the process. Re-use might require wastewater being blended with wastewater from other operations and/or freshwater. (Note that there may be recycling within an individual operation but here we consider only the net input and output from operations.)

(ii) *Regeneration re-use*: Wastewater can be regenerated by partial treatment to remove the contaminants, which would otherwise prevent its re-use, and then re-used in other operations. Again, re-use after regeneration might require blending with wastewater from

other operations and/or freshwater. Let us emphasize that when water is re-used after regeneration, in this case it does not re-enter processes in which it has previously been used.

(iii) *Regeneration recycling*: Wastewater can be regenerated to remove contaminants which have built up and then the water recycled. In this case water can re-enter processes in which it has previously been used. (Wang and Smith, 1994)

To incorporate above three possibilities the root of mathematical modeling and pinch technology were proposed.

## **2.1 Mathematical Modeling approach**

Takama *et al.* (1980) used mathematical programming to solve a refinery example. A superstructure of all water using operations and cleanup processes was set up and an optimization was then carried out to reduce the system structure (super structure) by removing irrelevant and uneconomical connections. (Savelski and Bagejewicz, 2000)

Later, El-Halwagi and Manousiouthakis (1990) automated the approach and introduced the concept of regeneration. In the first stage of their automated approach, a linear programming (LP) problem was formulated using thermodynamic constraints, whose solution determined the minimum cost and pinch points that limit the mass exchange between rich and lean streams. Then in the second stage a mixed integer linear program (MILP) transshipment problem was solved to identify the minimum number of mass exchange units. (Hallale *et al.*, 2000)

On the other hand, superstructure models present serious numerical difficulties. Due to the nonlinear nature of the constraints the straight use of Non Linear Programming (NLP) packages to solve the problem often renders infeasible solutions. Doyle and Smith (1997) proposed an iterative procedure to solve this bilinearly constrained problem.

Alva-Argaez et al. (1998) continued this line of work and proposed solving a two-phase procedure for the solution of a non-convex Mixed Integer Non Linear Programming (MINLP). Even after the problem has been successfully solved there is no guarantee about the optimality of the optimum. Finally, Huang et al. (1999) also presented a mathematical programming solution of the combined problem of water allocation and treatment. (Savelski and Bagejewicz, 2000)

## **2.2 Pinch Technology**

In the beginning, Pinch technology was initially used for the process of heat integration for the design of heat exchange networks to transfer energy from a set of hot streams to a set of cold process streams. A major breakthrough in this field was the identification of the pinch point temperature (Linhoff and Flower, 1978; Umeda et al, 1976). Linhoff et al. (1982) have applied the principles of thermodynamics and energy balance to systematically analyze heat flow across various temperature levels in a process. In this way, a temperature level, called the pinch point can be identified. The use of utilities is subject to certain constraints. Firstly, no heat is transferred across the pinch. Secondly, heat is added only above the pinch and lastly, cooling is done only below the pinch. In other words, hot process streams can be cooled more cost effectively above the pinch temperature by cold process streams as compared to cooling utility streams. Similarly, cold process streams can be heated below this point more effectively by using hot process streams than by using hot utility streams. Linhoff (1993) has

illustrated the use of pinch technology to calculate energy “targets,” such as the minimum hot and cold utilities required. A sample composite curve to illustrate the process is shown in Fig 2.1.

(Querzoli et al., 2003)

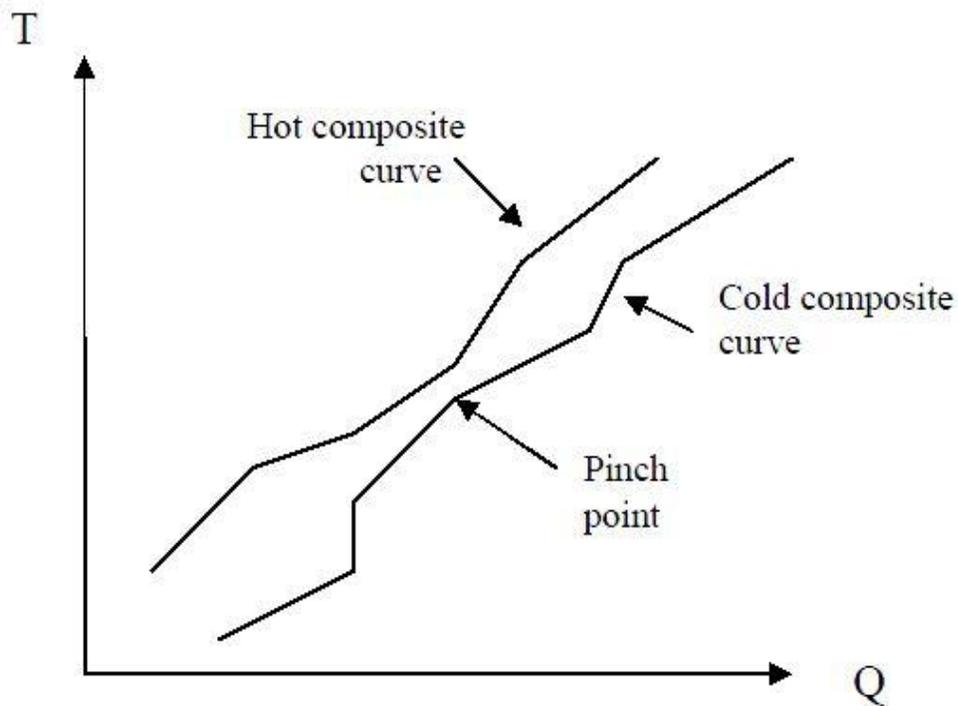


Figure 2.1 Composite Curve to determine pinch point temperature

The approach used in application of pinch technology to heat integration can be extended to mass integration. A mass exchange integration problem involves transferring mass from rich process streams (decreasing their concentrations) to lean process streams (increasing their concentrations) so that each stream reaches its desired concentration while minimizing waste production and utility consumption (including freshwater and mass separating agents) (Mann and Liu, 1999).

El-Halwagi and Manousiouthakis (1989) first introduced the concept of “mass transfer network”, where contaminants from a set of rich streams are transferred to a set of poor streams. Their approach was adapted from the methodology developed for heat exchanger networks by Linnhoff and Hindmarsh (1983). Based on the similar pattern as in heat integration El-Halwagi and Manousiouthakis (1989) showed how mass transfer composite curves could be plotted using a minimum composition difference. The mass transfer pinch can be located using this plot and the targets for the minimum flow rate of lean stream i.e. mass separating agent can be determined. A sample composite curve is presented in Fig. 2.2 to illustrate the method.

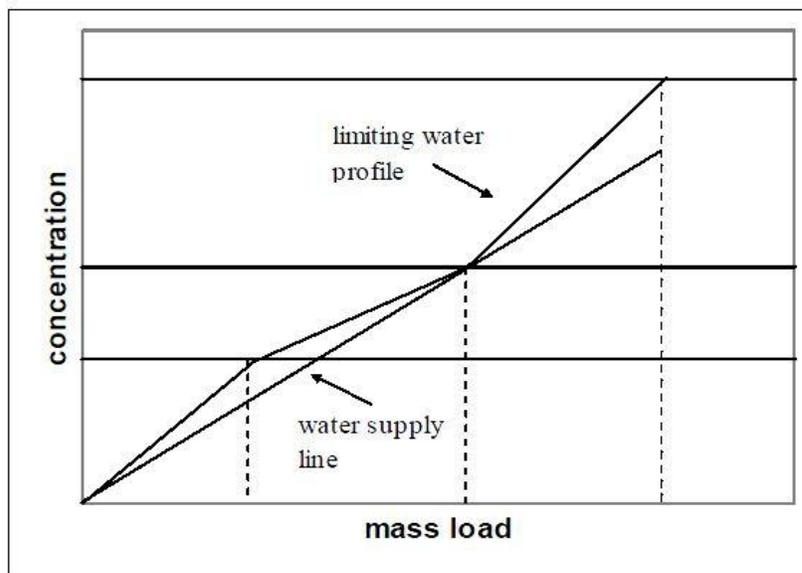


Figure 2.2 Composite curves to determine freshwater pinch concentration

Wang and Smith (1994) presented a method based on targeting and a design procedure based on heuristics similar to those used in heat exchanger network design. The targeting part of this procedure is in reality an application of mass exchange technology. Since mixing of lean streams was not introduced in the original work of El-Halwagi and Manousiouthakis (1989) or

the few immediate follow-up papers, Wang and Smith (1994) resorted to an ad-hoc design procedure based on the identified target. Despite these special approaches, the problem should be regarded as a mass exchanger network problem and not a separate area of research. Nevertheless, one cannot minimize the visionary work of Umeda (1980).

They proposed design methodology i.e. targeting minimum wastewater for single contaminants. The inlet and outlet concentration of contaminant in the process stream are specified by the process requirement, as is the mass of contaminant transferred. Specifying all this also specifies water flow rate. Limiting water profile i.e. in order to maximize the possibility of re-use of water from other operations to the given operation was drawn; water with highest possible inlet concentration was specified. Then specify the maximum possible outlet concentration which minimizes the water flow rate at maximum inlet concentration. This may not be the best possible design, any water supply line below limiting profile meets requirement of the process as presented in figures 2.3 and 2.4.

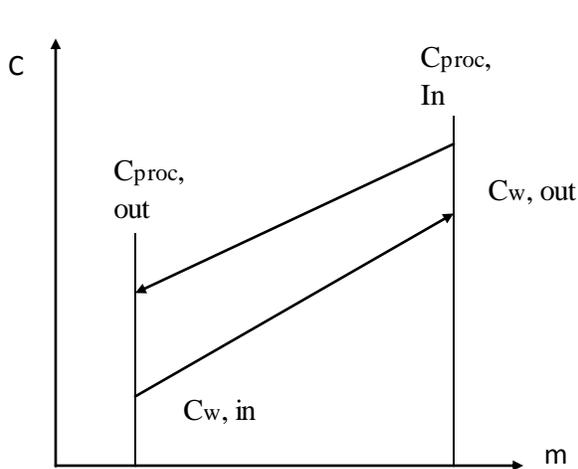


Figure 2.3 Concentration vs Mass of contaminants transferred for a process

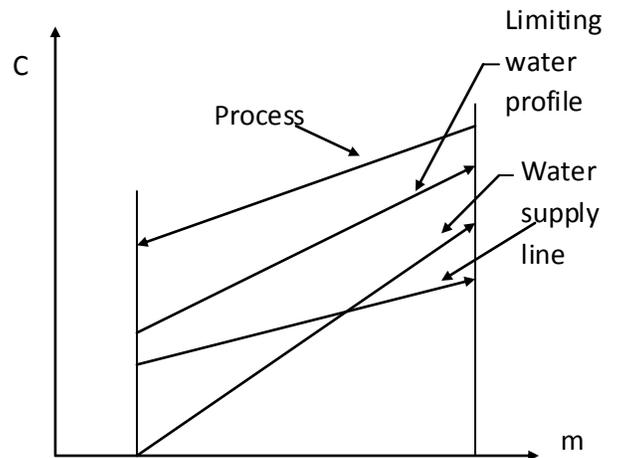


Figure 2.4 Limiting water profile curve

The approach to single contaminant problem discussed can be extended to multiple contaminants problem by incorporating inlet and outlet concentration shifts. It will apply to multiple contaminants if only one contaminant is key, providing the other contaminants do not interfere with the transfer of the key contaminant. The approach for multiple contaminants could be to target and design for the key contaminant and to simulate the performance for the non-key contaminants. However, it is unlikely that such an approach would be widely applicable. It will most often be necessary to take account of several (if not all) contaminants in targeting and design. (Wang and Smith, 1994)

Olesen and Polley (1997) recognized the difficulties of the design procedure proposed by Wang and Smith and introduced a simplified design procedure for single contaminant. However, this approach cannot handle more than four or five operations as stated by the authors, mostly because it is based on a special ad-hoc inspection procedure.

Kuo and Smith (1998) proposed another graphical design method that slightly improves the matching techniques used by Wang and Smith but left some unresolved issues that make its application somewhat uncertain even for a single contaminant. (Savelski and Bagejewicz, 2000)

In this work the concept of water reuse, regeneration reuse and regeneration recycle have been discussed to determine the minimum freshwater requirement for a water using system. The approach to solving single contaminant problems has been extended to multiple contaminant problems. The basic concepts embedded in ASPEN WATER are used for designing and then optimization of waterusing network which is now one of the most common and time saving option. Two industrial case studies involving multiple contaminant problems have been analyzed to illustrate the significance of the methods discussed.

### PROBLEM STATEMENT

The present work deals with the generation of water network with the best use of reuse, regeneration reuse and regeneration recycle. To apply these concepts two case studies are considered which are described below:

#### 3.1 Multiple contaminants: Starch industry

A case study for water using network of a Starch industry in the state of Gujarat, India, is undertaken with an aim to reduce demineralised water and freshwater flow rates and consequently the wastewater flowrate. The reduction in demineralised and freshwater consumptions will ultimately affect the cost of water use on per hour basis. The problem was identified as a multi contaminant, reuse and recycle problem. The freshwater consumption and demineralised water consumption were 100t/h and 51t/h respectively before modification and the network was dealing with three major contaminants such as total organic content (TOC), total dissolved solids (TDS) and total suspended solids (TSS). A water network is to be developed using ASPEN WATER and modified network is to be found out by simulation. (Dakwala *et al.*, 2009)

The Limiting process data, constraints associated with the process and the process flow sheet are given.

Table 3.1 Limiting Process data for starch industry

<b>Operation</b>	<b>Contaminant Type</b>	<b>Limiting Water Flow Rate (t/h)</b>	<b>Limiting Inlet Concentration (ppm)</b>	<b>Limiting Outlet Concentration (ppm)</b>
Reactor-1	TDS	15	1	140
	TSS		7	105
	TOC		2	15
Separators	TDS	15	1	205
	TSS		7	55
	TOC		2	40
Grinding Mill	TDS	10	1	410
	TSS		7	205
	TOC		2	55
Washing	TDS	11	1	5
	TSS		7	10
	TOC		2	5
Scrubbers	TDS	25	50	600
	TSS		220	230
	TOC		30	35
Starch Washing Screens	TDS	30	50	70
	TSS		220	300
	TOC		30	45
Cooling Tower-I	TDS	20	50	250
	TSS		220	1100
	TOC		30	150
Cooling Tower-II	TDS	25	50	150
	TSS		220	660
	TOC		30	90

Table 3.2 Constraints associated with water using networks

Unit	Water Flow Rate (t/h)		Maximum Inlet Concentration (ppm)			New Conn.
	Minimum	Maximum	TDS	TSS	TOC	
DM Water	4	75	1	7	2	Allowed
Freshwater	2	130	50	220	30	Allowed
Reactor-1	15	15	5	7	5	Banned
Separators	15	15	5	7	5	Banned
Grinding Mill	5	10	25	100	15	Allowed
Washing	5	11	30	130	20	Allowed
Scrubbers	20	30	200	210	50	Allowed
Starch Washing Screens	4	31	150	100	20	Allowed
Cooling Tower-I	8.5	8.5	475	300	100	Allowed
Cooling Tower-II	25	25	200	120	40	Allowed

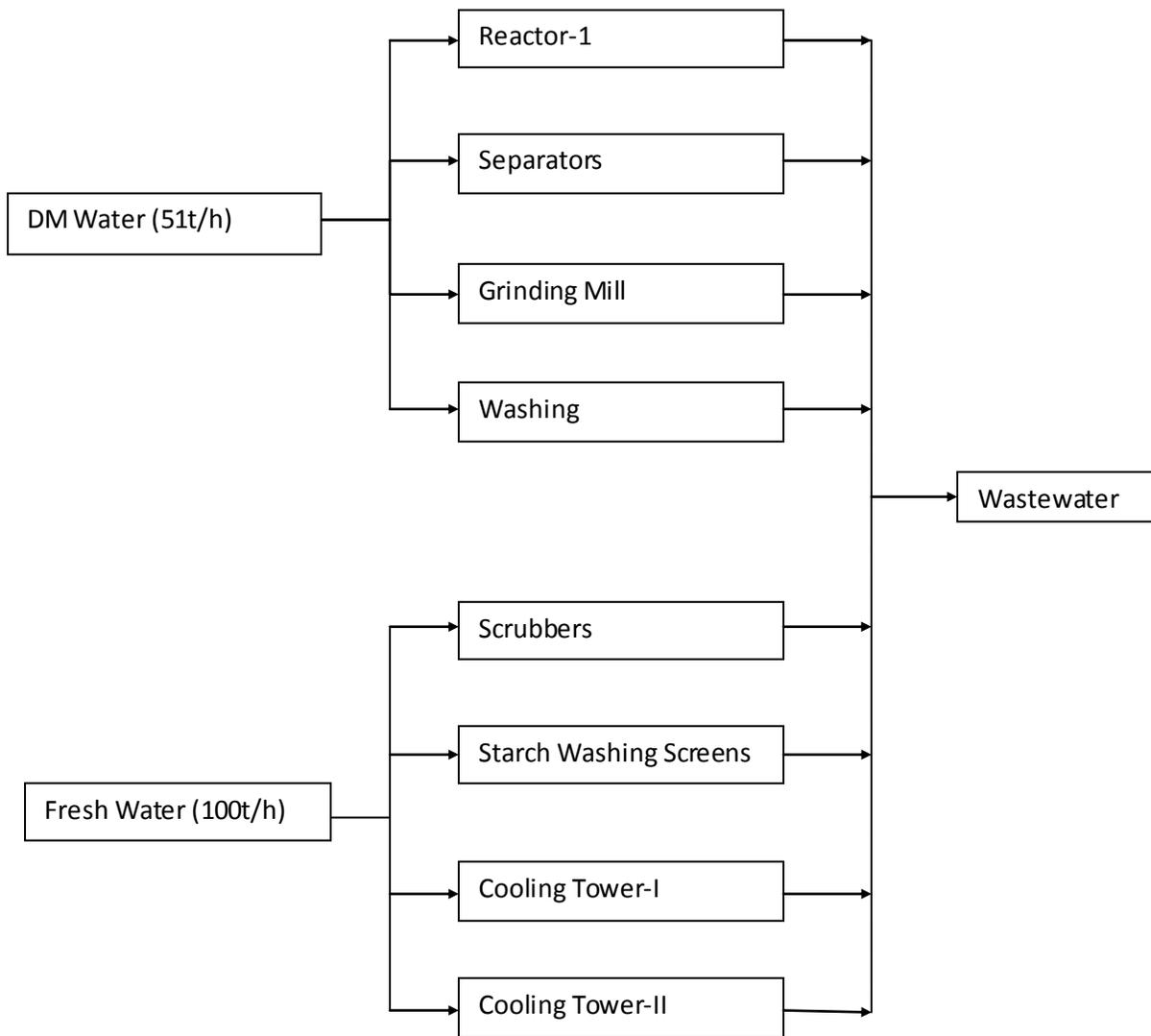


Figure 3.1 Initial network design for starch industry

All the data is available for carrying out necessary designing and optimization procedure.

### 3.2 Petroleum refining complex

A petroleum refinery case study is presented to deal with the problem of multiple contaminants in process plants. Three water using operations commonly found in the petroleum industry are considered. These include a distillation unit using live steam injection, a hydrodesulphurization (HDS) reactor and a desalter. The last two processes use water to wash out contaminants. The limiting process data for three contaminants are given in Table 3.2.

A water network is to be designed and optimized for lower water consumption. (Wang and Smith, 1994)

Table 3.3 Limiting Process data for Refinery Complex

Process Unit	Water flow rate (t/h)	Contaminants	Inlet Concentration (ppm)	Outlet Concentration (ppm)
1. Distillation	45	Hydrocarbon	0	15
		H <sub>2</sub> S	0	400
		Salt	45	80
2. HDS	34	Hydrocarbon	20	120
		H <sub>2</sub> S	300	12500
		Salt	45	180
3. Desalter	56	Hydrocarbon	120	220
		H <sub>2</sub> S	20	45
		Salt	200	9500

Input was taken as Freshwater with initial concentrations of contaminants as-

Hydrocarbon: 0 ppm, H<sub>2</sub>S: 0 ppm and Salt: 45 ppm (Freshwater has salt concentration of less than 500 ppm)

Network is to be designed keeping in mind reusing and recycling of water streams keeping in mind the concentrations of streams in effluent discharge.

### SOLUTION TECHNIQUES

This chapter lays out the basic principles for analyzing a water using operation and then compares the freshwater and wastewater flowrates for the systems with and without reuse. First, the system is defined as a mass transfer problem in which the contaminant is transferred from a contaminant rich process stream to a water stream. All constraints are to be satisfied for a successful run of optimization of network in an ASPEN WATER simulation. These constraints are given otherwise practical assumptions are to be made in case of limited data. Described below are the techniques used for minimization practices.

#### 4.1 Reducing generation of wastewater

**4.1.1 Reduction at source:** reduction in the consumption of water with changes or improvements in the processes or operating procedures. Some examples of this technique:

- Elimination of leakages
- Changes in operational procedures
- Reformulation of products
- Modification of equipment
- Purification of raw materials and supplies

**4.1.2 Reuse:** reuse of wastewater directly in another operation or process, till the contaminant level built up is not affecting the process.

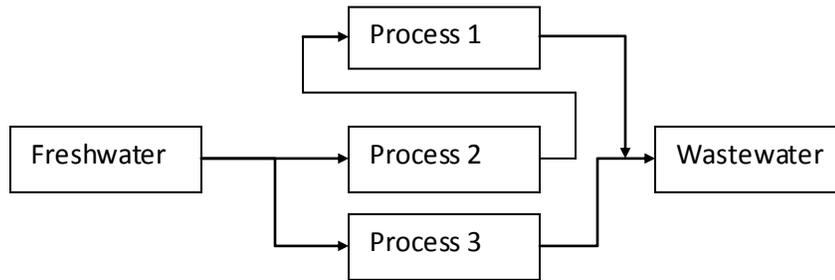


Figure 4.1 Reuse of wastewater from process 2 to process 1

**4.1.3 Reuse with regeneration:** total or partial removal of contaminants from the wastewater to reuse this stream in another operation or process. Regenerator is the equipment for the removal of the contaminant. (Fontana *et al.*, 2010)

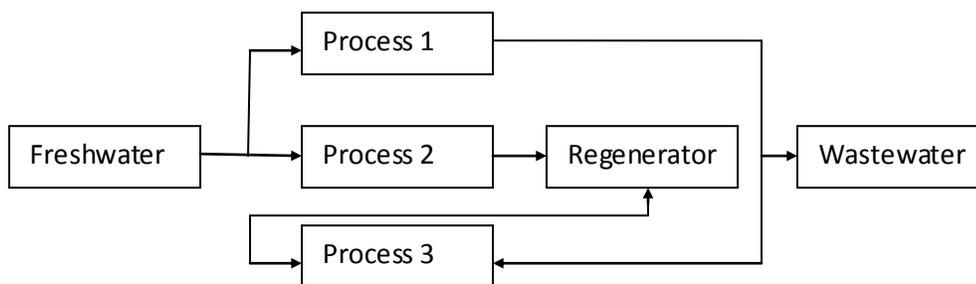


Figure 4.2 Regeneration of the wastewater from process 2 to be reused in process 3

**4.1.4 Recycling with regeneration:** total or partial removal of contaminants from the wastewater to reuse this same stream in the same operation or process

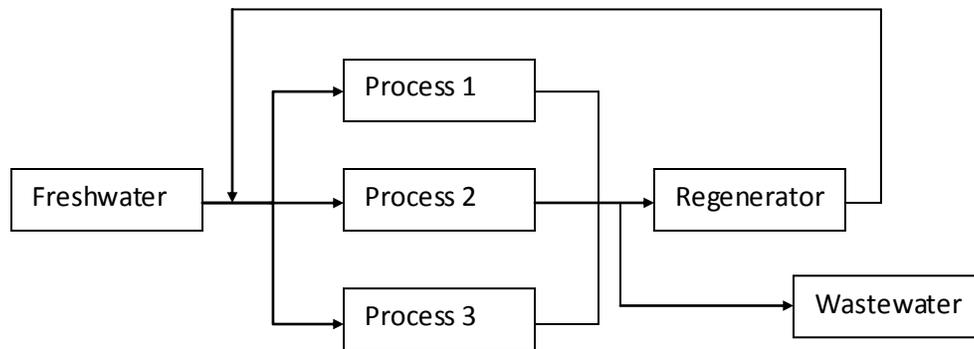


Figure 4.3 Regeneration of wastewater to be recycled in the same process

The application of the techniques described above has the following advantages:

- Reduction in the final wastewater flow generated and consequent reduction in cost of wastewater disposal.
- Reduction in the consumption of an exhaustible natural resource - water - reducing the cost of water intake.

The feasibility of the application of the techniques of reuse and recycling basically depend on (Fontana *et al.*, 2010):

- The availability of sources of wastewater with physical/chemical characteristics which are compatible with the water consumers.
- The economic viability of logistics between the source and consumer.

## **4.2 Key steps in Waste Water Minimization for Multiple Contaminant problems**

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

Step 1: The need of waste water minimization identified based on limited availability of freshwater, economic and regularity consideration.

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

Step 3: Now after getting all the data a flowsheet of the process is drawn which shows water balance diagram of the process.

Step 4: Key contaminants for the process are identified; these are the contaminants which are to be reduced so that the discharged waste water comes under the ability of treatment to meet the control standards for an industry.

Step 5: Now, the two types of approaches can be there for solving the wastewater minimization problems.

### 1. Heuristics approach:

It consists of following steps:

- Analysis of problem

- Determination of Reuse and Regeneration opportunities
- Selection of treatment operations based on constraints

## 2. Mathematical programming approach:

It has following steps:

- Definition of superstructure
- Mathematical optimization
- Analysis of solution

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

In case of a failure of initial model other different techniques are to be considered like reuse-regeneration or recycle-regeneration and the above steps are to be followed. The above steps are the basic approach to any industry which wants to implement a water minimization project. These steps are to be satisfied before successful implementation of any water minimization process.

### **4.3 ASPEN WATER Software**

The vision for the software has been “A single tool for integrated water management.” First, water users model what exists at present and reconcile any gaps or inconsistencies in the data. Second, the software identifies opportunities for improvement and helps set targets for these improvement options. Third, users check the technical feasibility and economics of the options open to them, and further optimize the one they like best.

Aspen Water enables the user to:

- Define what is happening now (by producing a current water and contaminant balance)
- Identify opportunities for improvement in a systematic way, such as water reuse and regeneration
- Test future scenarios (before addition of more units in present operations)

Using Aspen Water, a model of the site (or plant) water and effluent system in a flowsheeting environment is first produced using a drag-and-drop system. In constructing the flowsheet, in built models of water operations can be deployed such as cooling towers, process, boilers, vessels, pumps, and filters.

Aspen Water rigorously models water chemistry and energy issues. It contains data reconciliation capabilities that produce a water balance when not all data are available or when some data are conflicting. Once the balance is complete Aspen Water uses a Mixed Integer Linear Program (MILP) optimization routine to define all options for water re-use. Sensitivity analysis within Aspen Water, linked to a database of treatment technologies, allows you to define the most appropriate location (and the benefit) of treatment options within the overall water and effluent system.

### RESULTS AND DISCUSSIONS

#### 5.1 Multiple contaminants: Starch Industry

As discussed earlier the case study of starch industry in Chapter 3, the present chapter shows the results obtained using ASPEN WATER software for optimization of the given industrial network for finding a network using “minimum water costs” optimization. The original network was given in Chapter 3. Demineralised and Fresh water are used for the processes and the contaminants given were TDS, TSS and TOC.

In the given starch industry water using processes include following equipments:

1. Reactor
2. Separators
3. Grinding mill
4. Washing
5. Scrubbers (SCR)
6. Starch washing screens (SWS)
7. Cooling tower-I (CT-1)
8. Cooling tower-II (CT-2)

The initial network was designed in ASPEN WATER.

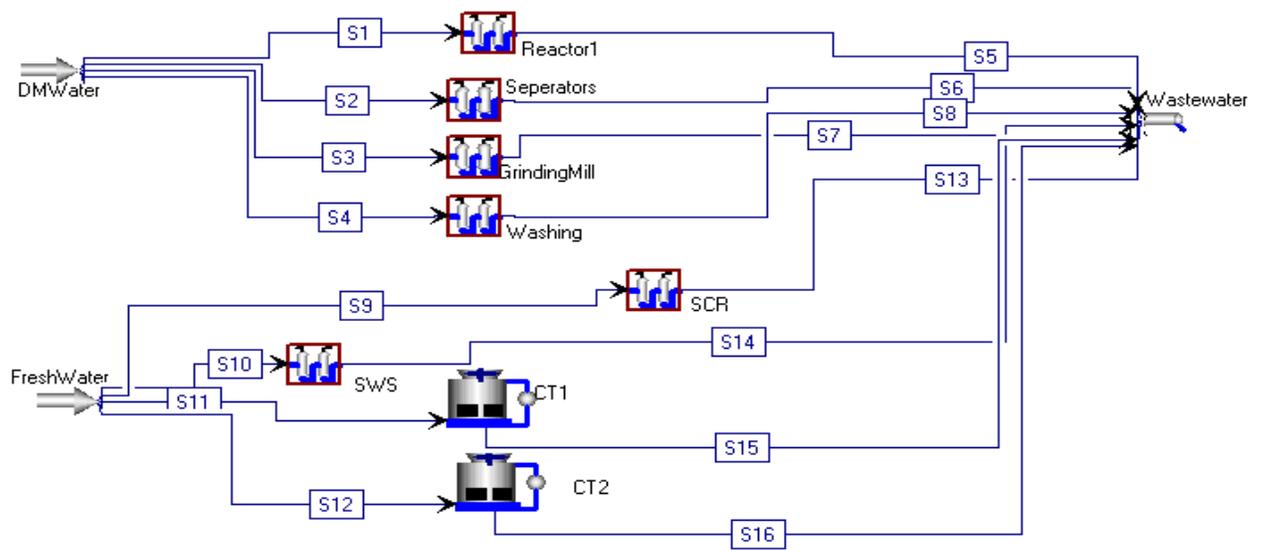


Figure 5.1 Initial water network for starch industry

Initial Flow rate for DM water is 51t/h and for Fresh water is 100t/h. The initial discharge report and contaminant report for wastewater is given in Table 5.1.

Table 5.1 Initial discharge report and contaminant report for starch industry

From Block	Stream Name	Flow Rate (t/h)	TDS (ppm)	TSS (ppm)	TOC (ppm)
Reactor-1	S5	15	140	105	15
Separators	S6	15	200	55	40
Grinding Mill	S7	10.01	410	205	55
Washing	S8	11	5	10	5
SCR	S13	25.01	600	230	35
SWS	S14	30	70	300	45
CT-1	S15	4.00	150	660	90
CT-2	S16	8.33	250	1100	150
<b>Mixed Total</b>		<b>118.35</b>	<b>241.77</b>	<b>246.83</b>	<b>42.29</b>

As seen in the table we have total initial discharge of wastewater without optimization as 118.35t/h and also the initial wastewater contaminant level with TDS- 241.77 ppm, TSS- 246.83 ppm and TOC- 42.29 ppm.

### 5.1.1 Results

Now, optimization was done to minimize the water costs as the Demineralised water costs around 2 Euros per ton and Fresh water costs around 0.1 Euros per ton. So cost per hour will be 102 Euros for DM water and 10 Euros for fresh water. Optimization was done keeping in mind the constraints given in Table 3.2.

The results of optimizations for “Minimize water costs” are given in Table 5.2. The optimized network is shown in Figure 5.2 the total numbers of new network connections are 22. The percentage of water costs savings is 45% on per hour basis. Cost details can be seen in Table 5.2.

Table 5.2 Cost of water per hour (optimized and initial)

<b>Cost item</b>	<b>Optimized Cost Euros</b>	<b>Base Cost Euros</b>
Water cost	61.96	112
Wastewater costs	20.656	52.291

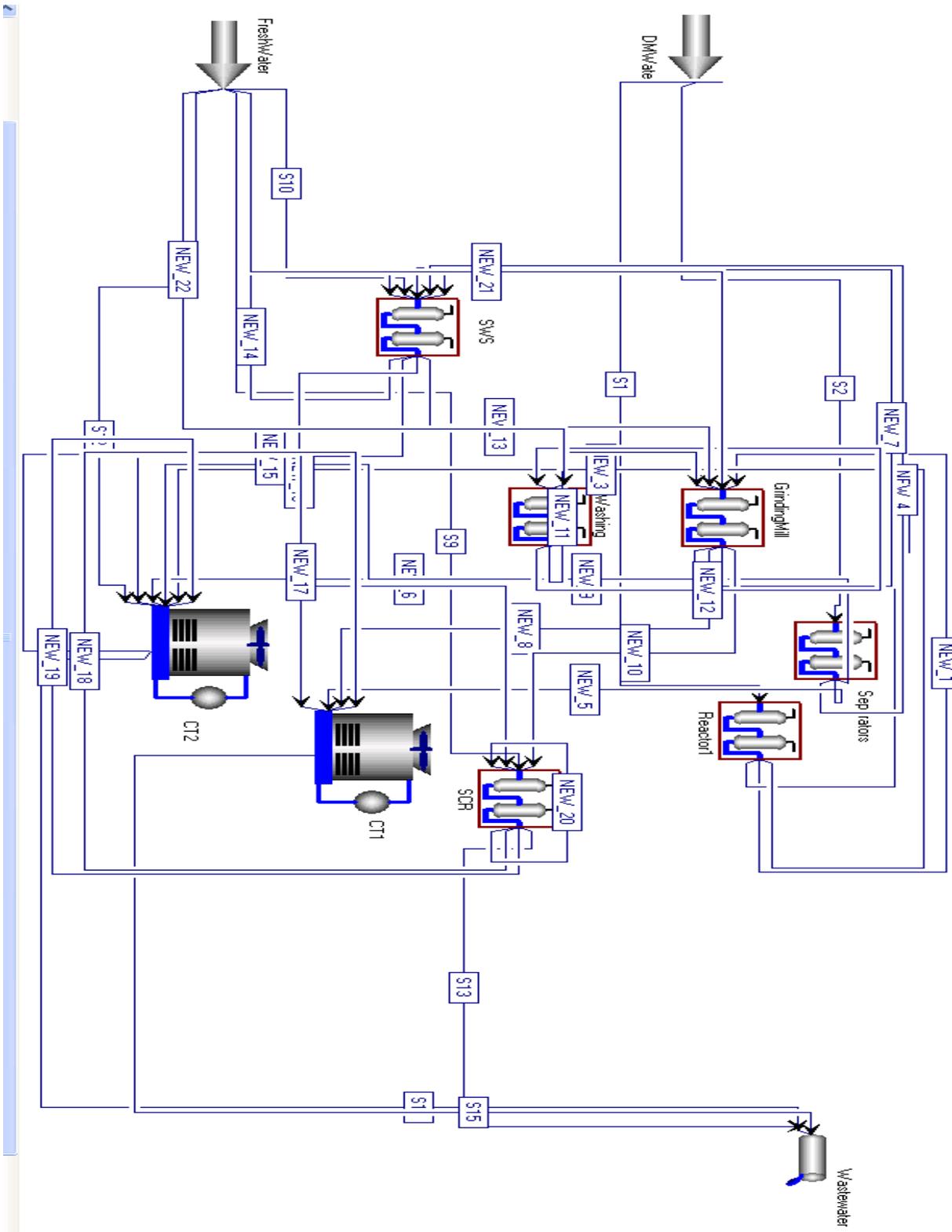


Figure 5.2 Optimized water network for starch industry

The final discharge report and contaminant report for wastewater is presented in Table 5.3 other details of the streams has been given in APPNEDIX A.

Table 5.3 Final discharge report and contaminant report for starch industry

<b>From Block</b>	<b>Stream Name</b>	<b>Flow Rate (t/h)</b>	<b>TDS (ppm)</b>	<b>TSS (ppm)</b>	<b>TOC (ppm)</b>
SCR	S13	15.82	600	230	35
CT-1	S15	4.79	2505.68	1487.71	332.24
CT-2	S16	1.49	640.12	562.26	119.67
<b>Mixed Total</b>		<b>22.1</b>	<b>1015.36</b>	<b>524.81</b>	<b>105.09</b>

### 5.1.2 Discussion

So, the results obtained were quite encouraging but few things are to be noted-when modifying an existing water network the piping and pumping costs for modifying the network are to be considered and the contaminant level at discharge should meet standards set by environmental agencies.

The process of reusing (use of water from one process to another) and recycling (use of outgoing water from a process in same process) were widely used for optimized network as it can be seen in Figure 5.2 also if the contaminant level of wastewater are acceptable to the industry our results are successful. Table 5.3 shows reduction of the wastewater flow. Table 5.4 shows savings of water.

Table 5.4 Savings report

Water Type	Initial Flow (t/h)	Optimized flow (t/h)	%Savings
Demineralised	51	30	41.17
Fresh	100	19.579	80.42
Wastewater (discharge)	118.35	22.1	81.32

Now, on comparing with the actual plant data available after four months of successful plant operation shows 26% and 66% of DM water and Fresh water decreased consumption respectively. We were still able to get a savings of 41% and 80% for DM water and Fresh water respectively for minimum water costs.

Table 5.5 Final water savings report

	DM Water (t/h)	Fresh Water (t/h)	Savings DM WATER (t/h)	Saving Fresh Water (t/h)
Before analysis	51	100	-	-
Using Aspen Water	30	19.579	21	80.42
Actual Results Plant	38	34	13	66

The wastewater discharge decreases after optimization which shows our target of reducing total water consumption and discharge is achieved using ASPEN WATER.

The step wise procedure of case study of starch industry is solved in Appendix A.

## 5.2 Petroleum refining complex

As described in Chapter 3 the refinery complex problem has three water using process: steam stripper, hydrodesulphurization unit and the Desalter unit. The initial freshwater usage is 135t/h with individual flow rates given in Table 3.3, along with limiting concentrations of the contaminants. The initial network designed for the problem by using ASPEN WATER:

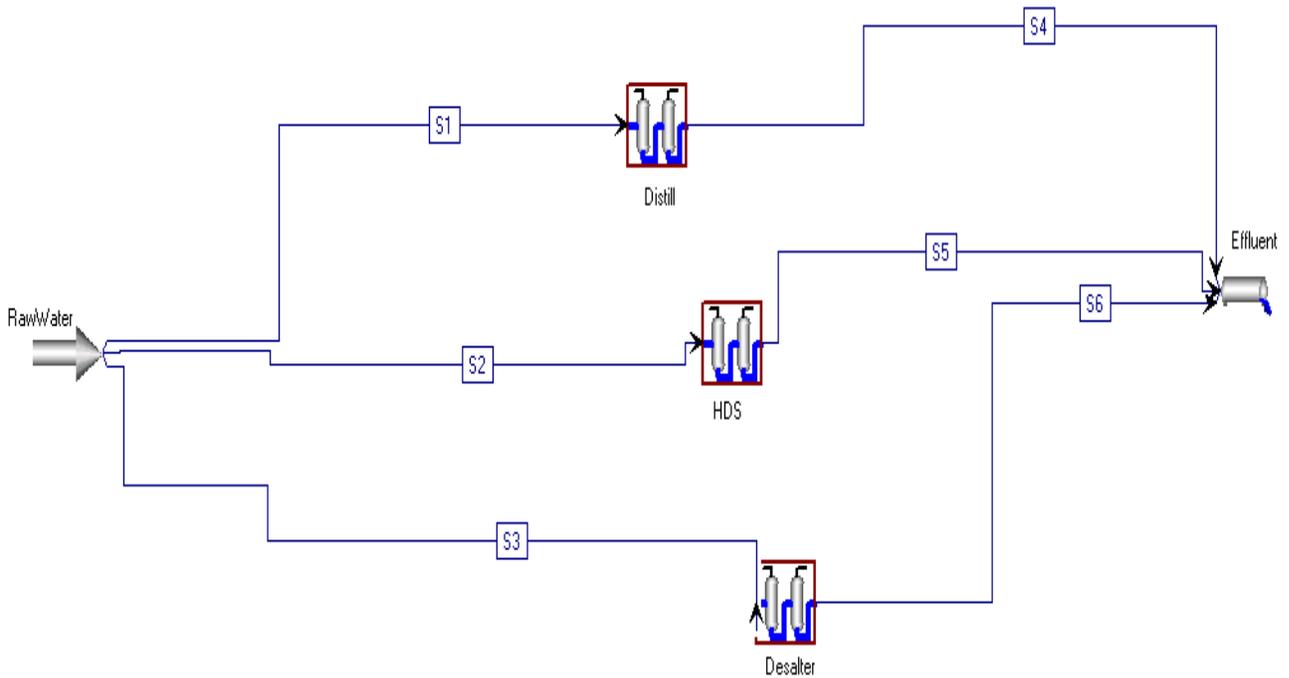


Figure 5.3 Initial water network for refinery complex

The individual water flows in various units are: Distill 45t/h, HDS 34t/h and Desalter 56t/h. The contaminants present here include: Hydrocarbons,  $H_2S$  and Salt. The initial discharge report and contaminant report was given for wastewater.

Table 5.6 Initial discharge report and contaminant report for refinery complex

From Block	Stream Name	Flow Rate(t/h)	Hydrocarbons (ppm)	H <sub>2</sub> S (ppm)	Salt (ppm)
Distill	S4	45.02	15	400	35
HDS	S5	34.43	100	12200	135
Desalter	S6	56.53	100	25	9300
<b>Mixed Total</b>		<b>135.98</b>	<b>71.86</b>	<b>3231.66</b>	<b>3912.15</b>

### 5.2.1 Result

The discharge is quite high with high contaminant concentration. So we need to optimize network so that we minimize water usage in the given problem and also try to decrease the contaminant concentrations if possible.

After Optimizations were done for “Minimize water use” the total numbers of new network connections are 5.

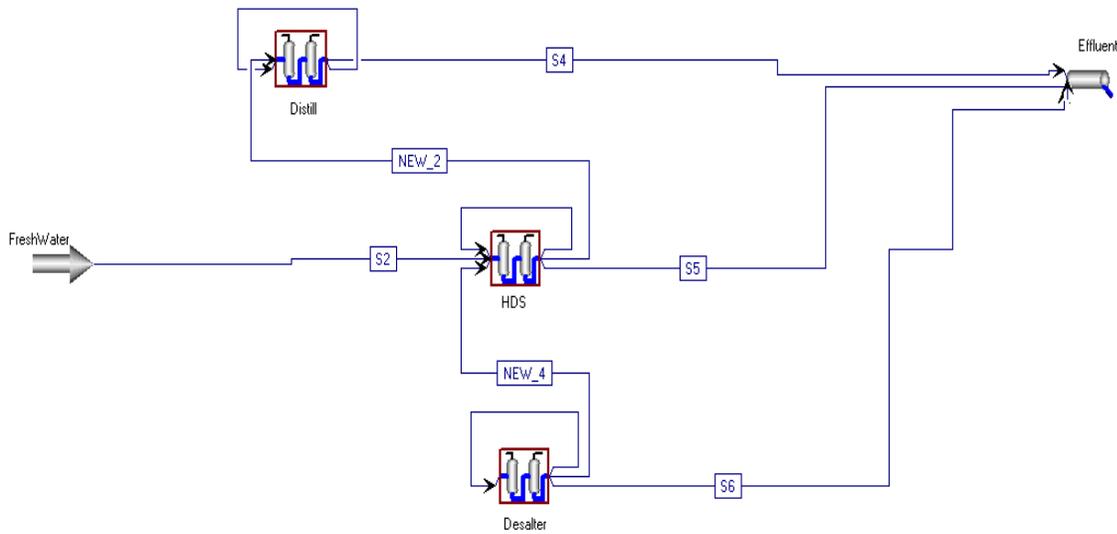


Figure 5.4 Optimized water network for refinery complex

The final discharge report and contaminant report for wastewater:

Table 5.7 Final discharge report and contaminant report for starch industry

From Block	Stream Name	Flow Rate	Hydrocarbons (ppm)	H <sub>2</sub> S (ppm)	Salt (ppm)
Distill	S4	19.90	15	400	35
HDS	S5	3.95	100	12200	135
Desalter	S6	0.0	100	25	9300
<b>Mixed Total</b>		<b>23.85</b>	<b>29.09</b>	<b>2356.03</b>	<b>51.58</b>

### 5.2.2 Discussion

The results got by optimizing the network were quite encouraging. Overall water usage was successfully brought down along with the contaminant concentration levels by using reuse and recycle techniques.

: Table 5.8 Final water savings report

Water Type	Initial Flow (t/h)	Optimized Flow (t/h)	Savings (t/h)
Fresh Water	135	23.798	111.2
Wastewater	135.98	23.85	112.13

The wastewater discharge decreases along with the contamination level of the contaminants, after optimization which shows our target of reducing water consumption and discharge is achieved. In terms of percentage we can bring down Fresh water consumption by about 82%.

### CONCLUSION

The methods of reuse, regeneration reuse and regeneration recycle have been discussed to reduce the freshwater requirement as well as wastewater generation in a wide range of processes. The final design of a water network is always subjected to constraints such as minimum mass transfer driving forces, equipment fouling due to action of various contaminants, etc. Therefore one needs to optimize network keeping in mind the costs involved in applying the optimized networks. The following conclusions can be drawn from the application of the methods discussed in this thesis to the industrial case studies (using ASPEN WATER):

1. There is a significant decrease in the minimum freshwater requirement of a system with reuse and recycle of wastewater as compared to systems without reuse.
2. The reduction in Demineralised water and Freshwater for starch industry is about 41% and 80% respectively with water cost savings of 45%.
3. The reduction in freshwater requirement with reuse and recycle for the petroleum refinery complex is about 82%.
4. The reduction of freshwater requirement by use of ASPEN WATER software leads to a decrease in the total annual operating cost of the system with condition that an industry is willing to bear some additional costs of piping and pumping.
5. A more environmental friendly industrial water network can be designed keeping in mind necessary steps for saving of water and reduction of effluent.

## REFERENCES

1. Alva-Argaez, A., Kokossis, A.C. and Smith R., “*Wastewater minimisation of industrial systems using an integrated approach*”, Computers Chem. Eng, vol. 22, pg 741-744, 1998.
2. Dakwala, M., Mohanty, B. and Bhargwa, R., “*A process integration approach to industrial water conservation: A case study for a starch industry*”, Dept. of Chem. Eng, IIT Roorkee, Journal of cleaner prod., vol.17, pg 1654-1662, 2009.
3. Doyle S.J. and Smith R., “*Targeting water reuse with multiple contaminants*”, Trans IChemE, Part B, vol. 75, pg 181-189, 1997.
4. El-Halwagi, M. M. and Manousiouthakis, V., “*Synthesis of mass exchange networks*”, AIChE Journal, vol. 8, pg 1233-1244, 1989.
5. Fontana, D., Kalid, R., Kiperstok, A and Silva, M. A. S., “*Methodology for wastewater minimization in industries in the petrochemical complex*”, Universidade Federal da Bahia Unidade de Insumos Básicos (UNIB) Braskem, 2010.
6. Gomes, F.S.J., Queiroz, M.F. and Perrosoa, L.P., “*Design procedure for water/wastewater minimization: Single Contaminant*”, Journal of cleaner prod., vol. 15, pg 474-485, 2005.
7. Hallale, N., and Fraser, D.M, “*Supertargeting for mass exchange networks Part I: Targeting and Design Techniques*”, Trans IChemE, vol. 78, part A, 2000.
8. Huang C.H., Chang C.T., Ling H.C. and Chang C.C., “*A mathematical programming model for water usage and treatment network design*”, Ind & Eng Chem. Res., 38, pg 2666-2679, 1999.

9. Kuo J. and Smith R., "*Designing for the interactions between water-use and effluent treatment*" Trans I Chem., vol. 76, Part A, pg 287-301, 1998.
10. Linnhoff, B., and Flower, J.R., "*Synthesis of Heat Exchanger Networks. Part-I Systematic generation of energy optimal networks*", AIChE Journal, vol. 24, pg 633-642, 1978.
11. Linnhoff, B., Townsend, D. W., Boland, D., Hewitt, G. F., Thomas, B. E. A., Guy, A. R. and Marshall, R. H. ,"*A user guide on process integration for the efficient use of energy*". IChemE, Rugby, UK, 1982.
12. Linnhoff, B., "*Pinch analysis: A state-of-the-art overview*", Trans IChemE, Part A, vol. 71, pg 503, 1993.
13. Mann, James G. and Liu, Y.A, "*Industrial Water Reuse and Wastewater Minimization*", McGraw Hill, 1999.
14. McIntyre, J.P., "*Industrial Water Reuse and Wastewater Minimization*", GE technical paper, 1993.
15. Olesen S.G. and Polley S.G., "*A simple methodology for the design of water networks handling single contaminants*", Trans I Chem, Part A, pg 420-426, 1997.
16. Querzoli, Adrian L., Hoadley , Andrew F. A and Dyson, T. E. S., "*Identification of Heat Integration Retrofit Opportunities for Crude Distillation and Residue Cracking Units*", Korean J. Chem. Eng, vol. 20 no.4, pg 635-641, 2003.

17. Savelski, M. J. and Bagejewicz, M. J., "*On the optimality conditions of water utilization systems in process plants with single contaminants*", Chem Eng.Sci. , vol.55, pg 5035-5048, 2000.
18. Savelski, M. J. and Bagejewicz, M. J., "*Design of water utilizing systems in process plants with single contaminant*", Waste management, vol. 20, pg 659-664, 2000.
19. Takama, N., Kuriyama, T., Shiroko, K. and Umeda, T., "*Optimal water allocation in a petroleum refinery*", Computers Chem. Eng., vol. 4, pg 251-258, 1980.
20. Wang, Y.P. and Smith, R., "*Wastewater minimization*", Chem Eng Sci, vol. 49 no.7, pg 981-1006, 1994.

# APPENDIX A

## DETAILED SOLUTION

The detailed solution for the case of starch industry is presented in this appendix.

The limiting process data was given in Table 3.1 and constraints to be applied were given in Table 3.2. Now steps for designing of network, entering of process data and running of simulation are as follow:

### A.1 Designing of water network

The interface of ASPEN WATER:

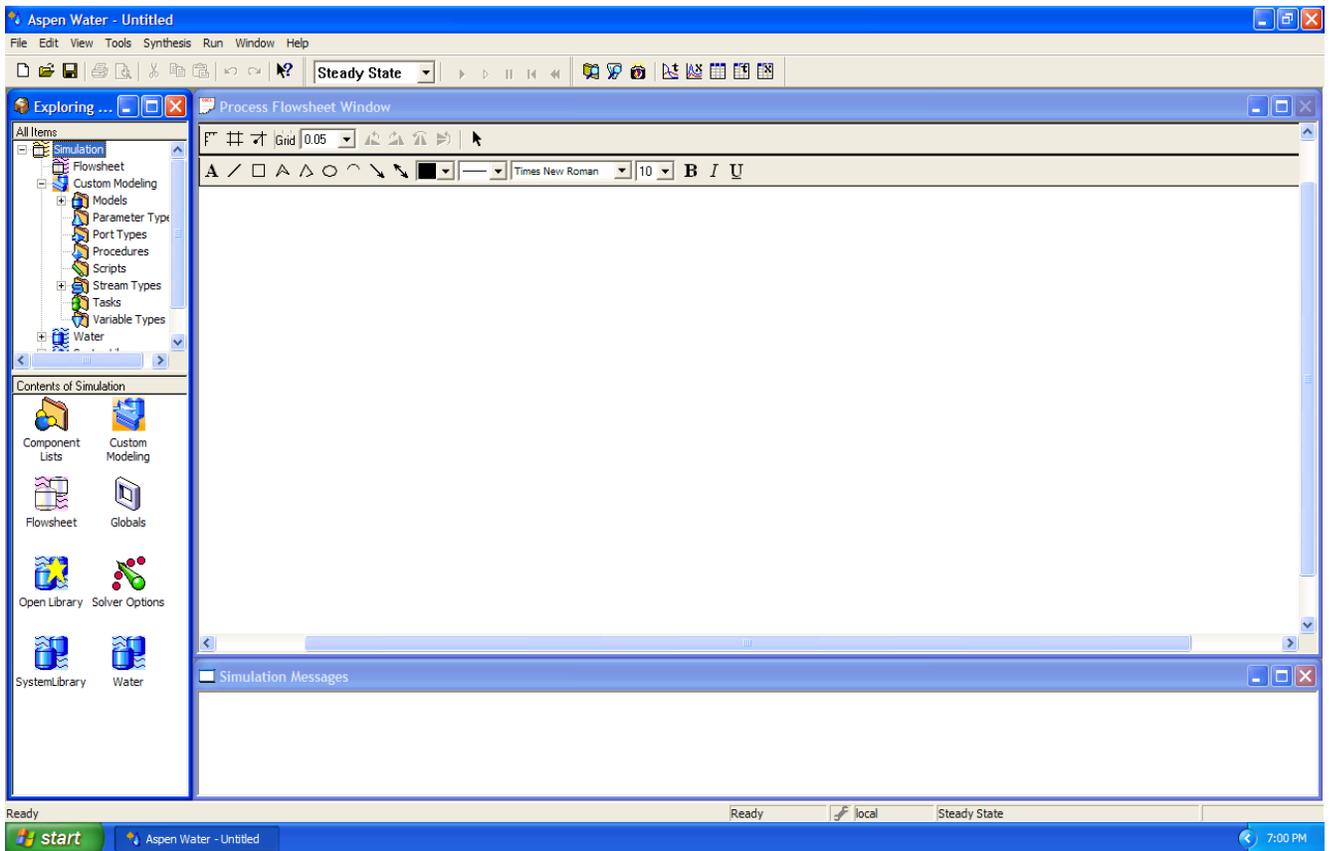


Figure A.1 ASPEN WATER interface

The steps followed in designing the water network Figure 5.1 in Chapter 5 are given below. Our flow sheet design is as follows (see figure A.2 for details):

1. The water models required for our flowsheet were under water\_models in All items pane.
2. First feed block was selected for DM water and then for Freshwater.
3. For the various units given we selected Process block under water\_models.
4. Stream connections were taken as measurement streams under stream type in All item pane.
5. Two cooling towers were selected under Utility equipment.
6. All connections were made and at the end connected to discharge block available in water\_models.

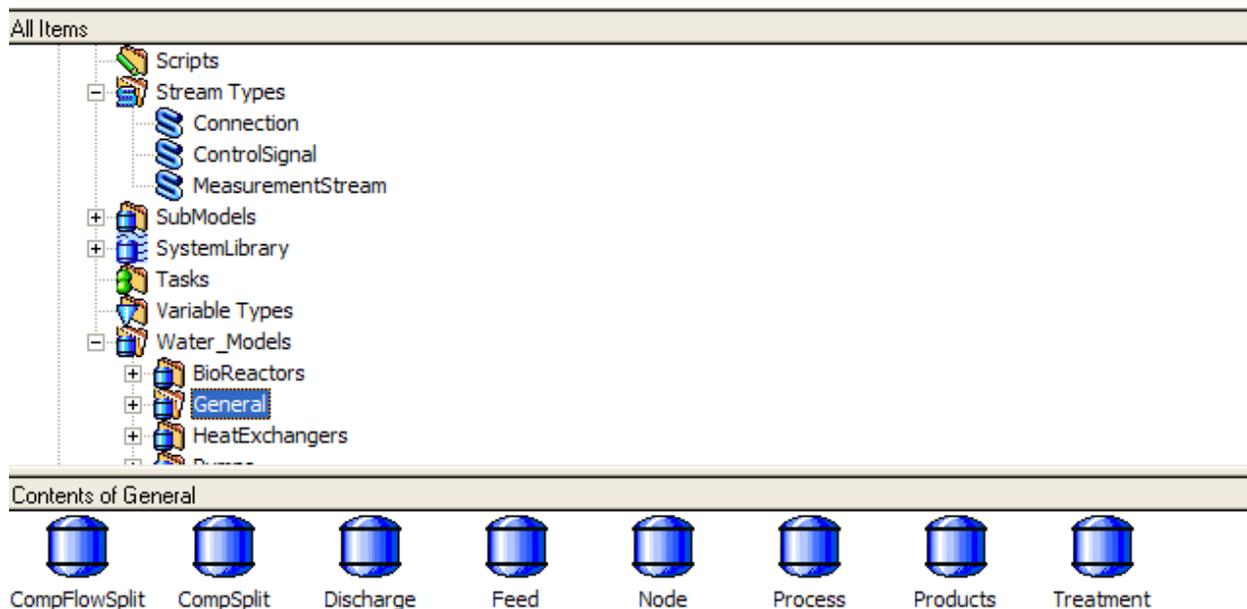


Figure A.2 All items pane with various models and stream types

A component list was initialized for various contaminants present in the problem to be solved.  
 (Note: Solids represent TDS)

## A.2 Entering process data

Now for entering the constraints we go to Edit Blocks under synthesis see Figure A.3. All flowrate constraints for DM water and Fresh water were entered along with individual process constraints for finding out optimum network for the given plant. (See Table 3.1 and 3.2)

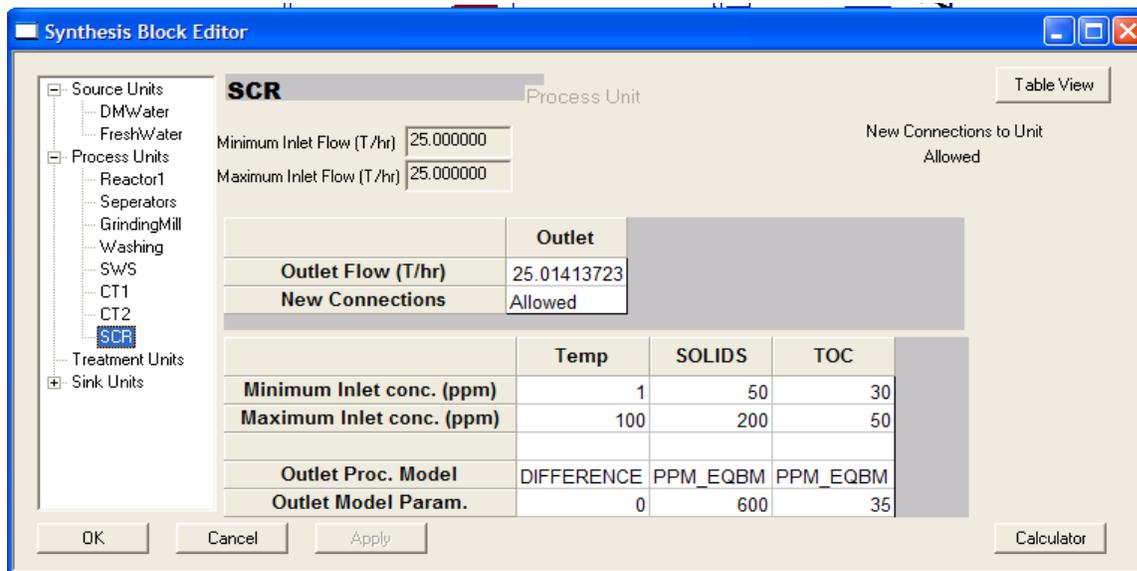


Figure A.3 Constraints input block

We entered all the data available to us and the unavailable data like the temperature was generated itself by ASPEN WATER for standard models.

## A.3 Optimization

Now the simulation was run. The given network was run for “minimum water costs”, the costs given in Euros as a standard for the software. For running simulation we go to synthesis in menu bar then click run optimization.

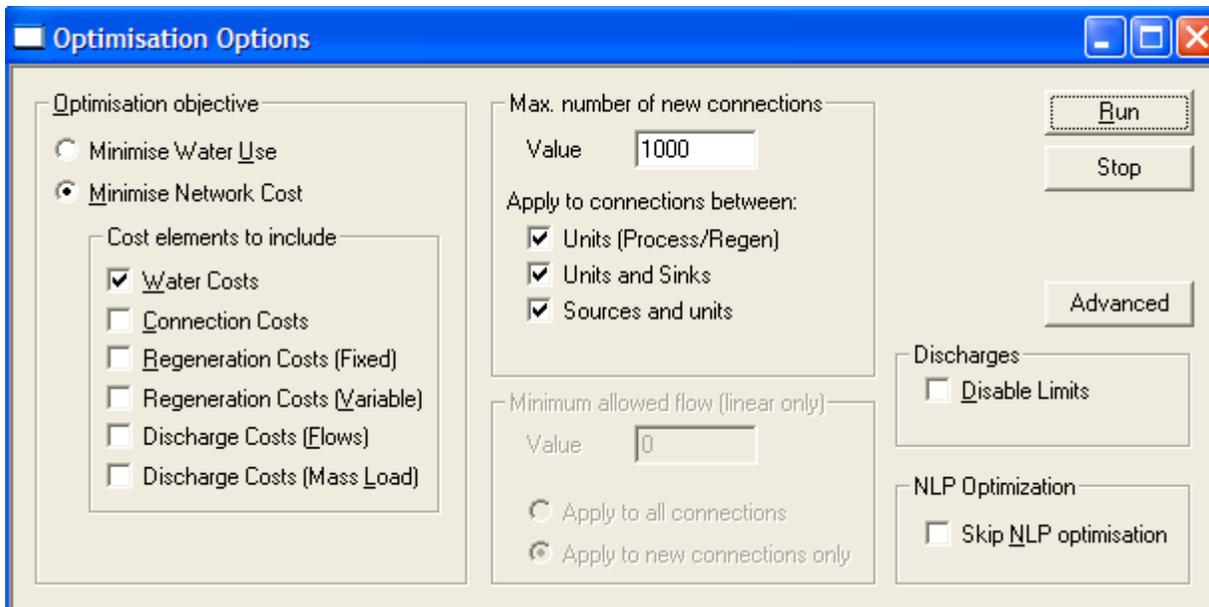


Figure A.4 Optimization options available

We see that the limit for new connection was set for 1000 and cost elements to include were only water costs. Other costs can also be selected if available.

#### A.4 Detailed Results

After the optimization was run large amount of data was generated regarding the number of new connections, discharge report, individual water usages for each unit which will be presented now.

The discharge reports have already been given earlier in Chapter 5 (see Table 5.1 and 5.3) and individual water usages will be given later here itself. The total number of new connections was found to be 22. The water requirement will now be presented in form of a table.

The data also includes the costs for water used in each unit also, which gives us the cost savings per hour basis. (Note: Cost of DM Water 2 Euros/ton and Fresh Water 0.1 Euros/ton)

Table A.1 Various cost data for various water sources

Cost item	Optimized Cost in Euros			Base Cost in Euros		
	Fixed	Variable	Total	Fixed	Variable	Total
<b>Water Sources</b>						
<b>DM Water</b>						
Flow cost	0.000	60.000	60.000	0.000	102.000	102.000
Conn. Cost	0.000	0.000	0.000	0.000	0.000	0.000
<b>Total Cost</b>	<b>0.000</b>	<b>60.000</b>	<b>60.000</b>	<b>0.000</b>	<b>102.000</b>	<b>102.000</b>
<b>Freshwater</b>						
Flow Cost	0.000	1.958	1.958	0.000	10.000	10.000
Conn. Cost	4.000	0.189	4.189	0.000	0.000	0.000
<b>Total Cost</b>	<b>4.000</b>	<b>2.146</b>	<b>6.146</b>	<b>0.000</b>	<b>10.000</b>	<b>10.000</b>
<b>Wastewater</b>						
Flow Cost	0.000	3.389	3.389	0.000	23.673	23.673
Solids Cost		17.267	17.267		28.618	28.618
TOC Cost		0.000	0.000		0.000	0.000
<b>Total Cost</b>	<b>0.000</b>	<b>20.656</b>	<b>20.656</b>	<b>0.000</b>	<b>52.291</b>	<b>52.291</b>

Table A.2 Flows from water Sources

Connection	Source Water of	To	Optimized Flow Rate (t/h)	Old Flow Rate (t/h)	Connection Cost Euros
	<b>DM Water</b>	Reactor1	15.000	15.000	0.000
		Separators	15.000	15.000	0.000
		Grinding Mill	0.000	10.000	0.000
		Washing	0.000	11.000	0.000
		<b>Total</b>	<b>30.000</b>	<b>51.000</b>	<b>0.000</b>
X	<b>Fresh Water</b>	Grinding Mill	3.316	0.000	2.066
X		Washing	6.111	0.000	2.122
		SWS	0.002	30.000	0.000
		CT1	0.000	20.000	0.000
		CT2	0.541	25.000	0.000
		SCR	9.608	25.000	0.000
		<b>Total</b>	<b>19.579</b>	<b>100.000</b>	<b>4.189</b>

Above table is for optimized flow from water sources. (Note: X denotes new connections)

Now for individual units:

Table A.3 Flow to individual units from outlet of an individual unit

Connection	From Outlets	To	Optimized Flow Rate (t/h)	Old Flow Rate (t/h)	Connection Cost Euros
X	Reactor-1	Grinding Mill	0.194	0.000	2.004
		Waste water	0.000	15.004	0.000
X		SWS	12.164	0.000	2.243
X		CT2	2.646	0.000	2.053
		<b>Total</b>	<b>15.004</b>	<b>15.004</b>	<b>6.300</b>
	Separators	Waste water	0.000	15.004	0.000
X		SWS	1.106	0.000	2.022
X		CT1	5.348	0.000	2.107
X		CT2	8.550	0.000	2.171
		<b>Total</b>	<b>15.004</b>	<b>15.004</b>	<b>6.300</b>
	Grinding Mill	Waste water	0.000	10.007	0.000
X		SWS	4.132	0.000	2.083
X		CT1	1.899	0.000	2.038
X		CT2	1.727	0.000	2.035
X		SCR	2.249	0.000	2.045
		<b>Total</b>	<b>10.007</b>	<b>10.007</b>	<b>8.200</b>
X	Washing	Grinding Mill	6.111	0.000	2.122
X		Washing	4.889	0.000	2.098
		Waste water	0.000	11.000	0.000
		<b>Total</b>	<b>11.000</b>	<b>11.000</b>	<b>4.220</b>
	SCR	Waste water	11.618	25.014	0.000
X		CT1	5.746	0.000	2.115
X		CT2	2.598	0.000	2.052
X		SCR	5.052	0.000	2.101
		<b>Total</b>	<b>25.014</b>	<b>25.014</b>	<b>6.268</b>
X	SWS	Grinding Mill	0.379	0.000	2.008
		Waste water	0.000	30.003	0.000
X		SWS	12.596	0.000	2.252

X		CT2	8.938	0.000	2.179
X		SCR	8.090	0.000	2.162
		<b>Total</b>	<b>30.003</b>	<b>30.003</b>	<b>8.600</b>
<b>Connection</b>					
	<b>From Outlet</b>	<b>To</b>	<b>Optimized Flow Rate (t/h)</b>	<b>Old Flow Rate (t/h)</b>	<b>Connection Cost Euros</b>
	CT1 Blowdown	Wastewater	4.000	4.000	0.000
		<b>Total</b>	<b>4.000</b>	<b>4.000</b>	<b>0.000</b>
	CT1 Evaporate	<b>Total</b>	<b>0.000</b>	<b>0.000</b>	<b>0.000</b>
	CT2 Blowdown	Wastewater	1.327	8.333	0.000
X		CT1	7.007	0.000	2.140
		<b>Total</b>	<b>8.333</b>	<b>8.333</b>	<b>2.140</b>
	CT1 Evaporate	<b>Total</b>	<b>0.000</b>	<b>0.000</b>	<b>0.000</b>

So the above given table shows the new connections along with the water costs for it. This is the result obtained from optimization of the network. Now, table for water units to individual unit and the discharge units are as follows:

Table A.4 Flow from one individual unit to other units

<b>Connection</b>	<b>To</b>	<b>From</b>	<b>Optimized Flow Rate (t/h)</b>	<b>Old Flow Rate (t/h)</b>	<b>Connection Cost Euros</b>
	Reactor-1	DMWater	15.000	15.000	0.000
		<b>Total</b>	<b>15.000</b>	<b>15.000</b>	<b>0.000</b>
	Separators	DMWater	15.000	15.000	0.000
		<b>Total</b>	<b>15.000</b>	<b>15.000</b>	<b>0.000</b>

Connection	To	From	Optimized Flow Rate (t/h)	Old Flow Rate (t/h)	Connection Cost Euros
	Grinding Mill	DMWater	0.000	10.000	0.000
X		FreshWater	3.316	0.000	2.066
X		Reactor1 Outlet	0.194	0.000	2.004
X		Washing Outlet	6.111	0.000	2.122
X		SWS Outlet	0.379	0.000	2.008
		<b>Total</b>	<b>10.000</b>	<b>10.000</b>	<b>8.200</b>
	Washing	DMWater	0.000	11.000	0.000
X		FreshWater	6.111	0.000	2.122
X		Washing Outlet	4.889	0.000	2.098
		<b>Total</b>	<b>11.000</b>	<b>11.000</b>	<b>4.220</b>
	SCR	FreshWater	9.608	25.000	0.000
X		Grinding Mill Outlet	2.249	0.000	2.045
X		SWS Outlet	8.090	0.000	2.162
X		SCR Outlet	5.052	0.000	2.101
		<b>Total</b>	<b>25.000</b>	<b>25.000</b>	<b>6.308</b>
	SWS	FreshWater	0.002	30.000	0.000
X		Reactor1 Outlet	12.164	0.000	2.243
X		Separators Outlet	1.106	0.000	2.022
X		Grinding Mill Outlet	4.132	0.000	2.083
X		SWS Outlet	12.596	0.000	2.252
		<b>Total</b>	<b>30.000</b>	<b>30.000</b>	<b>8.600</b>
	CT-1	FreshWater	0.000	20.000	0.000
X		Separators Outlet	5.348	0.000	2.107
X		Grinding Mill Outlet	1.899	0.000	2.038
X		CT2 Blowdown	7.007	0.000	2.140
X		SCR Outlet	5.746	0.000	2.115
		<b>Total</b>	<b>20.000</b>	<b>20.000</b>	<b>8.400</b>

Table A.4 continued...

Connection	To	From	Optimized Flow Rate (t/h)	Old Flow Rate (t/h)	Connection Cost Euros
	CT-2	Freshwater	0.541	25.000	0.000
X		Reactor1 Outlet	2.646	0.000	2.053
X		Separators Outlet	8.550	0.000	2.171
X		Grinding Mill Outlet	1.727	0.000	2.035
X		SWS Outlet	8.938	0.000	2.179
X		SCR Outlet	2.598	0.000	2.052
		<b>Total</b>	<b>25.000</b>	<b>25.000</b>	<b>10.489</b>

The discharge results were given earlier in Chapter 5 in section 5.1.2, along with the necessary optimized results which can lead to using of the current optimized network. All the necessary data has been analyzed.